Supporting Information for

Practical *N*-Alkylation *via* Homogeneous Iridium-Catalyzed Direct Reductive Amination

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CONTENTS

I. General remarks

All reactions were performed in the nitrogen–filled glovebox or under nitrogen using standard Schlenk techniques unless otherwise noted. Chemicals were purchased from Adamas, Energy Chemicals and other companies. Column chromatography was performed using silica gel 60 (200–300 mesh). ^{1}H NMR and ^{13}C NMR spectral data were obtaineded 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 GC on an Agilent 6890 Series instrument. New products were further characterized by ^{13}C NMR and HRMS. A positive ion mass spectrum of sample was acquired on a Thermo Scientific LTQ Orbitrap XL mass spectrometer with an electrospray ionization source.

II. Procedures for direct reductive amination

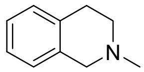
General Procedure. In a nitrogen–filled glovebox, $[Ir(cod)Cl]_2$ (2.0 mg, 3 μmol) and PPh_3 (3.5 mg, 13.2 μmol) were dissolved in anhydrous trifluoroethanol (2 mL) in a 10 mL vial equipped with a stir bar. The above solution was stirred at room temperature for 20 minutes to *in situ* generate the Ir-PPh_3 complex. To a 5mL vial equipped with a stir bar were added amine (0.3 mmol) and aldehyde (0.36 mmol) substrates, followed by the addition of anhydrous trifluoroethanol (1.5 mL) and the Ir-PPh_3 complex solution (10 μL, 0.01 mol%). The resulting vial was transferred to an autoclave, which was purged with H_2 3 times and then charged with H_2 (20 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.

For the reactions of ketones and amines, due to the low solubility of the Ir-BrettPhos and Ir-SPhos complexes in trifluoroethanol, THF was instead used to *in situ* generate the catalyst. For the DRA reactions of aldehydes and amines, the aldehyde/amine ratio is 1.2:1; For the DRA reactions of ketones and amines, the ketone/amine ratio is 1:1.2.

For the DRA reactions in Table 4, different sets of reaction conditions were adopted. For products **97**, **100** and **101**, the conditions were: catalyst 0.01 mol%, r.t., H_2 20 atm; For products **102**, the conditions were: catalyst 0.01 mol%, 40 °C, H_2 20 atm; For products **111** and **112**, the conditions were: catalyst 0.1 mol%, 50 °C, H_2 40 atm; For the rest products, the conditions were: catalyst 0.2 mol%, 50 °C, H_2 40 atm.

For the DRA reactions in Table 5, different sets of reaction conditions were adopted. In Table 5A and 5B sections, the conditions for the DRA reactions of aldehydes and amines were: Ir-PPh_3 0.01 mol%, r.t., H_2 20 atm; The conditions for the DRA reactions of ketones and amines were: Ir-BrettPhos 0.01 mol%, 40 °C, H_2 40 atm; For products **119** from the reaction of corresponding ketone and dimethylamine, the conditions were: Ir-SPhos 0.1 mol%, 60 °C, H_2 40 atm. In Table 5C section, for products **30**, the conditions were: Ir-BrettPhos 0.04 mol%, 40 °C, H_2 40 atm; For products **128**, the conditions were: Ir-PPh_3 0.04 mol%, 40 °C, H_2 40 atm; For products **129**, the conditions were: Ir-PPh_3 0.1 mol%, r.t., H_2 20 atm. In Table 5D section, the DRA reactions conditions were the same as for the corresponding racemic compounds.

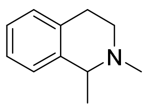
2-methyl-1,2,3,4-tetrahydroisoquinoline (2) [1]



2

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as yellow oil, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 42 mg, 95% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 6.99 (m, 4H), 3.68 – 3.54 (m, 2H), 2.94 (t, J = 6.0 Hz, 2H), 2.70 (t, J = 6.0 Hz, 2H), 2.46 (s, 3H).

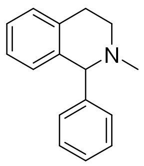
1,2-dimethyl-1,2,3,4-tetrahydroisoquinoline (3) [2]



3

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as yellow oil, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 46 mg, 95% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.12 (m, 4H), 3.67 (q, J = 6.8 Hz, 1H), 3.07 (m, 1H), 2.95 – 2.83 (m, 2H), 2.74 – 2.65 (m, 1H), 2.50 (d, J = 2.5 Hz, 3H), 1.41 (dd, J = 6.8, 2.5 Hz, 3H).

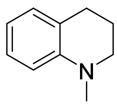
2-methyl-1-phenyl-1,2,3,4-tetrahydroisoquinoline (4) [2]



4

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as yellow solid, R_f = 0.7 (CH_2Cl_2:MeOH = 10:1), 64 mg, 95% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.28 (m, 5H), 7.10 (q, J = 8.4, 7.9 Hz, 2H), 6.97 (t, J = 7.5 Hz, 1H), 6.63 (d, J = 7.7 Hz, 1H), 4.23 (s, 1H), 3.27 (m, 1H), 3.18 – 3.06 (m, 1H), 2.82 (d, J = 16.2 Hz, 1H), 2.63 (m, 1H), 2.23 (s, 3H).

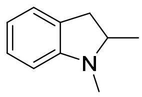
1-methyl-1,2,3,4-tetrahydroquinoline (5) [3]



5

Purified by column chromatography (silica gel, Petroleum ether:EtOAc = 50:1 with 0.1% Et_3N) afforded the product as brown liquid, R_f = 0.5 (Petroleum ether:EtOAc = 10:1), 44 mg, 99% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.06 (t, J = 7.9 Hz, 1H), 6.93 (d, J = 7.4 Hz, 1H), 6.65 – 6.47 (m, 2H), 3.22 – 3.13 (m, 2H), 2.85 (d, J = 2.6 Hz, 3H), 2.75 (t, J = 6.7 Hz, 2H), 1.96 (m, 2H).

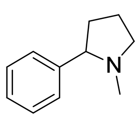
1,2-dimethylindoline (6) [4]



6

Purified by column chromatography (silica gel, Petroleum ether:EtOAc = 50:1 with 0.1% Et_3N) afforded the product as yellow oil, R_f = 0.6 (Petroleum ether:EtOAc = 10:1), 40 mg, 90% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.12 – 6.98 (m, 2H), 6.64 (t, J = 7.3 Hz, 1H), 6.43 (d, J = 7.8 Hz, 1H), 3.37 (m, 1H), 3.06 (dd, J = 15.3, 8.2 Hz, 1H), 2.69 (s, 3H), 2.58 (dd, J = 15.2, 10.5 Hz, 1H), 1.31 (d, J = 6.1 Hz, 3H).

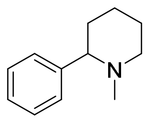
1-methyl-2-phenylpyrrolidine (7) [5]



7

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as yellow liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 48 mg, 99% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.21 (m, 5H), 3.25 (m, 1H), 3.04 (m, 1H), 2.29 (m, 1H), 2.17 (s, 4H), 2.02 – 1.91 (m, 1H), 1.87 – 1.72 (m, 2H).

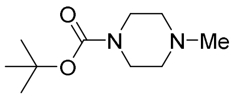
1-methyl-2-phenylpiperidine (8) [5]



8

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 30:1 with 0.1% Et_3N) afforded the product as yellow liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 50 mg, 95% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.19 (m, 5H), 3.11 – 3.01 (m, 1H), 2.77 (dd, J = 11.0, 3.0 Hz, 1H), 2.18 – 2.07 (m, 1H), 2.00 (s, 3H), 1.86 – 1.59 (m, 5H), 1.38 (m, 1H).

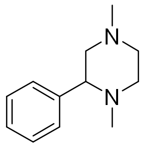
Tert-butyl 4-methylpiperazine-1-carboxylate (9) [6]



9

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 30:1 with 0.1% Et_3N) afforded the product as white solid, R_f = 0.7 (CH_2Cl_2:MeOH = 10:1), 59 mg, 99% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 3.44 (t, J = 5.1 Hz, 4H), 2.35 (t, J = 5.1 Hz, 4H), 2.29 (s, 3H), 1.46 (s, 9H).

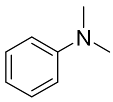
1,4-dimethyl-2-phenylpiperazine (10) [7]



10

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 56 mg, 98% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.24 (m, 5H), 3.07 (dd, J = 10.5, 3.0 Hz, 1H), 2.95 (m, 1H), 2.84 (m, 1H), 2.76 (m, 1H), 2.43 (m, 1H), 2.35 – 2.27 (m, 4H), 2.07 (d, J = 13.6 Hz, 4H).

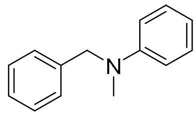
***N*,*N*-dimethyl aniline (11)** [8]



11

Purified by column chromatography (silica gel, Petroleum ether:EtOAc = 80:1 with 0.1% Et_3N) afforded the product as yellow liquid, R_f = 0.7 (Petroleum ether:EtOAc = 10:1), 34 mg, 94% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.27 – 6.64 (m, 5H), 2.91 (s, 6H).

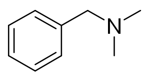
***N*-benzyl-*N*-methyl aniline (12)** [8]



12

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 55 mg, 93% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.48 – 6.56 (m, 10H), 4.51 (d, J = 2.7 Hz, 2H), 2.99 (d, J = 3.0 Hz, 3H).

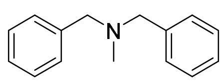
***N*,*N*-dimethyl-1-phenylmethanamine (13)** [9]



13

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 30:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.4 (CH_2Cl_2:MeOH = 10:1), 38 mg, 95% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.24 (m, 5H), 3.42 (s, 2H), 2.24 (s, 6H).

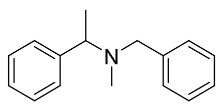
***N*-benzyl-*N*-methyl-1-phenylmethanamine (14)** [8]



14

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 62 mg, 98% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.42 – 7.14 (m, 10H), 3.51 (s, 4H), 2.18 (s, 3H).

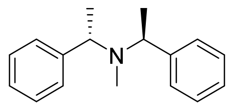
***N*-benzyl-*N*-methyl-1-phenylethan-1-amine (15)** [10]



15

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1). The yield from the reaction of *N*-benzyl-1-phenylethan-1-amine (30) and paraformaldehyde was 98% (62 mg). The yield from the reaction of *N*-methyl-1-phenylethan-1-amine and benzaldehyde was 96% (61 mg). ^1H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.08 (m, 10H), 3.60 – 3.44 (m, 2H), 3.21 (dd, J = 13.4, 2.6 Hz, 1H), 2.10 – 2.00 (m, 3H), 1.34 (dd, J = 7.0, 2.7 Hz, 3H).

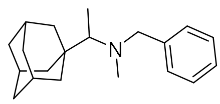
(*S*)-*N*-methyl-1-phenyl-*N*-((*S*)-1-phenylethyl)ethan-1-amine (16) [11]



16

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.4 (CH_2Cl_2:MeOH = 10:1), 71 mg, 99% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.39 – 7.17 (m, 10H), 3.81 (q, J = 6.8 Hz, 2H), 2.00 (s, 3H), 1.33 (d, J = 6.8 Hz, 6H).

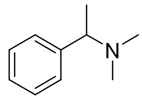
1-(adamantan-1-yl)-*N*-benzyl-*N*-methylethan-1-amine (17) [12]



17

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 83 mg, 98% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.44 – 7.16 (m, 5H), 3.70 (d, J = 13.8 Hz, 1H), 3.38 (d, J = 13.8 Hz, 1H), 2.20 (q, J = 7.1 Hz, 1H), 2.13 (s, 3H), 1.96 (p, J = 3.2 Hz, 3H), 1.69 (m, 9H), 1.52 (m, 3H), 0.95 (d, J = 7.1 Hz, 3H).

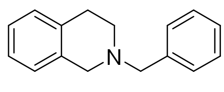
***N*, *N*-dimethyl-1-phenylethan-1-amine (18)** [10]



18

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.4 (CH_2Cl_2:MeOH = 10:1), 40 mg, 90% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.38 – 7.14 (m, 5H), 3.24 (q, J = 6.7 Hz, 1H), 2.19 (s, 6H), 1.37 (d, J = 6.6 Hz, 3H).

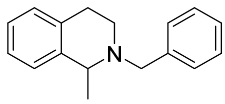
2-benzyl-1,2,3,4-tetrahydroisoquinoline (19) [8]



19

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as yellow oil, R_f = 0.7 (CH_2Cl_2:MeOH = 10:1), 66 mg, 98% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.41 – 7.24 (m, 5H), 7.15 – 7.02 (m, 3H), 7.00 – 6.91 (m, 1H), 3.67 (s, 2H), 3.62 (s, 2H), 2.88 (t, J = 5.9 Hz, 2H), 2.73 (t, J = 5.9 Hz, 2H).

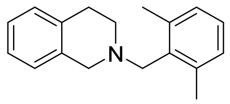
2-benzyl-1-methyl-1,2,3,4-tetrahydroisoquinoline (20) [13]



20

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as brown liquid, R_f = 0.7 (CH_2Cl_2:MeOH = 10:1), 66 mg, 92% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40 – 7.23 (m, 5H), 7.15 – 6.98 (m, 4H), 3.93 – 3.61 (m, 3H), 3.06 (m, 1H), 2.89 (m, 1H), 2.75 – 2.60 (m, 2H), 1.38 (d, J = 6.7 Hz, 3H).

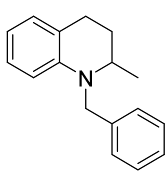
2-(2,6-dimethylbenzyl)-1,2,3,4-tetrahydroisoquinoline (21) [14]



21

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.6 (CH_2Cl_2: MeOH = 10:1), 66 mg, 88% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.16 – 6.90 (m, 7H), 3.63 (d, J = 2.3 Hz, 4H), 2.79 (t, J = 5.8 Hz, 2H), 2.69 (t, J = 5.8 Hz, 2H), 2.41 (s, 6H).

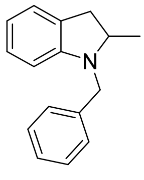
1-benzyl-2-methyl-1,2,3,4-tetrahydroquinoline (22) [15]



22

Purified by column chromatography (silica gel, Petroleum ether:EtOAc = 80:1 with 0.1% Et_3N) afforded the product as yellow liquid, R_f = 0.6 (Petroleum ether:EtOAc = 10:1), 61 mg, 86% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 – 7.15 (m, 5H), 7.08 – 6.82 (m, 2H), 6.56 (t, J = 7.2 Hz, 1H), 6.39 (d, J = 8.2 Hz, 1H), 4.50 (q, J = 17.3 Hz, 2H), 3.57 (m, 1H), 2.92 (m, 1H), 2.75 (m, 1H), 2.04 (m, 1H), 1.83 (m, 1H), 1.17 (d, J = 6.5 Hz, 3H).

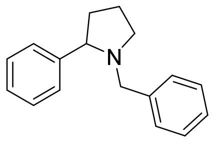
1-benzyl-2-methylindoline (23) [16]



23

Purified by column chromatography (silica gel, Petroleum ether:EtOAc = 80:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.5 (Petroleum ether:EtOAc = 10:1), 60 mg, 90% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.39 – 7.20 (m, 5H), 7.08 – 6.94 (m, 2H), 6.62 (m, 1H), 6.31 (d, J = 7.9 Hz, 1H), 4.36 (d, J = 16.1 Hz, 1H), 4.18 (d, J = 16.1 Hz, 1H), 3.72 (m, 1H), 3.16 (dd, J = 15.5, 8.6 Hz, 1H), 2.67 (dd, J = 15.4, 9.5 Hz, 1H), 1.29 (d, J = 6.1 Hz, 3H).

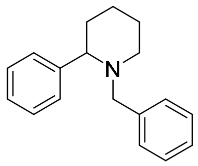
1-benzyl-2-phenylpyrrolidine (24) [17]



24

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 69 mg, 97% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.53 – 7.11 (m, 10H), 3.85 (d, J = 13.1 Hz, 1H), 3.35 (t, J = 8.2 Hz, 1H), 3.16 – 2.96 (m, 2H), 2.22 – 2.13 (m, 2H), 1.87 (m, 1H), 1.81 – 1.64 (m, 2H).

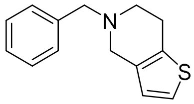
1-benzyl-2-phenylpiperidine (25) [17]



25

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as white solid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 75 mg, 99% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.47 – 7.17 (m, 10H), 3.76 (d, J = 13.4 Hz, 1H), 3.10 (dd, J = 11.1, 2.8 Hz, 1H), 2.96 (m, 1H), 2.80 (d, J = 13.5 Hz, 1H), 1.98 – 1.87 (m, 1H), 1.80 – 1.73 (m, 2H), 1.67 – 1.52 (m, 3H), 1.42 – 1.31 (m, 1H).

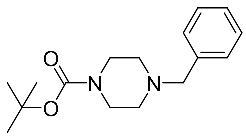
5-benzyl-4,5,6,7-tetrahydrothieno[3,2-c] pyridine (26) [18]



26

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 67 mg, 97% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.48 – 6.65 (m, 7H), 3.71 (s, 2H), 3.56 (d, J = 1.8 Hz, 2H), 2.84 (m, J = 30.8, 5.9 Hz, 4H).

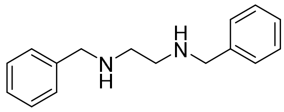
Tert-butyl 4-benzylpiperazine-1-carboxylate (27) [6]



27

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 80 mg, 97% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.21 (m, 5H), 3.50 (s, 2H), 3.42 (t, J = 5.1 Hz, 4H), 2.38 (t, J = 5.1 Hz, 4H), 1.45 (s, 9H).

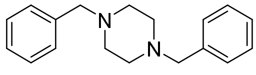
***N*^{1},*N*^{2}-dibenzylethane-1,2-diamine (28) [19]**



28

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 69 mg, 96% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.41 – 7.13 (m, 10H), 3.75 (s, 4H), 2.74 (s, 4H), 2.22 (d, J = 3.7 Hz, 2H).

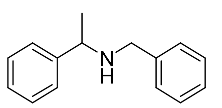
1,4-dibenzylpiperazine (29) [20]



29

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as light yellow solid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 70 mg, 88% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.41 – 7.19 (m, 10H), 3.50 (s, 4H), 2.47 (s, 8H).

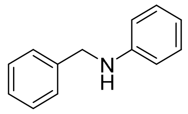
N-benzyl-1-phenylethan-1-amine (30) [21]



30

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1). The yield for the reaction of 1-phenylethan-1-amine and benzaldehyde was 94% (60 mg). The yield for the reaction of acetophenone and benzylamine was 96% (61 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.46 – 7.12 (m, 10H), 3.79 (t, J = 6.5 Hz, 1H), 3.61 (q, J = 13.2 Hz, 2H), 1.65 (s, 1H), 1.35 (t, J = 4.6 Hz, 3H).

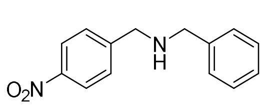
N-benzylaniline (31) [8]



31

Purified by column chromatography (silica gel, Petroleum ether:EtOAc = 50:1 with 0.1% Et_3N) afforded the product as white soild , R_f = 0.7 (Petroleum ether:EtOAc = 10:1), 54 mg, 98% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40 – 7.10 (m, 7H), 6.75 – 6.59 (m, 3H), 4.31 (s, 2H).

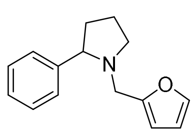
N-benzyl-1-phenylethan-1-amine (32) [8]



32

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1). 60 mg, 83% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.22 – 8.14 (m, 2H), 7.53 (d, J = 8.6 Hz, 2H), 7.34 (d, J = 5.2 Hz, 5H), 3.91 (s, 2H), 3.81 (s, 2H).

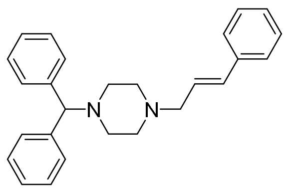
1-(furan-2-ylmethyl)-2-phenylpyrrolidine (33)



33

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 60:1 with 0.1% Et_3N) afforded the product as yellow liquid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 68 mg, 99% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.44 – 7.22 (m, 6H), 6.27 (m, 1H), 6.10 (d, J = 3.1 Hz, 1H), 3.75 (d, J = 14.2 Hz, 1H), 3.38 – 3.30 (m, 1H), 3.28 – 3.14 (m, 2H), 2.39 (q, J = 8.9 Hz, 1H), 2.23 – 2.09 (m, 1H), 2.00 – 1.84 (m, 1H), 1.82 – 1.71 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.00, 143.20, 141.76, 128.45, 127.57, 127.06, 109.97, 107.88, 68.68, 53.39, 49.29, 35.06, 22.25. HRMS (ESI) m/z calcd for $C_{15}H_{18}NO^+$ $(M+H)^+$ 228.13829, found 228.13818.

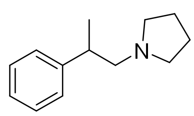
1-benzhydryl-4-cinnamylpiperazine (34) [22]



34

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as yellow liquid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 109 mg, 99% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40 (d, J = 7.6 Hz, 4H), 7.34 (d, J = 7.3 Hz, 2H), 7.27 – 7.11 (m, 9H), 6.49 (d, J = 15.8 Hz, 1H), 6.26 (m, 1H), 4.22 (s, 1H), 3.14 (d, J = 6.8 Hz, 2H), 2.48 (d, J = 31.8 Hz, 8H).

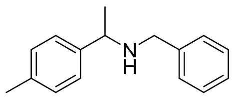
1-(2-phenylpropyl) pyrrolidine (35) [23]



35

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 54 mg, 95% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.25 (m, 5H), 3.05 – 2.93 (m, 1H), 2.77 (m, 1H), 2.55 (m, 5H), 1.77 (d, J = 5.7 Hz, 4H), 1.34 – 1.28 (m, 3H).

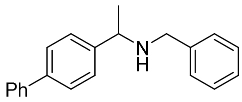
N-benzyl-1-(p-tolyl)ethan-1-amine (36) [24]



36

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.4 (CH_2Cl_2:MeOH = 10:1), 66 mg, 97% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 – 7.19 (m, 7H), 7.15 (d, J = 7.8 Hz, 2H), 3.77 (q, J = 6.6 Hz, 1H), 3.69 – 3.53 (m, 2H), 2.34 (s, 3H), 1.61 (s, 1H), 1.34 (d, J = 6.6 Hz, 3H).

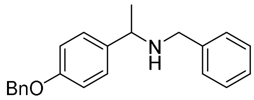
1-([1,1'-biphenyl]-4-yl)-N-benzylethan-1-amine (37) [25]



37

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as white solid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 75 mg, 87% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.63 – 7.54 (m, 4H), 7.46 – 7.39 (m, 4H), 7.36 – 7.20 (m, 6H), 3.85 (q, J = 6.6 Hz, 1H), 3.72 – 3.60 (m, 2H), 1.65 (s, 1H), 1.39 (d, J = 6.6 Hz, 3H).

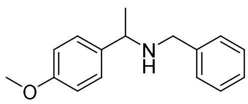
N-benzyl-1-(4-(benzyloxy)phenyl)ethan-1-amine (38) [26]



38

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as white solid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 94 mg, 99% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.47 – 7.41 (m, 2H), 7.40 – 7.34 (m, 2H), 7.34 – 7.19 (m, 8H), 6.99 – 6.92 (m, 2H), 5.05 (s, 2H), 3.76 (q, J = 6.6 Hz, 1H), 3.69 – 3.51 (m, 2H), 1.59 (s, 1H), 1.34 (d, J = 6.6 Hz, 3H).

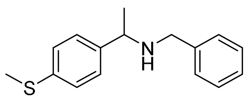
N-benzyl-1-(4-methoxyphenyl)ethan-1-amine (39) [21]



39

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 70 mg, 97% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.19 (m, 7H), 6.92 – 6.85 (m, 2H), 3.85 – 3.73 (m, 4H), 3.69 – 3.55 (m, 2H), 1.75 (s, 1H), 1.34 (d, J = 6.6 Hz, 3H).

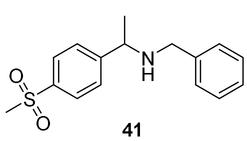
N-benzyl-1-(4-(methylthio)phenyl)ethan-1-amine (40)



40

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as light yellow solid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 76 mg, 99% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.26 (m, 9H), 3.77 (q, J = 6.6 Hz, 1H), 3.67 – 3.54 (m, 2H), 2.48 (s, 3H), 1.62 (s, 1H), 1.34 (d, J = 6.6 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-d) δ 142.67, 140.59, 128.42, 128.16, 127.33, 127.00, 126.92, 57.04, 51.66, 24.52, 16.13. HRMS (ESI) m/z calcd for $C_{16}H_{20}NS^+$ $(M+H)^+$ 258.13110, found 258.13120.

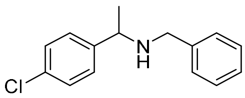
N-benzyl-1-(4-(methylsulfonyl)phenyl)ethan-1-amine (41)



41

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as yellow solid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 86 mg, 99% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.94 – 7.88 (m, 2H), 7.63 – 7.54 (m, 2H), 7.36 – 7.21 (m, 5H), 3.92 (q, J = 6.6 Hz, 1H), 3.68 – 3.55 (m, 2H), 3.06 (s, 3H), 1.78 (s, 1H), 1.36 (d, J = 6.6 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 152.39, 140.08, 139.06, 128.50, 128.08, 127.78, 127.68, 127.11, 57.28, 51.77, 44.57, 24.62. HRMS (ESI) m/z calcd for $C_{16}H_{20}NO_2S^+$ $(M+H)^+$ 290.12093, found 290.12057.

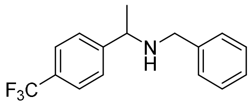
N-benzyl-1-(4-chlorophenyl)ethan-1-amine (42) [27]



42

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 60:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.4 (CH_2Cl_2:MeOH = 10:1), 68 mg, 92% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 – 7.19 (m, 9H), 3.78 (q, J = 6.6 Hz, 1H), 3.66 – 3.45 (m, 2H), 1.61 (s, 1H), 1.32 (d, J = 6.6 Hz, 3H).

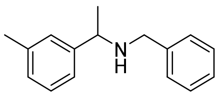
N-benzyl-1-(4-(trifluoromethyl)phenyl)ethan-1-amine (43) [24]



43

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 60:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 83 mg, 99% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.60 (d, J = 8.1 Hz, 2H), 7.48 (d, J = 8.1 Hz, 2H), 7.36 – 7.21 (m, 5H), 3.88 (q, J = 6.6 Hz, 1H), 3.61 (q, J = 13.2 Hz, 2H), 1.62 (s, 1H), 1.36 (d, J = 6.6 Hz, 3H).

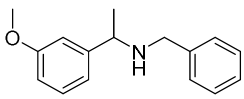
N-benzyl-1-(m-tolyl)ethan-1-amine (44) [24]



44

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 60:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 67 mg, 99% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.02 (m, 9H), 3.76 (q, J = 6.6 Hz, 1H), 3.69 – 3.54 (m, 2H), 2.35 (s, 3H), 1.61 (s, 1H), 1.35 (d, J = 6.6 Hz, 3H).

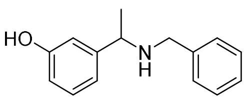
N-benzyl-1-(3-methoxyphenyl)ethan-1-amine (45) [24]



45

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 60:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 71 mg, 98% yield, colorless liquid. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.36 – 7.19 (m, 6H), 6.98 – 6.89 (m, 2H), 6.80 (m, 1H), 3.81 (s, 3H), 3.81 – 3.76 (m, 1H), 3.67 (d, J = 13.1 Hz, 1H), 3.59 (d, J = 13.1 Hz, 1H), 1.62 (s, 1H), 1.35 (d, J = 6.6 Hz, 3H).

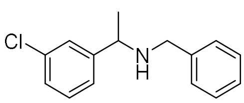
3-(1-(benzylamino)ethyl)phenol (46)



46

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as white solid, R_f = 0.4 (CH_2Cl_2:MeOH = 10:1), 61 mg, 89% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.23 – 7.05 (m, 6H), 6.80 – 6.58 (m, 3H), 4.73 (s, 2H), 3.68 (q, J = 6.6 Hz, 1H), 3.63 – 3.51 (m, 2H), 1.28 (d, J = 6.6 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.47, 146.72, 139.81, 129.72, 128.50, 128.33, 127.10, 119.12, 114.50, 113.49, 57.23, 51.48, 23.77. HRMS (ESI) m/z calcd for $C_{15}H_{18}NO^+$ $(M+H)^+$ 228.13829, found 228.13866.

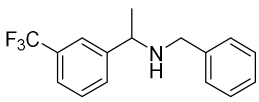
N-benzyl-1-(3-chlorophenyl)ethan-1-amine (47) [28]



47

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 69 mg, 93% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.39 – 7.17 (m, 9H), 3.77 (q, J = 6.6 Hz, 1H), 3.68 – 3.53 (m, 2H), 1.64 (s, 1H), 1.33 (d, J = 6.6 Hz, 3H).

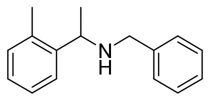
N-benzyl-1-(3-(trifluoromethyl)phenyl)ethan-1-amine (48)



48

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 83 mg, 99% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.64 (d, J = 1.9 Hz, 1H), 7.56 (d, J = 7.7 Hz, 1H), 7.53 – 7.48 (m, 1H), 7.44 (t, J = 7.6 Hz, 1H), 7.36 – 7.20 (m, 5H), 3.88 (q, J = 6.6 Hz, 1H), 3.70 – 3.53 (m, 2H), 1.61 (s, 1H), 1.36 (d, J = 6.6 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 146.73, 140.29, 130.81(q, $J_{C\text{-}F}$ = 32.3Hz), 130.21, 128.95, 128.48, 128.14, 127.05, 124.34 (q, $J_{C\text{-}F}$ = 272.7Hz), 123.86 (q, $J_{C\text{-}F}$ = 3Hz), 123.60 (q, $J_{C\text{-}F}$ = 4Hz), 57.30, 51.75, 24.60. HRMS (ESI) m/z calcd for $C_{16}H_{17}F_3N^+$ $(M+H)^+$ 280.13076, found 280.13071.

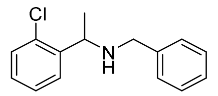
N-benzyl-1-(o-tolyl)ethan-1-amine (49) [29]



49

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.4 (CH_2Cl_2:MeOH = 10:1), 61 mg, 90% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.57 – 7.09 (m, 9H), 4.07 (q, J = 6.5 Hz, 1H), 3.71 – 3.56 (m, 2H), 2.26 (s, 3H), 1.62 (s, 1H), 1.31 (d, J = 6.5 Hz, 3H).

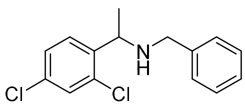
N-benzyl-1-(2-chlorophenyl)ethan-1-amine (50) [21]



50

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 73 mg, 99% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.61 (dd, J = 7.8, 1.7 Hz, 1H), 7.39 – 7.21 (m, 7H), 7.18 (td, J = 7.6, 1.7 Hz, 1H), 4.34 (q, J = 6.6 Hz, 1H), 3.70 – 3.55 (m, 2H), 1.66 (s, 1H), 1.35 (d, J = 6.6 Hz, 3H).

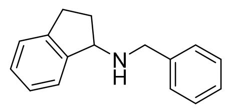
N-benzyl-1-(2,4-dichlorophenyl)ethan-1-amine (51) [30]



51

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 70:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 81 mg, 96% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.58 (d, J = 8.4 Hz, 1H), 7.43 – 7.18 (m, 7H), 4.29 (q, J = 6.5 Hz, 1H), 3.68 – 3.54 (m, 2H), 1.60 (s, 1H), 1.31 (d, J = 6.5 Hz, 3H).

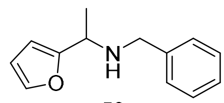
N-benzyl-2,3-dihydro-1H-inden-1-amine (52) [21]



52

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as yellow liquid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 64 mg, 95% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.46 – 7.28 (m, 5H), 7.28 – 7.15 (m, 4H), 4.29 (t, J = 6.6 Hz, 1H), 3.98 – 3.81 (m, 2H), 3.01 (m, 1H), 2.81 (m, 1H), 2.42 (m, 1H), 1.94 – 1.81 (m, 1H), 1.62 (s, 1H).

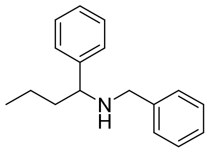
N-benzyl-1-(furan-2-yl)ethan-1-amine (53) [21]



53

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 60:1 with 0.1% Et_3N) afforded the product as yellow liquid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 60 mg, 99% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.53 – 7.10 (m, 6H), 6.32 (dd, J = 3.2, 1.8 Hz, 1H), 6.16 (d, J = 3.1 Hz, 1H), 3.88 (q, J = 6.8 Hz, 1H), 3.77 – 3.61 (m, 2H), 1.70 (s, 1H), 1.432 (d, J = 6.8 Hz, 3H).

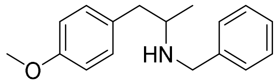
N-benzyl-1-phenylbutan-1-amine (54) [31]



54

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 60:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 67 mg, 94% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40 – 7.15 (m, 10H), 3.68 – 3.48 (m, 3H), 1.75 – 1.54 (m, 3H), 1.36 – 1.10 (m, 2H), 0.84 (t, J = 7.3 Hz, 3H).

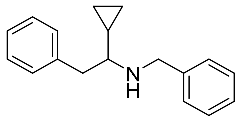
N-benzyl-1-(4-methoxyphenyl)propan-2-amine (55) [32]



55

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 70 mg, 92% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 – 7.15 (m, 5H), 7.09 – 7.03 (m, 2H), 6.84 – 6.78 (m, 2H), 3.87 – 3.68 (m, 5H), 2.93 – 2.83 (m, 1H), 2.69 (dd, J = 13.5, 7.1 Hz, 1H), 2.59 (dd, J = 13.5, 6.4 Hz, 1H), 1.55 (s, 1H), 1.08 (d, J = 6.2 Hz, 3H).

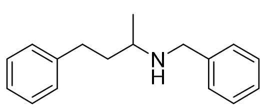
N-benzyl-1-cyclopropyl-2-phenylethan-1-amine (56)



56

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 70 mg, 93% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.12 – 6.93 (m, 10H), 3.74 (d, J = 13.4 Hz, 1H), 3.61 (d, J = 13.5 Hz, 1H), 2.75 (dd, J = 13.5, 5.1 Hz, 1H), 2.62 (dd, J = 13.5, 7.8 Hz, 1H), 1.82 (m, 1H), 1.56 (s, 1H), 0.58 (m, 1H), 0.42 – 0.32 (m, 1H), 0.26 – 0.17 (m, 1H), -0.04 (s, 1H), -0.22 (m, 1H). ^{13}C NMR (101 MHz, Chloroform-d) δ 138.58, 137.32, 127.37, 126.24, 126.21, 125.77, 124.64, 124.05, 61.60, 49.49 , 39.93, 14.04, 2.74. HRMS (ESI) m/z calcd for $C_{18}H_{22}N^+$ $(M+H)^+$ 252.17468, found 252.17499.

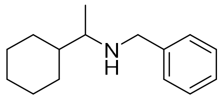
N-benzyl-4-phenylbutan-2-amine (57) [33]



57

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 68 mg, 95% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.32 – 7.21 (m, 7H), 7.20 – 7.12 (m, 3H), 3.86 – 3.69 (m, 2H), 2.67 (m, 3H), 1.81 (m, 1H), 1.66 (m, 1H), 1.43 (s, 1H), 1.14 (d, J = 6.3 Hz, 3H).

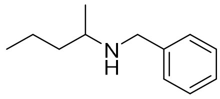
N-benzyl-1-cyclohexylethan-1-amine (58) [34]



58

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 58 mg, 89% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40 – 7.17 (m, 5H), 3.84 (d, J = 13.0 Hz, 1H), 3.71 (d, J = 13.1 Hz, 1H), 2.50 (m, J = 6.4, 5.0 Hz, 1H), 1.85 – 1.58 (m, 5H), 1.45 – 1.07 (m, 6H), 1.02 (d, J = 6.5 Hz, 4H).

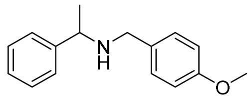
N-benzylpentan-2-amine (59) [35]



59

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.7 (CH_2Cl_2:MeOH = 10:1), 51 mg, 95% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.32 (d, J = 4.4 Hz, 4H), 7.26 – 7.20 (m, 1H), 3.86 – 3.70 (m, 2H), 2.69 (p, J = 6.1 Hz, 1H), 1.53 (s, 1H), 1.49 – 1.44 (m, 1H), 1.34 (m, 3H), 1.08 (d, J = 6.3 Hz, 3H), 0.94 – 0.87 (m, 3H).

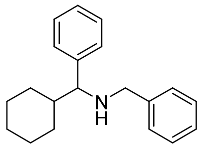
_N_-(4-methoxybenzyl)-1-phenylethan-1-amine (60) [24]



60

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 67 mg, 92% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.42 – 7.13 (m, 7H), 6.90 – 6.76 (m, 2H), 3.78 (s, 4H), 3.55 (q, J = 12.9 Hz, 2H), 1.64 (s, 1H), 1.35 (d, J = 6.5 Hz, 3H).

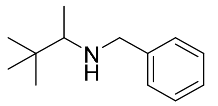
_N_-benzyl-1-cyclohexyl-1-phenylmethanamine (61) [36]



61

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 60:1 with 0.1% Et_3N) afforded the product as yellow liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 75 mg, 90% yield, light yellow liquid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.19 (m, 10H), 3.63 (d, J = 13.2 Hz, 1H), 3.44 (d, J = 13.2 Hz, 1H), 3.36 (d, J = 7.2 Hz, 1H), 1.98 – 0.77 (m, 11H).

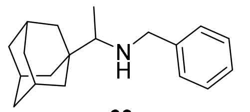
_N_-benzyl-3,3-dimethylbutan-2-amine (62) [21]



62

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 53 mg, 93 yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.38 – 7.19 (m, 5H), 3.93 (d, J = 13.2 Hz, 1H), 3.66 (d, J = 13.2 Hz, 1H), 2.29 (q, J = 6.5 Hz, 1H), 1.01 (d, J = 6.4 Hz, 3H), 0.88 (s, 9H).

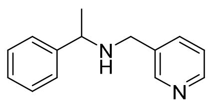
1-(adamantan-1-yl)-_N_-benzylethan-1-amine (63) [37]



63

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 80 mg, 99% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.44 – 7.21 (m, 5H), 3.92 (d, J = 13.2 Hz, 1H), 3.64 (d, J = 13.2 Hz, 1H), 1.96 (p, J = 3.2 Hz, 3H), 1.72 – 1.57 (m, 10H), 1.47 (m, 3H), 1.19 (s, 1H), 0.98 (d, J = 6.5 Hz, 3H).

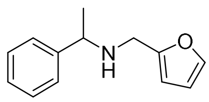
1-phenyl-_N_-(pyridin-3-ylmethyl)ethan-1-amine (64) [38]



64

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 60:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.4 (CH_2Cl_2:MeOH = 10:1), 54 mg, 85% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.60 – 7.16 (m, 9H), 3.80 (q, J = 6.6 Hz, 1H), 3.68 – 3.58 (m, 2H), 1.94 (s, 1H), 1.38 (d, J = 6.6 Hz, 3H).

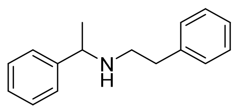
_N_-(furan-2-ylmethyl)-1-phenylethan-1-amine (65) [39]



65

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.4 (CH_2Cl_2:MeOH = 10:1), 59 mg, 97% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.46 – 7.14 (m, 6H), 6.29 (dd, J = 3.2, 1.9 Hz, 1H), 6.15 – 6.03 (m, 1H), 3.78 (q, J = 6.6 Hz, 1H), 3.69 – 3.53 (m, 2H), 1.75 (s, 1H), 1.36 (d, J = 6.5 Hz, 3H).

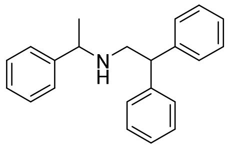
_N_-phenethyl-1-phenylethan-1-amine (66) [39]



66

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 66 mg, 98% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.39 – 7.06 (m, 10H), 3.76 (q, J = 6.6 Hz, 1H), 2.84 – 2.64 (m, 4H), 1.46 (s, 1H), 1.32 (d, J = 6.6 Hz, 3H).

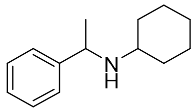
2,2-diphenyl-*N*-(1-phenylethyl)ethan-1-amine (67) [40]



67

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 90 mg, 99% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 – 7.13 (m, 15H), 4.16 (t, J = 7.6 Hz, 1H), 3.77 (q, J = 6.6 Hz, 1H), 3.15 – 2.99 (m, 2H), 1.27 (d, J = 6.6 Hz, 3H).

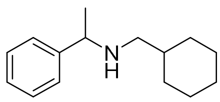
***N*-(1-phenylethyl)cyclohexanamine (68)** [39]



68

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 59 mg, 97% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40 – 7.18 (m, 5H), 3.96 (q, J = 6.6 Hz, 1H), 2.27 (m, 1H), 1.98 (d, J = 13.0 Hz, 1H), 1.80 – 1.45 (m, 5H), 1.34 (d, J = 6.6 Hz, 3H), 1.22 – 0.95 (m, 5H).

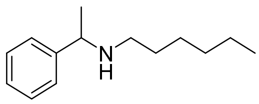
***N*-(cyclohexylmethyl)-1-phenylethan-1-amine (69)** [39]



69

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 63 mg, 96% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.39 – 7.17 (m, 5H), 3.72 (q, J = 6.6 Hz, 1H), 2.34 (dd, J = 11.5, 6.2 Hz, 1H), 2.23 (dd, J = 11.5, 7.1 Hz, 1H), 1.78 – 1.60 (m, 5H), 1.51 – 1.36 (m, 2H), 1.34 (d, J = 6.6 Hz, 3H), 1.29 – 1.06 (m, 3H), 0.93 – 0.78 (m, 2H).

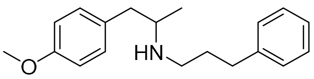
***N*-(1-phenylethyl)hexan-1-amine (70)** [41]



70

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 56 mg, 91% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.19 (m, 5H), 3.75 (q, J = 6.6 Hz, 1H), 2.45 (m, 2H), 1.53 – 1.17 (m, 12H), 0.86 (t, J = 6.8 Hz, 3H).

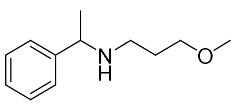
***N*-(1-(4-methoxyphenyl)propan-2-yl)-3-phenylpropan-1-amine (71)** [42]



71

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 77 mg, 91% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.24 (m, 2H), 7.19 – 7.05 (m, 5H), 6.86 – 6.80 (m, 2H), 3.76 (s, 3H), 2.82 (m, 1H), 2.72 – 2.49 (m, 6H), 1.75 (m, 2H), 1.53 (s, 1H), 1.03 (d, J = 6.2 Hz, 3H).

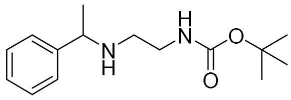
3-methoxy-*N*-(1-phenylethyl)propan-1-amine (72) [41]



72

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.4 (CH_2Cl_2:MeOH = 10:1), 56 mg, 96% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.39 – 7.19 (m, 5H), 3.76 (q, J = 6.6 Hz, 1H), 3.41 (m, 2H), 3.30 (s, 3H), 2.55 (m, 2H), 1.79 (s, 1H), 1.74 (p, J = 6.7 Hz, 2H), 1.36 (d, J = 6.6 Hz, 3H).

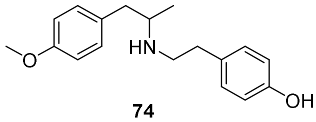
Tert-butyl (2-((1-phenylethyl)amino)ethyl)carbamate (73) [43]



73

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as white solid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 75 mg, 95% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.20 (m, 5H), 3.76 (q, J = 6.6 Hz, 1H), 3.16 (m, 2H), 2.71 – 2.48 (m, 2H), 1.54 (s, 1H), 1.44 (s, 9H), 1.35 (d, J = 6.6 Hz, 3H).

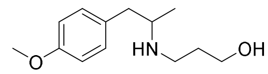
4-(2-((1-(4-methoxyphenyl)propan-2-yl)amino)ethyl)phenol (74)



74

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 83 mg, 97% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.03 – 6.64 (m, 8H), 5.26 (s, 2H), 3.76 (s, 3H), 3.02 – 2.54 (m, 7H), 1.09 (d, J = 6.4 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.13, 155.51, 130.68, 130.13, 129.85, 129.67, 116.01, 113.97, 55.27, 54.76, 48.15, 41.99, 34.57, 19.48. HRMS (ESI) m/z calcd for $C_{18}H_{24}NO_2^+$ $(M+H)^+$ 286.18016, found 286.18088.

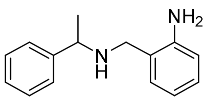
3-((1-(4-methoxyphenyl)propan-2-yl)amino)propan-1-ol (75)



75

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 60:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 64 mg, 96% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.12 – 6.79 (m, 4H), 3.77 (d, J = 11.4 Hz, 5H), 3.21 (s, 2H), 2.93 – 2.75 (m, 3H), 2.66 (dd, J = 13.5, 6.8 Hz, 1H), 2.57 (dd, J = 13.5, 6.5 Hz, 1H), 1.66 (p, J = 5.7 Hz, 2H), 1.06 (d, J = 6.3 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.11, 130.90, 130.20, 113.86, 63.82, 55.22, 54.89, 46.91, 42.42, 31.27, 19.89. HRMS (ESI) m/z calcd for $C_{13}H_{22}NO_2^+$ $(M+H)^+$ 224.16451, found 224.16464.

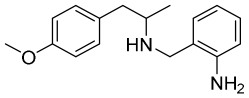
2-(((1-phenylethyl)amino)methyl)aniline (76) [44]



76

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as white solid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 62 mg, 91% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.21 (m, 5H), 7.06 (m, 1H), 6.93 (m, 1H), 6.64 (t, J = 7.5 Hz, 2H), 4.19 (s, 2H), 3.76 (q, J = 6.6 Hz, 1H), 3.61 (d, J = 1.3 Hz, 2H), 1.37 (d, J = 6.7 Hz, 3H).

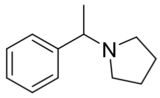
2-(((1-(4-methoxyphenyl)propan-2-yl)amino)methyl)aniline (77)



77

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 73 mg, 90% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.11 – 6.57 (m, 8H), 4.55 (s, 2H), 3.86 (d, J = 12.3 Hz, 1H), 3.78 (s, 3H), 3.68 (d, J = 12.3 Hz, 1H), 2.89 (h, J = 6.4 Hz, 1H), 2.62 (m, 2H), 1.10 (d, J = 6.3 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.00, 146.99, 131.54, 130.26, 129.67, 128.25, 124.44, 117.68, 115.72, 113.74, 55.28, 54.46, 50.63, 42.73, 20.27. HRMS (ESI) m/z calcd for $C_{17}H_{23}N_2O^+$ $(M+H)^+$ 271.18049, found 271.18051.

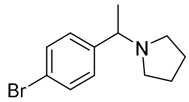
1-(1-phenylethyl)pyrrolidine (78) [41]



78

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 48 mg, 91% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.38 – 7.20 (m, 5H), 3.23 (q, J = 6.6 Hz, 1H), 2.64 – 2.56 (m, 2H), 2.41 (m, 2H), 1.84 – 1.72 (m, 4H), 1.43 (d, J = 6.6 Hz, 3H).

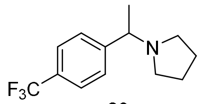
1-(1-(4-bromophenyl)ethyl)pyrrolidine (79) [45]



79

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 60:1 with 0.1% Et_3N) afforded the product as brown liquid, R_f = 0.4 (CH_2Cl_2:MeOH = 10:1), 73 mg, 96% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.46 – 7.39 (m, 2H), 7.25 – 7.19 (m, 2H), 3.17 (q, J = 6.6 Hz, 1H), 2.54 (m, 2H), 2.41 – 2.29 (m, 2H), 1.84 – 1.66 (m, 4H), 1.38 (d, J = 6.6 Hz, 3H).

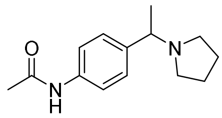
1-(1-(4-(trifluoromethyl)phenyl)ethyl)pyrrolidine (80) [45]



80

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 60:1 with 0.1% Et_3N) afforded the product as yellow liquid, R_f = 0.4 (CH_2Cl_2:MeOH = 10:1), 71 mg, 97% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.56 (d, J = 7.7 Hz, 2H), 7.46 (d, J = 7.9 Hz, 2H), 3.23 (q, J = 6.5, 4.7 Hz, 1H), 2.45 (m, 4H), 1.86 – 1.68 (m, 4H), 1.39 (m, 3H).

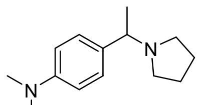
***N*-(4-(1-(pyrrolidin-1-yl)ethyl)phenyl)acetamide (81)**



81

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as white solid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 65 mg, 93% yield, white solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.97 (s, 1H), 7.53 – 7.24 (m, 4H), 3.22 (q, J = 6.6 Hz, 1H), 2.59 (m, 2H), 2.41 (m, 2H), 2.16 (s, 3H), 1.86 – 1.67 (m, 4H), 1.41 (d, J = 6.6 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.63, 140.69, 136.94, 127.79, 120.00, 65.52, 52.94, 24.50, 23.39, 22.77. HRMS (ESI) m/z calcd for $C_{14}H_{21}N_2O^+$ $(M+H)^+$ 233.16484, found 233.16505.

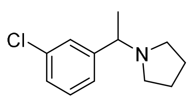
***N*,*N*-dimethyl-4-(1-(pyrrolidin-1-yl)ethyl)aniline (82)**



82

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 65 mg, 99% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.20 (d, J = 8.2 Hz, 2H), 6.69 (d, J = 8.3 Hz, 2H), 3.14 (q, J = 6.6 Hz, 1H), 2.92 (s, 6H), 2.56 (m, 2H), 2.38 (m, 2H), 1.77 (d, J = 3.7 Hz, 4H), 1.40 (d, J = 6.6 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 128.01, 112.44, 65.21, 52.95, 40.75, 23.41, 22.88. HRMS (ESI) m/z calcd for $C_{14}H_{23}N_2^+$ $(M+H)^+$ 219.18558, found 219.18532.

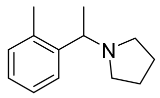
1-(1-(3-chlorophenyl)ethyl)pyrrolidine (83) [45]



83

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 60:1 with 0.1% Et_3N) afforded the product as brown liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 60 mg, 96% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.18 (m, 4H), 3.17 (m, 1H), 2.55 (q, J = 6.7 Hz, 2H), 2.38 (q, J = 5.4, 3.8 Hz, 2H), 1.77 (h, J = 3.0 Hz, 4H), 1.38 (m, 3H).

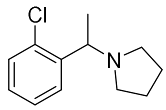
1-(1-(o-tolyl)ethyl)pyrrolidine (84) [45]



84

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.4 (CH_2Cl_2:MeOH = 10:1), 56 mg, 99% yield. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.60 – 7.00 (m, 4H), 3.45 (q, J = 6.5 Hz, 1H), 2.53 (m, 2H), 2.42 (m, 2H), 2.34 (s, 3H), 1.81 – 1.70 (m, 4H), 1.32 (d, J = 6.6 Hz, 3H).

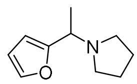
1-(1-(2-chlorophenyl)ethyl)pyrrolidine (85) [45]



85

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as yellow liquid, R_f = 0.4 (CH_2Cl_2:MeOH = 10:1), 61 mg, 97% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.63 (d, J = 7.8 Hz, 1H), 7.29 (dd, J = 21.4, 7.4 Hz, 2H), 7.14 (t, J = 7.7 Hz, 1H), 3.83 (m, 1H), 2.53 (m, 4H), 1.78 (h, J = 2.9 Hz, 4H), 1.36 (m, 3H).

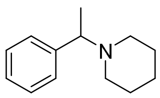
1-(1-(furan-2-yl)ethyl)pyrrolidine (86)



86

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as brown liquid, R_f = 0.3 (CH_2Cl_2:MeOH = 10:1), 49 mg, 99% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.33 (d, J = 1.6 Hz, 1H), 6.29 (p, J = 1.2 Hz, 1H), 6.13 (d, J = 3.2 Hz, 1H), 3.55 (q, J = 6.8 Hz, 1H), 2.59 (m, 2H), 2.50 – 2.42 (m, 2H), 1.81 – 1.71 (m, 4H), 1.45 (d, J = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.14, 141.20, 109.70, 105.86, 56.58, 51.47, 23.34, 19.06. HRMS (ESI) m/z calcd for $C_{10}H_{16}NO^+$ $(M+H)^+$ 166.12264, found 166.12271.

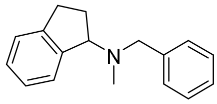
1-(1-phenylethyl)piperidine (87) [39]



87

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 56 mg, 92% yield. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.33 – 7.19 (m, 5H), 3.39 (q, J = 6.8 Hz, 1H), 2.37 (m, 4H), 1.55 (m, 4H), 1.38 (m, 5H).

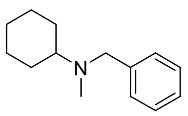
***N*-benzyl-*N*-methyl-2,3-dihydro-1H-inden-1-amine (88)** [46]



88

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as brown liquid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 65 mg, 91% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.49 – 7.44 (m, 1H), 7.38 (d, J = 6.9 Hz, 2H), 7.31 (m, 2H), 7.26 – 7.19 (m, 4H), 4.48 (t, J = 7.3 Hz, 1H), 3.61 (d, J = 13.2 Hz, 1H), 3.44 (d, J = 13.3 Hz, 1H), 2.95 (m, 1H), 2.82 (m, 1H), 2.18 (s, 3H), 2.14 – 2.07 (m, 2H).

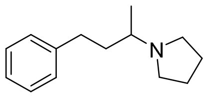
***N*-benzyl-*N*-methylcyclohexanamine (89)** [47]



89

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 60 mg, 98% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.17 (m, 5H), 3.56 (s, 2H), 2.44 (m, 1H), 2.19 (s, 3H), 1.92 – 1.75 (m, 4H), 1.66 – 1.57 (m, 1H), 1.35 – 1.06 (m, 5H).

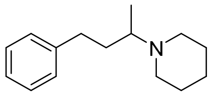
1-(4-phenylbutan-2-yl)pyrrolidine (90) [45]



90

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as yellow liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 60 mg, 99% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.06 (m, 5H), 2.72 (m, 1H), 2.62 – 2.51 (m, 5H), 2.34 (m, 1H), 1.92 (m, 1H), 1.81 – 1.62 (m, 5H), 1.15 (d, J = 6.4 Hz, 3H).

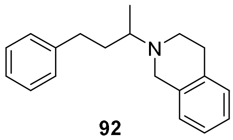
1-(4-phenylbutan-2-yl)piperidine (91) [48]



91

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as brown liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 63 mg, 96% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.31 – 7.13 (m, 5H), 2.72 – 2.47 (m, 5H), 2.41 (m, 2H), 1.89 (m, 1H), 1.65 – 1.49 (m, 5H), 1.42 (p, J = 6.0 Hz, 2H), 1.01 (d, J = 6.6 Hz, 3H).

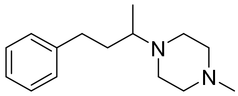
2-(4-phenylbutan-2-yl)-1,2,3,4-tetrahydroisoquinoline (92) [49]



92

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as brown liquid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 79 mg, 99% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.29 – 6.97 (m, 9H), 3.82 – 3.60 (m, 2H), 2.90 – 2.60 (m, 7H), 1.95 (m, 1H), 1.65 (m, 1H), 1.07 (d, J = 6.5 Hz, 3H).

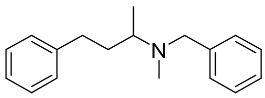
1-methyl-4-(4-phenylbutan-2-yl)piperazine (93) [48]



93

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 63 mg, 91% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.33 – 7.14 (m, 5H), 2.77 – 2.32 (m, 11H), 2.29 (s, 3H), 1.85 (m, 1H), 1.56 (m, 1H), 1.00 (d, J = 6.5 Hz, 3H).

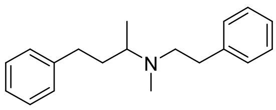
***N*-benzyl-*N*-methyl-4-phenylbutan-2-amine (94) [48]**



94

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.4 (CH_2Cl_2:MeOH = 10:1), 74 mg, 98% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.40 – 7.08 (m, 10H), 3.60 (d, J = 13.4 Hz, 1H), 3.45 (d, J = 13.3 Hz, 1H), 2.92 – 2.61 (m, 3H), 2.14 (s, 3H), 1.89 (m, 1H), 1.58 (m, 1H), 1.02 (dd, J = 6.6, 1.6 Hz, 3H).

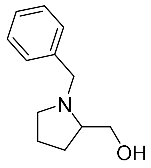
***N*-methyl-*N*-phenethyl-4-phenylbutan-2-amine (95) [50]**



95

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 79 mg, 99% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.30 – 7.09 (m, 10H), 2.80 – 2.50 (m, 7H), 2.27 (s, 3H), 1.85 – 1.74 (m, 1H), 1.57 – 1.46 (m, 1H), 0.95 (d, J = 6.6 Hz, 3H).

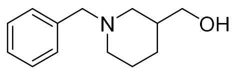
(1-benzylpyrrolidin-2-yl)methanol (96) [51]



96

Purified by column chromatography (silica gel, CH_2Cl_2 : MeOH = 30 : 1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.7 (CH_2Cl_2:MeOH = 10:1), 55 mg, 95% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.27 – 7.08 (m, 5H), 3.86 (d, J = 12.9 Hz, 1H), 3.53 (dd, J = 10.8, 3.8 Hz, 1H), 3.34 (dd, J = 10.8, 2.5 Hz, 1H), 3.25 (d, J = 13.0 Hz, 1H), 3.02 (s, 1H), 2.85 (m, 1H), 2.61 (m, 1H), 2.23 – 2.11 (m, 1H), 1.87 – 1.66 (m, 2H), 1.57 (m, 2H).

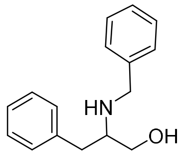
(1-benzylpiperidin-3-yl)methanol (97) [52]



97

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 59 mg, 95% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.19 (m, 5H), 3.58 – 3.38 (m, 5H), 2.85 (dd, J = 11.4, 3.6 Hz, 1H), 2.63 (dd, J = 10.9, 5.7 Hz, 1H), 2.09 (t, J = 9.8 Hz, 1H), 1.95 (t, J = 10.1 Hz, 1H), 1.83 – 1.62 (m, 3H), 1.56 (m, 1H), 1.08 (dd, J = 11.4, 7.7 Hz, 1H).

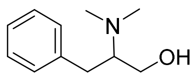
2-(benzylamino)-3-phenylpropan-1-ol (98) [53]



98

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as white solid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 64 mg, 89% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.42 – 7.18 (m, 10H), 4.68 (s, 1H), 3.80 (s, 2H), 3.67 (dd, J = 10.9, 3.8 Hz, 1H), 3.40 (dd, J = 10.9, 5.5 Hz, 1H), 3.02 – 2.95 (m, 1H), 2.82 (m, 2H).

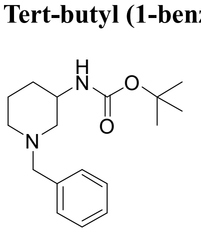
2-(dimethylamino)-3-phenylpropan-1-ol (99) [54]



99

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as white solid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 50 mg, 93% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.30 – 7.10 (m, 5H), 3.42 – 3.28 (m, 2H), 3.18 (s, 1H), 2.94 – 2.81 (m, 2H), 2.33 (s, 6H).

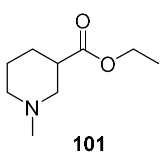
Tert-butyl (1-benzylpiperidin-3-yl)carbamate (100) [55]



100

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.7 (CH_2Cl_2:MeOH = 10:1), 86 mg, 99% yield.^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.39 – 7.17 (m, 5H), 5.05 (s, 1H), 3.74 (s, 1H), 3.45 (s, 2H), 2.60 – 2.12 (m, 4H), 1.75 – 1.47 (m, 4H), 1.43 (s, 9H).

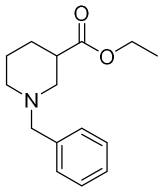
Ethyl 1-methylpiperidine-3-carboxylate (101) [56]



101

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 47 mg, 92% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 4.13 (m, 2H), 2.94 (d, J = 11.3 Hz, 1H), 2.71 (d, J = 11.3 Hz, 1H), 2.57 (m, 1H), 2.28 (d, J = 2.8 Hz, 3H), 2.10 (t, J = 10.9 Hz, 1H), 1.95 (t, J = 11.1 Hz, 2H), 1.73 (m, 1H), 1.67 – 1.52 (m, 1H), 1.47 – 1.35 (m, 1H), 1.30 – 1.21 (m, 3H).

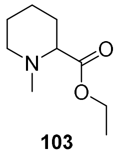
Ethyl 1-benzylpiperidine-3-carboxylate (102) [51]



102

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 70 mg, 94% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.42 – 7.15 (m, 5H), 4.10 (m, 2H), 3.51 (m, 2H), 2.94 (d, *J* = 11.1 Hz, 1H), 2.71 (d, *J* = 10.9 Hz, 1H), 2.57 (m, 1H), 2.22 (t, *J* = 10.7 Hz, 1H), 2.04 (d, *J* = 2.8 Hz, 1H), 1.96 – 1.86 (m, 1H), 1.71 (m, 1H), 1.64 – 1.38 (m, 2H), 1.22 (m, 3H).

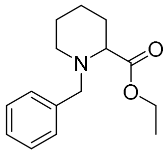
Ethyl 1-methylpiperidine-2-carboxylate (103) [56]



103

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 47 mg, 91% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 4.20 – 4.08 (m, 2H), 2.98 – 2.89 (m, 1H), 2.71 (m, 1H), 2.57 (m, 1H), 2.28 (s, 3H), 2.10 (t, *J* = 10.8 Hz, 1H), 1.95 (m, 2H), 1.73 (m, 1H), 1.58 (m, 1H), 1.46 – 1.34 (m, 1H), 1.25 (t, *J* = 7.1 Hz, 3H).

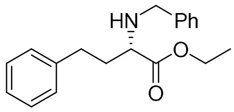
Ethyl 1-benzylpiperidine-2-carboxylate (104) [51]



104

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 70 mg, 95% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.18 (m, 5H), 4.26 – 4.12 (m, 2H), 3.80 (d, *J* = 13.2 Hz, 1H), 3.39 (d, *J* = 13.3 Hz, 1H), 3.13 (m, 1H), 2.97 – 2.89 (m, 1H), 2.13 (m, 1H), 1.90 – 1.74 (m, 2H), 1.65 – 1.49 (m, 3H), 1.35 (m, 1H), 1.27 (t, *J* = 7.2 Hz, 3H).

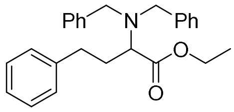
Ethyl (*S*)-2-(benzylamino)-4-phenylbutanoate (105) [57]



105

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 100:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.8 (CH_2Cl_2:MeOH = 10:1), 81 mg, 91% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.07 (m, 10H), 4.16 (q, *J* = 7.1 Hz, 2H), 3.81 (d, *J* = 12.9 Hz, 1H), 3.61 (d, *J* = 12.9 Hz, 1H), 3.25 (dd, *J* = 7.6, 5.8 Hz, 1H), 2.72 (m, 2H), 1.92 – 1.82 (m, 2H), 1.25 (t, *J* = 7.2 Hz, 3H).

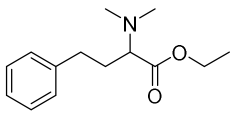
Ethyl 2-(dibenzylamino)-4-phenylbutanoate (106) [58]



106

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 100:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.9 (CH_2Cl_2:MeOH = 10:1), 113 mg, 97% yield, colorless liquid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.44 – 6.98 (m, 15H), 4.21 (m, 2H), 3.97 (dd, *J* = 13.8, 6.8 Hz, 2H), 3.66 – 3.54 (m, 2H), 3.38 (q, *J* = 7.4 Hz, 1H), 2.79 (m, 1H), 2.47 (m, 1H), 2.03 (p, *J* = 7.6 Hz, 2H), 1.32 (q, *J* = 6.7 Hz, 3H).

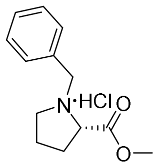
Ethyl 2-(dimethylamino)-4-phenylbutanoate (107) [59]



107

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 80:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.8 (CH_2Cl_2:MeOH = 10:1), 62 mg, 88% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.32 – 7.13 (m, 5H), 4.18 (m, 2H), 3.12 (t, *J* = 7.4 Hz, 1H), 2.65 (t, *J* = 7.9 Hz, 2H), 2.35 (s, 6H), 2.09 – 1.89 (m, 2H), 1.28 (t, *J* = 7.1 Hz, 3H).

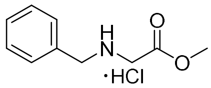
Methyl benzyl-*L*-prolinate (108) [60]



108

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.7 (CH_2Cl_2:MeOH = 10:1), 64 mg, 98% yield, 99% *ee* for (*S*)-117. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.17 (m, 5H), 3.88 (d, *J* = 12.8 Hz, 1H), 3.63 (s, 3H), 3.56 (d, *J* = 12.7 Hz, 1H), 3.24 (m, 1H), 3.04 (m, 1H), 2.42 – 2.34 (m, 1H), 2.12 (m, 1H), 2.00 – 1.70 (m, 3H). The enantiomeric excess was determined by HPLC on OJ-H column, hexane: isopropanol = 90: 10; flow rate = 1 mL/min; UV detection at 220 nm;

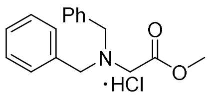
Methyl benzylglycinate (109) [61]



109

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 60:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.4 (CH_2Cl_2:MeOH = 10:1), 51 mg, 94% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.19 (m, 5H), 3.79 (s, 2H), 3.70 (s, 3H), 3.40 (s, 2H), 2.02 (s, 1H).

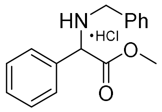
Methyl dibenzylglycinate (110) [62]



110

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 60:1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.8 (CH_2Cl_2:MeOH = 10:1), 73 mg, 90% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.41 – 7.21 (m, 10H), 3.80 (s, 4H), 3.67 (s, 3H), 3.30 (s, 2H).

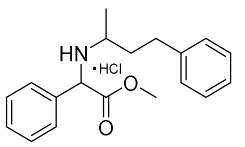
Methyl 2-(benzylamino)-2-phenylacetate (111) [63]



111

Purified by column chromatography (silica gel, Petroleum ether : EtOAc = 20 : 1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.5 (Petroleum ether:EtOAc = 10:1), 71 mg, 93% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.44 – 7.15 (m, 10H), 4.39 (s, 1H), 3.71 (d, *J* = 1.6 Hz, 2H), 3.65 (s, 3H), 2.31 (s, 1H).

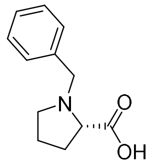
Methyl 2-phenyl-2-((4-phenylbutan-2-yl)amino)acetate (112)



112

Purified by column chromatography (silica gel, Petroleum ether : EtOAc = 20 : 1 with 0.1% Et_3N) afforded the product as colorless liquid, R_f = 0.5 (Petroleum ether:EtOAc = 10:1), 81 mg, 91% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.43 – 7.02 (m, 10H), 4.48 (d, *J* = 1.5 Hz, 1H), 3.67 (d, *J* = 2.6 Hz, 3H), 2.75 – 2.52 (m, 3H), 2.00 (s, 1H), 1.87 – 1.59 (m, 2H), 1.09 (dd, *J* = 6.3, 2.4 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.95, 142.31, 128.76, 128.73, 128.37, 128.35, 128.33, 128.04, 127.53, 127.36, 125.77, 125.72, 62.87, 62.73, 52.30, 52.23, 50.57, 50.13, 38.86, 38.51, 32.12, 32.10, 20.47, 20.23. HRMS (ESI) m/z calcd for $C_{19}H_{24}NO_2^+$ $(M+H)^+$ 298.18016, found 298.18076.

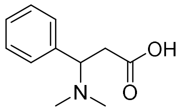
Benzyl-*L*-proline (113) [51]



113

Purification procedures: The solvent was removed under reduced pressure. The residue was rinses with *n*-hexane (2 mL*2), and filtered under reduced pressure to obtain the product as white solid. R_f = 0.3 (CH_2Cl_2:MeOH = 10:1), 61 mg, 99% yield, 99% *ee* for (*S*)-**122**. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.49 – 7.32 (m, 5H), 4.28 (dd, *J* = 71.5, 13.0 Hz, 2H), 3.82 (dd, *J* = 9.1, 6.4 Hz, 1H), 3.68 (m, 1H), 2.88 (m, 1H), 2.42 – 2.18 (m, 2H), 2.12 – 1.84 (m, 2H).

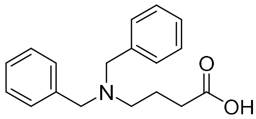
3-(dimethylamino)-3-phenylpropanoic acid (114) [64]



114

Purification procedures: The solvent was removed under reduced pressure. The residue was rinses with *n*-hexane (2 mL*2), and filtered under reduced pressure to obtain the product as white solid. R_f = 0.3 (CH_2Cl_2:MeOH = 10:1), 57 mg, 99% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 13.03 (s, 1H), 7.54 – 7.19 (m, 5H), 4.29 (dd, J = 11.5, 4.4 Hz, 1H), 3.07 (dd, J = 16.6, 11.3 Hz, 1H), 2.62 (dd, J = 16.6, 4.4 Hz, 1H), 2.42 (s, 6H).

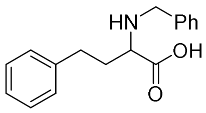
4-(dibenzylamino)butanoic acid (115) [65]



115

Purification procedures: The solvent was removed under reduced pressure. The residue was rinses with *n*-hexane (2 mL*2), and filtered under reduced pressure to obtain the product as white solid. R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 77 mg, 90% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 11.45 (s, 1H), 7.51 – 7.22 (m, 10H), 3.72 (s, 4H), 2.66 (t, J = 6.0 Hz, 2H), 2.27 (t, J = 6.4 Hz, 2H), 1.80 (p, J = 6.1 Hz, 2H).

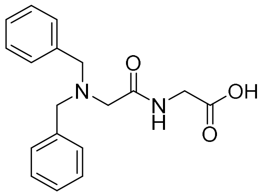
2-(benzylamino)-4-phenylbutanoic acid (116) [66]



116

Purification procedures: The solvent was removed under reduced pressure. The residue was rinses with *n*-hexane (2 mL*2), and filtered under reduced pressure to obtain the product as white solid. R_f = 0.2 (CH_2Cl_2:MeOH = 10:1), 78 mg, 96% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 12.31 (s, 1H), 7.50 – 6.90 (m, 10H), 4.16 (d, J = 56.6 Hz, 2H), 3.79 (t, J = 6.1 Hz, 1H), 2.80 – 2.56 (m, 2H), 2.19 (q, J = 7.6 Hz, 2H).

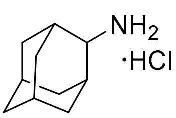
Dibenzylglycylglycine (117) [67]



117

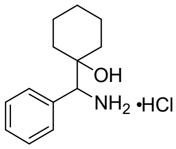
Purification procedures: The solvent was removed under reduced pressure. The residue was rinses with *n*-hexane:CH_2Cl_2 = 50:1 (2 mL*3), and filtered under reduced pressure to obtain the product as white solid. R_f = 0.4 (CH_2Cl_2:MeOH = 10:1), 88 mg, 94% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 11.19 – 10.74 (m, 1H), 7.86 (t, J = 4.8 Hz, 1H), 7.38 (d, J = 7.3 Hz, 4H), 7.27 (m, 6H), 3.94 (d, J = 4.8 Hz, 2H), 3.85 (s, 4H), 3.37 (s, 2H).

Adamantan-2-aminium chloride (120) [68]



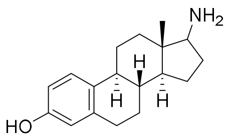
Purified by treatment with ethereal HCl (4.0 M) to form the corresponding HCl salt, white powder, 54.6 mg, 97% yield. ^1H NMR (400 MHz, DMSO-d_6) δ 8.42 (s, 3H), 3.26 (s, 1H), 2.12 – 2.01 (m, 4H), 1.86 – 1.66 (m, 8H), 1.53 (d, J = 12.9 Hz, 2H).

(1-hydroxycyclohexyl)(phenyl)methanamine hydrochloride (121) [68]



Purified by treatment with ethereal HCl (4.0 M) to form the corresponding HCl salt, white powder, 63.8 mg, 88% yield. ^1H NMR (400 MHz, DMSO-d_6) δ 8.47 (s, 3H), 7.52 – 7.43 (m, 2H), 7.43 – 7.33 (m, 3H), 5.03 (s, 1H), 4.11 (s, 1H), 1.82 – 0.94 (m, 10H).

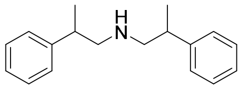
Estrone-NH$_2$ (122) [68]



122

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 5:1) afforded the product as off-white solid. R_f = 0.4 (CH_2Cl_2:MeOH = 10:1), 73 mg, 90% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.05 (d, J = 8.5 Hz, 1H), 6.58 – 6.38 (m, 2H), 3.38 (s, 2H), 3.05 (t, J = 8.9 Hz, 1H), 2.81 – 2.63 (m, 2H), 2.27 (m, 1H), 2.17 – 1.94 (m, 3H), 1.83 – 1.66 (m, 2H), 1.65 – 1.52 (m, 1H), 1.29 (q, J = 11.1, 8.9 Hz, 6H), 0.74 (s, 3H).

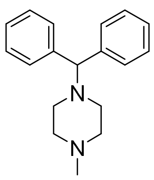
Bis(2-phenylpropyl)amine (124) [69]



124

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 20:1 with 0.1% Et_3N) afforded the product as colorless liquid. R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 70 mg, 92% yield. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.30 – 7.07 (m, 10H), 2.95 – 2.66 (m, 6H), 1.55 (s, 1H), 1.19 (dd, J = 6.9, 3.8 Hz, 6H).

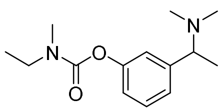
Cyclizine (125) [70]



125

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as white solid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 79 mg, 99% yield. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.44 – 7.38 (m, 4H), 7.25 (t, J = 7.6 Hz, 4H), 7.18 – 7.12 (m, 2H), 4.21 (s, 1H), 2.43 (s, 8H), 2.27 (s, 3H).

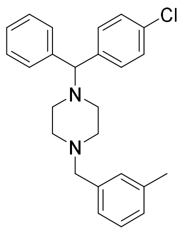
Rivastigmine (126) [71]



126

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.3 (CH_2Cl_2:MeOH = 10:1), 72 mg, 96% yield, the yield obtained from the reaction of 3-[1-(Methyamino)ethyl]phenyl N-ethyl-N-methyl carbamate [67] and Paraformaldehyde, 65 mg, 87% yield, the yield obtained from the reaction of Ethyl-methyl-carbamic acid 3-acetyl-phenyl ester [67] and dimethylamine methanol solution, ^{1}H NMR (400 MHz, Chloroform-d) δ 7.33 – 6.97 (m, 4H), 3.43 (m, 2H), 3.25 (q, J = 6.7 Hz, 1H), 3.02 (d, J = 29.4 Hz, 3H), 2.20 (s, 6H), 1.36 (d, J = 6.7 Hz, 3H), 1.21 (m, 3H).

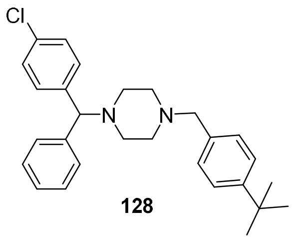
Ancolan (127) [72]



127

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as white solid, R_f = 0.4 (CH_2Cl_2:MeOH = 10:1), 110 mg, 94% yield. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.37 – 7.31 (m, 4H), 7.27 – 7.13 (m, 6H), 7.06 (dd, J = 22.6, 7.7 Hz, 3H), 4.20 (s, 1H), 3.47 (s, 2H), 2.46 (s, 8H), 2.31 (s, 3H).

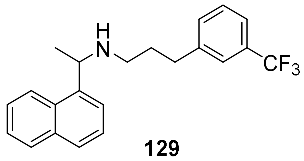
Buclizine (128) [72]



128

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as white solid, R_f = 0.4 (CH_2Cl_2:MeOH = 10:1), 123 mg, 95% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.28 (m, 6H), 7.24 – 7.13 (m, 7H), 4.19 (s, 1H), 3.47 (s, 2H), 2.43 (d, J = 23.4 Hz, 8H), 1.29 (s, 9H).

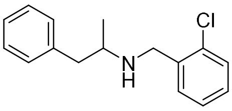
Cinacalcet (129) [73]



129

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.4 (CH_2Cl_2:MeOH = 10:1), 101 mg, 94% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.22 – 8.15 (m, 1H), 7.87 (dd, J = 7.5, 1.9 Hz, 1H), 7.74 (d, J = 8.2 Hz, 1H), 7.64 (dd, J = 7.3, 1.2 Hz, 1H), 7.54 – 7.38 (m, 5H), 7.37 – 7.26 (m, 2H), 4.62 (q, J = 6.6 Hz, 1H), 2.78 – 2.54 (m, 4H), 1.83 (p, J = 7.4 Hz, 2H), 1.49 (d, J = 6.5 Hz, 3H).

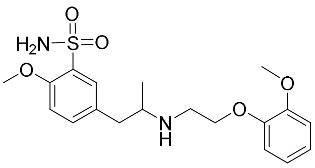
Clobenzorex (130) [74]



130

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.4 (CH_2Cl_2:MeOH = 10:1), 72 mg, 92% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.33 – 7.10 (m, 9H), 3.94 – 3.79 (m, 2H), 2.90 (h, J = 6.4 Hz, 1H), 2.80 – 2.60 (m, 2H), 1.69 (s, 1H), 1.11 (d, J = 6.2 Hz, 3H).

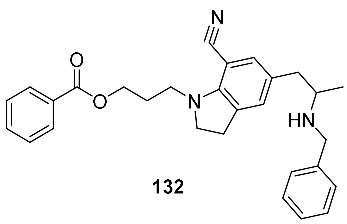
Tamsulosin analog (131) [75]



131

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as white solid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 110 mg, 93% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.57 (d, J = 2.3 Hz, 1H), 7.38 (dd, J = 8.4, 2.3 Hz, 1H), 7.12 – 6.84 (m, 7H), 3.98 (m, 2H), 3.87 (s, 3H), 3.72 (s, 3H), 2.98 – 2.70 (m, 4H), 2.49 – 2.42 (m, 1H), 1.69 (s, 1H), 0.92 (d, J = 6.1 Hz, 3H).

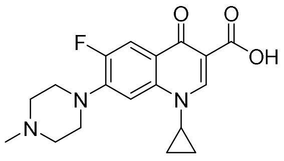
Silodosin derivative (132) [76]



132

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as yellow liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 135 mg, 99% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.09 – 8.04 (m, 2H), 7.55 (t, J = 7.3 Hz, 1H), 7.43 (t, J = 7.6 Hz, 2H), 7.31 (m, 2H), 7.23 (m, 3H), 6.92 (d, J = 8.6 Hz, 2H), 4.48 (t, J = 6.3 Hz, 2H), 3.88 – 3.70 (m, 4H), 3.58 (t, J = 8.7 Hz, 2H), 2.94 (t, J = 8.7 Hz, 2H), 2.83 (p, J = 6.4 Hz, 1H), 2.59 (dd, J = 13.7, 6.8 Hz, 1H), 2.46 (dd, J = 13.7, 6.5 Hz, 1H), 2.16 (p, J = 6.6 Hz, 2H), 1.67 (s, 1H), 1.06 (d, J = 6.2 Hz, 3H).

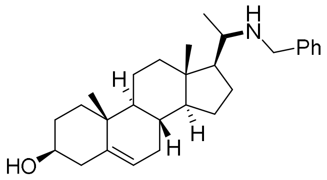
1-cyclopropyl-6-fluoro-7-(4-methylpiperazin-1-yl)-4-oxo-1,4-dihydroquinoline-3-carboxylic acid (133) [77]



133

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as white solid, R_f = 0.3 (CH_2Cl_2:MeOH = 10:1), 101 mg, 98% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.73 (s, 1H), 7.96 (d, *J* = 13.1 Hz, 1H), 7.36 (d, *J* = 7.2 Hz, 1H), 3.57 (tt, *J* = 7.2, 4.0 Hz, 1H), 3.37 (t, *J* = 4.9 Hz, 4H), 2.66 (t, *J* = 4.8 Hz, 4H), 2.40 (s, 3H), 1.46 – 1.14 (m, 5H).

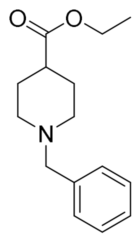
Pregnenolone + Benzylamine (134) [78]



134

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as white solid, R_f = 0.4 (CH_2Cl_2:MeOH = 10:1), 121 mg, 99% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.20 (m, 5H), 5.34 (m, 1H), 3.89 (d, *J* = 12.8 Hz, 1H), 3.62 (d, *J* = 12.8 Hz, 1H), 3.51 (m, 1H), 2.59 (m, 1H), 2.32 – 2.18 (m, 2H), 2.03 – 1.78 (m, 5H), 1.74 – 1.32 (m, 10H), 1.27 – 1.18 (m, 1H), 1.16 (d, *J* = 6.1 Hz, 3H), 1.14 – 1.02 (m, 3H), 1.00 (s, 3H), 0.94 (m, 1H), 0.66 (s, 3H).

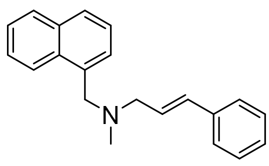
Donepezil intermediate (135) [51]



135

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 40:1 with 0.1% Et_3N) afforded the product as yellow liquid, R_f = 0.5 (CH_2Cl_2:MeOH = 10:1), 70 mg, 95% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.32 (m, 1H), 7.31 – 7.29 (m, 3H), 7.27 – 7.21 (m, 1H), 4.11 (q, *J* = 7.1 Hz, 2H), 3.47 (s, 2H), 2.83 (m, 2H), 2.26 (m, 1H), 2.01 (m, 2H), 1.93 – 1.64 (m, 4H), 1.23 (t, *J* = 7.1 Hz, 3H).

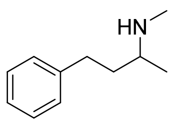
Naftifine (136) [79]



136

Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 50:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.6 (CH_2Cl_2:MeOH = 10:1), 83 mg, 96% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.37 – 8.29 (m, 1H), 7.92 – 7.85 (m, 1H), 7.81 (m, 1H), 7.59 – 7.38 (m, 6H), 7.37 – 7.30 (m, 2H), 7.28 – 7.23 (m, 1H), 6.66 – 6.55 (m, 1H), 6.41 (m, 1H), 3.99 (s, 2H), 3.32 (m, 2H), 2.31 (s, 3H).

***N*-methyl-4-phenylbutan-2-amine (139) [80]**

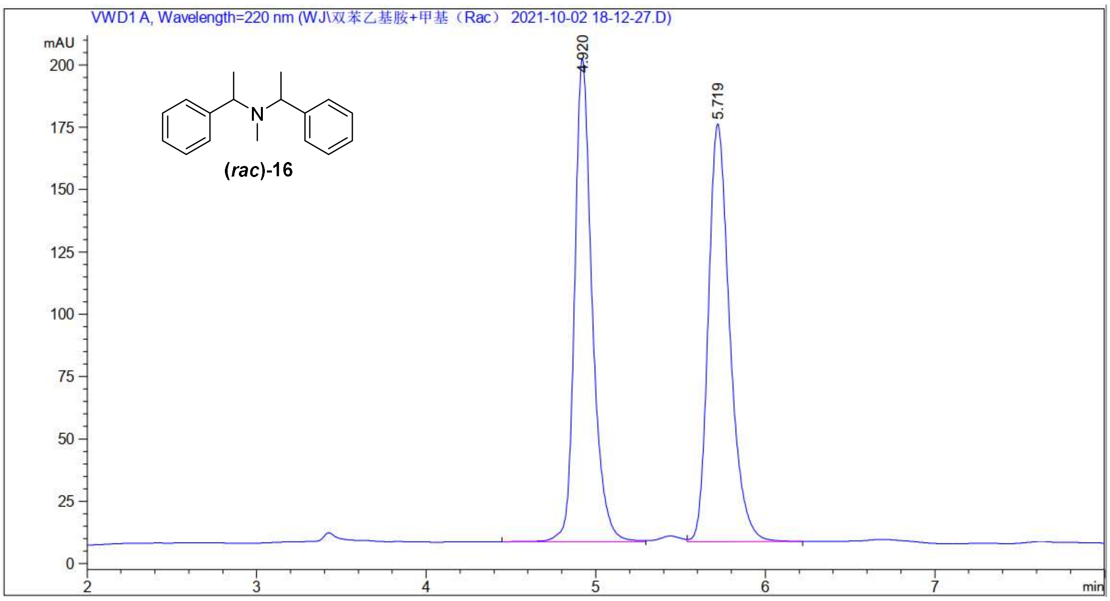


139

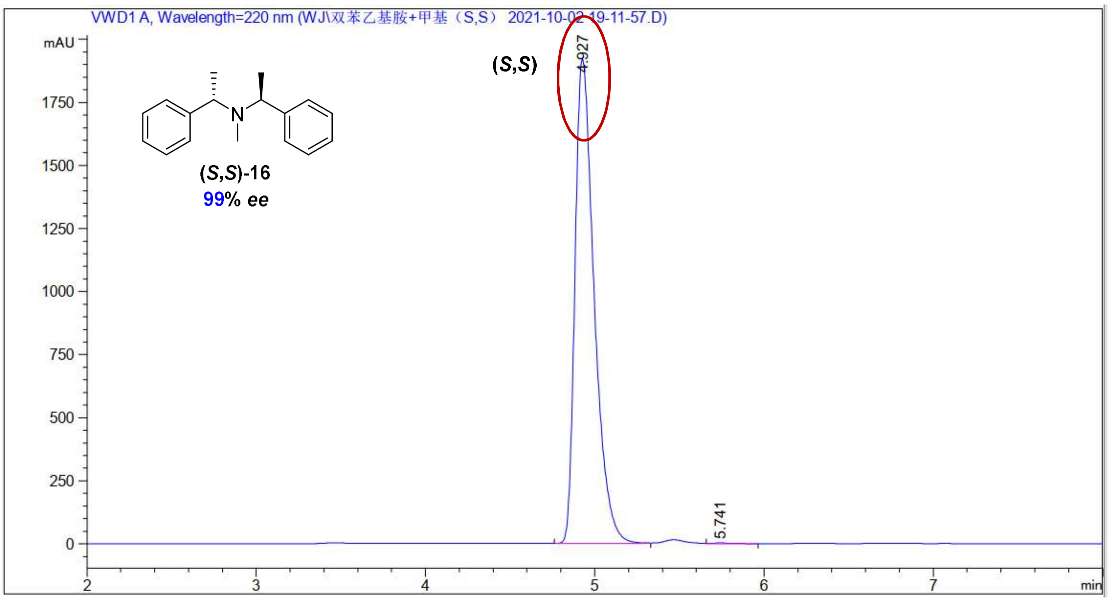
Purified by column chromatography (silica gel, CH_2Cl_2:MeOH = 30:1 with 0.1% Et_3N) afforded the product as light yellow liquid, R_f = 0.3 (CH_2Cl_2:MeOH = 10:1), 42 mg, 86% yield, the yield obtained from the reaction of Benzyl acetone and Methylamine ethanol solution. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.32 – 7.12 (m, 5H), 2.71 – 2.53 (m, 3H), 2.39 (s, 3H), 2.03 (s, 1H), 1.79 (m, 1H), 1.61 (m, 1H), 1.09 (d, J = 6.3 Hz, 3H).

III. GC and HPLC spectra

(*S,S*)-bis(1-phenylethyl)amine ((*S,S*)-16): 99% *ee*. HPLC conditions: OJ-3, hexane: isopropanol = 90: 10, 1 mL/min, 220 nm, 4.9 min (*S,S*), 5.7 min (*R,R*).

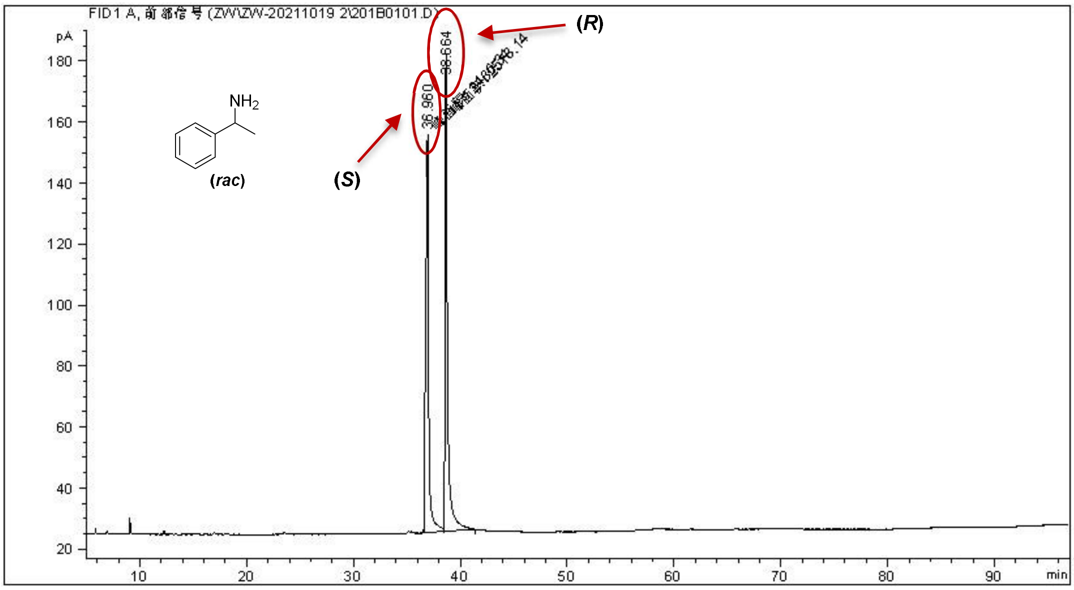


#	[min]		[min]	[mAU*s]	[mAU]	%
1	4.920	BV	0.1090	1393.29761	193.62140	48.6346
2	5.719	VB	0.1345	1471.52771	167.44519	51.3654

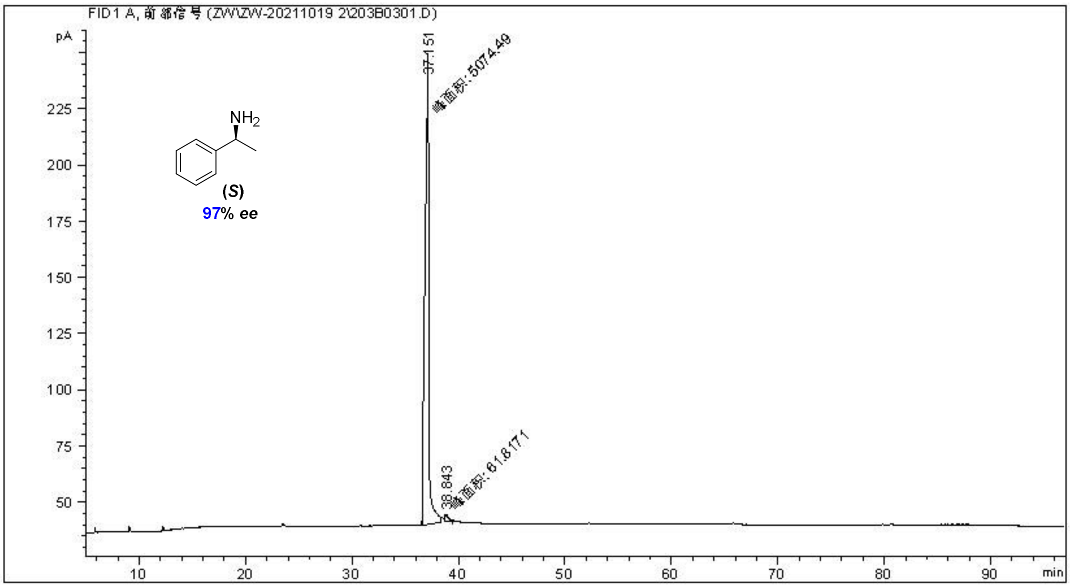


#	[min]		[min]	[mAU*s]	[mAU]	%
1	4.927	VV	0.1197	1.50930e4	1920.67334	99.8836
2	5.741	VB	0.1203	17.59029	2.17696	0.1164

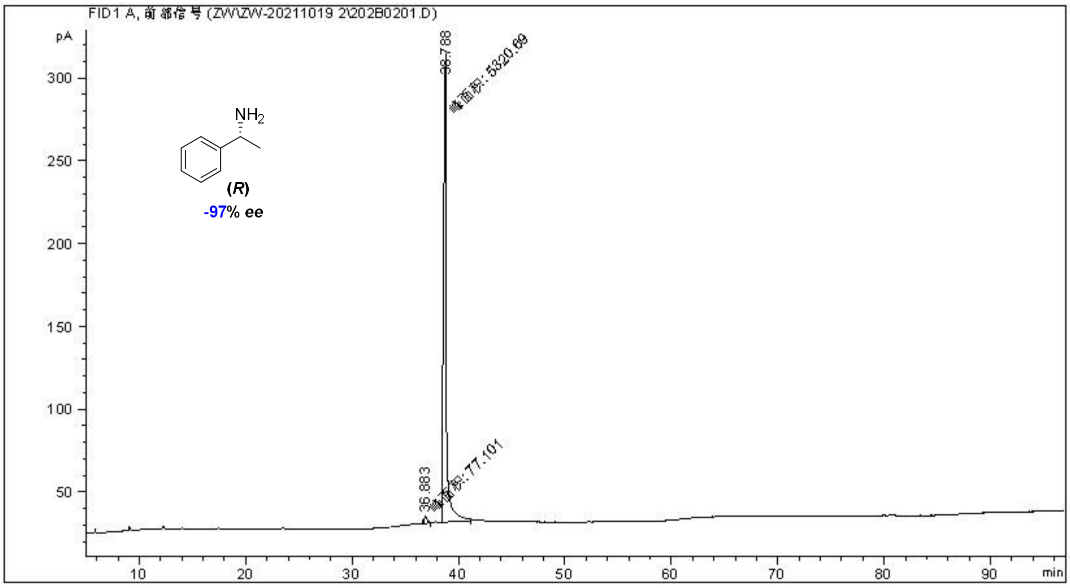
(***S***)-***N*-benzyl-1-phenylethan-1-amine ((*S*)-30)**, 97% *ee*; (***R***)-***N*-benzyl-1-phenylethan-1-amine ((*R*)-30)**, 96% *ee*. *ee* values were determined after acetylation by HPLC. The *ee* values for starting materials (*S*)-1-phenylethan-1-amine and (*R*)-1-phenylethan-1-amine was both 97%, which was determined by GC. GC conditions for 1-phenylethan-1-amine starting material: CP-7502, Chiralsil Dex CP, from 100 °C to 170 °C at 1 °C/min， 0.5 mL/min, 37.0 min (*S*), 38.7 min (*R*). HPLC conditions: AD-H, hexane: isopropanol = 90: 10, 1 mL/min, 220 nm, 8.1 (*R*), 9.4 (*S*).



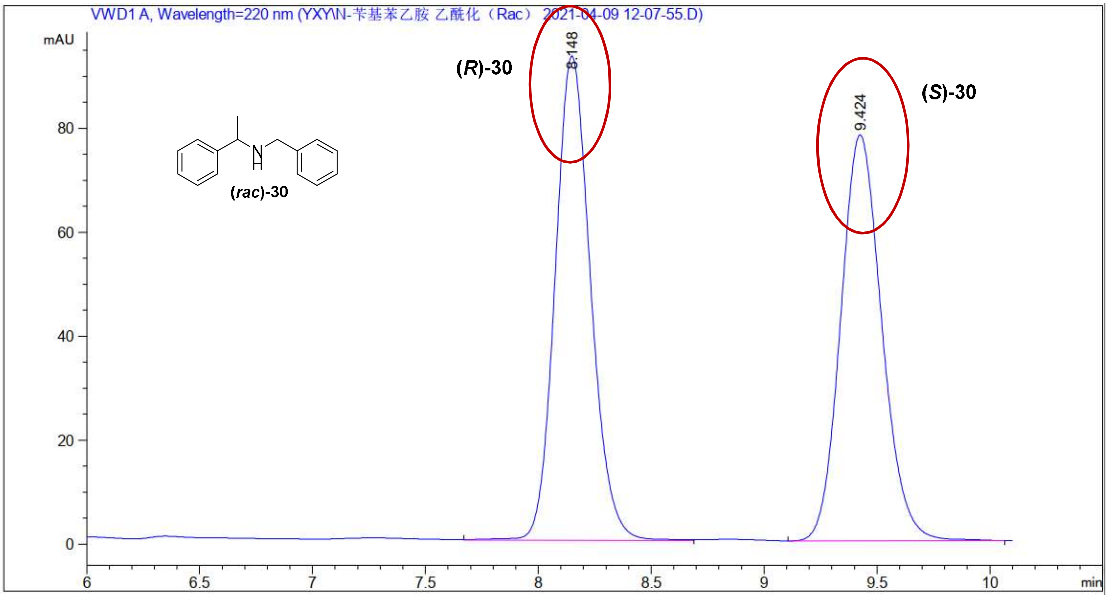
#	[min]		[min]	[pA*s]	[pA]	%
1	36.960	MF	0.3161	2480.34302	130.75916	49.62191
2	38.664	FM	0.2678	2518.14014	156.68954	50.37809



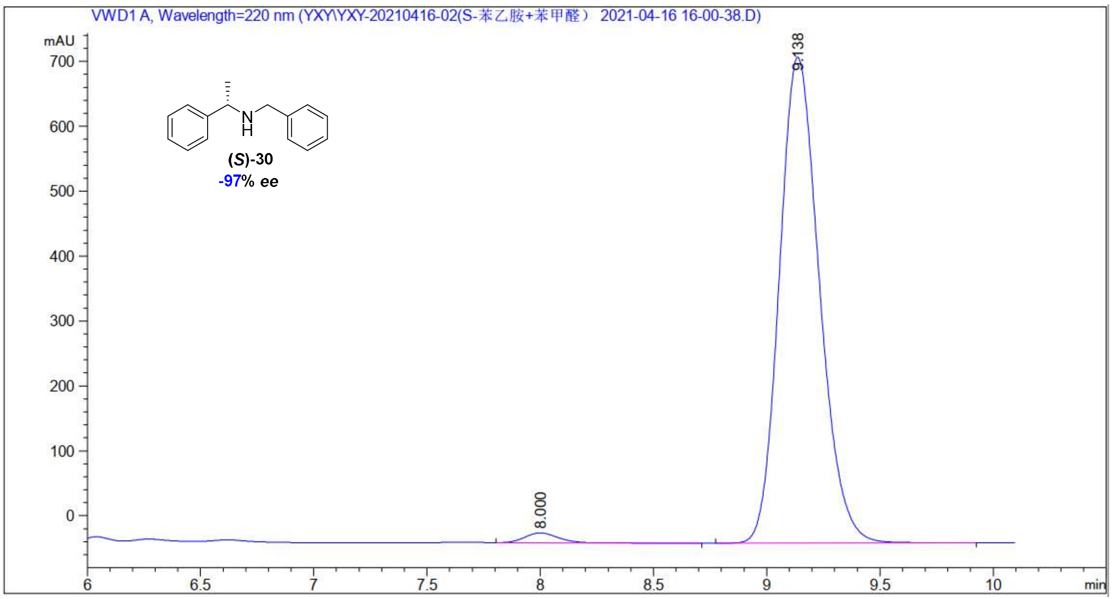
#	[min]		[min]	[pA*s]	[pA]	%
1	37.151	MM	0.4044	5074.49414	209.14543	98.79647
2	38.843	MM	0.3234	61.81708	3.18618	1.20353



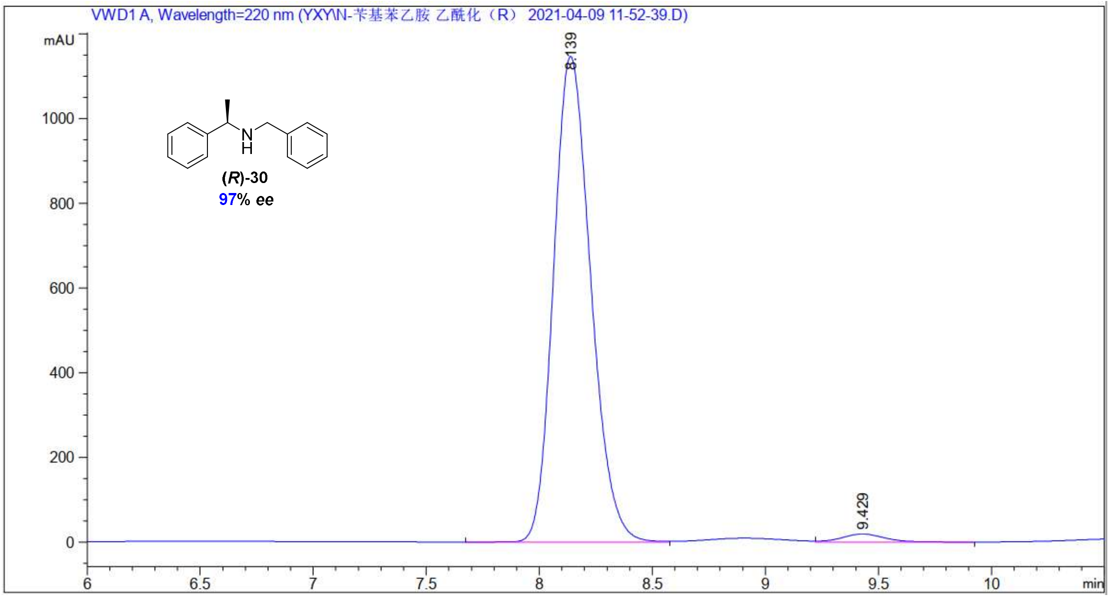
#	[min]		[min]	[pA*s]	[pA]	%
1	36.883	MM	0.2920	77.10102	4.40143	1.42838
2	38.788	MM	0.3137	5320.69385	282.66525	98.57162



#	[min]		[min]	[mAU*s]	[mAU]	%
1	8.148	VV	0.1674	1017.96710	93.18456	50.7383
2	9.424	BB	0.1977	988.34363	78.08629	49.2617

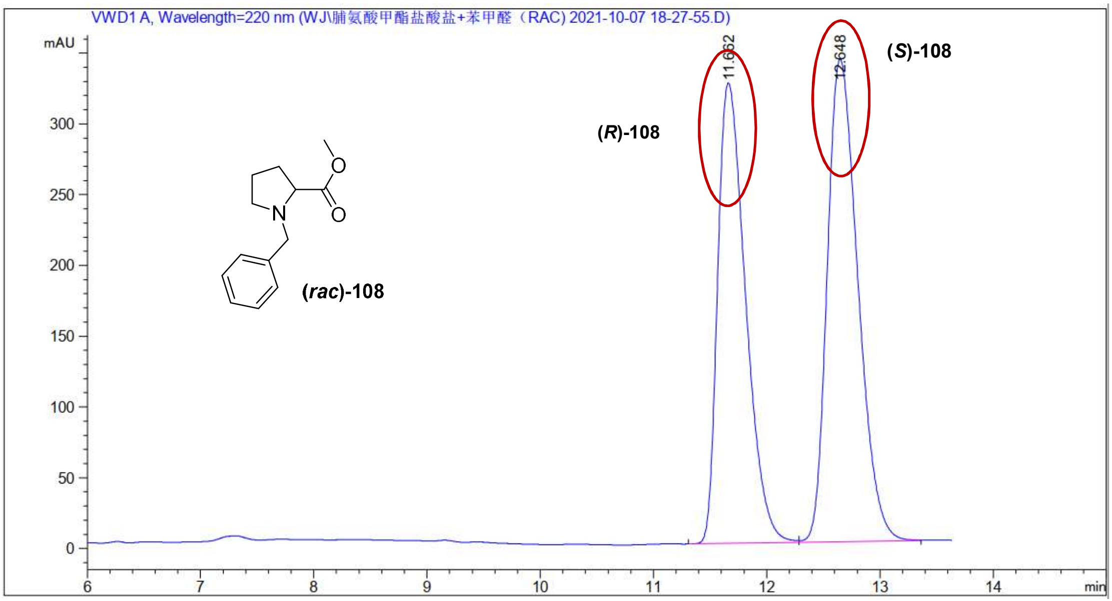


#	[min]		[min]	[mAU*s]	[mAU]	%
1	8.000	VB	0.1622	160.71053	15.34349	1.7223
2	9.138	BB	0.1910	9170.25195	748.18610	98.2777

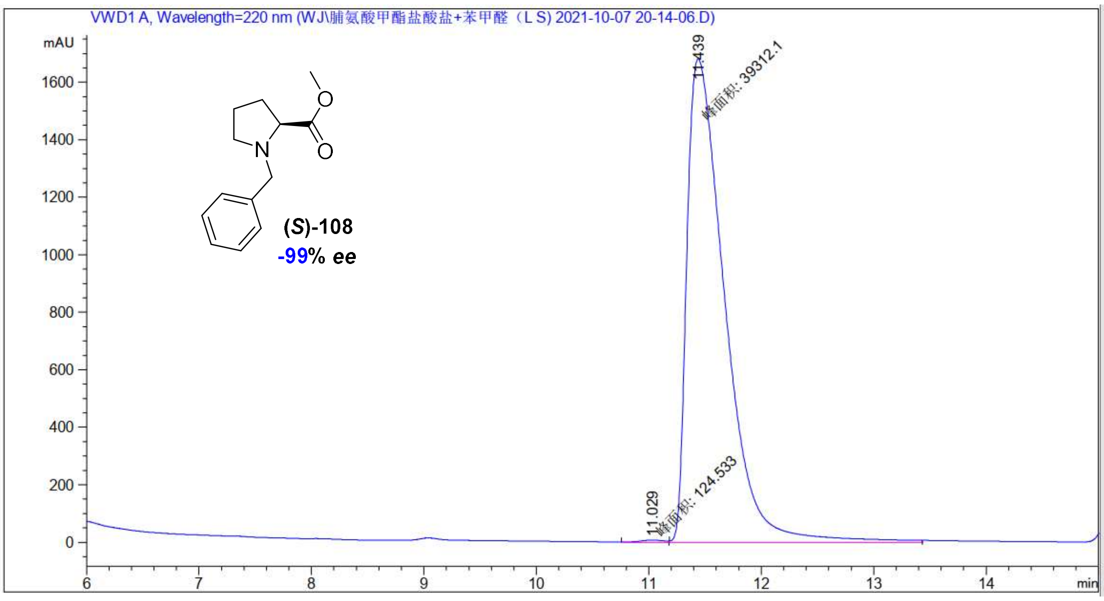


#	[min]		[min]	[mAU*s]	[mAU]	%
1	8.139	BV	0.1794	1.31081e4	1146.41858	98.1447
2	9.429	VB	0.1999	247.78821	19.03142	1.8553

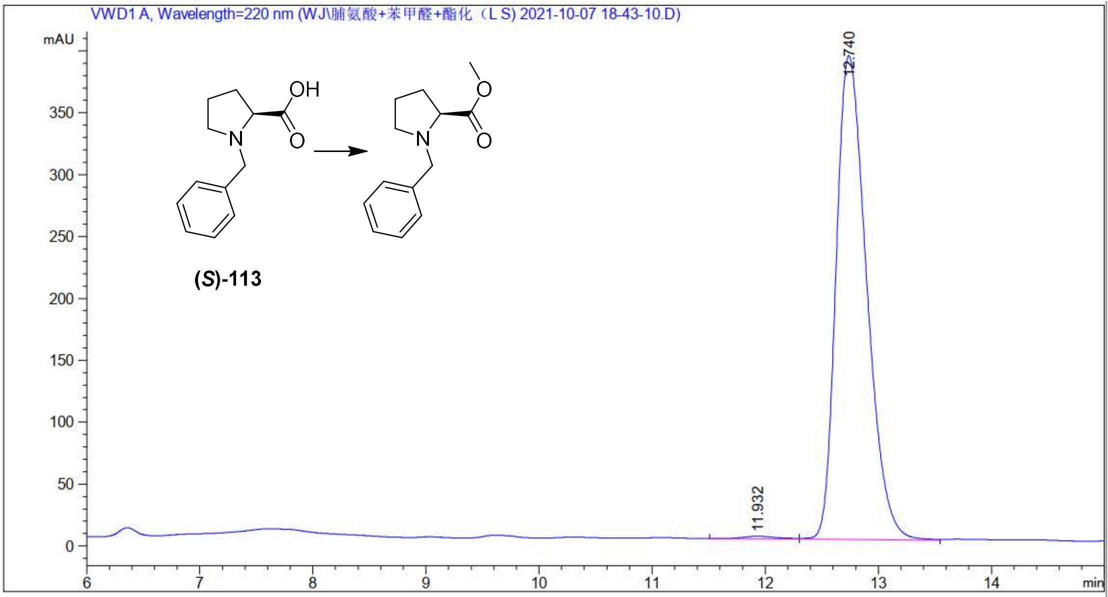
***L*-*N*-benzyl-proline methyl ester (108)**: 99% *ee*; For *L*-*N*-benzyl-proline **113**, the product was converted to the corresponding methyl ester, 99% *ee*. HPLC conditions: OJ-H, hexane: isopropanol = 90: 10; 1 mL/min; 220 nm, 11.7 min (*R*), 12.6 min (*S*).



#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.662	BV	0.2654	5559.07324	325.28293	46.4471
2	12.648	VV	0.2912	6409.54736	341.11859	53.5529

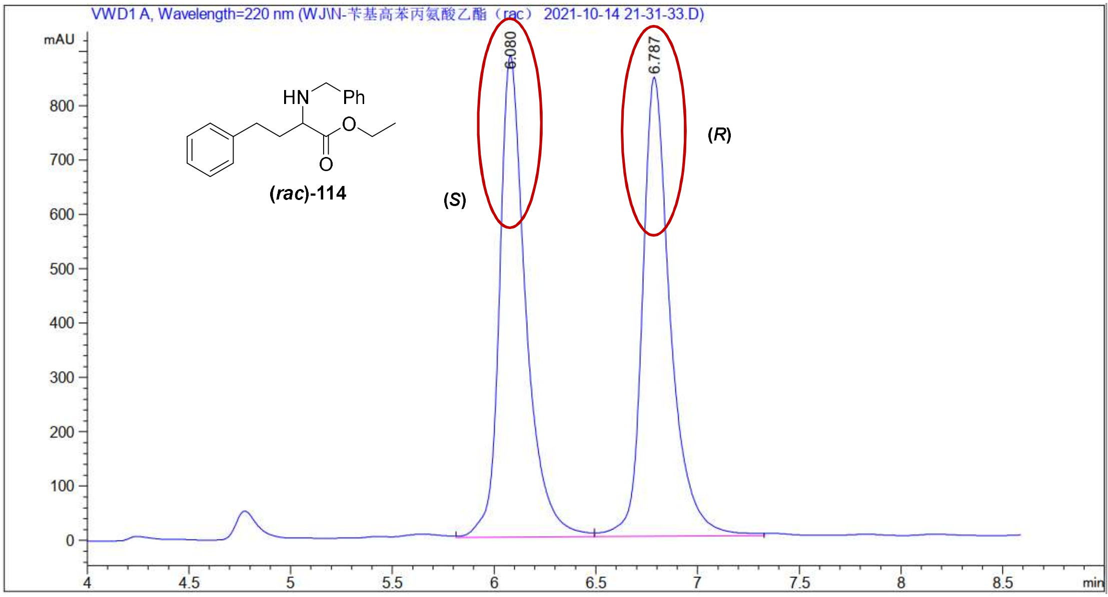


#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.029	MM	0.2589	124.53283	8.01824	0.3158
2	11.439	MM	0.3895	3.93121e4	1681.98865	99.6842

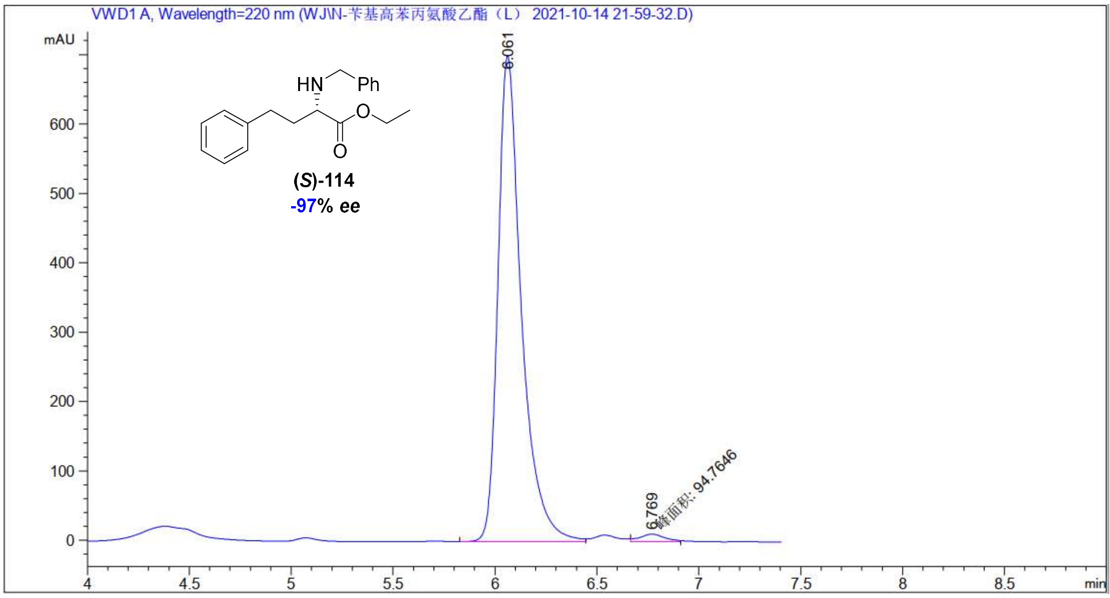


#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.932	BV	0.3156	46.66255	2.14653	0.6329
2	12.740	VV	0.2926	7325.91846	390.93369	99.3671

***N*-benzyl-*L*-homophenylalanine ethyl ester (105)**: *ee* was determined after acetylation, 97% *ee*. HPLC conditions: IB-3, hexane: isopropanol = 90: 10; 1 mL/min; 220 nm, 6.1 min (*S*), 6.8 min (*R*).



#	[min]		[min]	[mAU*s]	[mAU]	%
1	6.080	VV	0.1341	7986.02539	886.62610	49.6391
2	6.787	VV	0.1439	8102.14014	844.57239	50.3609



#	[min]		[min]	[mAU*s]	[mAU]	%
1	6.061	BV	0.1197	5623.92480	700.41327	98.3429
2	6.769	MF	0.1429	94.76461	11.05337	1.6571

IV. Time-conversion plot

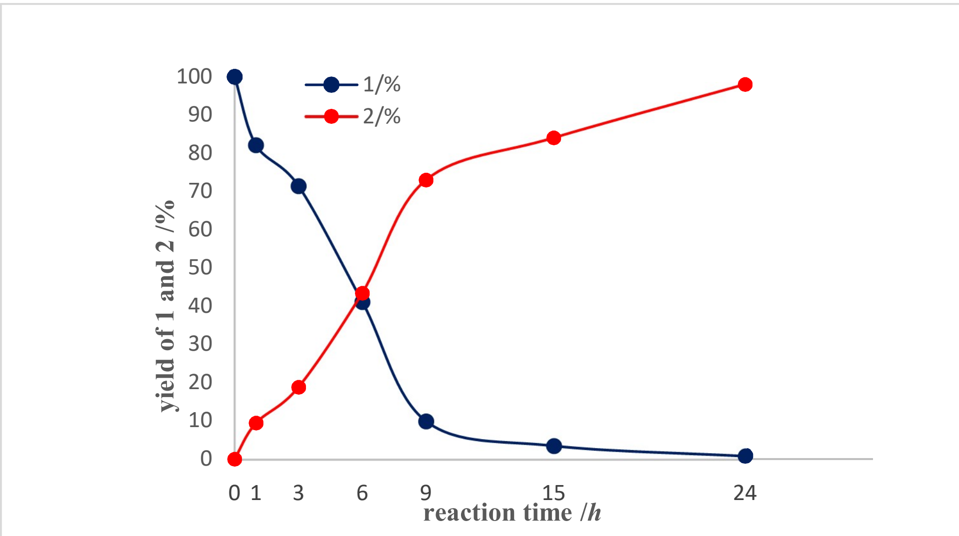


Figure S1. The time-conversion plot for the DRA reaction of **1** and paraformaldehyde. Reaction conditions: **1**/[Ir]/$(CH_2O)_n$ = 1:0.005:1.2, [Ir]/PPh_3 = 1:2.2; **1** 0.2 mmol, CF_3CH_2OH 2 mL, H_2 20 atm, r.t., 24 h.

Table S1. Data for the time-conversion plot.

Entry	time/*h*	remaining of **1** (%)	yield of **2** (%)
1	0	100	0
2	1	82	9
3	3	71	19
4	6	41	43
5	9	10	73
6	15	3.6	84
7	24	0.9	98

V. DFT calculations

All calculations were performed using Gaussian 09 software[81] with the density functional theory (DFT). Optimizations of intermediates and transition states were carried out at the B3LYP-D3 level of theory with the 6-31G(d,p) basis set for C, P, N, O, F, Cl, H and LANL2DZ for Ir. The vibrational frequencies were also computed at the same level so as to confirm the stationary points as transition states (one and only one imaginary frequency) or minima (zero imaginary frequency). Single point energy calculations were performed on optimized geometries in 2,2,2-triFluoroEthanol solvent using the IEFPCM model at the B3LYP-D3 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 Energies of the optimized structures were obtained from the thermal correction to Gibbs Free Energy in frequency analysis and the single point energy.

VI. References:

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VII. Cartesian coordinates of DFT-computed structures.

Complex I

E(RB3LYP) = -3091.10373046

Thermal correction to Gibbs Free Energy= 0.535429

G = -3090.568301

Cl	0.62227300	-2.79390000	-1.82459000
Ir	-0.17612600	-0.85064300	-0.59692500
P	1.86745300	-0.28256500	0.04012000
C	3.01236200	-1.69952800	0.34727500
C	2.49229800	-2.87664300	0.90330300
C	4.39518500	-1.58237800	0.15426500
C	3.34484200	-3.92157300	1.25593900
H	1.41957600	-2.97541100	1.03231300
C	5.24508700	-2.63394800	0.50130700
H	4.81113900	-0.67766800	-0.27775300
C	4.72192500	-3.80436700	1.05318700
H	2.93092600	-4.83339600	1.67685700
H	6.31492300	-2.53783600	0.33777300
H	5.38402700	-4.62317500	1.32087900
C	2.72576900	0.72551200	-1.23539300
C	2.87114300	2.11600500	-1.16204800
C	3.10370600	0.05563100	-2.41355800
C	3.41729600	2.82343600	-2.23596700
H	2.54363400	2.65870000	-0.28401800
C	3.65309400	0.76543300	-3.47840100
H	2.94443700	-1.01596800	-2.49484600
C	3.81630400	2.15222400	-3.39091300
H	3.51715200	3.90268100	-2.16468500
H	3.94640900	0.23725600	-4.38122400
H	4.24213700	2.70451400	-4.22409900
C	2.06364400	0.57011200	1.66620300
C	1.11093200	0.28599700	2.65465800
C	3.15363300	1.39015000	1.98938700
C	1.20982700	0.85538600	3.92428700
H	0.28177600	-0.36772300	2.41023100
C	3.24749600	1.96836100	3.25602100
H	3.92536500	1.58957600	1.25365800
C	2.27159100	1.71214400	4.22286200
H	0.45029900	0.63764100	4.66966400
H	4.08630000	2.61849300	3.48861000
H	2.34657300	2.16801200	5.20610800
P	-1.24139400	1.03512900	0.00822500

C	-2.17965600	1.08164600	1.60263300
C	-2.39813100	-0.13560400	2.26236200
C	-2.70432500	2.26050400	2.15751900
C	-3.12201200	-0.17598800	3.45486500
H	-1.98648800	-1.04466800	1.83915900
C	-3.42433100	2.21978800	3.35218500
H	-2.54262100	3.21236600	1.66125700
C	-3.63355700	1.00127700	4.00367900
H	-3.28333100	-1.12805400	3.95223600
H	-3.81999900	3.13910100	3.77489500
H	-4.19237300	0.97179700	4.93491700
C	-0.37204200	2.67611000	0.00578800
C	-0.21413900	3.39865800	-1.18653100
C	0.19908900	3.19182100	1.18105600
C	0.48871200	4.60351500	-1.20324100
H	-0.64027400	3.02826700	-2.11124400
C	0.90934700	4.39283300	1.16156000
H	0.09354800	2.65967700	2.11799000
C	1.05627800	5.10452000	-0.03066300
H	0.59745700	5.14572500	-2.13797800
H	1.34930100	4.76441900	2.08226600
H	1.60693500	6.04082700	-0.04549500
C	-2.56896100	1.30439600	-1.27227000
C	-2.22618100	1.08303500	-2.62185600
C	-3.89028300	1.64997000	-0.96407300
C	-3.18267500	1.20837800	-3.63100600
H	-1.20605000	0.79417200	-2.86815300
C	-4.84623400	1.77320300	-1.97634500
H	-4.18527900	1.81015200	0.06687400
C	-4.49851000	1.55275200	-3.30930100
H	-2.89874800	1.03592200	-4.66548000
H	-5.86838900	2.03523500	-1.71761100
H	-5.24604700	1.64534500	-4.09190100
C	-2.87660300	-3.38105000	0.28958700
C	-2.58235900	-3.01982100	-1.15279400
H	-3.49147900	-3.21690800	-1.72818500
H	-1.75169300	-3.63342300	-1.50969300
F	-3.84558100	-2.60618500	0.81803400
F	-1.79226600	-3.26985700	1.08455700
F	-3.29316400	-4.66420300	0.33828700
O	-2.25569600	-1.62875600	-1.21661300
H	-2.39964200	-1.29735900	-2.11559500

Complex II

E(RB3LYP) = -3092.32260054

Thermal correction to Gibbs Free Energy= 0.552844

G = -3091.769757

Cl	-1.09074700	-2.56745600	-1.92131600
Ir	0.11211300	-0.59093600	-1.05604000
P	-1.96883300	-0.01276700	0.06320200
C	-3.51515100	-0.23567300	-0.91239800
C	-3.46156600	-0.27049600	-2.31105500
C	-4.76274600	-0.26578100	-0.26986900
C	-4.64127700	-0.33593400	-3.05509700
H	-2.49983400	-0.27263400	-2.80950600
C	-5.93806700	-0.34113000	-1.01520900
H	-4.81450800	-0.23463700	0.81469500
C	-5.87846800	-0.37463000	-2.41108900
H	-4.58910600	-0.37008700	-4.13943600
H	-6.89841200	-0.37112700	-0.50809500
H	-6.79425100	-0.43298200	-2.99278100
C	-2.17889200	-1.09169000	1.52946900
C	-1.51983900	-0.78937600	2.73105800
C	-2.77584600	-2.35473700	1.37787000
C	-1.48970700	-1.71484800	3.77305500
H	-1.01611200	0.16135600	2.85142700
C	-2.73518300	-3.28113700	2.42161300
H	-3.25398900	-2.61823300	0.44049000
C	-2.09762000	-2.96330100	3.62305300
H	-0.97809400	-1.45942800	4.69674500
H	-3.20110900	-4.25383500	2.29176100
H	-2.06920800	-3.68647200	4.43329600
C	-2.22791600	1.72532200	0.61322500
C	-1.82131900	2.72160700	-0.28767900
C	-2.82437100	2.10231900	1.82252300
C	-1.97241800	4.07091700	0.02873600
H	-1.35828000	2.43706200	-1.22614400
C	-2.97008300	3.45387300	2.14244900
H	-3.15743700	1.34496800	2.52429400
C	-2.53729700	4.44029300	1.25288100
H	-1.62882100	4.82701000	-0.67105900
H	-3.42152500	3.73581600	3.08975000
H	-2.64509600	5.49027300	1.50970100
P	1.52725700	0.97012700	-0.20216700
C	1.53439400	2.65549300	-0.96673700

C	1.14833400	2.78049500	-2.30974000
C	1.96074500	3.80318800	-0.27944800
C	1.16009600	4.02516300	-2.94048500
H	0.82946300	1.89962900	-2.85580200
C	1.96520100	5.04807700	-0.90878200
H	2.27304800	3.73906700	0.75657400
C	1.55976600	5.16439800	-2.23975300
H	0.85257200	4.10213600	-3.97930700
H	2.28478500	5.92712000	-0.35635000
H	1.56038000	6.13478600	-2.72783400
C	1.31504200	1.26044900	1.61728900
C	1.87143500	0.32651200	2.50798400
C	0.54109500	2.30439000	2.14529100
C	1.66670900	0.43394900	3.88193400
H	2.48635000	-0.48124600	2.12987500
C	0.33976100	2.41496000	3.52336300
H	0.08414400	3.03445300	1.49088700
C	0.89900800	1.48183300	4.39660600
H	2.10864600	-0.29985600	4.54964800
H	-0.26985000	3.22890800	3.90320900
H	0.73868300	1.56829500	5.46735900
C	3.33871500	0.53837900	-0.25273700
C	3.81788800	-0.54204200	-1.00390200
C	4.25905600	1.31679100	0.47162200
C	5.18315800	-0.84321300	-1.02485100
H	3.11959700	-1.15583700	-1.56045200
C	5.61960400	1.02057100	0.44413300
H	3.91278700	2.15136800	1.07166500
C	6.08670900	-0.06390800	-0.30457200
H	5.53189800	-1.69154400	-1.60661200
H	6.31519100	1.63323300	1.01061400
H	7.14734300	-0.29792300	-0.32177600
H	1.31480500	-1.08671700	-1.97408800
H	-0.25304500	0.32766200	-2.24928400
C	2.08933600	-3.96459000	-0.24243500
C	1.79410000	-2.89472100	0.79757500
H	2.59016600	-2.15270200	0.74942200
H	1.80901000	-3.38797800	1.77653200
F	2.30162600	-3.47240100	-1.47100600
F	1.07445700	-4.85089900	-0.31162700
F	3.20613800	-4.63162900	0.13421800
O	0.56159400	-2.22681200	0.60109600
H	-0.12358800	-2.86327000	0.31414100

OS-III

E(RB3LYP) = -2640.56637129
Thermal correction to Gibbs Free Energy= 0.517564
G = -2640.048807

Cl	-1.68516900	-1.56013300	-2.94433200
Ir	0.02284000	-0.62504400	-1.43297300
P	-1.80933200	0.00161000	0.05398100
C	-3.31280100	0.70197600	-0.74609000
C	-3.25629600	1.20554400	-2.05131900
C	-4.49644100	0.84309200	-0.00317700
C	-4.37317700	1.83477000	-2.60563400
H	-2.35448800	1.08235100	-2.63751700
C	-5.61113100	1.46355000	-0.56346400
H	-4.54647700	0.46565800	1.01400200
C	-5.55013700	1.96181900	-1.86789800
H	-4.32221500	2.21466400	-3.62182200
H	-6.52377900	1.56136100	0.01763300
H	-6.41858700	2.44622800	-2.30558200
C	-2.40376300	-1.43817000	1.02273200
C	-1.66658300	-1.87790000	2.13511700
C	-3.46191700	-2.22748500	0.54785600
C	-2.00319500	-3.06763800	2.77830900
H	-0.82581800	-1.29942300	2.49820200
C	-3.79062100	-3.42112300	1.19324700
H	-4.01565500	-1.91849100	-0.33179000
C	-3.06792900	-3.84210400	2.31086000
H	-1.42479800	-3.38898500	3.63986600
H	-4.61011300	-4.02507400	0.81459800
H	-3.32694800	-4.77202200	2.80904000
C	-1.48280700	1.35148000	1.26609800
C	-0.77411500	2.45904000	0.77777700
C	-1.92620900	1.35789600	2.59446500
C	-0.48123000	3.53991000	1.60809300
H	-0.42717000	2.45854500	-0.24896600
C	-1.62822600	2.43779800	3.42827900
H	-2.48549900	0.51536800	2.98679700
C	-0.89901200	3.52570700	2.94174500
H	0.09080500	4.37587700	1.21680100
H	-1.96544900	2.42712200	4.46112600
H	-0.66261600	4.35929300	3.59692800
P	1.85994200	0.01863700	-0.21033300
C	2.34158400	1.79984500	-0.23942900

C	2.02909700	2.54796100	-1.38452800
C	3.04986800	2.42119600	0.80121700
C	2.39211900	3.89187700	-1.47519100
H	1.48753700	2.07494600	-2.19632500
C	3.40610700	3.76713700	0.71159500
H	3.31066800	1.86834200	1.69648200
C	3.07415600	4.50815000	-0.42403300
H	2.13661000	4.45684300	-2.36680500
H	3.94136800	4.23573500	1.53245200
H	3.34870000	5.55693700	-0.49080600
C	1.74174600	-0.46590800	1.57215000
C	1.98192100	-1.81473200	1.88944900
C	1.31671600	0.39915700	2.59061100
C	1.81231400	-2.28219300	3.19091400
H	2.30926400	-2.50220100	1.11528700
C	1.15508700	-0.07051400	3.89675400
H	1.09706500	1.43708400	2.37783100
C	1.40136300	-1.40893300	4.20227900
H	2.00227800	-3.32770400	3.41505600
H	0.81941700	0.61726800	4.66676200
H	1.27080900	-1.77162800	5.21769900
C	3.45480000	-0.81854300	-0.66647700
C	3.54430800	-1.70466000	-1.74586200
C	4.60271300	-0.57608800	0.10834500
C	4.75671600	-2.33155700	-2.04875300
H	2.66593800	-1.90097400	-2.34926600
C	5.81025400	-1.19836600	-0.19631700
H	4.55465000	0.09576500	0.95837600
C	5.89058900	-2.07979800	-1.27864100
H	4.80772000	-3.01620700	-2.89035300
H	6.68783200	-0.99820500	0.41177200
H	6.83234900	-2.56636200	-1.51603000
H	1.02556900	-0.88956100	-2.65019300
H	-0.10836500	0.77816000	-2.12217700
H	-0.07671600	-2.23824300	-0.48069100
H	0.38093800	-2.41869100	-1.12702100

OS-TS1

E(RB3LYP) = -3005.69280355

Thermal correction to Gibbs Free Energy= 0.656123

G = -3005.036681

Imaginary frequency: -1156.5001

Cl	-1.70524000	-0.34299200	-2.89123600
Ir	0.18366600	-0.29620500	-1.26709000
P	-0.78202500	1.67715200	-0.20716800
C	-1.19782600	3.09939100	-1.31298700
C	-1.09091300	2.97819700	-2.70438100
C	-1.56138700	4.34121000	-0.76051600
C	-1.36233400	4.07623300	-3.52567500
H	-0.81084500	2.02739100	-3.13974500
C	-1.83743200	5.43110400	-1.58344300
H	-1.61609300	4.45792000	0.31784400
C	-1.73892000	5.29929000	-2.97164300
H	-1.27878300	3.96792900	-4.60333900
H	-2.11866800	6.38336700	-1.14214400
H	-1.94894000	6.14958900	-3.61492100
C	-2.30395000	1.37342800	0.79424700
C	-2.21410100	0.38080400	1.78489000
C	-3.49234500	2.10541500	0.67632200
C	-3.26811400	0.16061400	2.66825200
H	-1.31034600	-0.21079300	1.86934100
C	-4.55517400	1.87281600	1.55537700
H	-3.59043500	2.86334900	-0.09267600
C	-4.44192900	0.91076100	2.55981600
H	-3.17284700	-0.60514200	3.43267200
H	-5.47051200	2.44946100	1.45313900
H	-5.26688800	0.73681500	3.24500600
C	0.27312400	2.59072300	1.01584800
C	1.52985000	3.01797900	0.56174500
C	-0.09731300	2.87685500	2.33621400
C	2.41719000	3.67052700	1.41462200
H	1.81865500	2.82479000	-0.46421100
C	0.78540100	3.54572600	3.18913800
H	-1.06463700	2.56409200	2.71210800
C	2.04868500	3.93089400	2.73803100
H	3.39767500	3.95868700	1.04721500
H	0.48432300	3.75610700	4.21199100
H	2.73872000	4.43527900	3.40861700
P	1.93438200	-0.72523500	0.08811700

C	3.43195000	0.35804500	0.10078700
C	3.69725900	1.15923400	-1.01680000
C	4.36628200	0.31451300	1.14654400
C	4.85496600	1.93738200	-1.06934400
H	2.98092200	1.17779300	-1.83263600
C	5.51630600	1.10156600	1.09883100
H	4.19503400	-0.32958600	2.00309500
C	5.76059700	1.92018700	-0.00687700
H	5.04477700	2.55992800	-1.93910000
H	6.22413000	1.07170300	1.92240300
H	6.65747700	2.53215800	-0.04366400
C	1.40429700	-0.88279300	1.84875600
C	0.61395300	-1.99263500	2.20103800
C	1.59583500	0.13319900	2.79229000
C	0.05027300	-2.09211300	3.47037700
H	0.42671300	-2.77244700	1.46986800
C	1.01879100	0.03779700	4.06186100
H	2.17053700	1.01584000	2.53848600
C	0.24974100	-1.07175700	4.40684400
H	-0.55506500	-2.95749800	3.72489900
H	1.16376000	0.84818100	4.76954400
H	-0.19947200	-1.14120700	5.39336100
C	2.80267800	-2.33699500	-0.24408300
C	3.10112600	-2.66910100	-1.57540000
C	3.25765200	-3.18075200	0.77927400
C	3.81603900	-3.82765100	-1.87518800
H	2.75192100	-2.02387800	-2.37478300
C	3.96378200	-4.34808100	0.47623500
H	3.05805700	-2.93756900	1.81711200
C	4.24251200	-4.67661700	-0.85031400
H	4.03474900	-4.06984900	-2.91140000
H	4.29665000	-4.99759300	1.28113400
H	4.79104900	-5.58446100	-1.08500100
H	0.73591100	-1.47923300	-2.17834600
H	1.02238600	0.65758800	-2.25304300
H	-0.80760900	-1.30720300	-0.23133600
H	-0.97416000	-2.16353200	-0.76919800
C	-5.61784200	-3.38311000	1.05164900
C	-4.48047700	-4.01774300	0.56118700
H	-6.71124300	-1.52797700	1.16160200
C	-5.82197600	-2.02558500	0.78489200
C	-3.52860600	-3.29251100	-0.17868900
C	-3.74241800	-1.92816400	-0.45062600
C	-4.89217500	-1.30835300	0.02802400

H	-3.04226500	-1.37236900	-1.06689300
H	-5.05073100	-0.25674300	-0.18077100
C	-2.35331100	-3.99564000	-0.68101000
N	-1.28057800	-3.41733000	-1.07763800
C	-0.16527800	-4.15293700	-1.64359500
H	0.73031200	-3.97699300	-1.04283900
H	-0.37085000	-5.22799500	-1.70239900
H	-4.32055700	-5.07605800	0.75429800
H	-6.34591600	-3.94326200	1.63084300
H	0.03543800	-3.75286000	-2.64123000
H	-2.41363900	-5.09063400	-0.72382700

OS-IV

E(RB3LYP) = -3005.70004265
Thermal correction to Gibbs Free Energy= 0.661075
G = -3005.038968

Cl	-1.85894900	-0.49098000	-2.77146600
Ir	0.10795000	-0.35648000	-1.19379100
P	-0.74531300	1.70062200	-0.25409100
C	-1.20096500	3.04659800	-1.44131100
C	-1.16480000	2.82332300	-2.82320100
C	-1.51121000	4.33376700	-0.96586900
C	-1.45713500	3.86423400	-3.70935500
H	-0.91295000	1.84009000	-3.19912700
C	-1.80752100	5.36724000	-1.85205400
H	-1.50587100	4.53119900	0.10202400
C	-1.78300600	5.13248800	-3.22989400
H	-1.42760500	3.67627700	-4.77896200
H	-2.04574100	6.35578500	-1.46884300
H	-2.00858500	5.93836800	-3.92326600
C	-2.19110000	1.58272400	0.89555600
C	-2.03901600	0.72497500	1.99820700
C	-3.37336000	2.32643400	0.78010100
C	-3.01011400	0.66531100	2.99537800
H	-1.14934300	0.11292400	2.07753100
C	-4.35717300	2.25168000	1.77286100
H	-3.52598800	2.97632100	-0.07419800
C	-4.17061500	1.43802100	2.89199500
H	-2.85773700	0.01019600	3.84837300
H	-5.26547400	2.83942600	1.67110400

H	-4.92913500	1.39494900	3.66886400
C	0.44949500	2.67278800	0.78286600
C	1.69864500	2.92957400	0.19900500
C	0.19315600	3.16271200	2.06968800
C	2.68755900	3.62044800	0.89563800
H	1.89567100	2.56285900	-0.80076600
C	1.17955900	3.86789500	2.76532000
H	-0.76491600	2.98133100	2.54337900
C	2.43135700	4.08813100	2.18819100
H	3.65881600	3.77358200	0.43439000
H	0.96868700	4.23629400	3.76584800
H	3.20058600	4.62247300	2.73885400
P	1.86119500	-0.79239500	0.13456000
C	3.45690300	0.13051100	-0.05367000
C	3.71365900	0.79699300	-1.25806500
C	4.45499500	0.09626300	0.93240400
C	4.92970600	1.45346900	-1.45714900
H	2.94253000	0.80821900	-2.02355100
C	5.66465000	0.76197700	0.73742600
H	4.28759400	-0.44465900	1.85841900
C	5.90305900	1.44790200	-0.45642200
H	5.11245100	1.97275200	-2.39384300
H	6.42255100	0.74141600	1.51563000
H	6.84604900	1.96592400	-0.60790200
C	1.45308200	-0.69688600	1.93391200
C	0.61368800	-1.68858100	2.47420600
C	1.81101100	0.39155000	2.73779700
C	0.17059800	-1.60709100	3.79203200
H	0.29409500	-2.51513700	1.84840700
C	1.35021500	0.48146200	4.05463100
H	2.42826700	1.18821100	2.34015600
C	0.53638200	-0.51583300	4.58791900
H	-0.47261500	-2.38539700	4.19320300
H	1.62271100	1.34644500	4.65155300
H	0.18056600	-0.44310500	5.61176900
C	2.56825100	-2.51149500	-0.03247200
C	2.75749600	-3.03974500	-1.31964500
C	3.03194700	-3.24973000	1.06594400
C	3.36526100	-4.28228100	-1.50041600
H	2.41979000	-2.47027200	-2.17939300
C	3.63217700	-4.49888400	0.88528400
H	2.92379500	-2.85911000	2.07161300
C	3.79731800	-5.02226800	-0.39663600
H	3.50364800	-4.67040600	-2.50602700

H	3.97240100	-5.05945300	1.75175300
H	4.26490500	-5.99289200	-0.53638800
H	0.62616000	-1.59366600	-2.05236800
H	0.92418500	0.54245000	-2.30458000
H	-0.78496300	-1.32990500	-0.11805300
H	-1.25296900	-2.40904500	-1.11289400
C	-5.53825200	-3.46056400	1.29960200
C	-4.57129400	-4.05211400	0.49645900
H	-6.34847400	-1.59927400	2.02802800
C	-5.58783500	-2.06533700	1.40789600
C	-3.62970100	-3.25100400	-0.18252000
C	-3.68931200	-1.84580900	-0.07634300
C	-4.67631900	-1.26599500	0.71420600
H	-3.00791000	-1.21889100	-0.64155300
H	-4.72939400	-0.18693300	0.78477600
C	-2.64604300	-3.91162300	-1.01185200
N	-1.56632000	-3.36579900	-1.45810100
C	-0.63819800	-3.98924800	-2.38986800
H	0.34376500	-4.07367600	-1.91897700
H	-1.00667900	-4.97238800	-2.69184900
H	-4.53147000	-5.13409500	0.39654200
H	-6.25591900	-4.07750500	1.83148900
H	-0.55163700	-3.32458600	-3.25309400
H	-2.83108300	-4.94820400	-1.29833200

OS-TS2

E(RB3LYP) = -3005.69828840

Thermal correction to Gibbs Free Energy= 0.661344

G = -3005.036944

Imaginary frequency: -74.6347

Cl	1.68109500	0.68393400	-2.91609900
Ir	-0.19561600	0.32424000	-1.23606600
P	1.08146800	-1.37738600	-0.13739600
C	2.34761400	-2.18608700	-1.21458600
C	3.60027700	-1.57988100	-1.38949000
C	2.05442500	-3.34442900	-1.94532300
C	4.54417400	-2.12698000	-2.25630000
H	3.83626300	-0.67763100	-0.83813700
C	2.99662500	-3.88890100	-2.81970600
H	1.09053500	-3.82889400	-1.83320900

C	4.24477200	-3.28507800	-2.97630700
H	5.50960000	-1.64290000	-2.37705300
H	2.75298400	-4.78940900	-3.37673700
H	4.97723600	-3.71101000	-3.65631900
C	2.06959600	-0.95075700	1.37028800
C	1.66632100	0.15615000	2.12671300
C	3.15760500	-1.71889000	1.81956600
C	2.30493200	0.46583900	3.32747700
H	0.85696900	0.77436500	1.75833300
C	3.81306300	-1.39307200	3.00779300
H	3.49344600	-2.57151300	1.23765900
C	3.37971200	-0.30540700	3.77137900
H	1.96320000	1.31725500	3.90799800
H	4.65444400	-1.99432300	3.34203800
H	3.88161600	-0.06055100	4.70393700
C	0.08230800	-2.83093100	0.44101200
C	-1.03872000	-3.18635400	-0.32498800
C	0.34305300	-3.53936500	1.62298500
C	-1.89483500	-4.20671400	0.09073900
H	-1.25298500	-2.62239000	-1.22514400
C	-0.51387700	-4.55981400	2.03962100
H	1.19363400	-3.27694100	2.24133900
C	-1.63933900	-4.89119000	1.28067700
H	-2.77480800	-4.43846400	-0.50217200
H	-0.30680300	-5.08924600	2.96593000
H	-2.31346200	-5.67386900	1.61770700
P	-2.05122700	0.41200600	0.01782800
C	-3.41216300	-0.79126500	-0.34997000
C	-3.54865800	-1.25240300	-1.66735600
C	-4.32572700	-1.23227000	0.62033000
C	-4.56207700	-2.15117600	-2.00108100
H	-2.82919800	-0.92633200	-2.41235200
C	-5.33499300	-2.13743200	0.28618300
H	-4.24642000	-0.88064300	1.64340200
C	-5.45306900	-2.60305200	-1.02443500
H	-4.64924500	-2.50481700	-3.02468500
H	-6.02511800	-2.47988500	1.05228200
H	-6.23503300	-3.31168800	-1.28329400
C	-1.81520700	0.25640200	1.85074300
C	-1.58836700	1.39813700	2.63552200
C	-1.72166100	-1.00475400	2.45935300
C	-1.26137500	1.27980700	3.98669200
H	-1.66100900	2.38458200	2.19064600
C	-1.38977300	-1.12117700	3.80920400

H	-1.90853200	-1.90292700	1.88533500
C	-1.15391000	0.01902500	4.57742900
H	-1.09082800	2.17549100	4.57816200
H	-1.30873000	-2.10993900	4.25088400
H	-0.88983100	-0.07281400	5.62711400
C	-2.94603000	2.04350400	-0.08241800
C	-2.20381900	3.21995100	-0.26854100
C	-4.33528900	2.14560700	0.07393100
C	-2.83128300	4.46499200	-0.28901100
H	-1.13207200	3.12808700	-0.39900200
C	-4.96502000	3.39230700	0.04160600
H	-4.93618100	1.25373300	0.21115100
C	-4.21684200	4.55614400	-0.13721300
H	-2.24031800	5.36720800	-0.43004200
H	-6.04411400	3.45043400	0.15403800
H	-4.70895100	5.52445000	-0.16177300
H	-1.00674000	1.35411900	-2.16617300
H	-0.74239100	-0.82448300	-2.29379400
H	0.40288300	1.59167600	-0.29367400
H	1.82147600	2.56054600	-2.39617600
C	3.84811900	3.35776000	2.22724100
C	2.85394700	3.80349300	1.36308900
H	5.45219300	1.94844100	2.51278500
C	4.68732600	2.31310700	1.83479600
C	2.69519900	3.21367700	0.09431700
C	3.54494200	2.15826200	-0.29407300
C	4.53037300	1.71661100	0.57911900
H	3.39868700	1.66466100	-1.24920700
H	5.17300300	0.89113100	0.29150900
C	1.65553600	3.75331800	-0.75786700
N	1.44690500	3.47216000	-2.00251600
C	0.31147600	3.97185800	-2.76668100
H	-0.13762000	4.83290700	-2.26715600
H	0.64827000	4.25247500	-3.76700400
H	2.19157700	4.60990000	1.66745300
H	3.96226800	3.81375000	3.20553600
H	-0.41748900	3.15654000	-2.83928300
H	1.02326400	4.52970700	-0.32573400

OS-TS2'

E(RB3LYP) = -3005.68813424
Thermal correction to Gibbs Free Energy= 0.661609
G = -3005.026525
Imaginary frequency: -94.6418

Cl	0.22549800	-3.19915600	-0.57716100
Ir	0.30877000	-0.65338600	-0.44861800
P	-1.97736100	-0.77847300	0.15769300
C	-3.02507800	-1.99777800	-0.75928000
C	-2.64066700	-2.41324200	-2.03953100
C	-4.25768300	-2.42470200	-0.24213100
C	-3.47420400	-3.24596200	-2.78792900
H	-1.68428800	-2.08515100	-2.43024000
C	-5.08530300	-3.26285900	-0.98863100
H	-4.56962400	-2.10681700	0.74806500
C	-4.69483400	-3.67529000	-2.26503500
H	-3.16390600	-3.56634200	-3.77890700
H	-6.03501400	-3.59087700	-0.57486400
H	-5.33984800	-4.32787400	-2.84725100
C	-2.20557300	-1.23618600	1.92150300
C	-2.18121400	-0.26144300	2.92976000
C	-2.20176100	-2.59250300	2.28501300
C	-2.18782800	-0.63402800	4.27378400
H	-2.14578400	0.78959900	2.67364900
C	-2.20638600	-2.96038000	3.63019900
H	-2.17725100	-3.35750600	1.51606200
C	-2.20463200	-1.98372700	4.62914400
H	-2.17015000	0.13721800	5.03873500
H	-2.20534400	-4.01355300	3.89742600
H	-2.20793700	-2.27384300	5.67632900
C	-3.01821200	0.72014000	-0.13979800
C	-2.75861700	1.42689400	-1.32294300
C	-4.05880300	1.15048700	0.69350600
C	-3.48808700	2.57064500	-1.64512200
H	-1.96172900	1.08576200	-1.97260300
C	-4.78645300	2.29865300	0.37413200
H	-4.29157400	0.60570000	1.60193400
C	-4.49657900	3.01829000	-0.78784900
H	-3.25074100	3.11868000	-2.55253700
H	-5.57954500	2.63290600	1.03757800
H	-5.05809900	3.91741700	-1.02612800
P	0.73784400	1.51957100	-0.09541100

C	0.36899300	2.73719000	-1.44517600
C	0.25898100	2.26318500	-2.75908000
C	0.23373700	4.11622500	-1.21134600
C	-0.00459400	3.14081300	-3.81193400
H	0.34607600	1.19376800	-2.92986500
C	-0.03405900	4.99285800	-2.26365200
H	0.32899000	4.50912300	-0.20470300
C	-0.15907000	4.50680400	-3.56690900
H	-0.09802700	2.75466400	-4.82334200
H	-0.14735900	6.05464700	-2.06345700
H	-0.37382500	5.18893400	-4.38489900
C	-0.06933200	2.26792800	1.40350600
C	0.47449200	1.99929300	2.66990600
C	-1.25511900	3.01478200	1.33093100
C	-0.13355100	2.48435400	3.82632500
H	1.37459700	1.40285100	2.75814100
C	-1.86645300	3.49666600	2.49113800
H	-1.72075800	3.21757500	0.37507000
C	-1.30663600	3.23860700	3.74241100
H	0.30675800	2.26473400	4.79470000
H	-2.78946200	4.06235000	2.40615400
H	-1.78240200	3.61395000	4.64410700
C	2.53374900	1.86407500	0.26583700
C	3.25597600	0.94415200	1.04423300
C	3.18025100	3.03489000	-0.15895300
C	4.57132800	1.21230400	1.42327800
H	2.78043600	0.01430200	1.33648500
C	4.50660100	3.28715500	0.19934500
H	2.66068400	3.75676400	-0.77751400
C	5.20339100	2.38317000	1.00116100
H	5.10435800	0.49059600	2.03331700
H	4.99043900	4.19634900	-0.14733000
H	6.23145500	2.58607200	1.28906800
H	0.83505400	-0.87835300	1.10975400
H	-0.14598100	-0.57598200	-2.07028000
H	2.03589400	-3.34899200	-1.73889500
H	1.87965500	-0.69370300	-0.91043400
C	6.13718700	-1.77933800	0.68196500
C	5.36474800	-1.53754400	-0.45119900
H	6.19909800	-2.69970700	2.62926900
C	5.60465200	-2.52272600	1.73744200
C	4.07157500	-2.07747900	-0.55394500
C	3.53263000	-2.81666900	0.51545300
C	4.30055700	-3.02517400	1.65622700

H	2.50658900	-3.16784900	0.46692600
H	3.87692500	-3.57661300	2.48978800
C	3.34699400	-1.84489500	-1.79804300
N	2.53947700	-2.69875500	-2.36790100
C	1.75579300	-2.34356300	-3.54453800
H	0.89909600	-1.73970300	-3.20351600
H	2.36994800	-1.76271800	-4.23662500
H	5.76437700	-0.93455300	-1.26181900
H	7.14113700	-1.37195200	0.74944500
H	1.41080800	-3.25614600	-4.03198800
H	3.65848600	-0.99894500	-2.40749700

Complex IS-III

E(RB3LYP) = -3004.52415832
Thermal correction to Gibbs Free Energy= 0.647202
G = -3003.876956

Cl	0.32247700	-2.88178000	-1.85097600
Ir	-0.29065300	-0.81946500	-0.64420900
P	2.11632300	-0.43842900	-0.07351200
C	3.15090000	-1.91012200	0.35865100
C	3.39148800	-2.87941500	-0.63108000
C	3.65309600	-2.12289800	1.65117900
C	4.11126900	-4.03438000	-0.32565300
H	3.00270200	-2.73575700	-1.63144500
C	4.36760900	-3.28373500	1.95346000
H	3.49094200	-1.38389600	2.42819200
C	4.59716000	-4.24372200	0.96694200
H	4.28505700	-4.77470900	-1.10117600
H	4.74927700	-3.43184600	2.96000300
H	5.15385000	-5.14662100	1.20206600
C	3.10834900	0.32863800	-1.43205400
C	2.49278700	1.25336700	-2.28602200
C	4.48406900	0.08417700	-1.58098000
C	3.23150800	1.92240300	-3.26187100
H	1.43496700	1.45373100	-2.18883500
C	5.21982800	0.74710700	-2.56421800
H	4.98270300	-0.62555000	-0.92985500
C	4.59600000	1.66966900	-3.40687100
H	2.73275400	2.64074400	-3.90575900
H	6.28137100	0.54127400	-2.67020800

H	5.17040300	2.18503500	-4.17169900
C	2.47678200	0.68915500	1.34774000
C	1.64011100	0.60318200	2.46884800
C	3.50600400	1.64151100	1.34733500
C	1.80395900	1.45876000	3.55819200
H	0.82674400	-0.11011100	2.46759200
C	3.67107500	2.50164300	2.43452600
H	4.16266100	1.73063800	0.48923200
C	2.81780300	2.41905100	3.53826000
H	1.12060400	1.39146400	4.39935900
H	4.46401000	3.24435800	2.41518800
H	2.94122200	3.10058600	4.37514800
P	-1.19676200	1.16364200	0.01525000
C	-1.50522100	1.49148000	1.81311500
C	-1.66029100	0.39950800	2.67899500
C	-1.61159200	2.78886200	2.34059800
C	-1.91023600	0.59572300	4.03775600
H	-1.55474400	-0.60586100	2.28709700
C	-1.85401200	2.98559300	3.70074700
H	-1.49206500	3.64958900	1.69124900
C	-2.00360300	1.88990000	4.55365400
H	-2.02459200	-0.26327700	4.69282700
H	-1.92395800	3.99604900	4.09325100
H	-2.19118700	2.04451100	5.61238900
C	-0.26294000	2.66625300	-0.54065800
C	-0.47560900	3.18136900	-1.82996300
C	0.75376300	3.22680900	0.24671300
C	0.31949500	4.21664300	-2.32210500
H	-1.25851000	2.77247800	-2.45880900
C	1.54905900	4.26068100	-0.24907600
H	0.93359000	2.86208600	1.24946000
C	1.33993300	4.75581200	-1.53598200
H	0.13987400	4.59996500	-3.32260800
H	2.33913200	4.66589000	0.37583600
H	1.96465000	5.55523700	-1.92362600
C	-2.86658300	1.49270400	-0.74636400
C	-3.12752200	1.01897900	-2.04300900
C	-3.86109300	2.23115100	-0.08894600
C	-4.34297600	1.29324400	-2.66938600
H	-2.38319500	0.41473800	-2.54925700
C	-5.08366900	2.49312600	-0.71323600
H	-3.69886900	2.59634800	0.91845500
C	-5.32690000	2.02984900	-2.00685000
H	-4.52424000	0.91546700	-3.67137600

H	-5.84486500	3.05864000	-0.18295800
H	-6.27774400	2.23370900	-2.49102700
H	0.00640100	-0.05967100	-1.98008600
H	-1.71887100	-1.14112300	-1.23429200
C	-5.29201500	-3.65996800	-0.60290600
C	-4.03596000	-3.88962200	-0.04524900
H	-6.78380000	-2.18053300	-1.08979300
C	-5.80252200	-2.36053200	-0.65976100
C	-3.25952600	-2.81869000	0.42858000
C	-3.79114600	-1.52302300	0.38248400
C	-5.05415500	-1.29428300	-0.15490500
H	-3.21953400	-0.69825300	0.77702100
H	-5.44110400	-0.28137200	-0.19092900
C	-1.94470800	-3.13227800	1.00000400
N	-0.87386100	-2.42155800	0.97892400
C	0.28871500	-3.02325200	1.63525100
H	0.77196100	-2.28346400	2.27598500
H	0.02090700	-3.89930000	2.24013800
H	-3.63926900	-4.90054000	0.00214900
H	-5.87281700	-4.49294600	-0.98781100
H	0.99940400	-3.32167200	0.86258400
H	-1.89493400	-4.11680800	1.48315000

IS-TS1

E(RB3LYP) = -3004.48423403
Thermal correction to Gibbs Free Energy= 0.646194
G = -3003.838040
Imaginary frequency: -199.1268

Cl	1.00103600	-2.59748000	-2.20738700
Ir	0.00511200	-0.84221000	-0.76358200
P	2.13411400	-0.29273300	0.02782600
C	3.20266900	-1.76373700	0.35419300
C	3.82402400	-2.41609600	-0.72339300
C	3.38352600	-2.26958800	1.64939300
C	4.60695100	-3.54812100	-0.50473100
H	3.69016100	-2.04272100	-1.73062600
C	4.16167700	-3.40897500	1.86284800
H	2.92641000	-1.77766200	2.50010400
C	4.77412500	-4.05161500	0.78704400
H	5.07865100	-4.04184400	-1.34918400

H	4.29076600	-3.78756800	2.87282500
H	5.38055700	-4.93748500	0.95347400
C	3.19397800	0.74930400	-1.05978900
C	2.60539400	1.63042700	-1.97448700
C	4.59399000	0.73905100	-0.92816300
C	3.39568700	2.49237900	-2.73579200
H	1.53050000	1.64198900	-2.09176700
C	5.38176300	1.59730900	-1.69466100
H	5.06838300	0.05844400	-0.22892900
C	4.78373700	2.47814000	-2.59952000
H	2.91885300	3.17437700	-3.43332900
H	6.46241100	1.57540600	-1.58613900
H	5.39896500	3.14584900	-3.19617800
C	2.17791300	0.58536400	1.64602000
C	1.26237900	0.17089000	2.62308600
C	3.05037000	1.64532100	1.93168400
C	1.19804500	0.81940900	3.85634200
H	0.58527200	-0.64532300	2.39712200
C	2.98644300	2.29160200	3.16691400
H	3.75730100	1.98759900	1.18504300
C	2.05569400	1.88715000	4.12760100
H	0.45697500	0.50808200	4.58558300
H	3.65739600	3.12069000	3.37384100
H	1.99723400	2.40431100	5.08107800
P	-1.21901100	0.97687500	-0.05153400
C	-1.79289600	1.15266500	1.68803200
C	-1.90647000	-0.00204700	2.47254400
C	-2.17470300	2.39294400	2.22715600
C	-2.39329400	0.08353400	3.77807500
H	-1.58458800	-0.95400200	2.05369500
C	-2.65256700	2.47384000	3.53495300
H	-2.09577500	3.29533300	1.62967500
C	-2.76391300	1.31824500	4.31327600
H	-2.47749000	-0.81867700	4.37805000
H	-2.93936600	3.43814100	3.94464300
H	-3.13766600	1.38340100	5.33146200
C	-0.39497800	2.59803000	-0.38598400
C	-0.51494600	3.23078800	-1.63238900
C	0.45594000	3.16001600	0.57778000
C	0.21731300	4.38451200	-1.91433300
H	-1.17707100	2.82561600	-2.38869300
C	1.19243400	4.30916600	0.29021900
H	0.54584500	2.70679300	1.55684300
C	1.08109800	4.92218400	-0.95792100

H	0.11184100	4.86167900	-2.88455000
H	1.85701400	4.71627900	1.04642900
H	1.65869100	5.81396700	-1.18307400
C	-2.78828200	1.09260200	-1.03094100
C	-2.75193800	0.83562800	-2.41318200
C	-4.00987300	1.44554700	-0.44177800
C	-3.90276600	0.96890700	-3.18919900
H	-1.82499000	0.51169000	-2.87423300
C	-5.16314200	1.56055500	-1.21951900
H	-4.07408800	1.61300100	0.62643600
C	-5.11232700	1.33410300	-2.59474300
H	-3.85443500	0.77268000	-4.25652800
H	-6.10423800	1.81990800	-0.74347900
H	-6.01120600	1.42754700	-3.19760400
H	0.24369600	0.05907600	-2.05302100
H	-1.44396700	-1.60753300	-1.34464400
C	-5.34454100	-1.88579700	-1.10931800
C	-3.97460800	-2.06054900	-1.28071400
H	-6.97008500	-1.79041000	0.30792800
C	-5.90192200	-1.93527100	0.17221000
C	-3.14037900	-2.28285200	-0.17729500
C	-3.70690900	-2.35916000	1.09800400
C	-5.08069700	-2.17781300	1.27329200
H	-3.06175700	-2.57230500	1.94205400
H	-5.50703800	-2.23012000	2.27128200
C	-1.66251100	-2.53776700	-0.37876100
N	-0.79498500	-2.40310000	0.69523500
C	0.07480800	-3.55461900	0.93751000
H	0.85963300	-3.26439900	1.63976700
H	-0.50468700	-4.36631100	1.40289700
H	-3.54059500	-1.99778400	-2.27468700
H	-5.97453500	-1.69256900	-1.97200700
H	0.55952400	-3.94512200	0.03343700
H	-1.48322900	-3.39674200	-1.04397900

Complex IS-IV

E(RB3LYP) = -3004.48458595
Thermal correction to Gibbs Free Energy= 0.645011
G = -3003.839575

Cl	0.95295300	-2.49751000	-2.33095800
Ir	0.02179500	-0.77559100	-0.81575600
P	2.11832900	-0.34231200	0.03426000
C	3.11521200	-1.86497400	0.34531900
C	3.72376700	-2.52349500	-0.73591900
C	3.26291100	-2.39574800	1.63469900
C	4.46161800	-3.68689000	-0.52616200
H	3.61419600	-2.13066600	-1.73857700
C	3.99583400	-3.56622700	1.83878300
H	2.81359500	-1.90052000	2.48736400
C	4.59566500	-4.21515300	0.75967500
H	4.92414500	-4.18522400	-1.37293000
H	4.09919100	-3.96458800	2.84404800
H	5.16683700	-5.12543000	0.91889800
C	3.24590200	0.69514000	-0.98520300
C	2.71255800	1.67390600	-1.83231600
C	4.64184700	0.59207900	-0.85488100
C	3.55438900	2.53865700	-2.53182600
H	1.64060300	1.75692400	-1.94375600
C	5.48104500	1.45359900	-1.56132700
H	5.07369400	-0.16115200	-0.20465200
C	4.93905600	2.43031400	-2.40039500
H	3.12043700	3.29637400	-3.17720600
H	6.55816700	1.35931500	-1.45689600
H	5.59468100	3.10002300	-2.94992300
C	2.13813800	0.48541500	1.67844500
C	1.18369600	0.07424100	2.61929500
C	3.04103200	1.50389500	2.01651300
C	1.10992300	0.69004100	3.86870900
H	0.48617800	-0.71207500	2.35354400
C	2.96769200	2.11583600	3.26858500
H	3.78000700	1.84045700	1.29868800
C	1.99742300	1.71812100	4.19243200
H	0.33990700	0.38425400	4.56984800
H	3.66239400	2.91319800	3.51739500
H	1.93240300	2.20961000	5.15897900
P	-1.16877300	1.04770800	-0.05032400
C	-1.78139400	1.16365800	1.67950500
C	-1.99224600	-0.03133700	2.38005800
C	-2.10625900	2.38806700	2.28692700
C	-2.51771500	-0.00004600	3.67257500
H	-1.70729600	-0.97210700	1.91023100
C	-2.62166000	2.41308200	3.58294100
H	-1.95499400	3.32074200	1.75353300

C	-2.82947000	1.21863100	4.27818200
H	-2.67884600	-0.93235600	4.20704200
H	-2.86347500	3.36471800	4.04764400
H	-3.23322100	1.24105100	5.28673400
C	-0.31489800	2.66268600	-0.32028400
C	-0.41105900	3.33329800	-1.54890600
C	0.53892000	3.17776700	0.66664400
C	0.34630100	4.47989000	-1.79057400
H	-1.07232600	2.96125200	-2.32300100
C	1.29993900	4.32039600	0.41937700
H	0.61339300	2.69191200	1.63122600
C	1.21133400	4.97224900	-0.81089400
H	0.25947500	4.98695900	-2.74735100
H	1.96620000	4.69198100	1.19224100
H	1.80811400	5.85876200	-1.00458500
C	-2.71979700	1.20783900	-1.05284400
C	-2.67435000	0.96406800	-2.43717200
C	-3.94142000	1.57537600	-0.47143200
C	-3.81919800	1.11061300	-3.22030800
H	-1.74571600	0.64027300	-2.89485000
C	-5.08767100	1.70623800	-1.25649100
H	-4.00997300	1.74443900	0.59631900
C	-5.03011600	1.48112700	-2.63195500
H	-3.76471000	0.92106700	-4.28851000
H	-6.02883600	1.97599500	-0.78646600
H	-5.92422000	1.58386000	-3.24035500
H	0.29442700	0.18097500	-2.07048600
H	-1.53311500	-1.57096200	-1.39045200
C	-5.45674700	-1.78529200	-1.02475800
C	-4.09312200	-1.91362900	-1.27855200
H	-7.01643800	-1.90528200	0.46292700
C	-5.95393600	-2.01085700	0.26189200
C	-3.20613100	-2.25922400	-0.25200900
C	-3.71203900	-2.50374800	1.02838100
C	-5.07839300	-2.37605000	1.28555700
H	-3.02173900	-2.79395600	1.81292900
H	-5.45773800	-2.56175100	2.28678600
C	-1.72856600	-2.45523500	-0.53990300
N	-0.82315500	-2.34675100	0.53824200
C	-0.02849400	-3.54824900	0.77813600
H	0.70758900	-3.33621500	1.55784200
H	-0.67198900	-4.36260000	1.14673300
H	-3.70882500	-1.71827400	-2.27550100
H	-6.12771400	-1.49444000	-1.82738900

H	0.51315600	-3.91001300	-0.10694400
H	-1.56444600	-3.32251100	-1.19948400

IS-TS2

E(RB3LYP) = -3004.47532211

Thermal correction to Gibbs Free Energy= 0.646411

G = -3003.828911

Imaginary frequency: -944.3121

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Ir	0.61078500	0.11340400	-0.66663800
P	-0.46663000	-1.82406200	-0.01511600
C	0.71730300	-3.12214500	0.56075000
C	2.01136200	-2.76436300	0.95770400
C	0.29302700	-4.44910400	0.72575700
C	2.87316200	-3.72078400	1.49533200
H	2.34540400	-1.74127700	0.83657600
C	1.16016000	-5.40628400	1.25204000
H	-0.71354100	-4.73704500	0.43742400
C	2.45332900	-5.04418700	1.63731400
H	3.87422600	-3.42660300	1.79745400
H	0.82441100	-6.43338700	1.36422000
H	3.12749300	-5.79016400	2.04877700
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C	-1.02619700	-1.05323400	2.58500100
C	-2.73841000	-2.47072800	1.64425400
C	-1.74609500	-0.95733400	3.77438100
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C	-3.45820700	-2.38059400	2.83769700
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C	-2.97427500	-1.61249900	3.89894000
H	-1.35243000	-0.36108500	4.59226700
H	-4.40315100	-2.90811700	2.93392200
H	-3.54453900	-1.53406800	4.82016800
C	-1.47816000	-2.63727400	-1.31741700
C	-0.91688800	-3.59915500	-2.17174300
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C	-1.65593200	-4.10498900	-3.24157500

H	0.09979700	-3.93709000	-2.01182600
C	-3.51396200	-2.68497700	-2.64331600
H	-3.22270000	-1.41844500	-0.94220200
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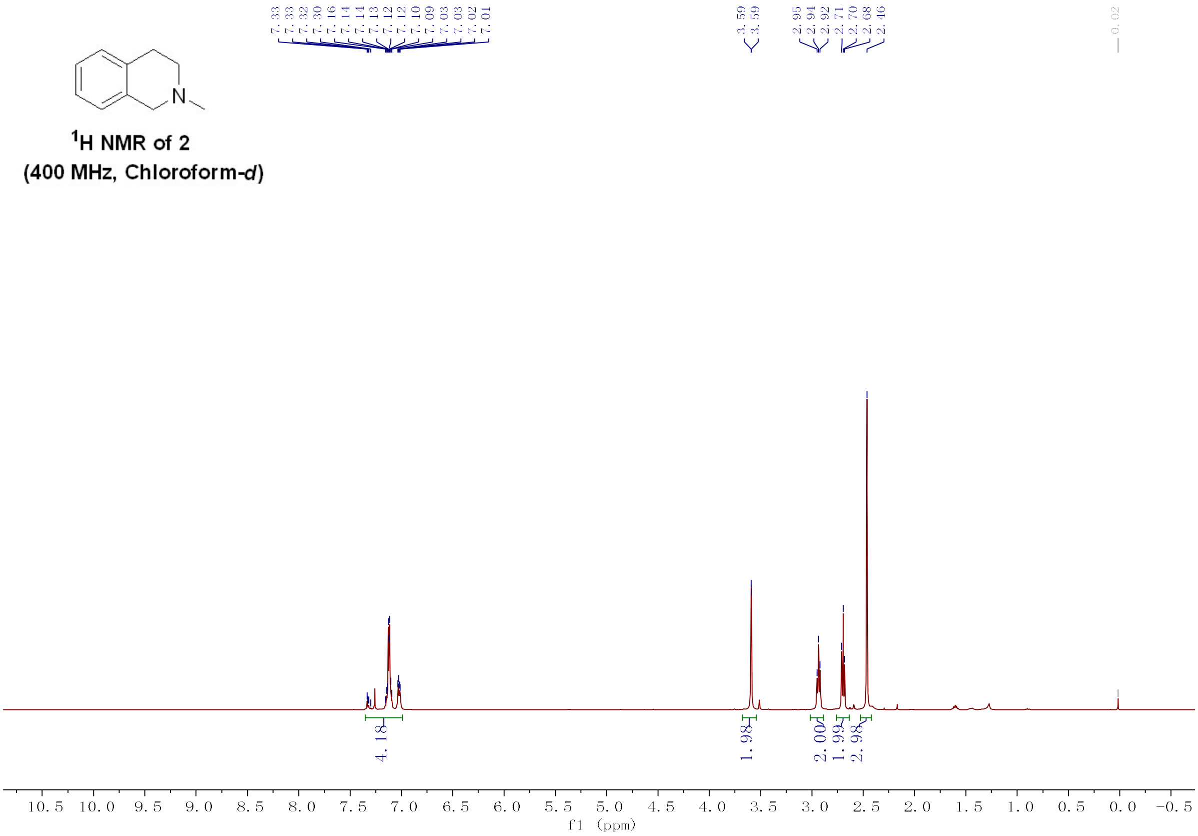
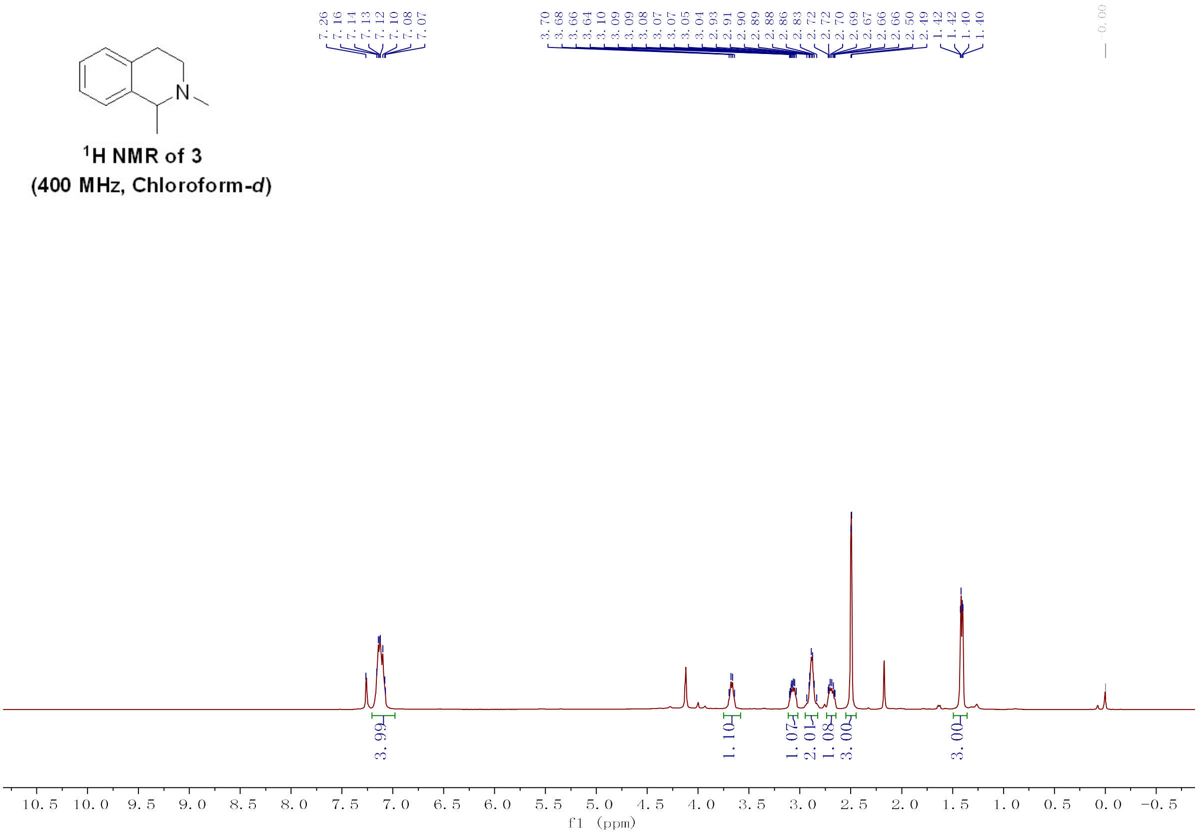
H	-1.20863900	-4.84820900	-3.89529900
H	-4.51992000	-2.31557000	-2.82129400
H	-3.52609600	-4.04891900	-4.31521400
P	-0.90870300	1.63783000	0.09054700
C	-0.82172800	3.20289900	-0.91206600
C	-0.37065400	3.12403000	-2.23995700
C	-1.21927200	4.44768100	-0.40532500
C	-0.32911500	4.26432900	-3.04223600
H	-0.01801200	2.17641700	-2.63221300
C	-1.16783800	5.58852800	-1.20803400
H	-1.55056100	4.54287100	0.62200500
C	-0.72586800	5.50041600	-2.52867100
H	0.02607700	4.18542000	-4.06562600
H	-1.46909200	6.54750000	-0.79598000
H	-0.68406200	6.38977600	-3.15096800
C	-2.68118500	1.17370000	-0.19314300
C	-3.49916100	0.64217900	0.81566300
C	-3.20725100	1.30047300	-1.49040800
C	-4.81338900	0.26239100	0.53495600
H	-3.11903700	0.51068700	1.82083700
C	-4.51914900	0.91980200	-1.76732400
H	-2.59370800	1.70022800	-2.28983400
C	-5.32932100	0.40118700	-0.75400000
H	-5.42424100	-0.15440400	1.32993300
H	-4.90570100	1.02638800	-2.77650200
H	-6.35179800	0.10437200	-0.96900300
C	-0.87240400	2.22099200	1.84637800
C	0.29627900	2.02516100	2.59714300
C	-1.96372200	2.86173000	2.45660900
C	0.37288900	2.45157600	3.92307600
H	1.14116400	1.51771800	2.14332000
C	-1.88962100	3.28336500	3.78473800
H	-2.88236300	3.01784100	1.90096800
C	-0.72183300	3.07809000	4.52205800
H	1.28596800	2.28742900	4.48773600
H	-2.74632600	3.76939300	4.24256900
H	-0.66599400	3.40358300	5.55682800
H	1.78936500	0.59063400	0.31039900
H	3.22502000	0.50175100	-2.36596200
C	6.45112200	1.35635000	0.71899800

C	5.46456800	1.75837800	-0.18632700
H	7.30236600	-0.29552000	1.81459700
C	6.53364800	0.02096200	1.11477000
C	4.53953200	0.84010100	-0.69988600
C	4.64339700	-0.50433500	-0.30745100
C	5.63086600	-0.90921700	0.59041800
H	3.95224000	-1.22804100	-0.72561300
H	5.70573900	-1.95726400	0.86979500
C	3.41478500	1.27605500	-1.62501400
N	2.16187700	1.57914100	-0.91377300
C	2.25875400	2.87120400	-0.24668700
H	1.38570800	3.07836800	0.36683900
H	3.14118000	2.93752300	0.40750200
H	5.41798000	2.79686000	-0.50606000
H	7.15730200	2.08513300	1.10833500
H	2.32942600	3.68408200	-0.98712900
H	3.72098600	2.18535000	-2.16681900

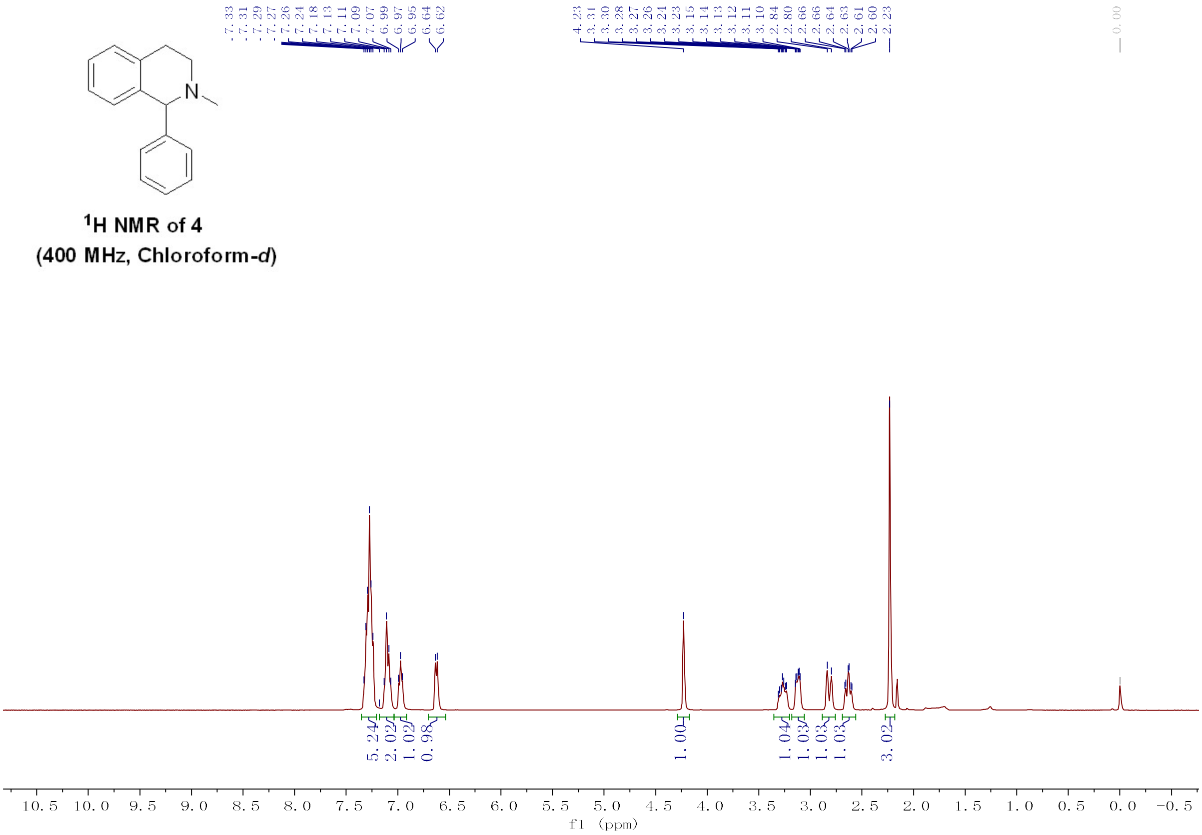
VIII. NMR & HRMS spectra



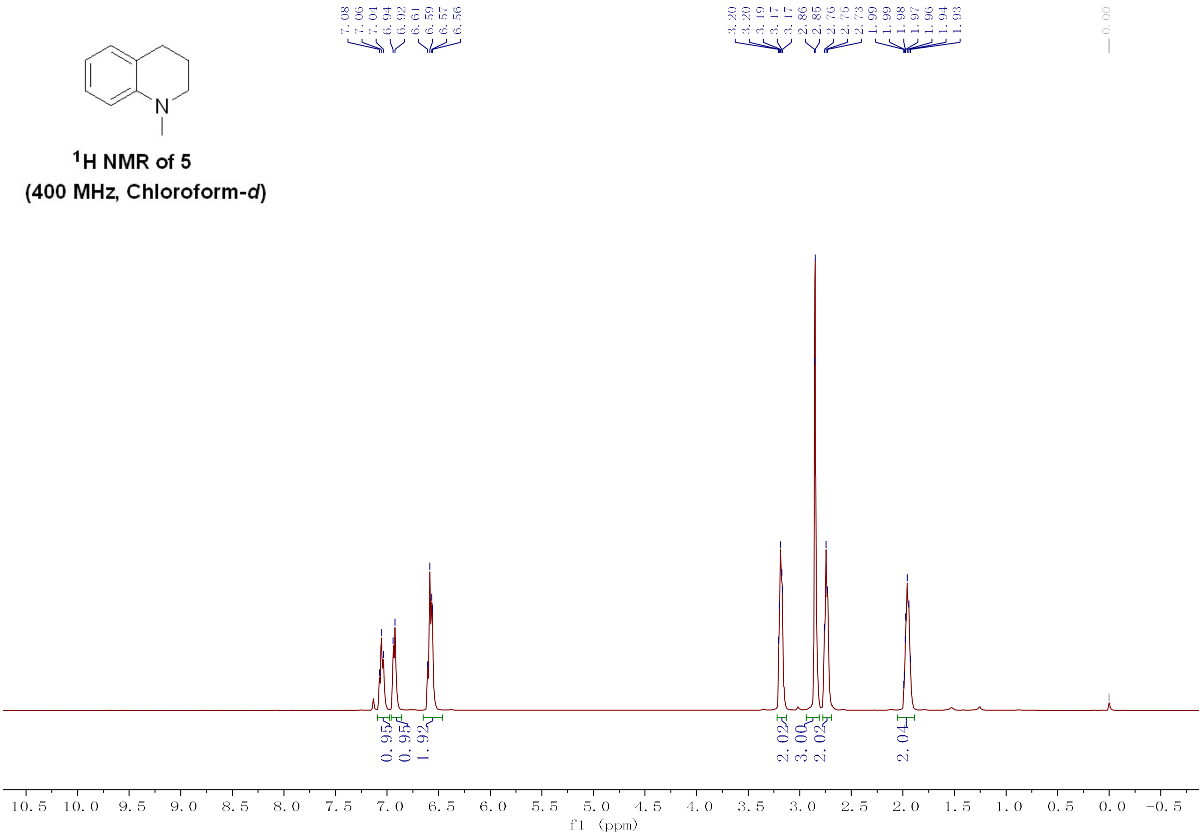
^{1}H NMR of 2
(400 MHz, Chloroform-*d*)



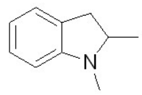
^{1}H NMR of 3
(400 MHz, Chloroform-*d*)



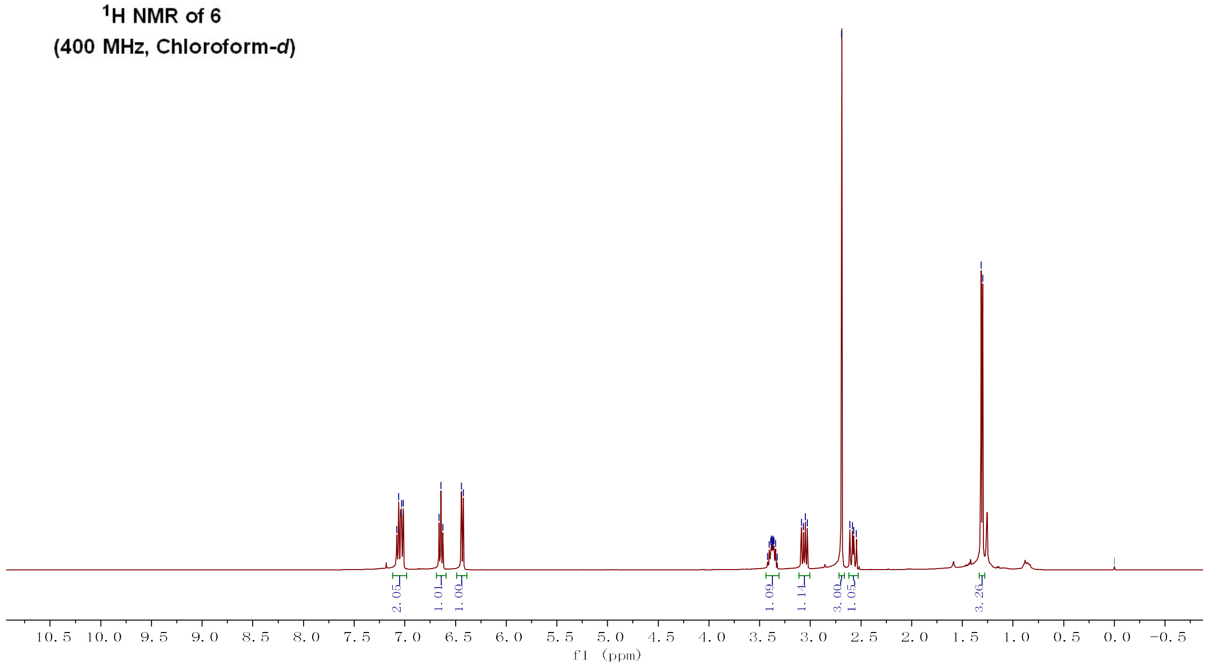
^{1}H NMR of 4
(400 MHz, Chloroform-*d*)

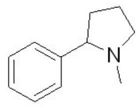


^{1}H NMR of 5
(400 MHz, Chloroform-*d*)

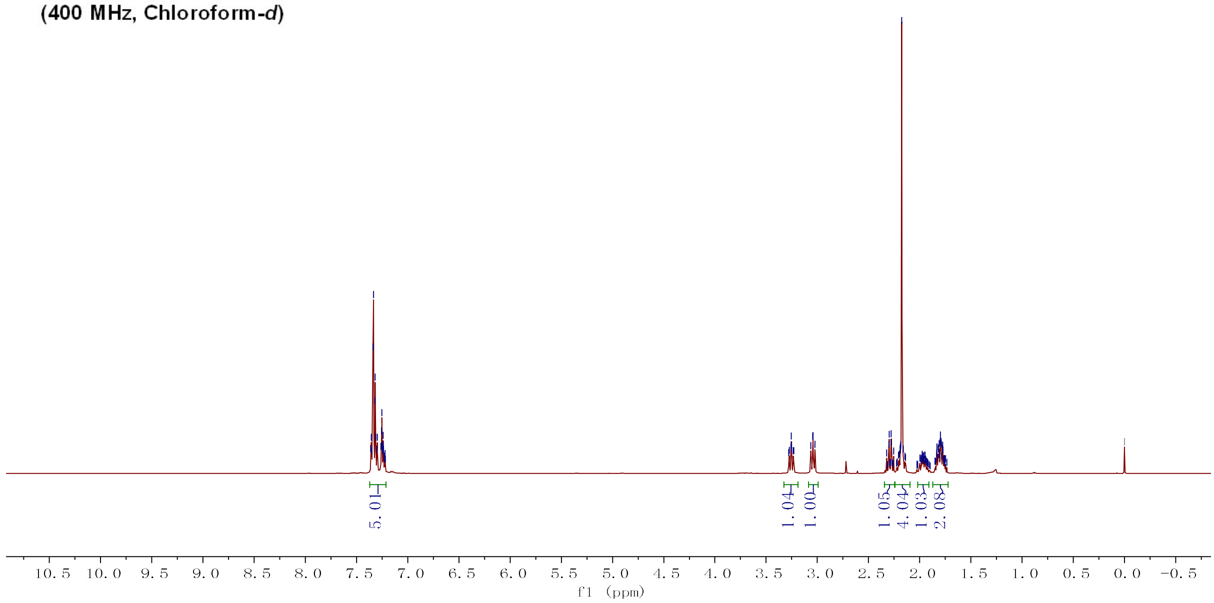


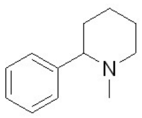
^{1}H NMR of 6
(400 MHz, Chloroform-*d*)



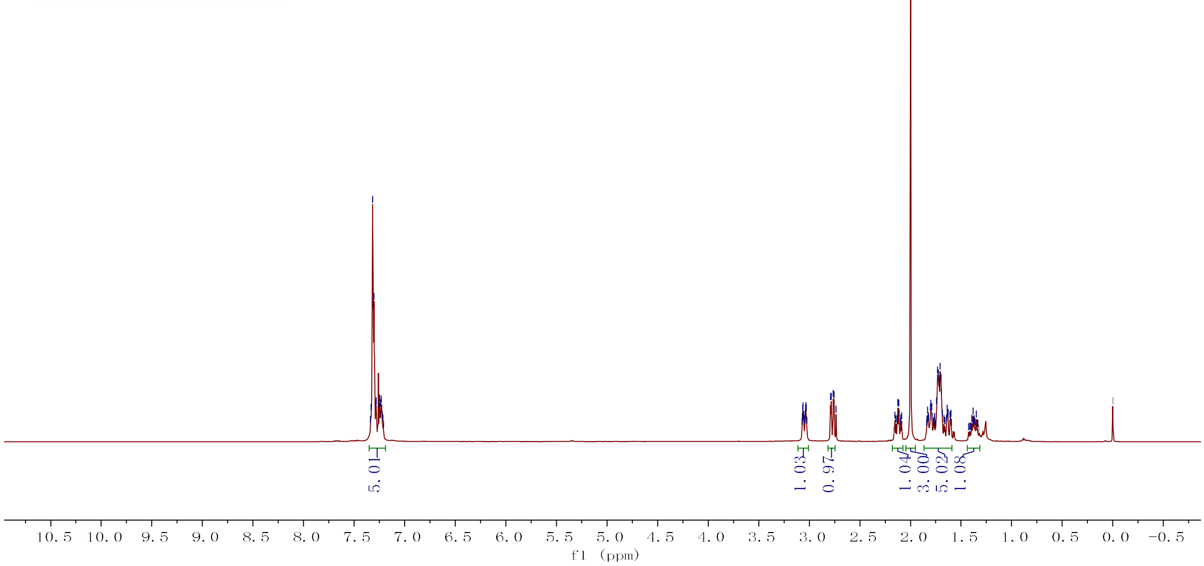


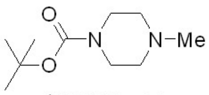
^{1}H NMR of 7
(400 MHz, Chloroform-*d*)



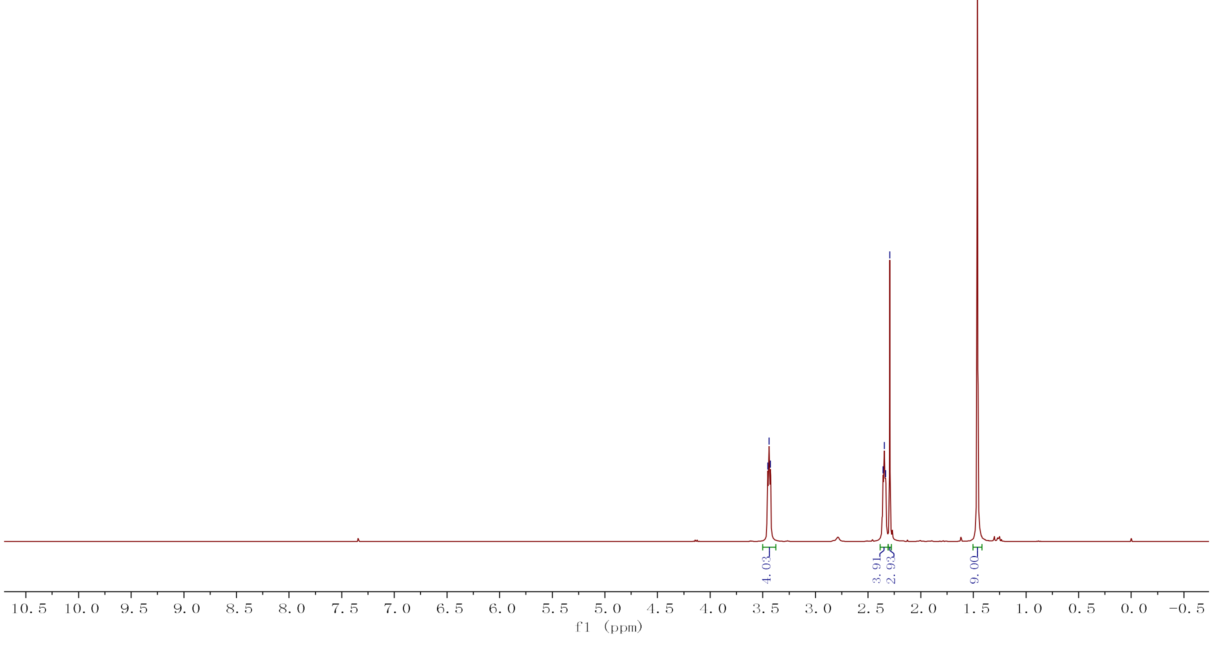


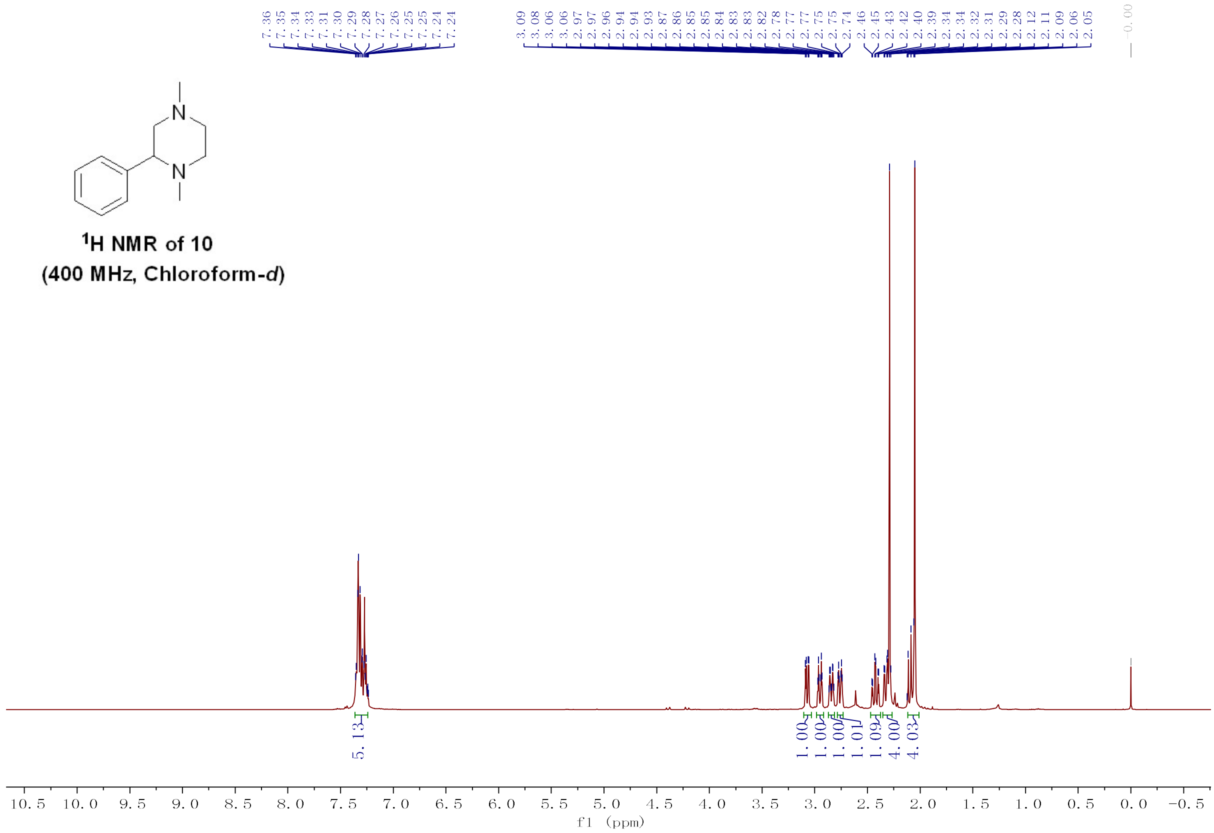
^{1}H NMR of 8
(400 MHz, Chloroform-*d*)



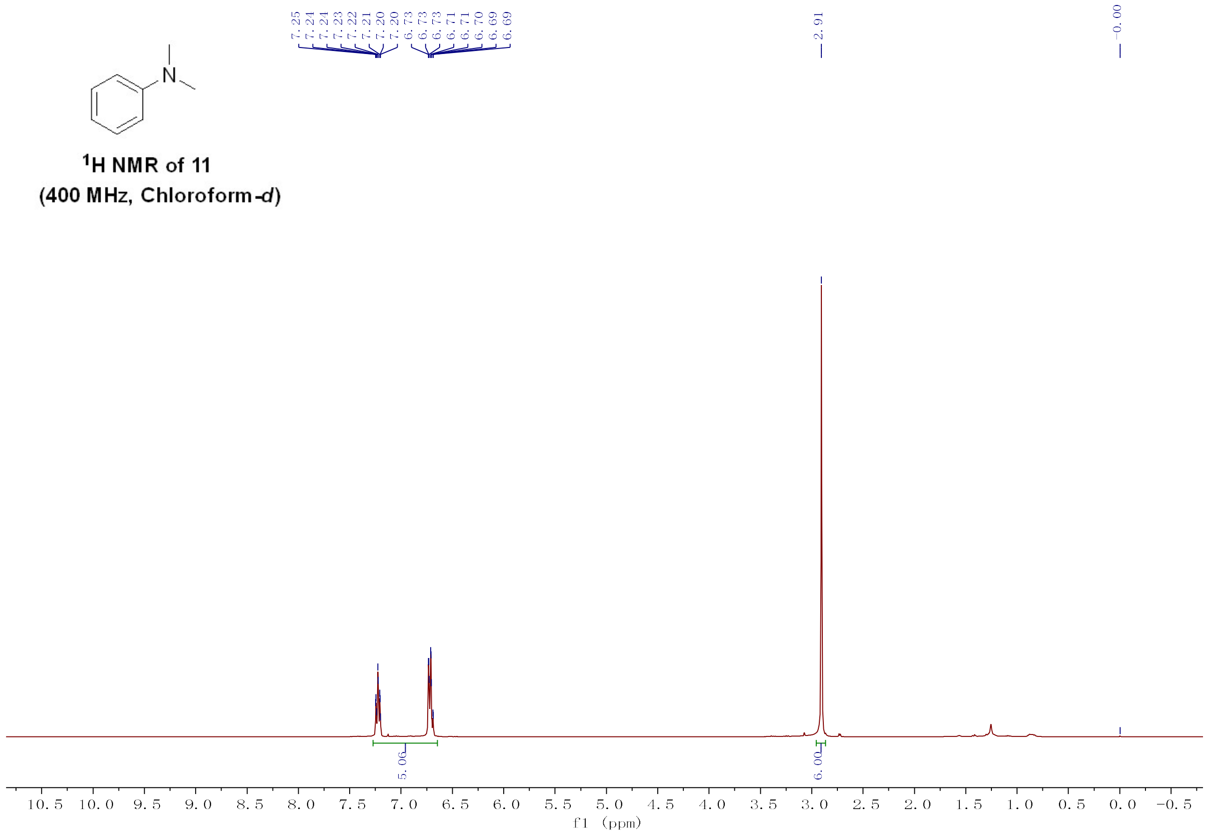


^{1}H NMR of 9
(400 MHz, Chloroform-*d*)

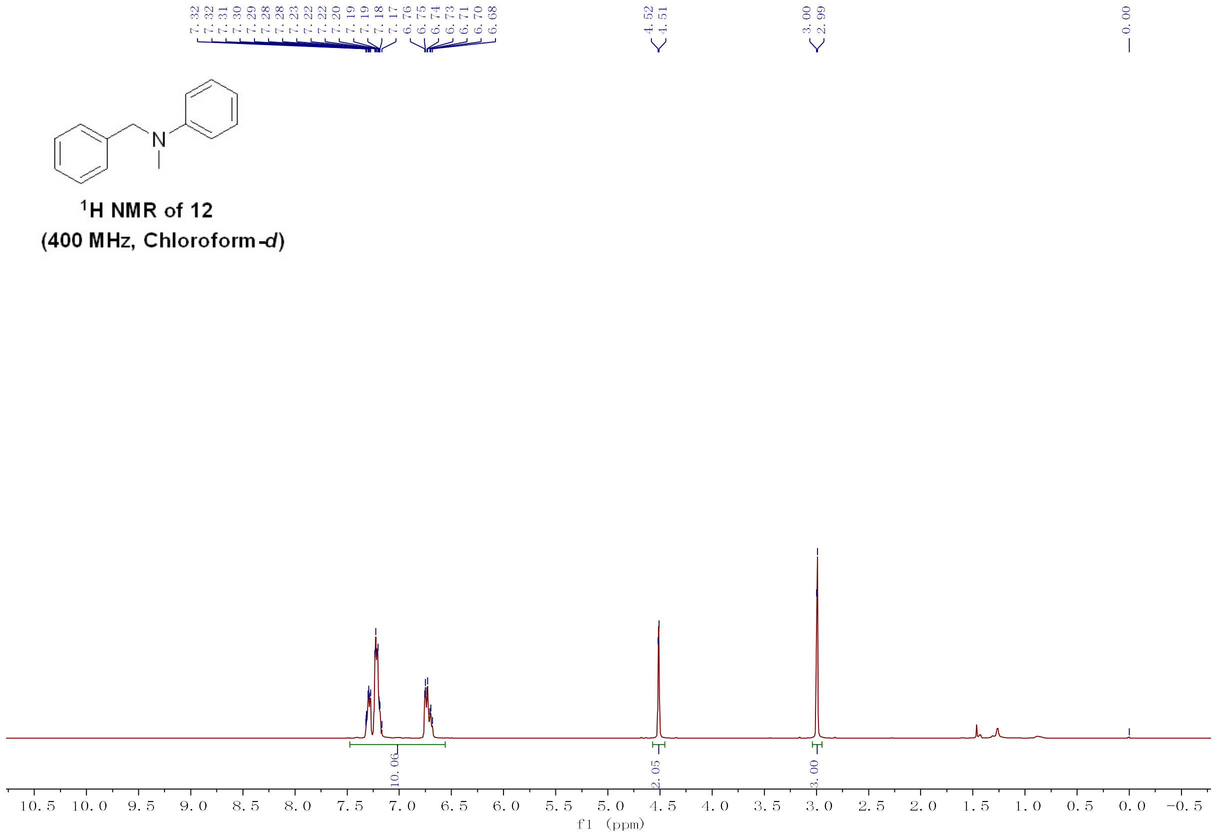




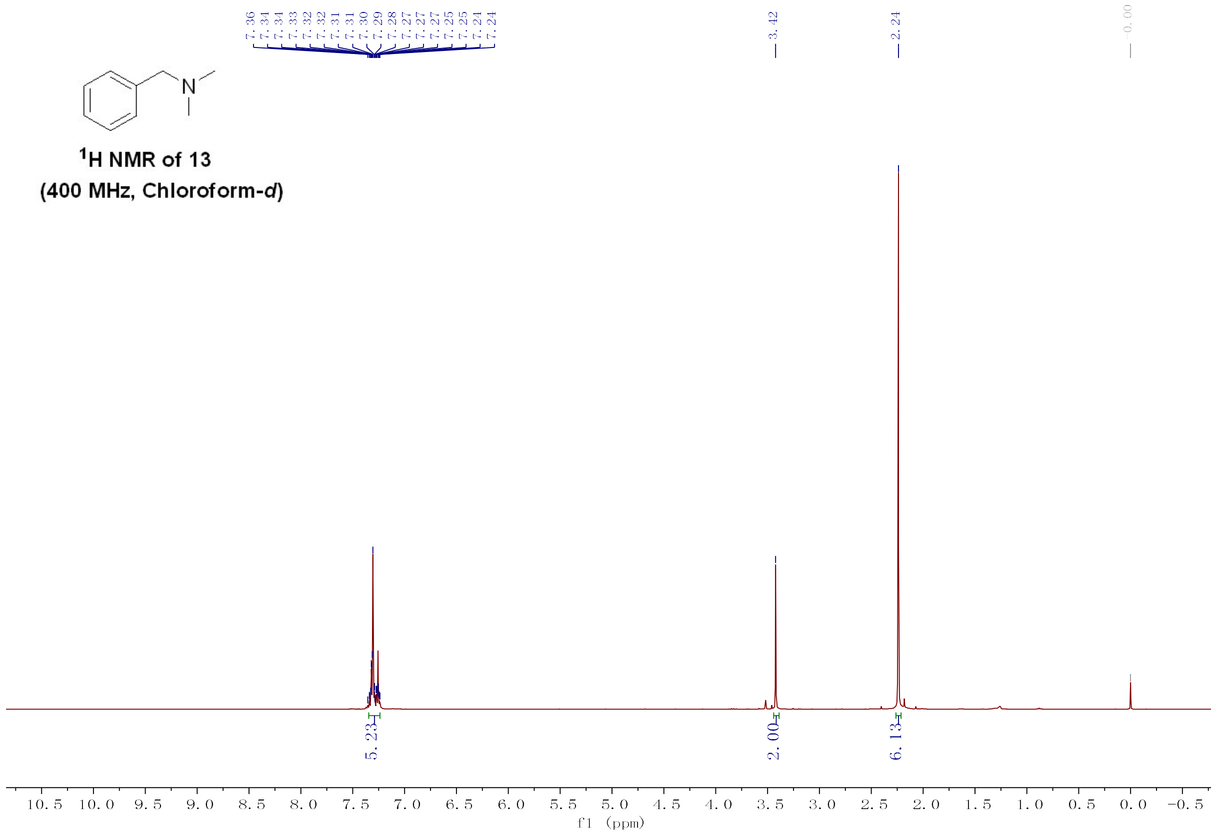
^{1}H NMR of 10
(400 MHz, Chloroform-*d*)



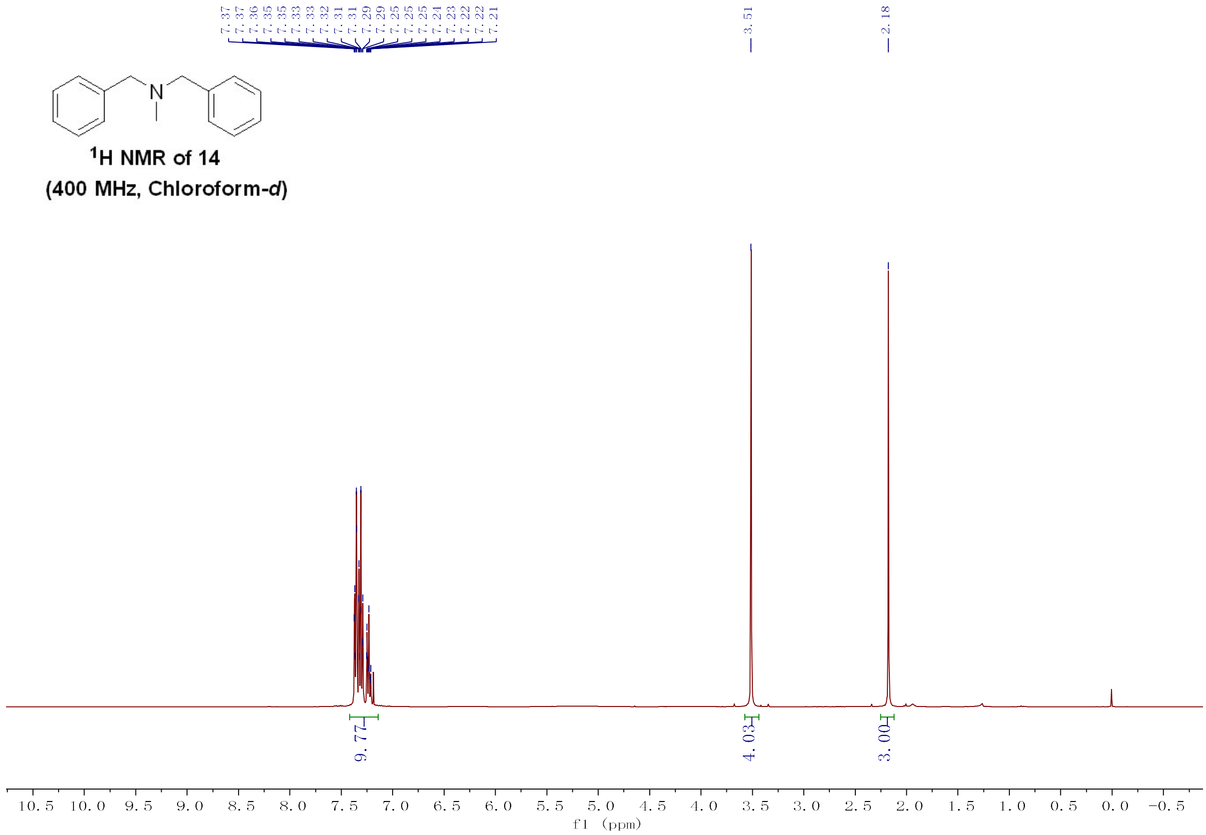
^{1}H NMR of 11
(400 MHz, Chloroform-*d*)



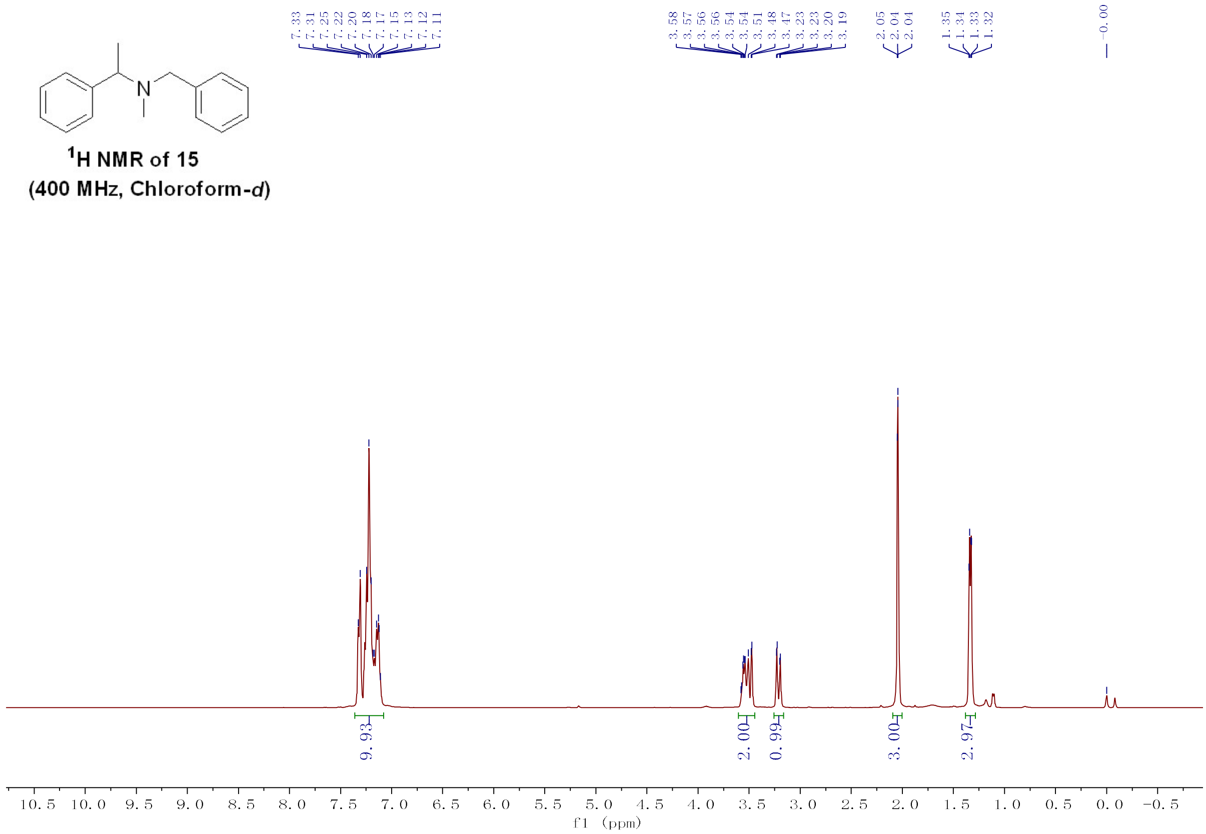
^{1}H NMR of 12
(400 MHz, Chloroform-*d*)



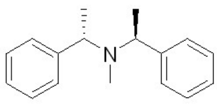
^{1}H NMR of 13
(400 MHz, Chloroform-*d*)



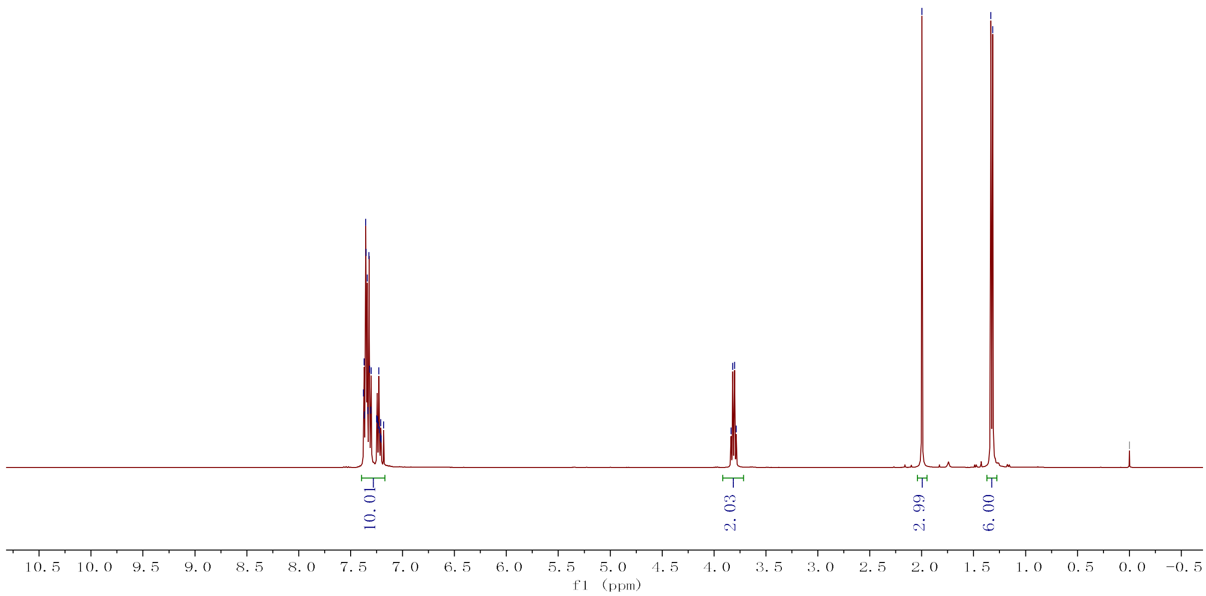
7.37 7.37 7.36 7.35 7.33 7.33 7.32 7.31 7.31 7.29 7.29 7.25 7.25 7.25 7.24 7.23 7.22 7.22 7.21
3.51
2.18
N
¹H NMR of 14
(400 MHz, Chloroform-*d*)
9.77
4.03
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

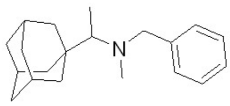


7.33 7.31 7.25 7.22 7.20 7.18 7.17 7.15 7.13 7.12 7.11
3.58 3.57 3.56 3.54 3.54 3.51 3.48 3.47 3.23 3.23 3.20 3.19
2.05 2.04 2.04
1.35 1.34 1.33 1.32
-0.00
N
¹H NMR of 15
(400 MHz, Chloroform-*d*)
9.93
2.00
0.99
3.00
2.97
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

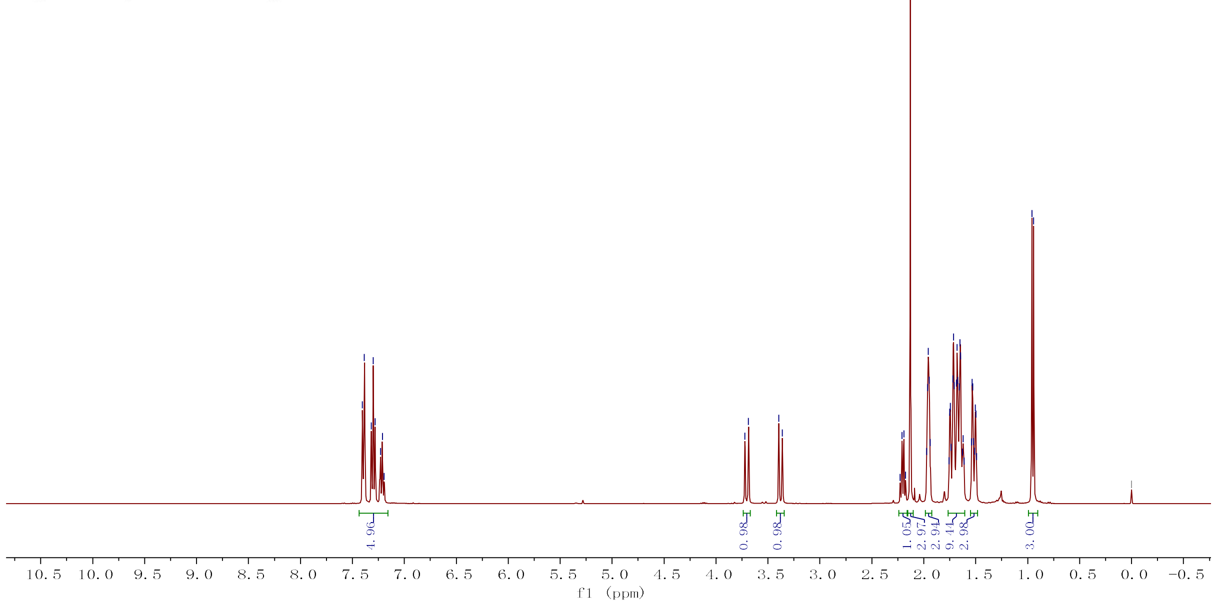


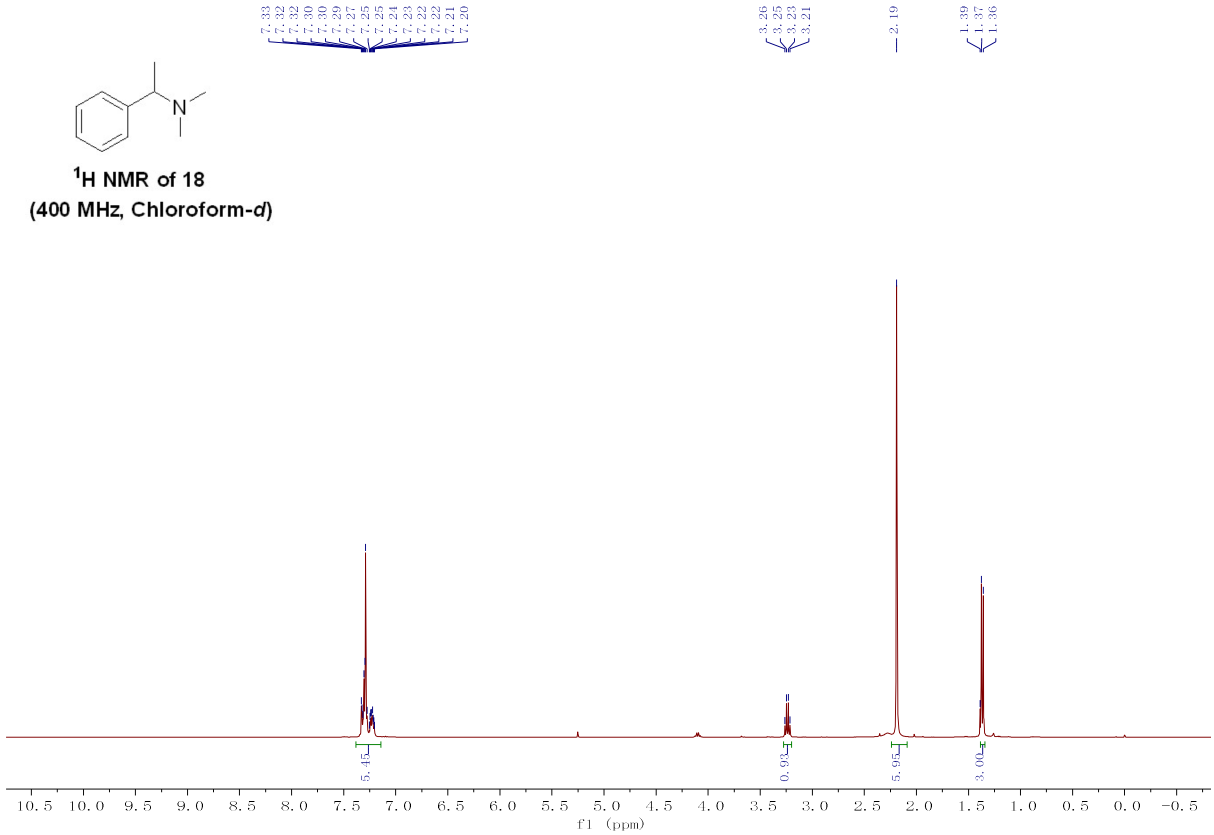
^{1}H NMR of 16
(400 MHz, Chloroform-*d*)



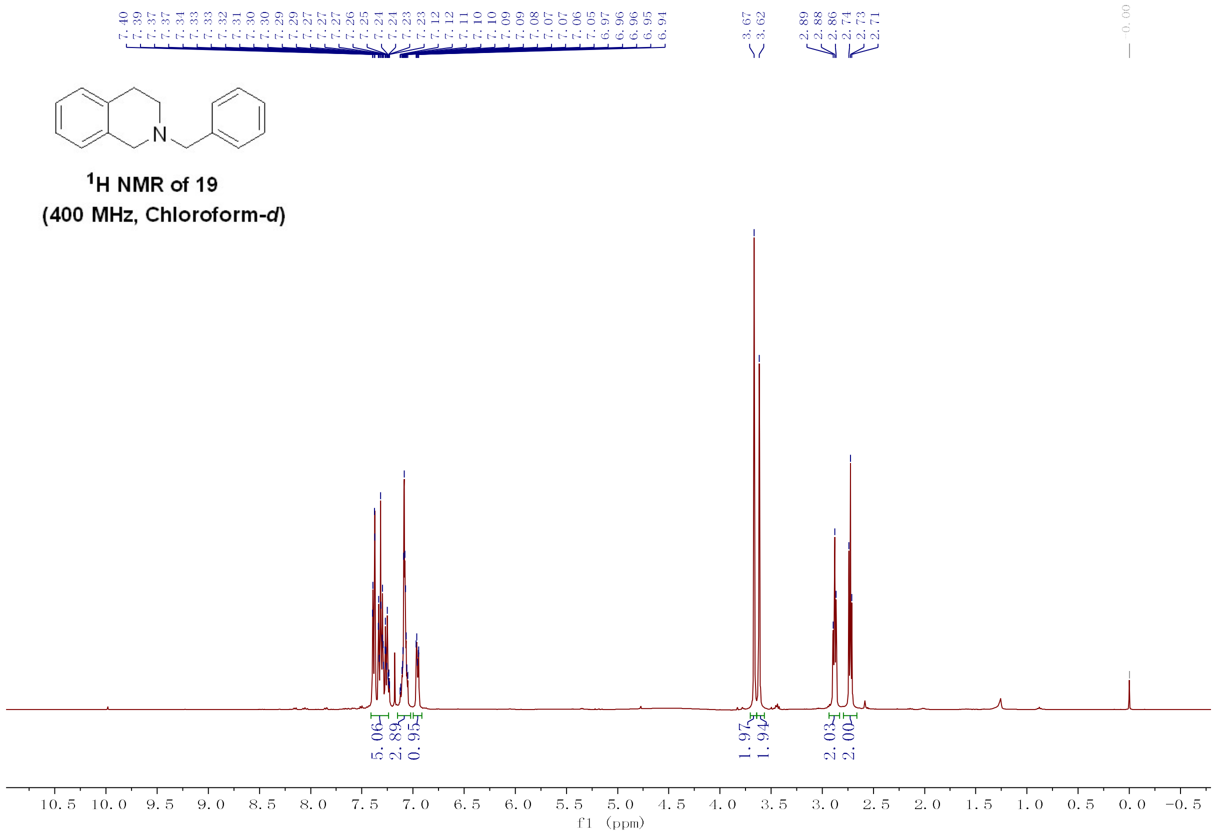


^{1}H NMR of 17
(400 MHz, Chloroform-*d*)

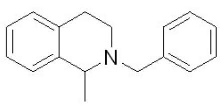




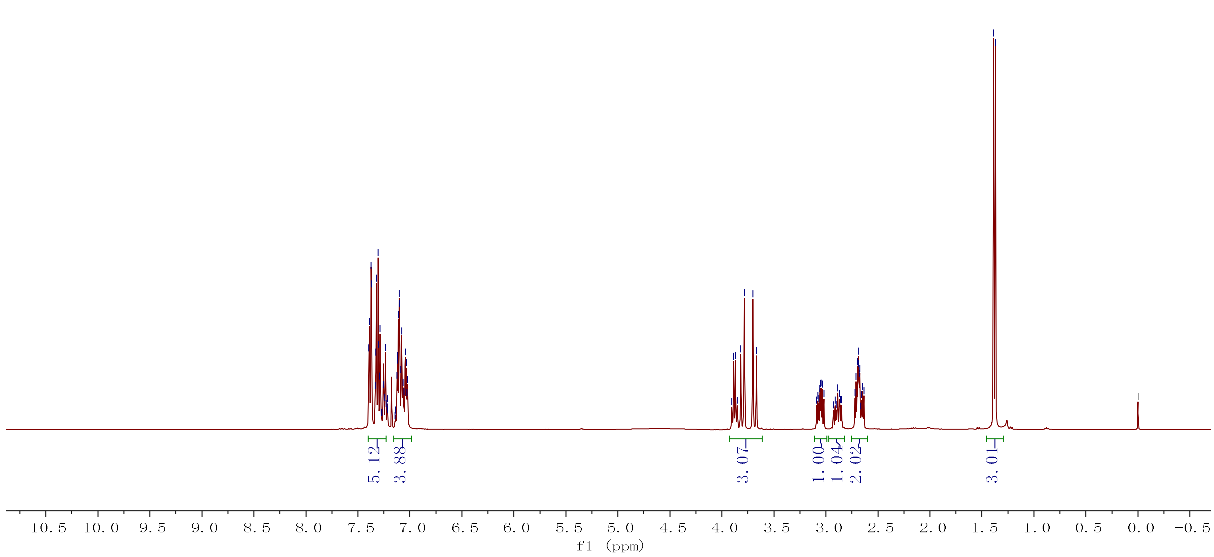
^{1}H NMR of 18
(400 MHz, Chloroform-*d*)

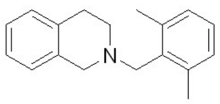


^{1}H NMR of 19
(400 MHz, Chloroform-*d*)

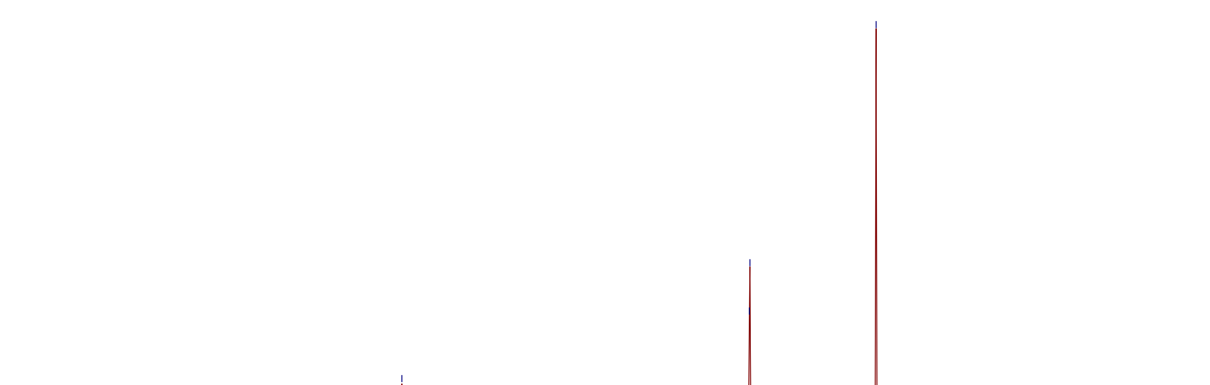


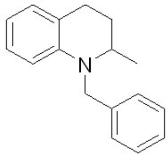
^{1}H NMR of 20
(400 MHz, Chloroform-*d*)



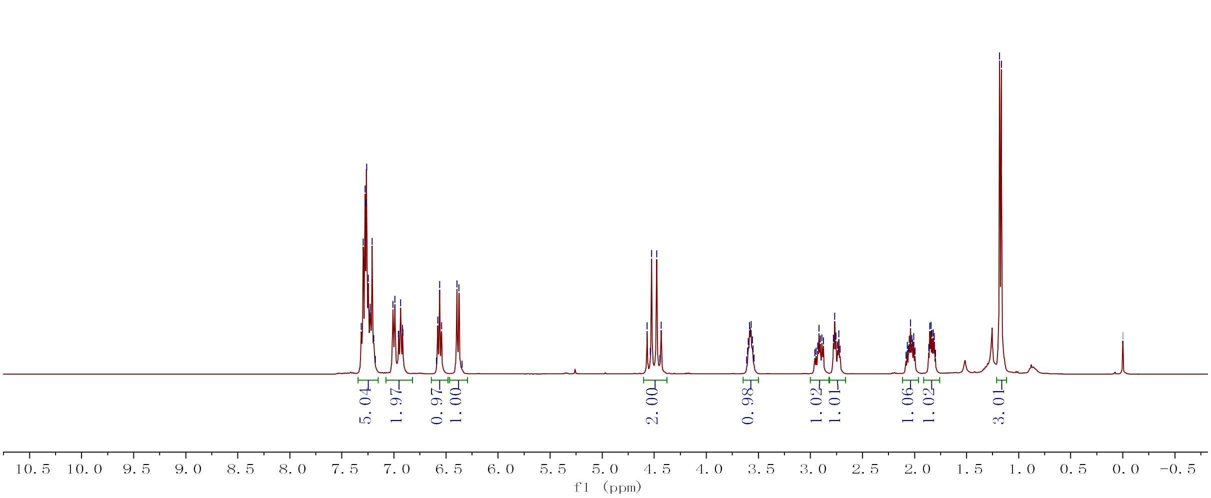


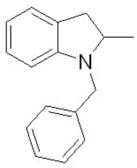
^{1}H NMR of 21
(400 MHz, Chloroform-*d*)



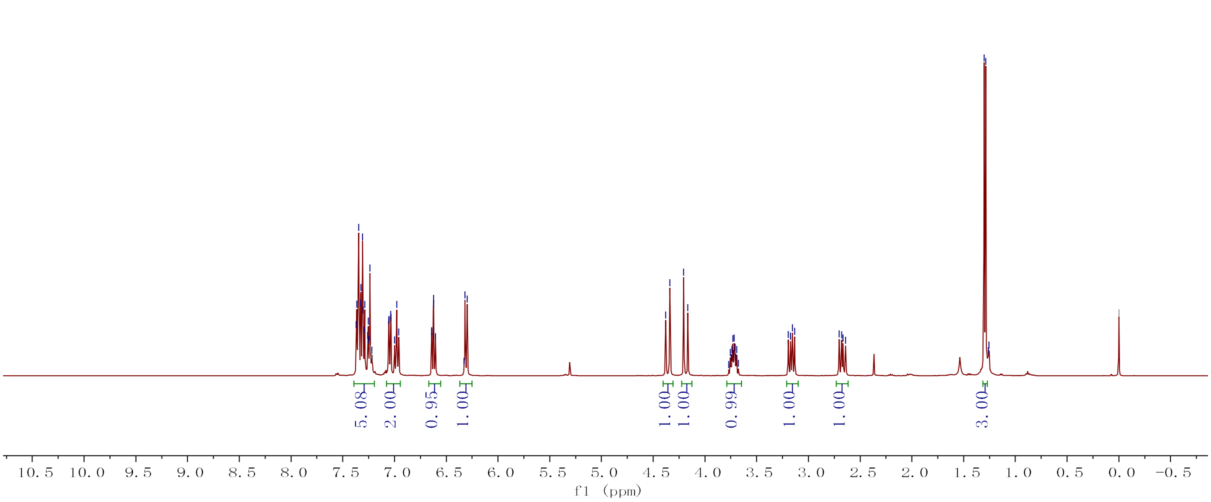


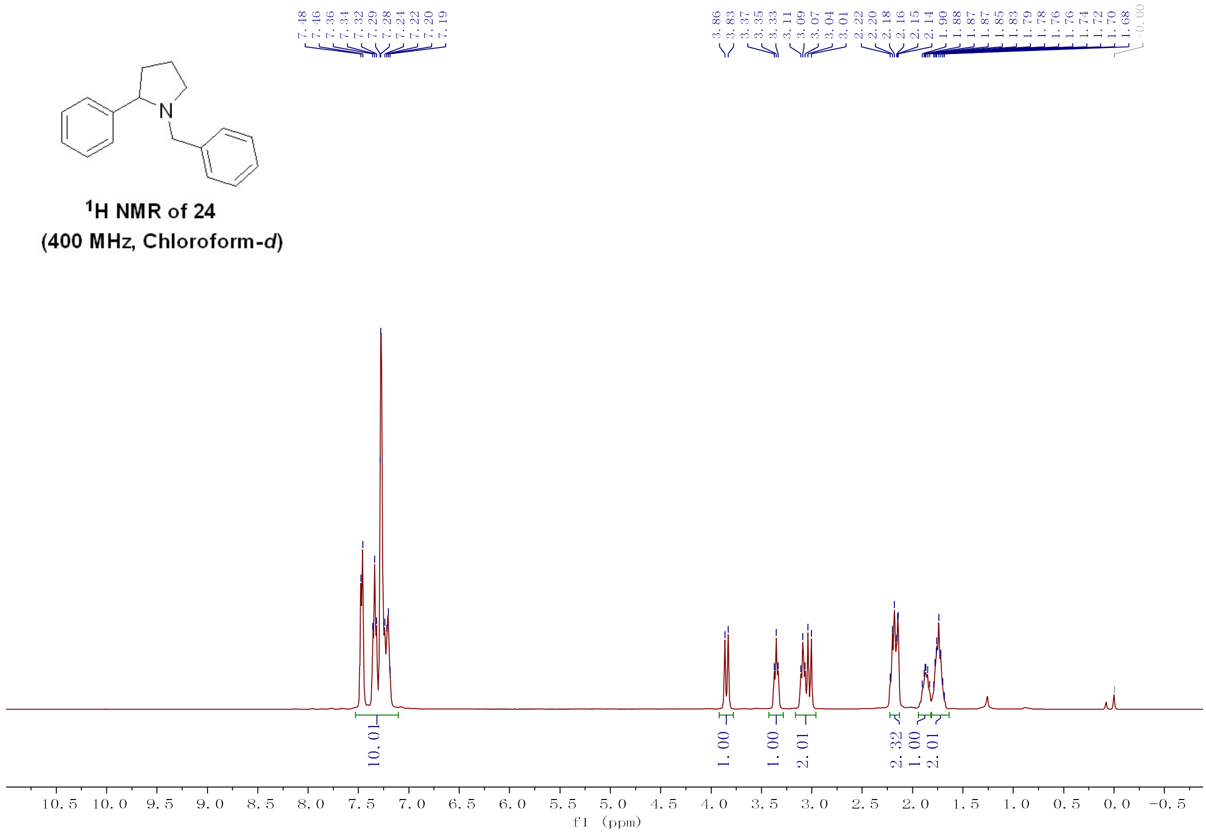
[1]H NMR of 22
(400 MHz, Chloroform-*d*)



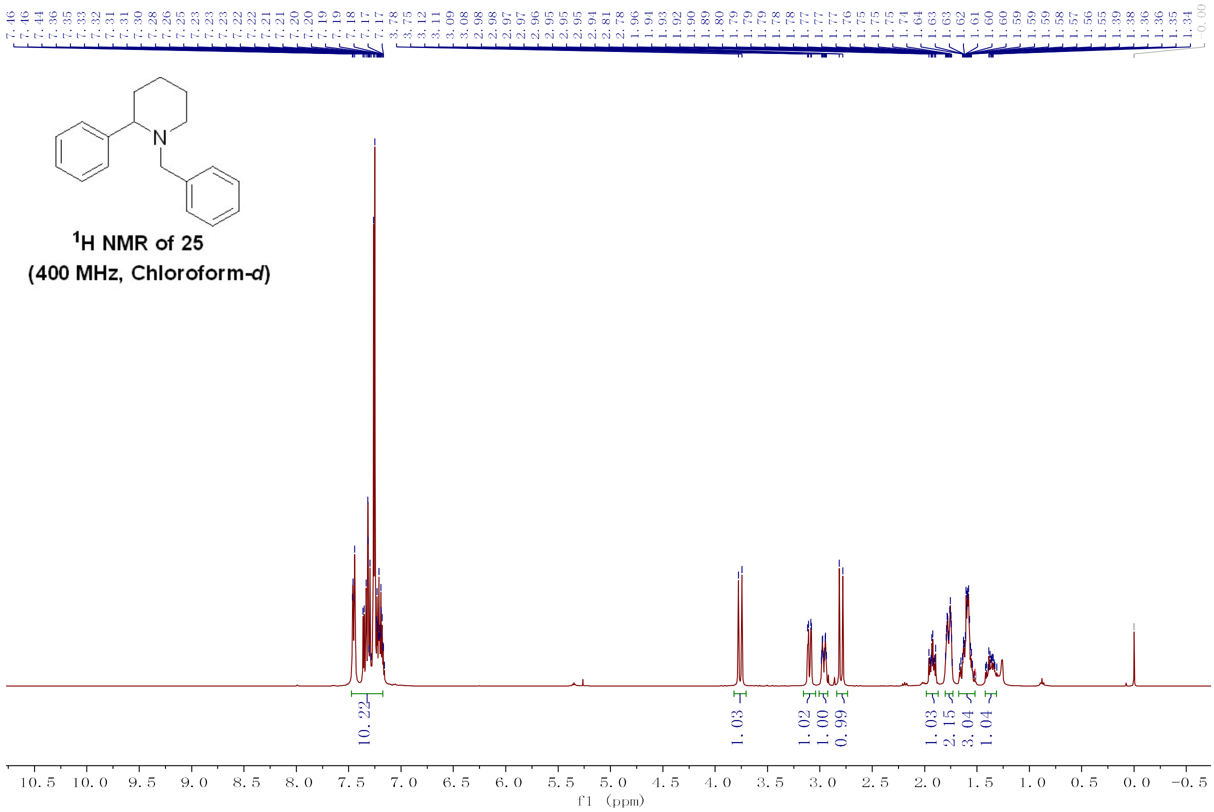


[1]H NMR of 23
(400 MHz, Chloroform-*d*)

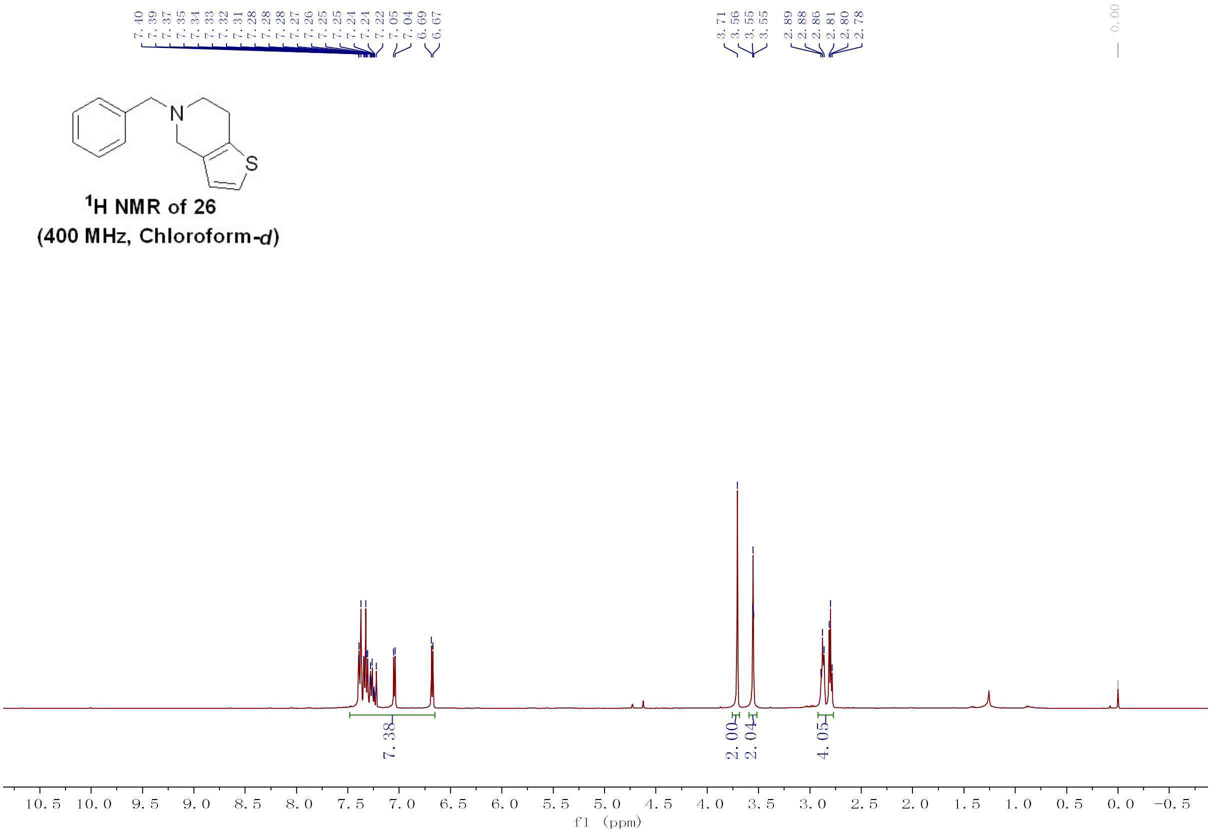




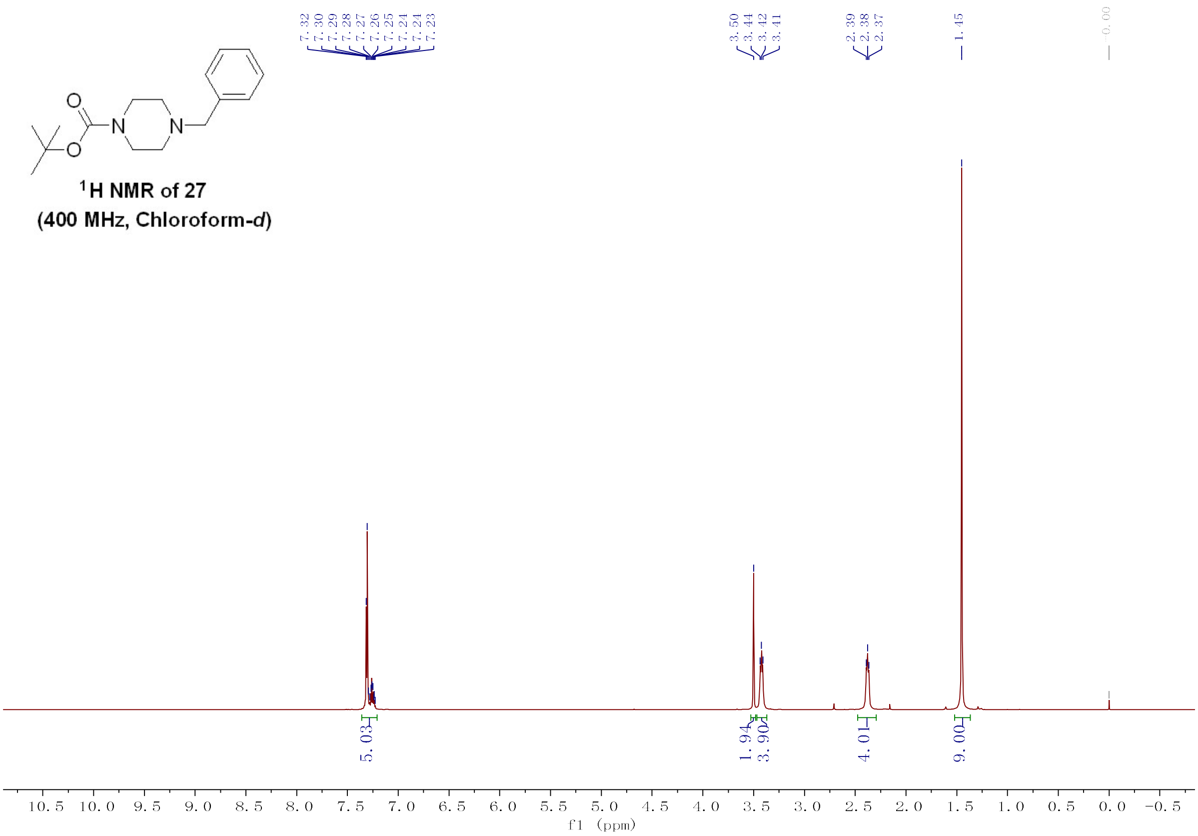
^{1}H NMR of 24
(400 MHz, Chloroform-*d*)



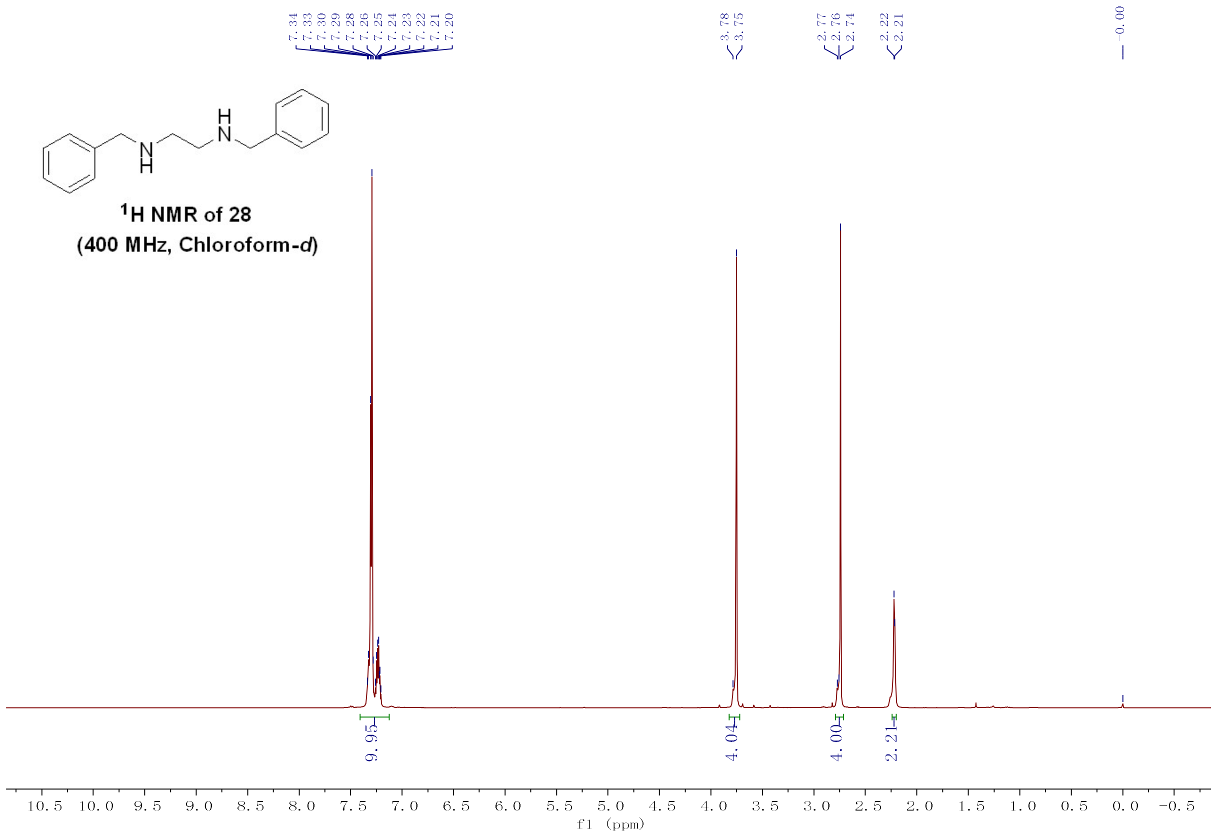
^{1}H NMR of 25
(400 MHz, Chloroform-*d*)



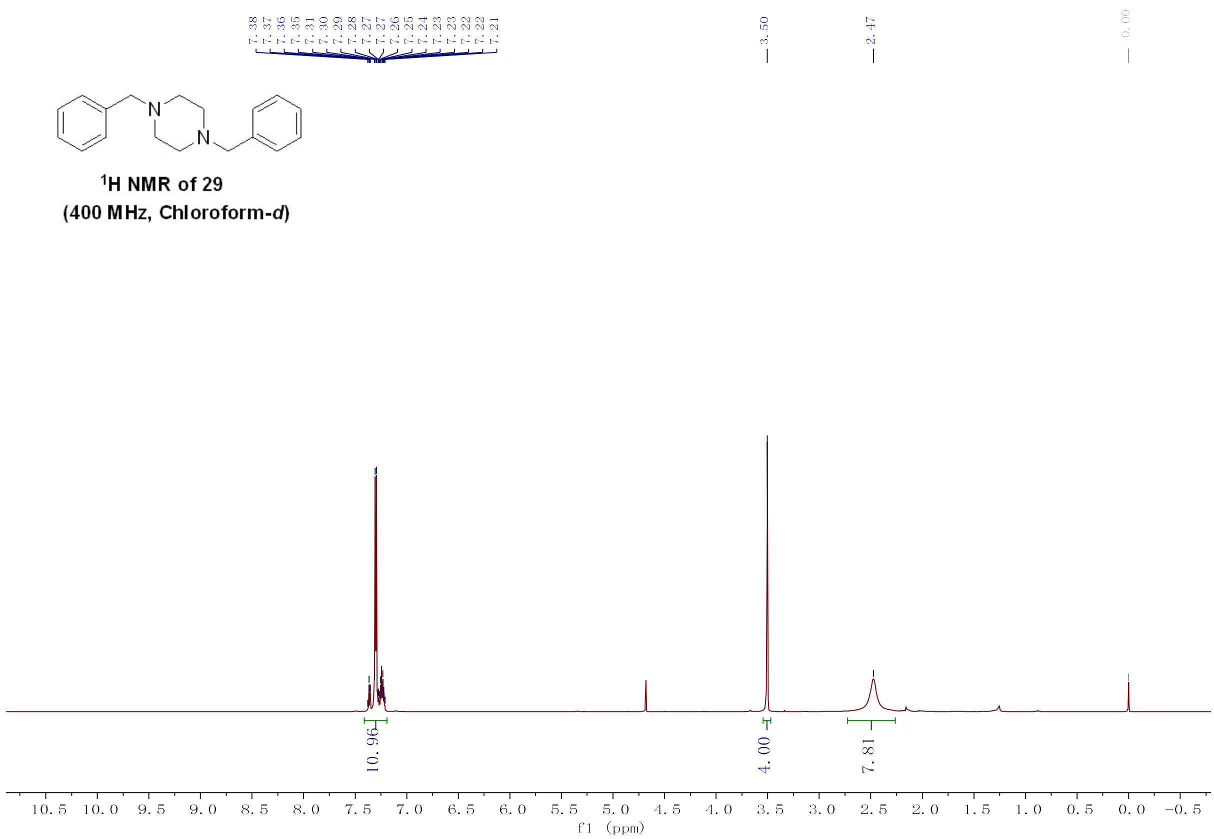
^{1}H NMR of 26
(400 MHz, Chloroform-*d*)



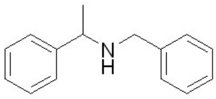
^{1}H NMR of 27
(400 MHz, Chloroform-*d*)



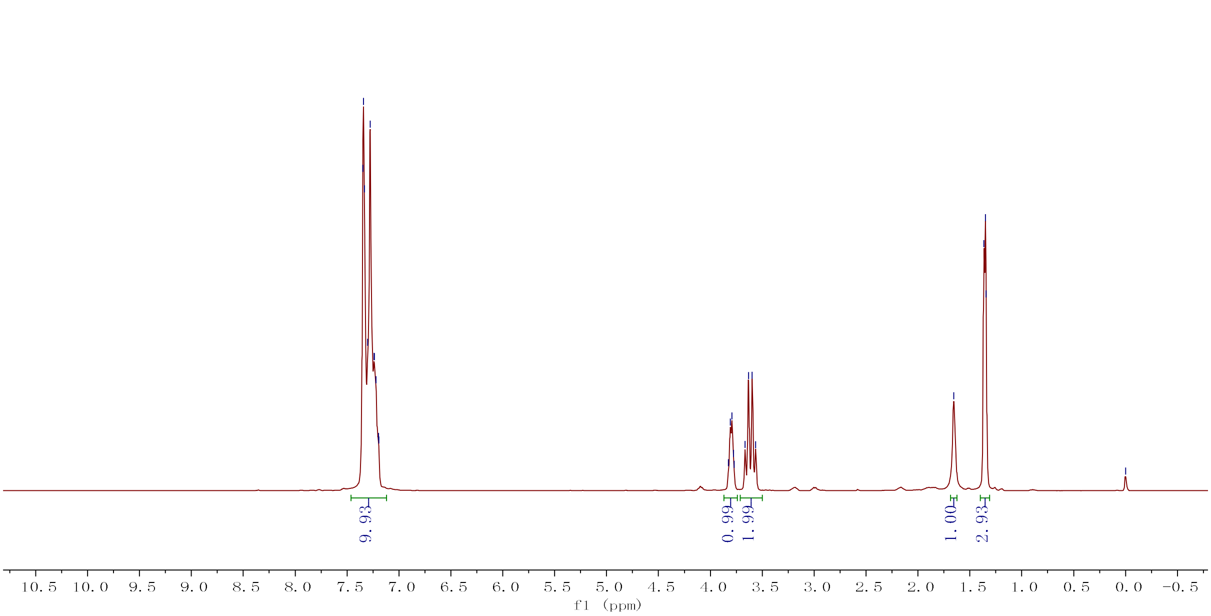
^{1}H NMR of 28
(400 MHz, Chloroform-*d*)

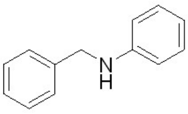


^{1}H NMR of 29
(400 MHz, Chloroform-*d*)

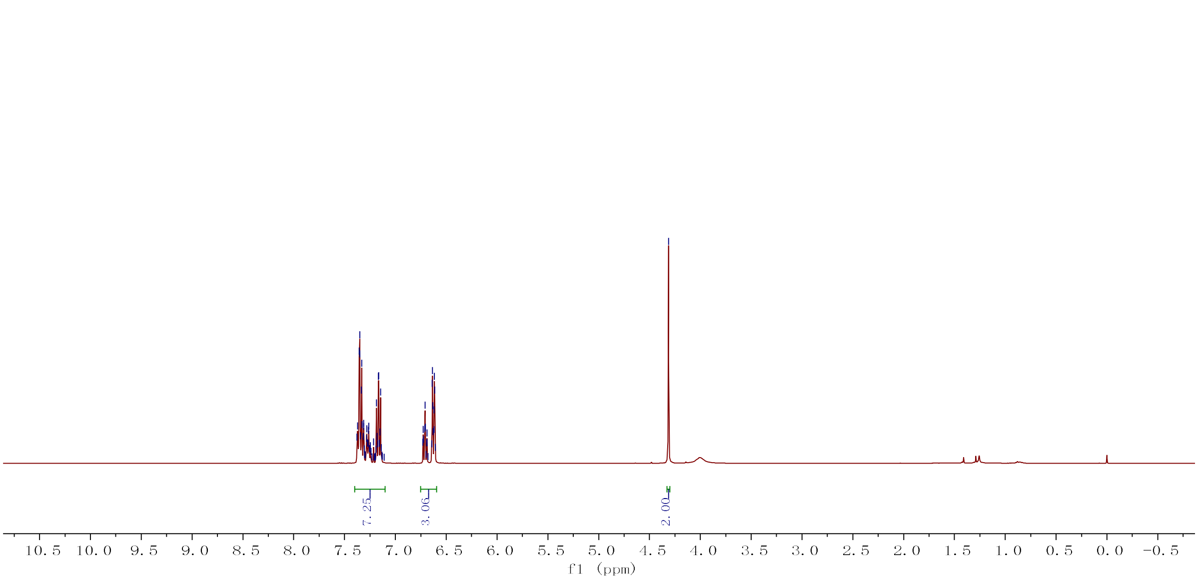


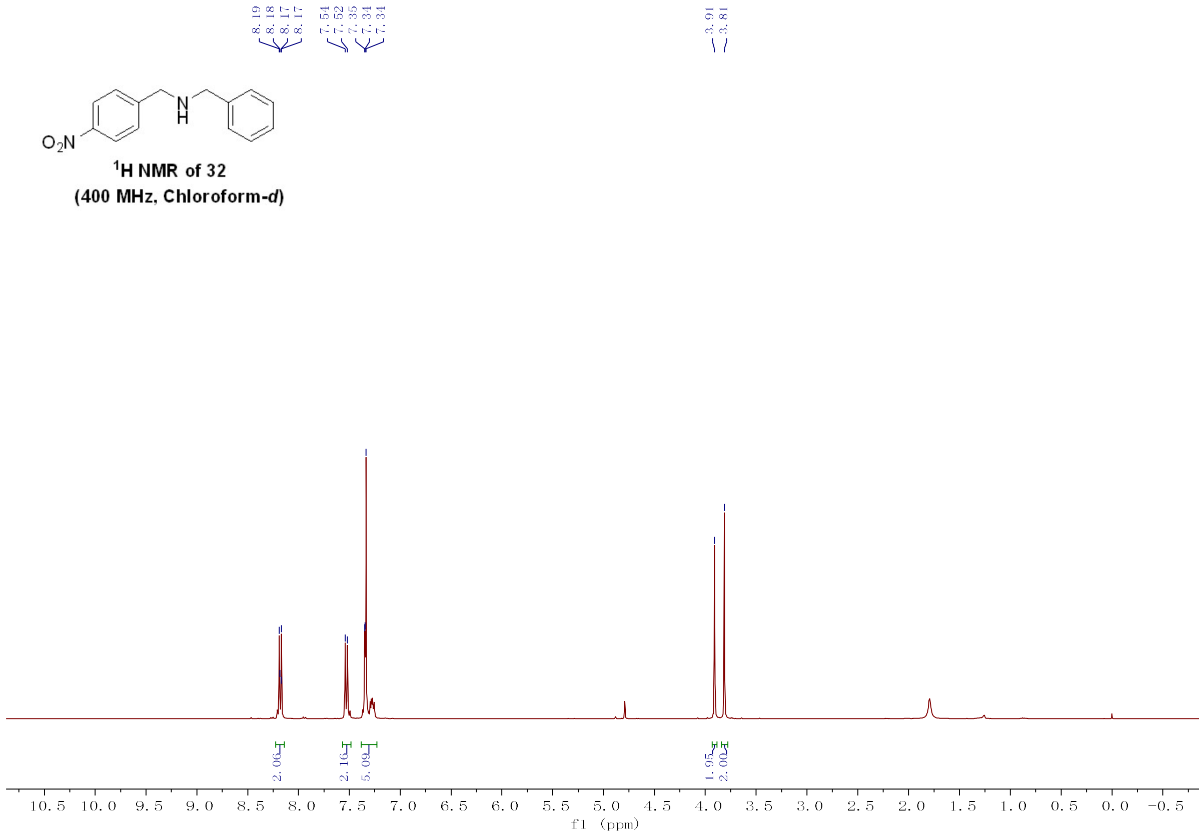
^{1}H NMR of 30
(400 MHz, Chloroform-*d*)



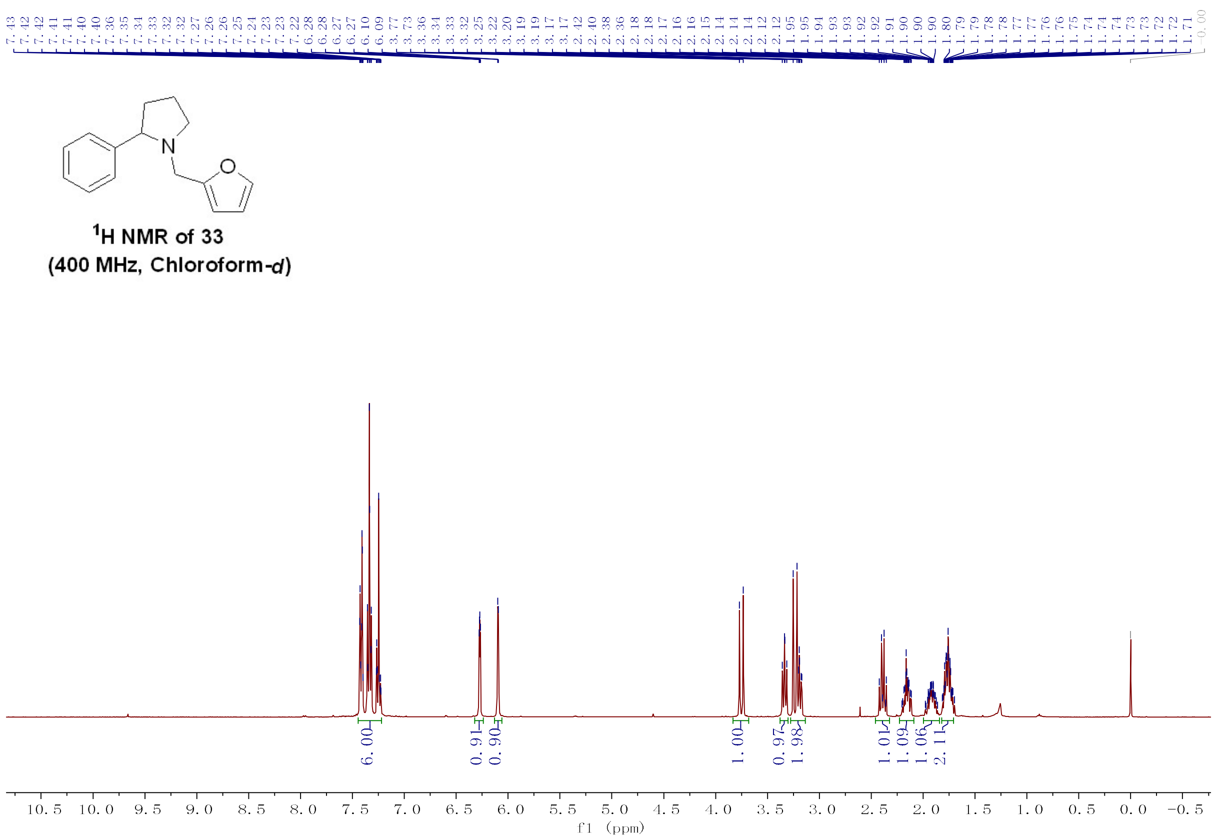


^{1}H NMR of 31
(400 MHz, Chloroform-*d*)

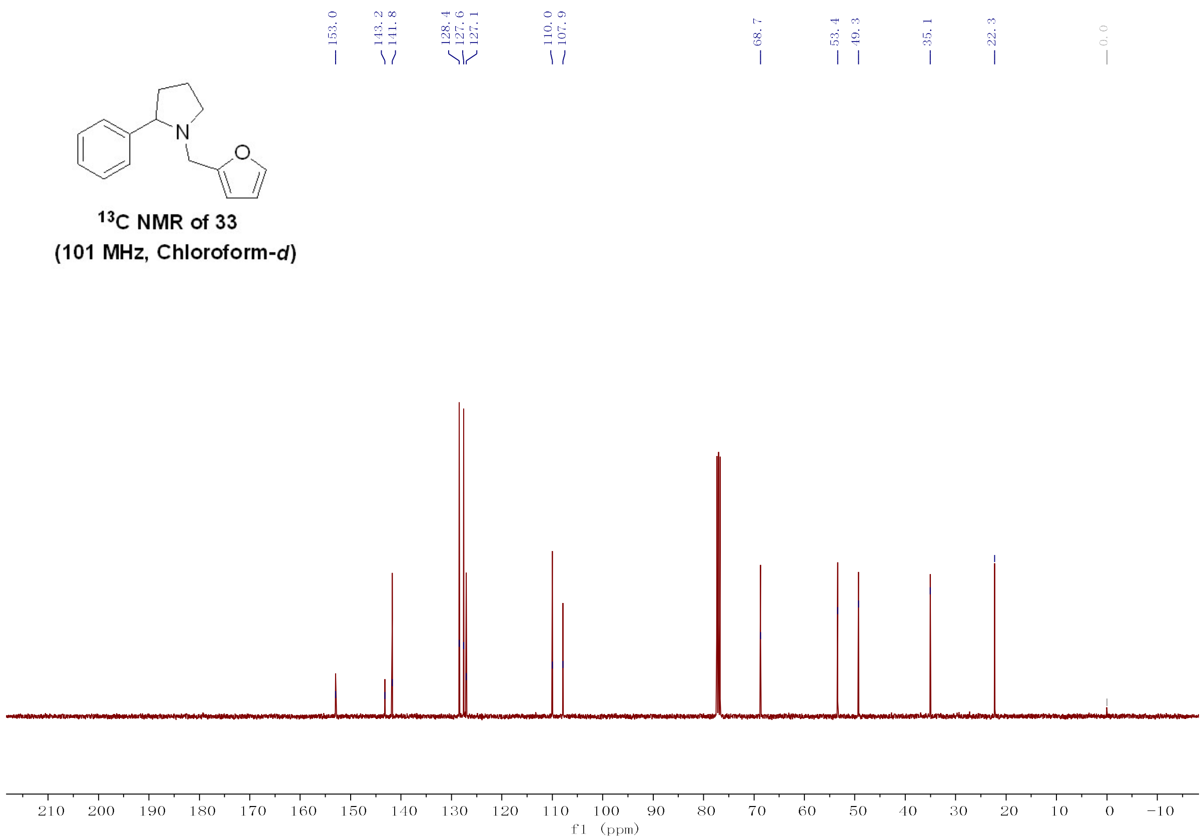




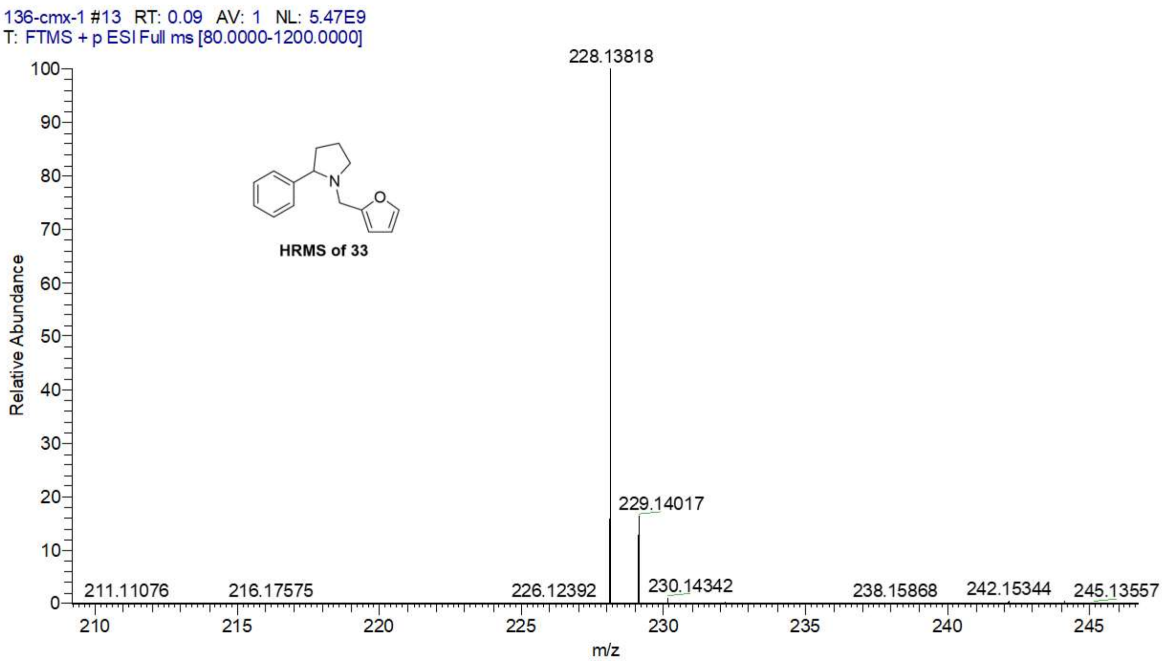
^{1}H NMR of 32
(400 MHz, Chloroform-*d*)



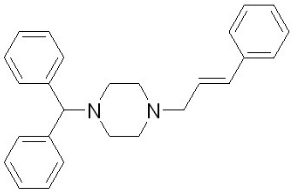
^{1}H NMR of 33
(400 MHz, Chloroform-*d*)



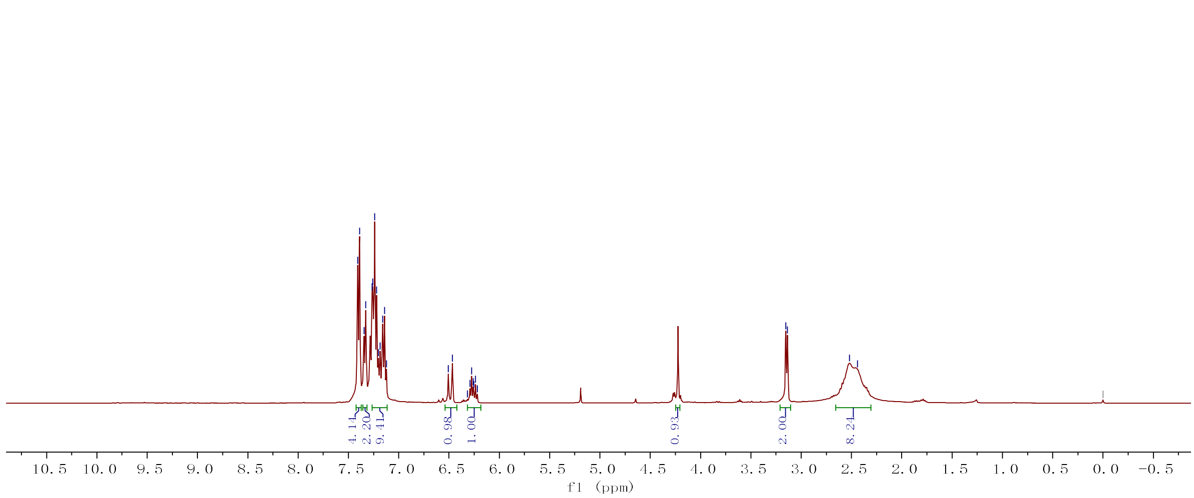
153.0
143.2
141.8
128.4
127.6
127.1
110.0
107.9
68.7
53.4
49.3
35.1
22.3
0.0
N
O
^{13}C NMR of 33
(101 MHz, Chloroform-*d*)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

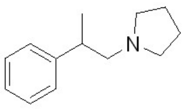


136-cmx-1 #13 RT: 0.09 AV: 1 NL: 5.47E9
T: FTMS + p ESI Full ms [80.0000-1200.0000]
228.13818
N
O
HRMS of 33
Relative Abundance
229.14017
211.11076
216.17575
226.12392
230.14342
238.15868
242.15344
245.13557
m/z

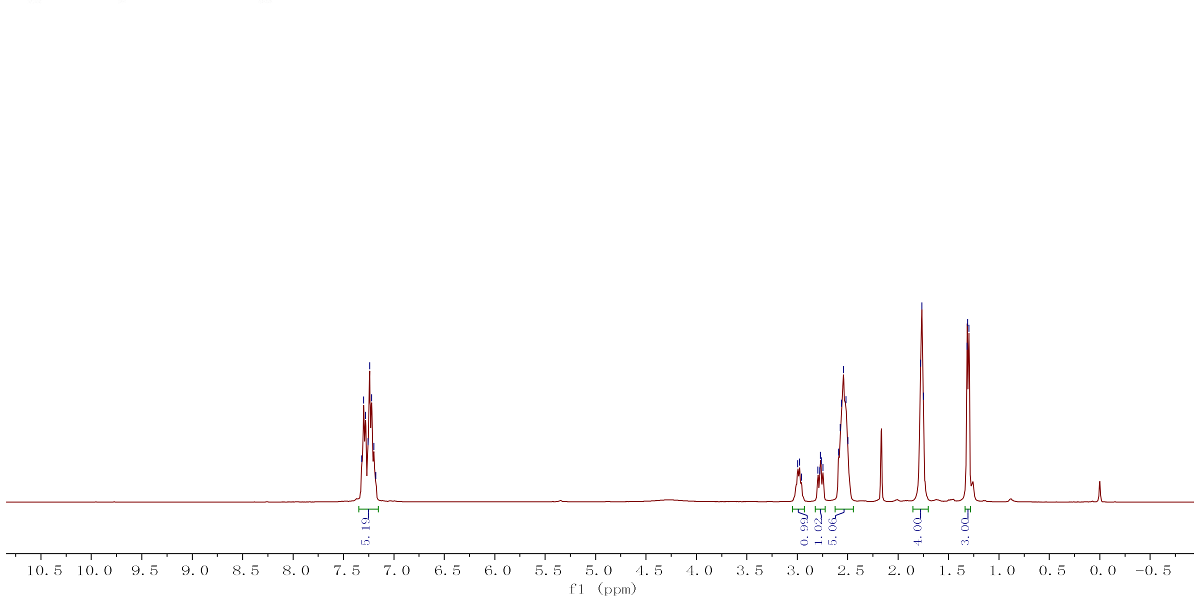


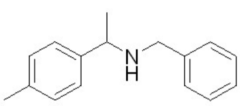
^{1}H NMR of 34
(400 MHz, Chloroform-*d*)

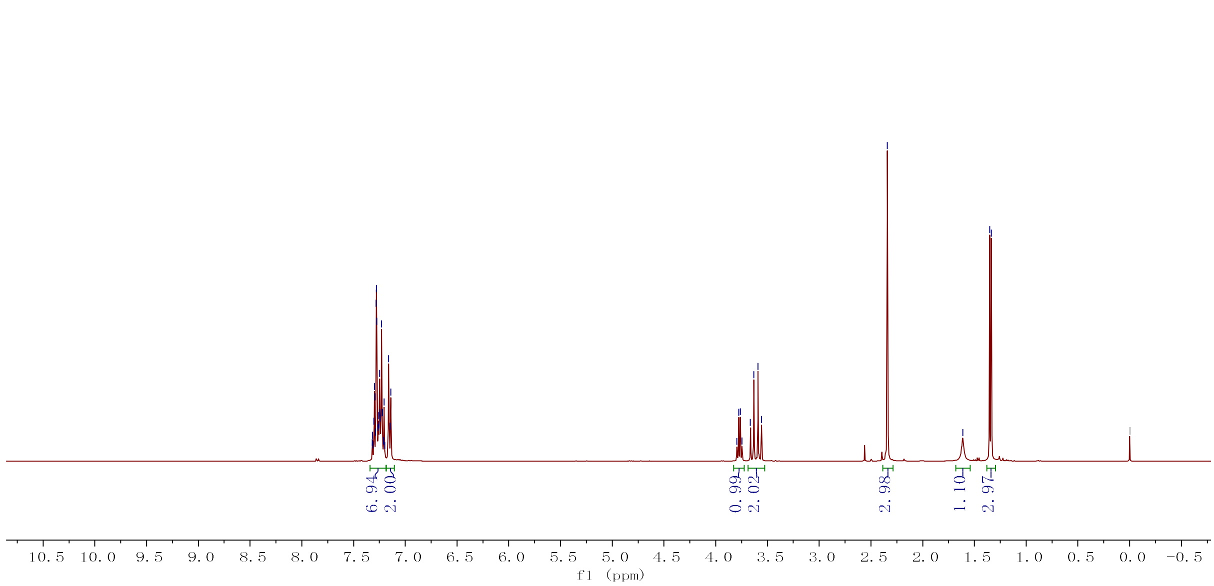




^{1}H NMR of 35
(400 MHz, Chloroform-*d*)

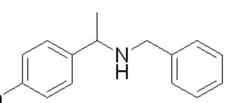




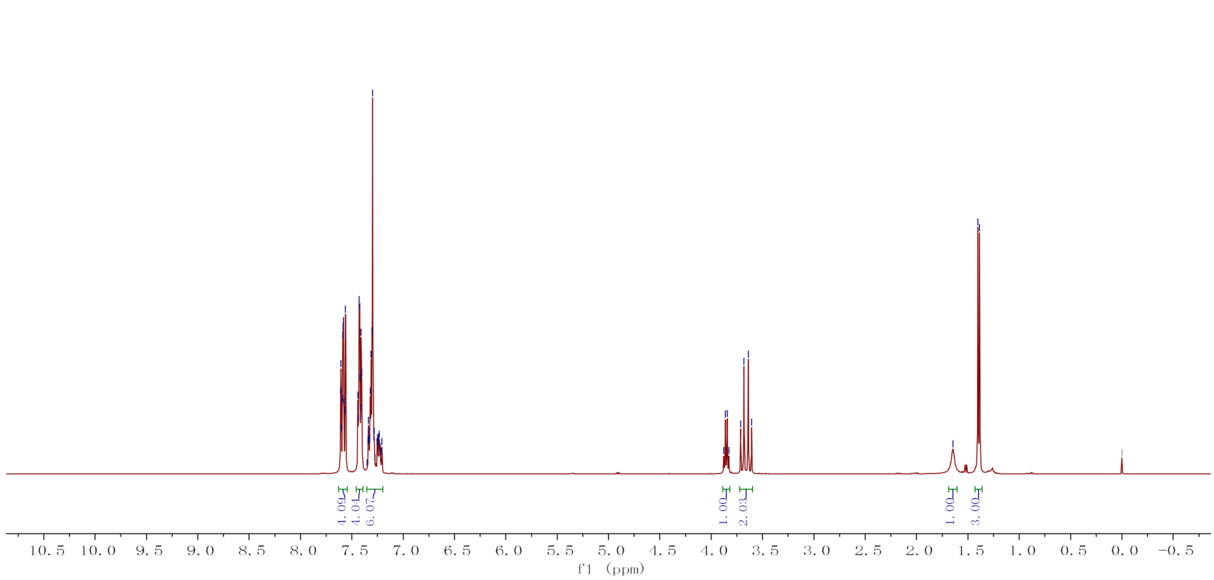


^{1}H NMR of 36

(400 MHz, Chloroform-*d*)

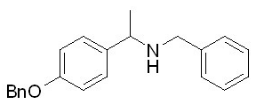


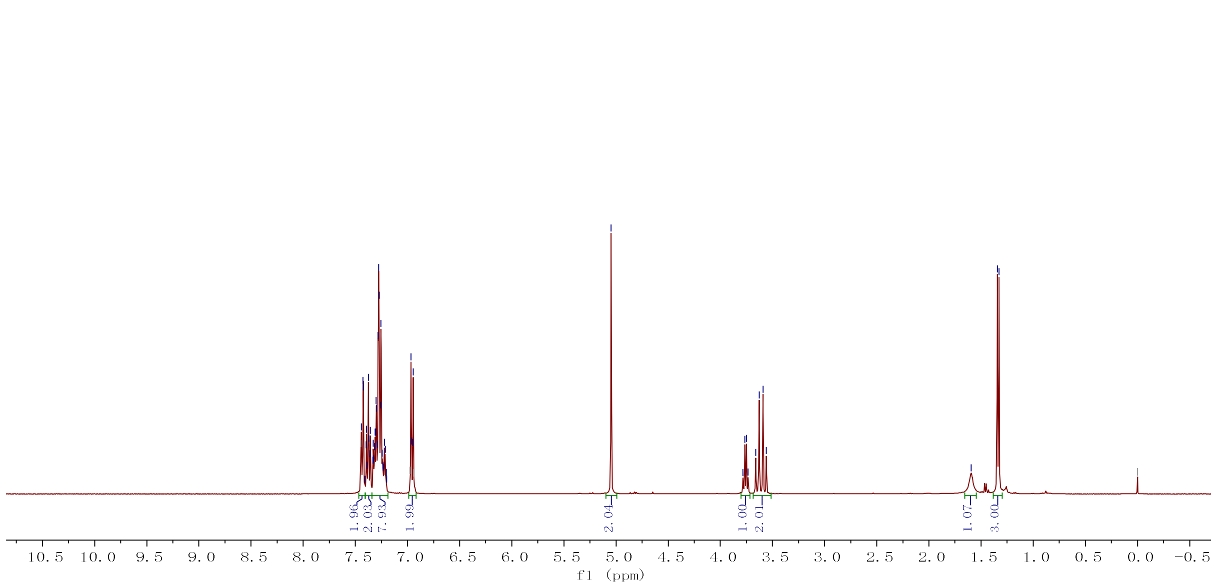
Ph



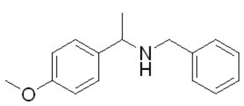
^{1}H NMR of 37

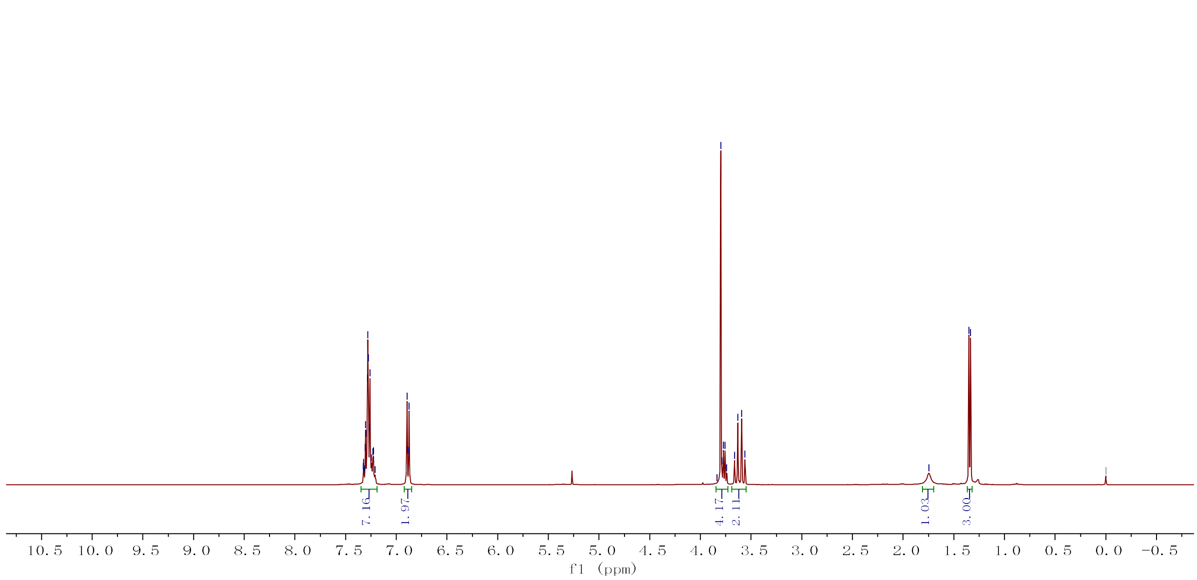
(400 MHz, Chloroform-*d*)



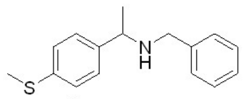


^{1}H NMR of 38
(400 MHz, Chloroform-*d*)

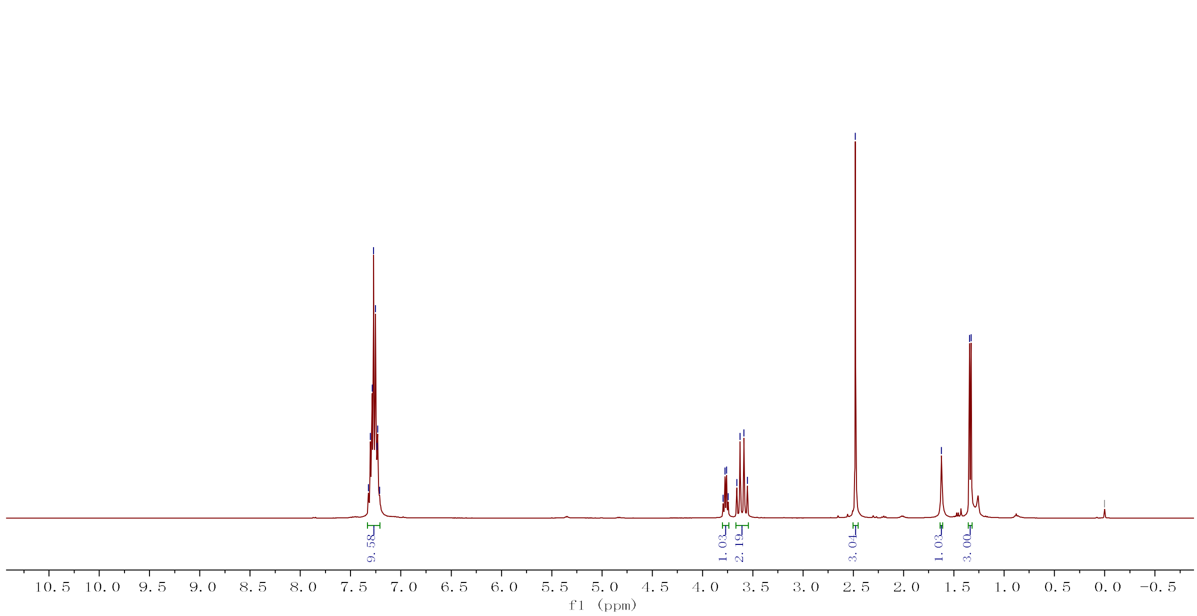


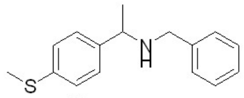


^{1}H NMR of 39
(400 MHz, Chloroform-*d*)

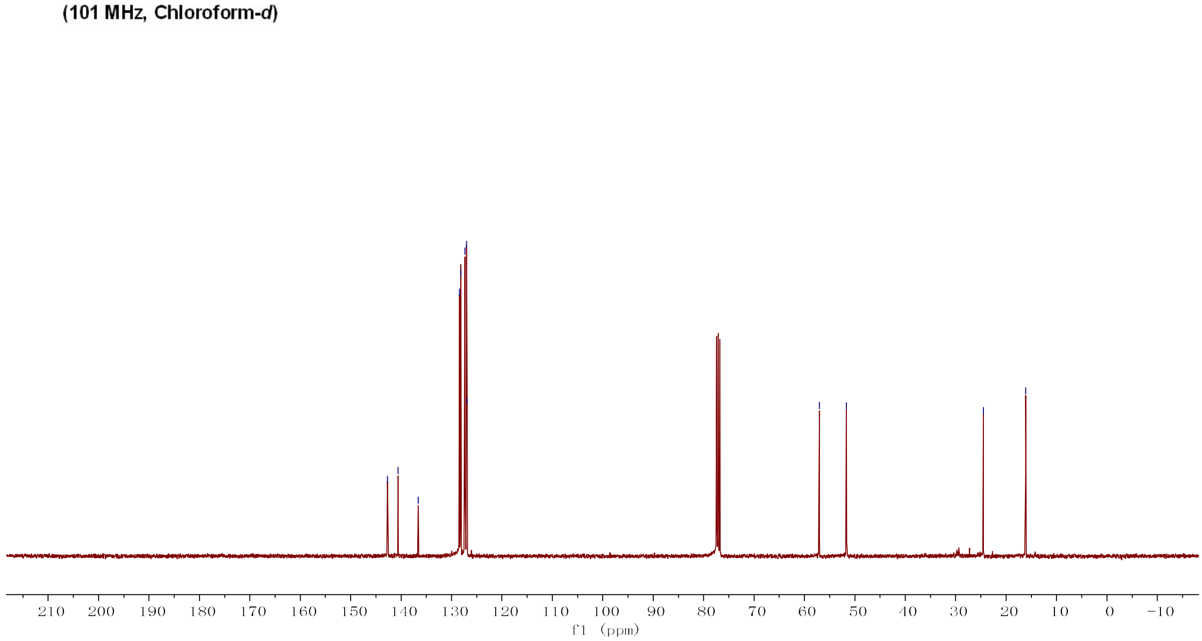


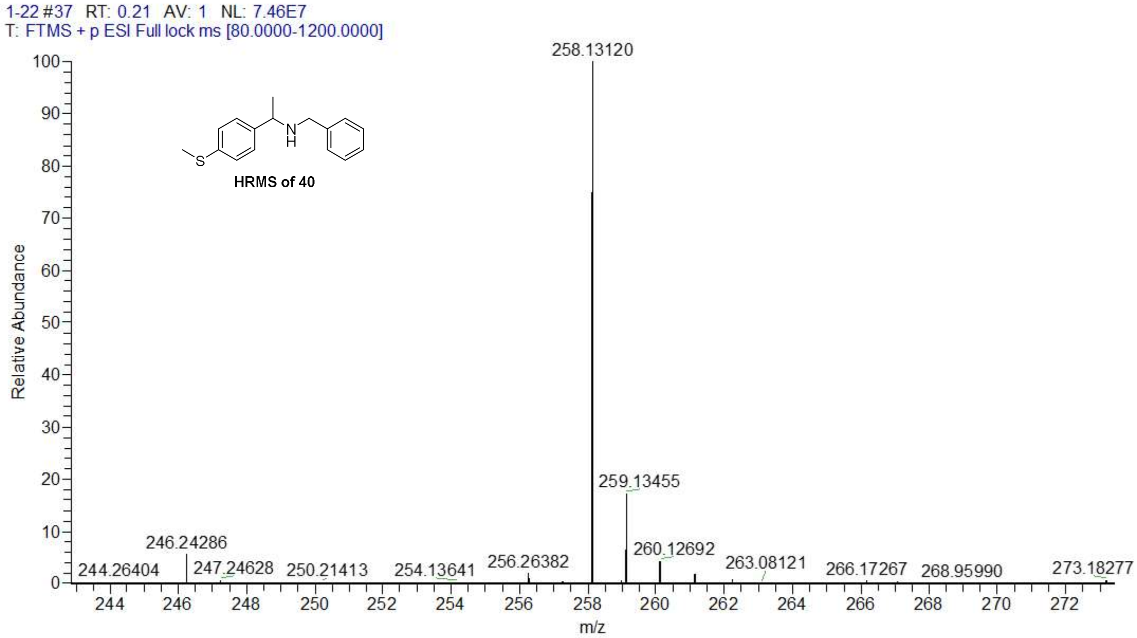
^{1}H NMR of 40
(400 MHz, Chloroform-*d*)

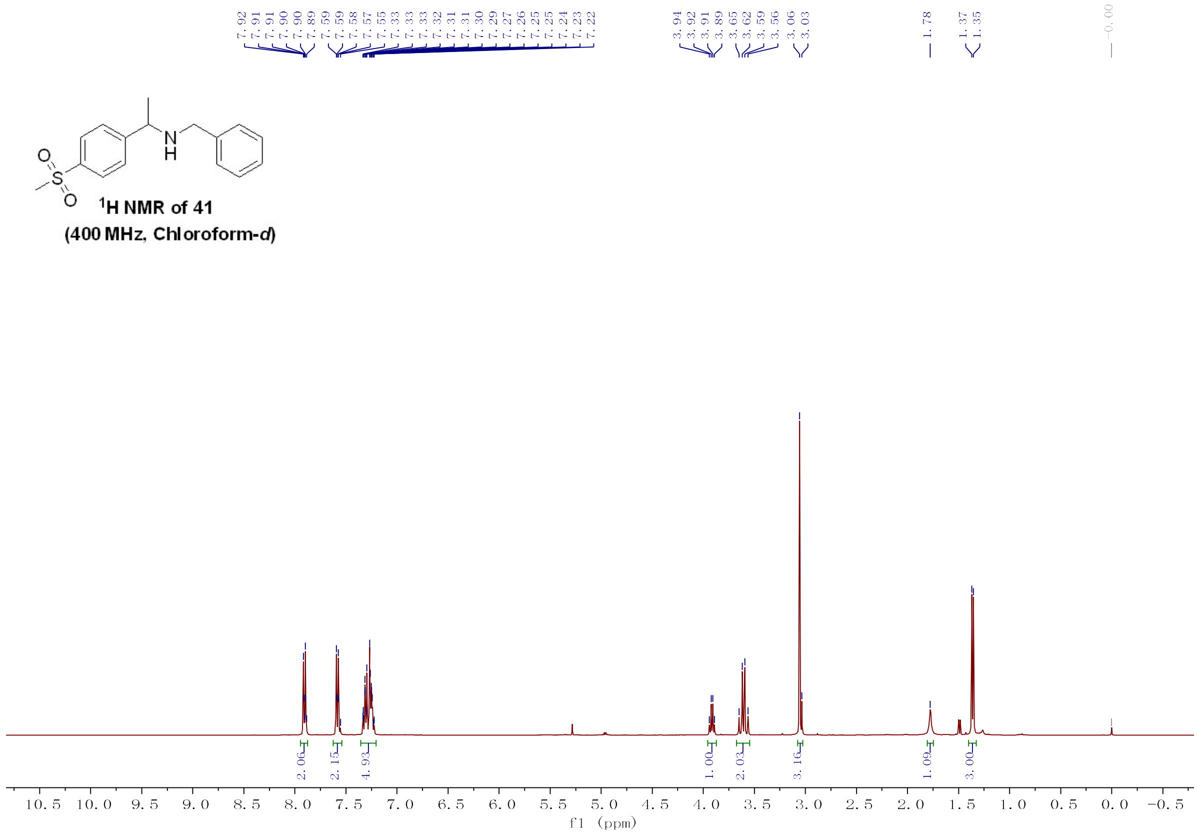


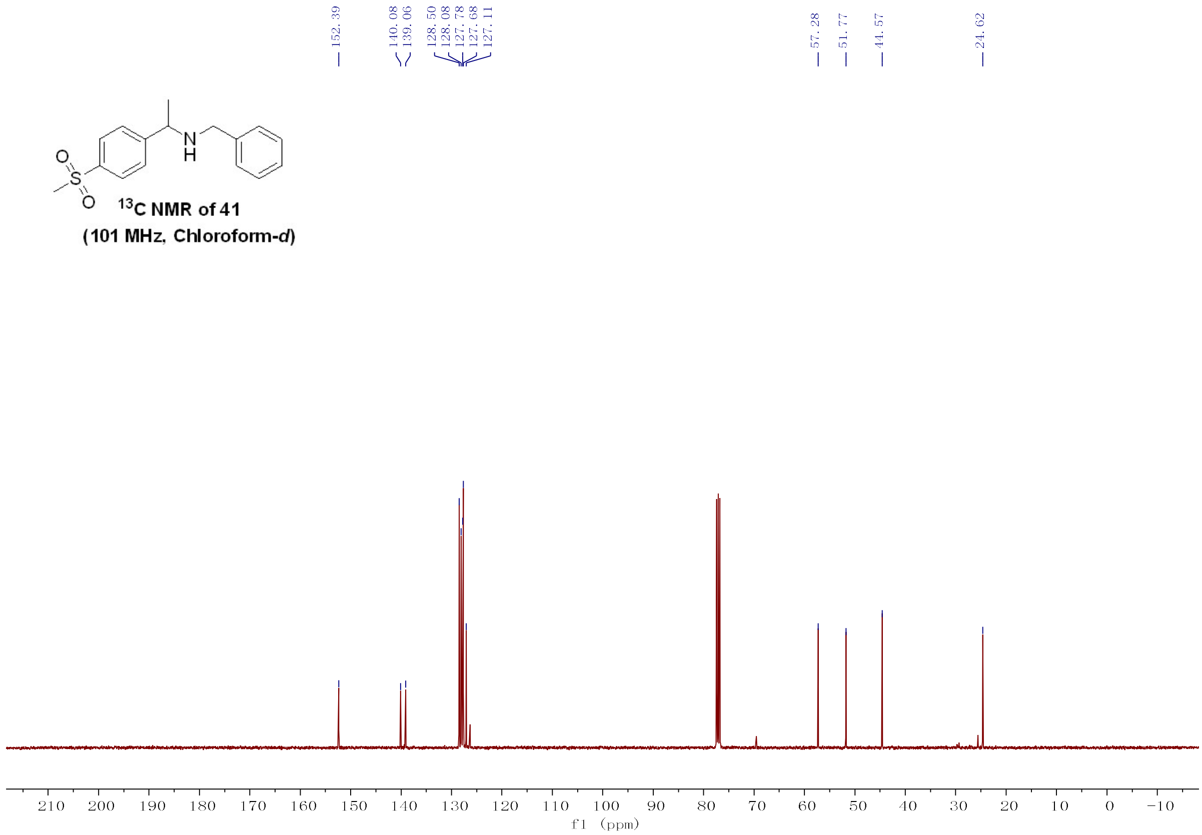


^{13}C NMR of 40
(101 MHz, Chloroform-*d*)

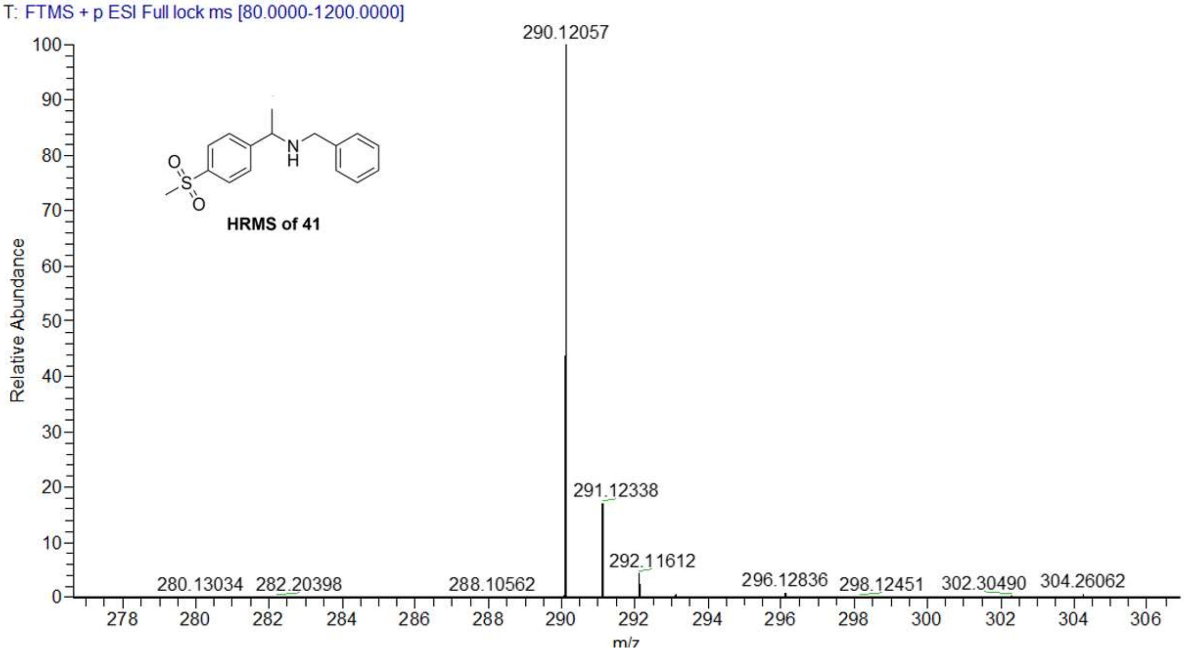



1-22 #37 RT: 0.21 AV: 1 NL: 7.46E7
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]
258.13120
259.13455
260.12692
246.24286
244.26404
247.24628
250.21413
254.13641
256.26382
263.08121
266.17267
268.95990
273.18277
Relative Abundance
m/z
HRMS of 40

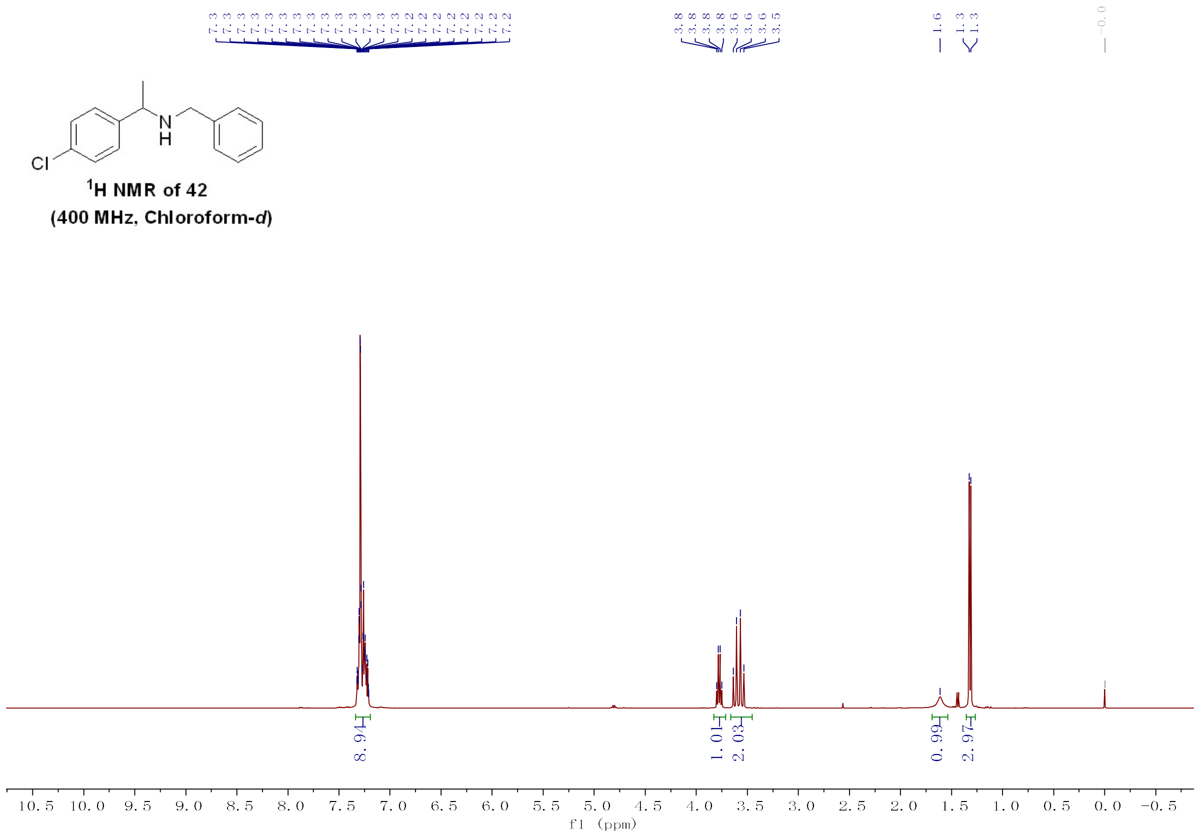

^{1}H NMR of 41
(400 MHz, Chloroform-d)
7.92 7.91 7.91 7.90 7.90 7.89 7.59 7.59 7.58 7.57 7.55 7.33 7.33 7.33 7.32 7.32 7.31 7.31 7.30 7.29 7.27 7.26 7.25 7.25 7.24 7.23 7.22
3.94 3.92 3.91 3.89 3.65 3.62 3.59 3.56 3.06 3.03
1.78
1.37 1.35
0.00
2.06 2.15 4.93 1.00 2.03 3.16 1.09 3.00
f1 (ppm)

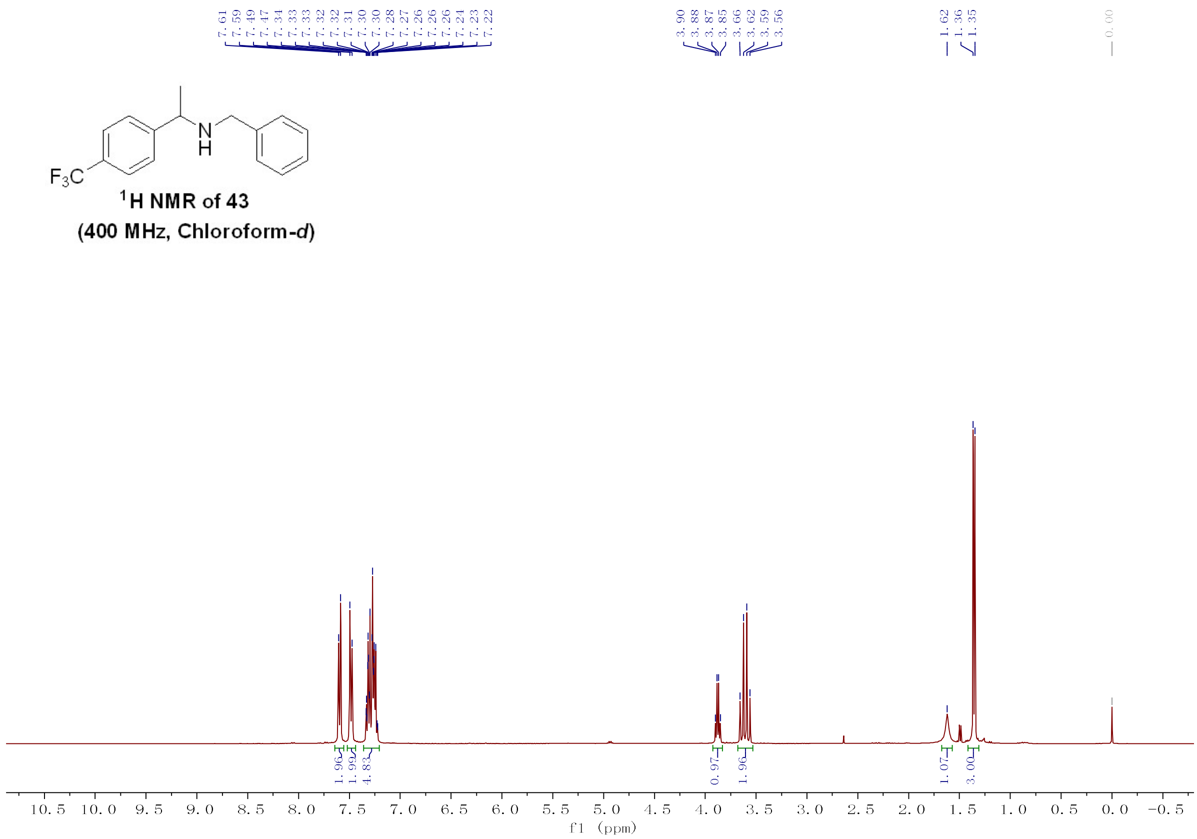


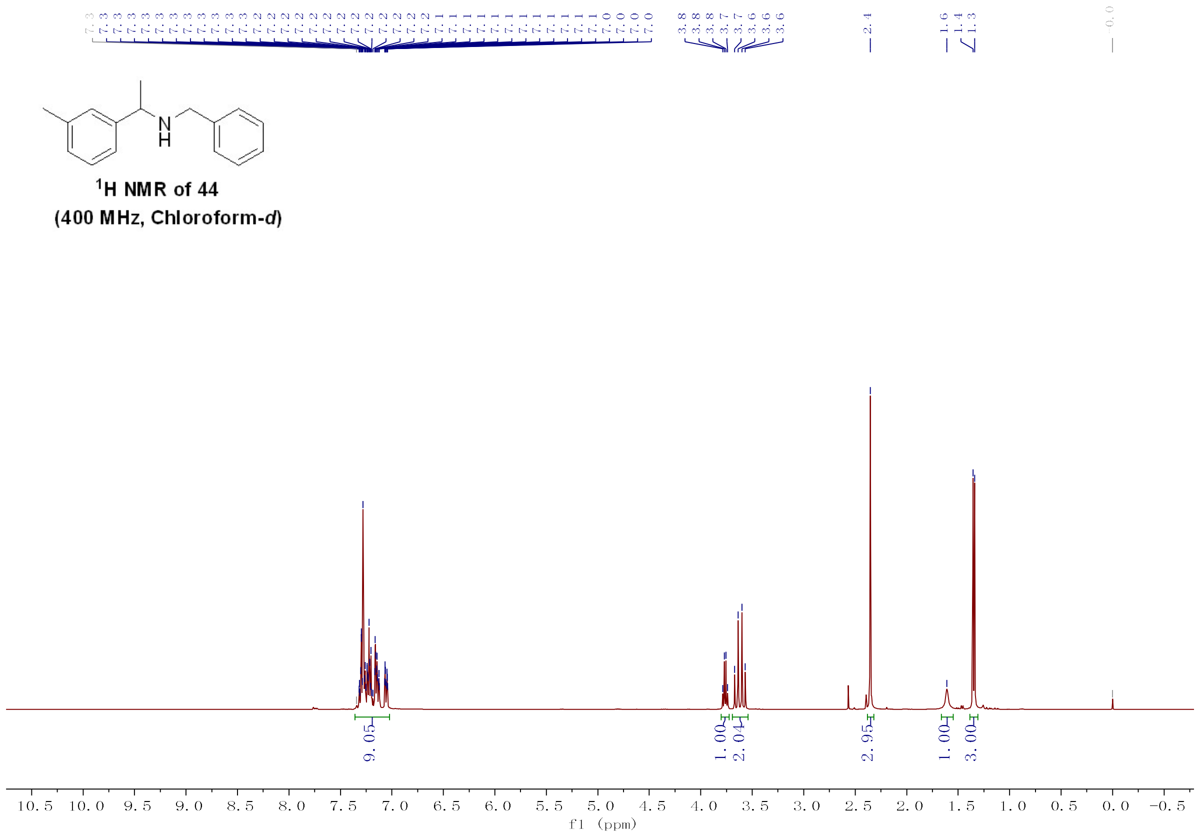
^{13}C NMR of 41
(101 MHz, Chloroform-*d*)

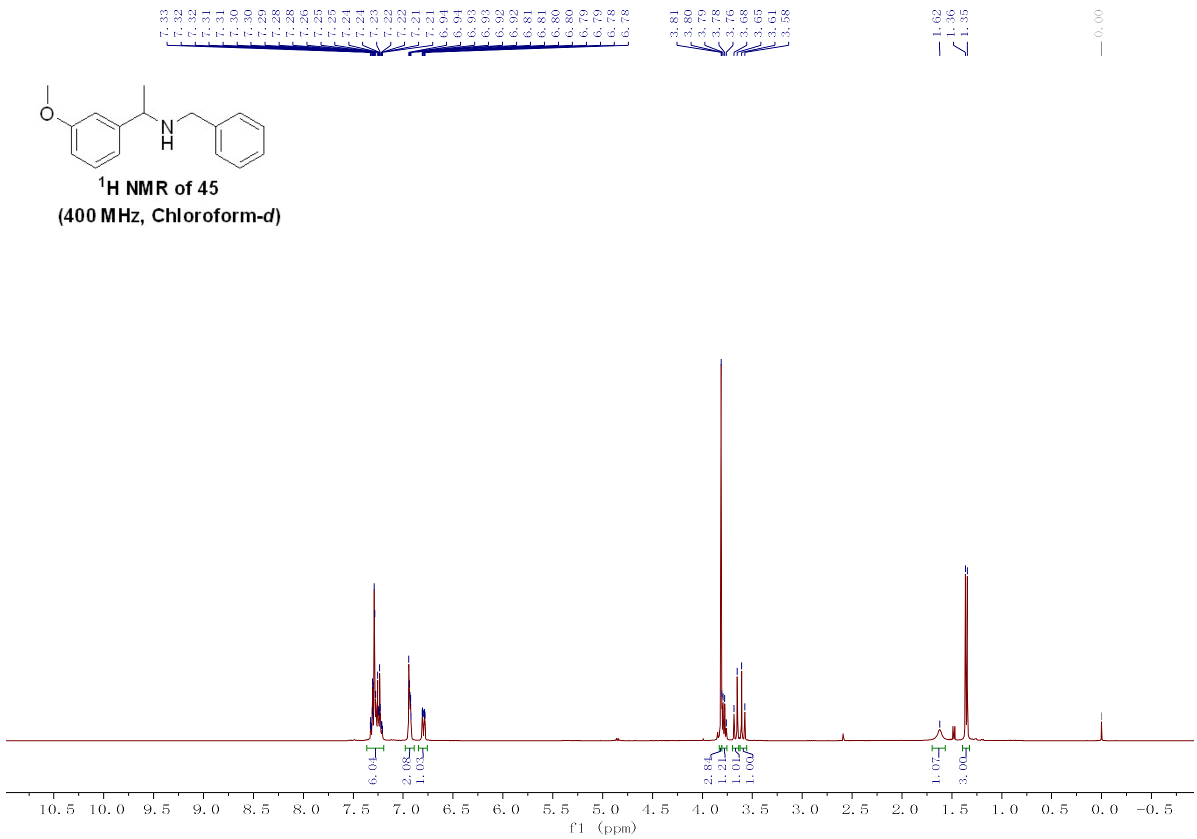


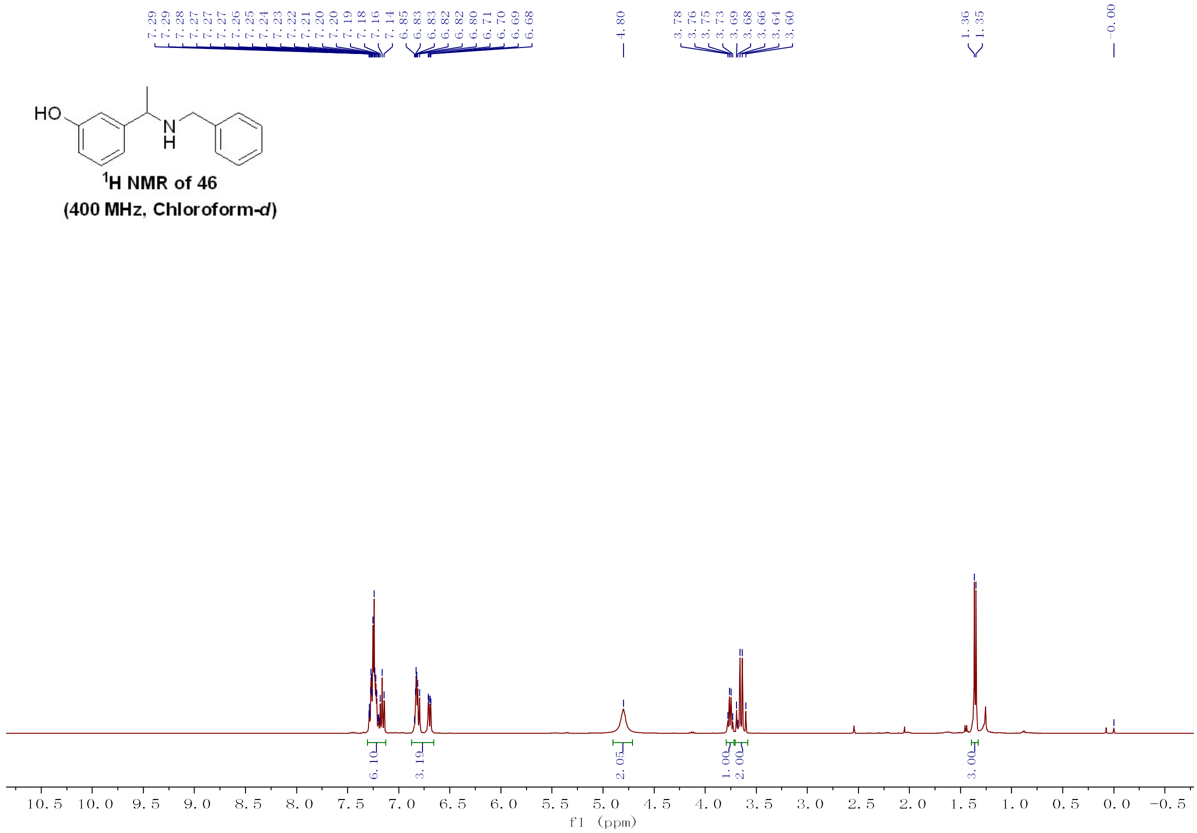
HRMS of 41


Cl
N
H
1H NMR of 42
(400 MHz, Chloroform-d)
8.94
1.01
2.03
0.99
2.97
f1 (ppm)

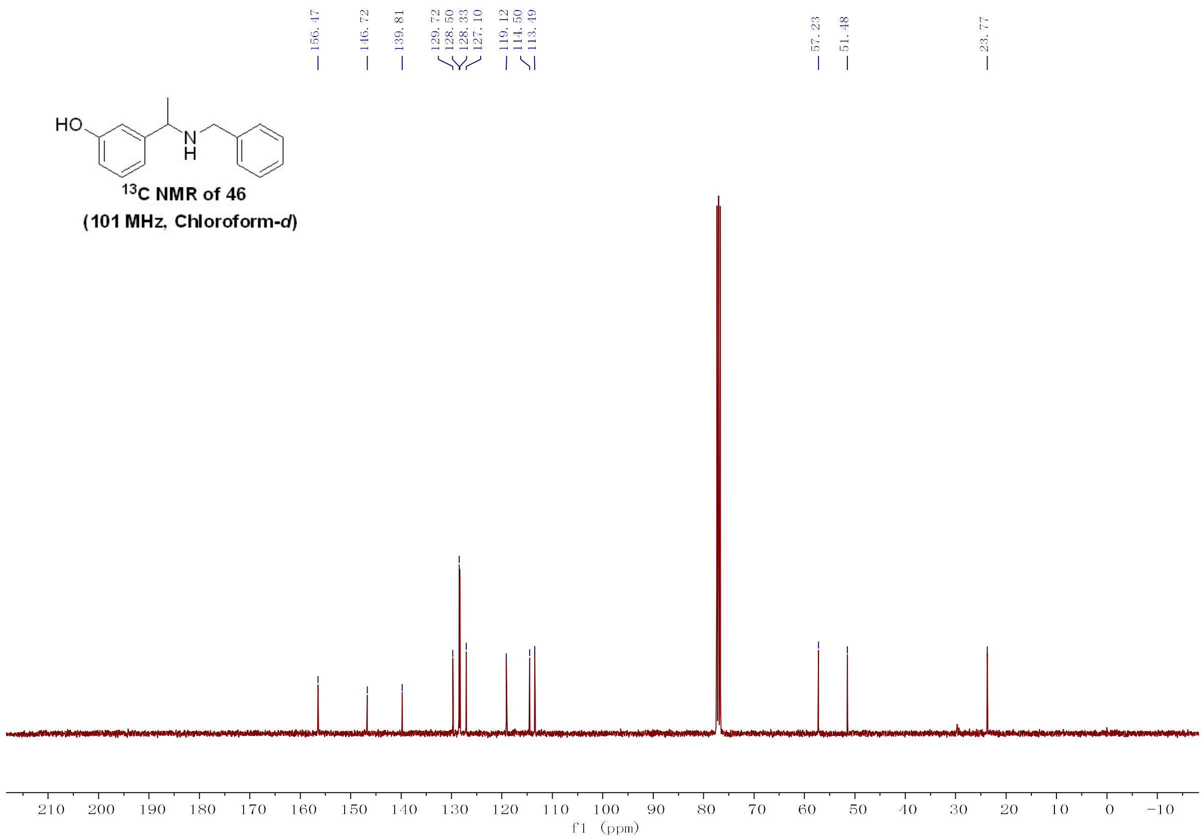

7.61
7.59
7.49
7.47
7.34
7.33
7.32
7.31
7.30
7.30
7.28
7.27
7.26
7.26
7.24
7.23
7.22
3.90
3.88
3.87
3.85
3.66
3.62
3.59
3.56
1.62
1.36
1.35
0.00
F3C
N
H
1H NMR of 43
(400 MHz, Chloroform-d)
1.96
1.99
4.83
0.97
1.96
1.07
3.00
f1 (ppm)


^{1}H NMR of 44
(400 MHz, Chloroform-*d*)
f1 (ppm)

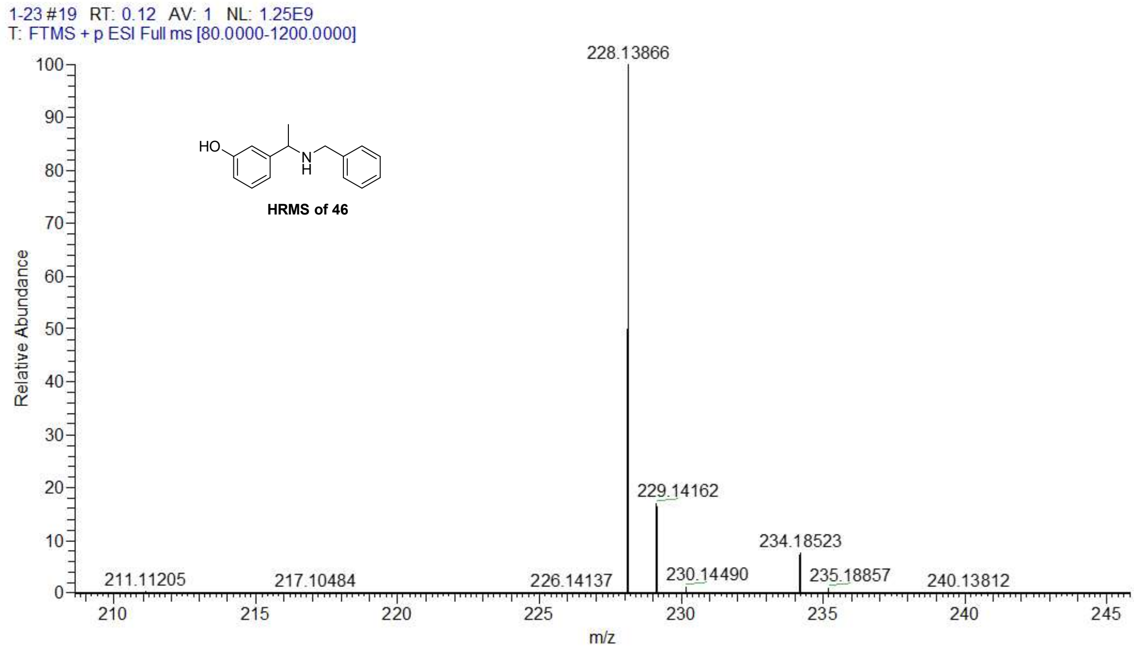

^{1}H NMR of 45
(400 MHz, Chloroform-*d*)
f1 (ppm)

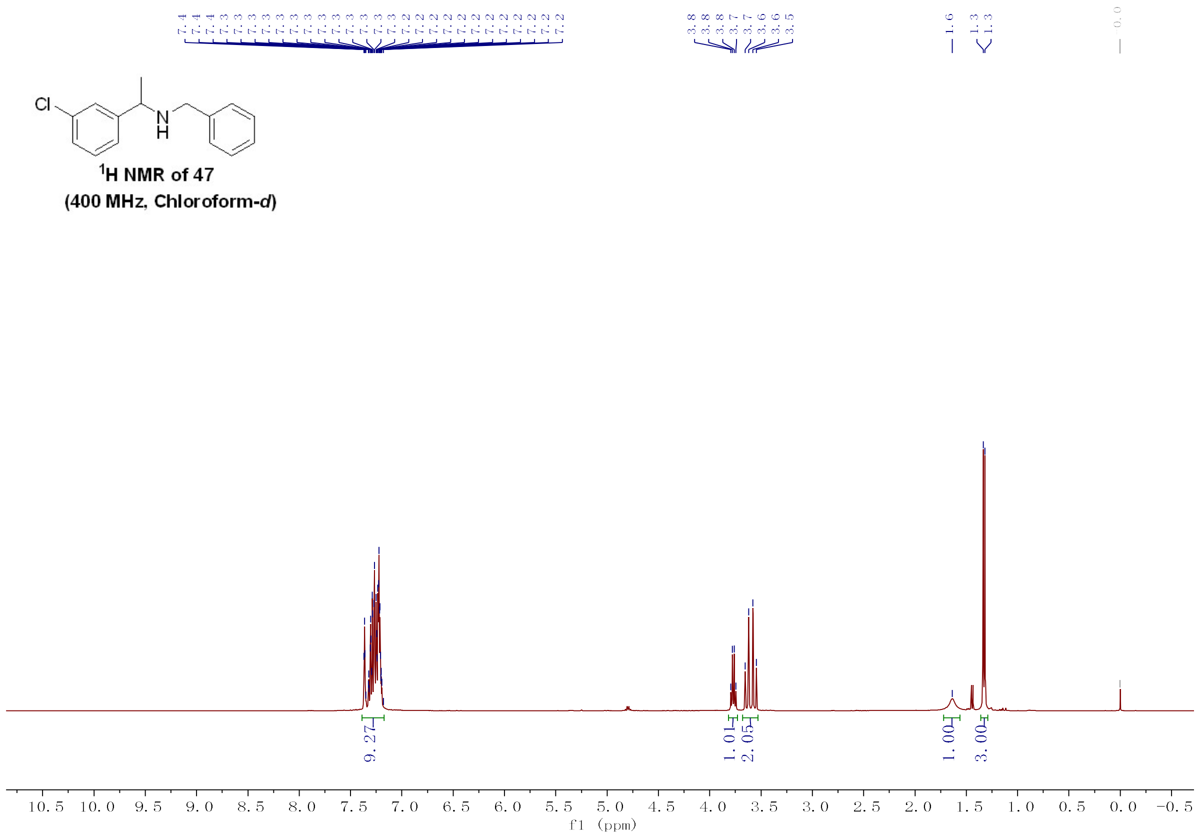


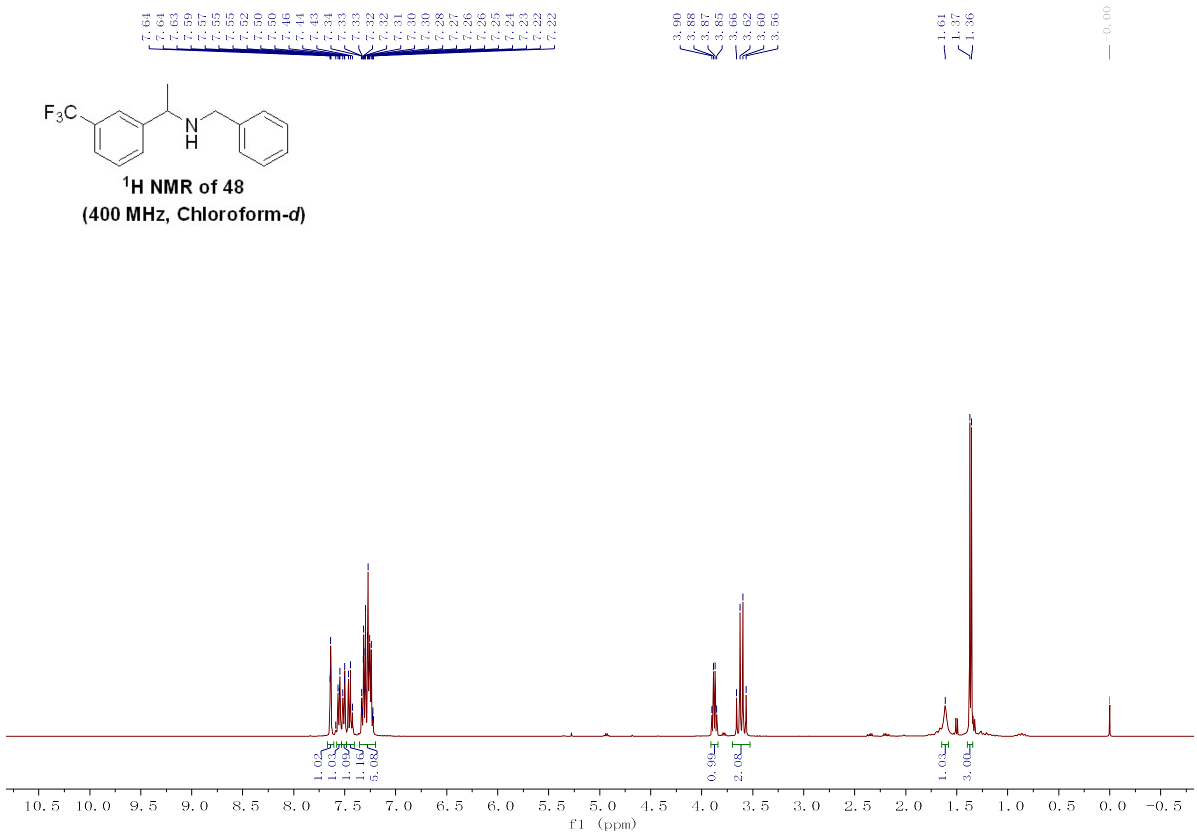
^{1}H NMR of 46
(400 MHz, Chloroform-*d*)



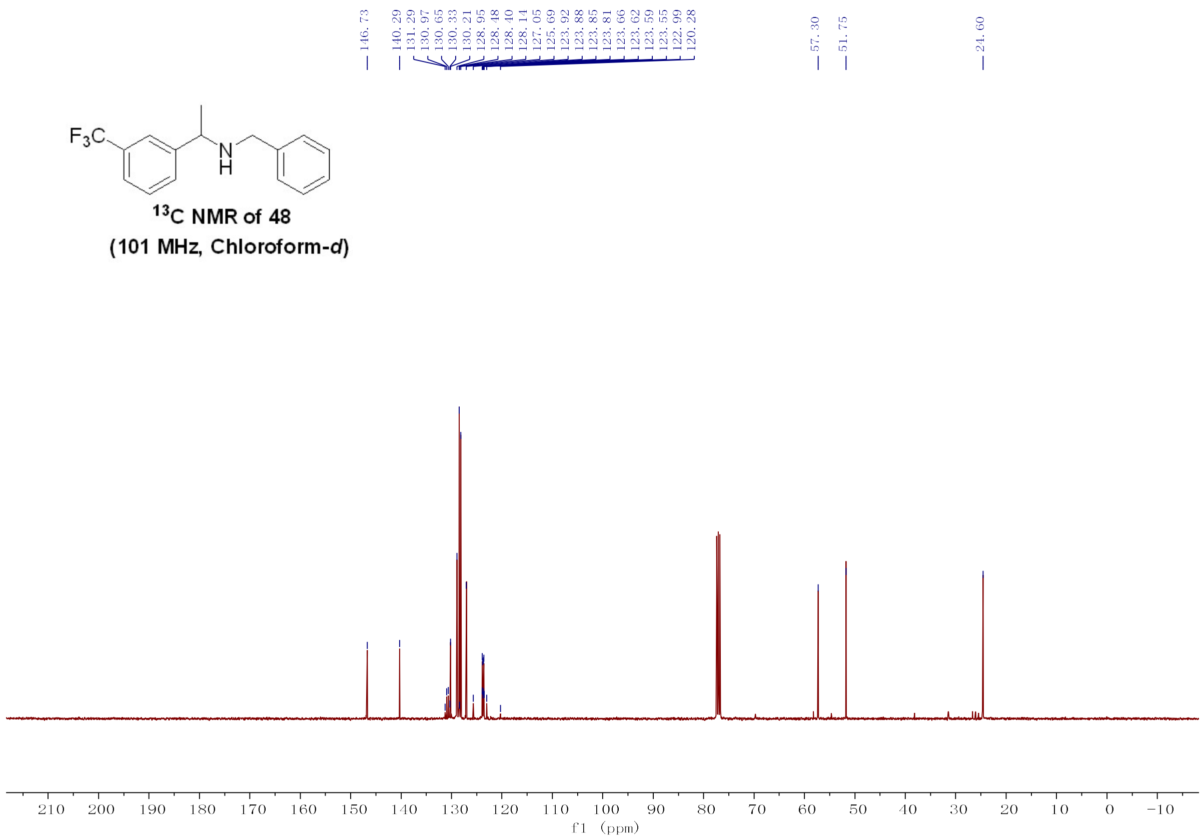
^{13}C NMR of 46
(101 MHz, Chloroform-*d*)


1-23 #19 RT: 0.12 AV: 1 NL: 1.25E9
T: FTMS + p ESI Full ms [80.0000-1200.0000]
HO
N
H
HRMS of 46
228.13866
229.14162
234.18523
211.11205
217.10484
226.14137
230.14490
235.18857
240.13812
Relative Abundance
m/z

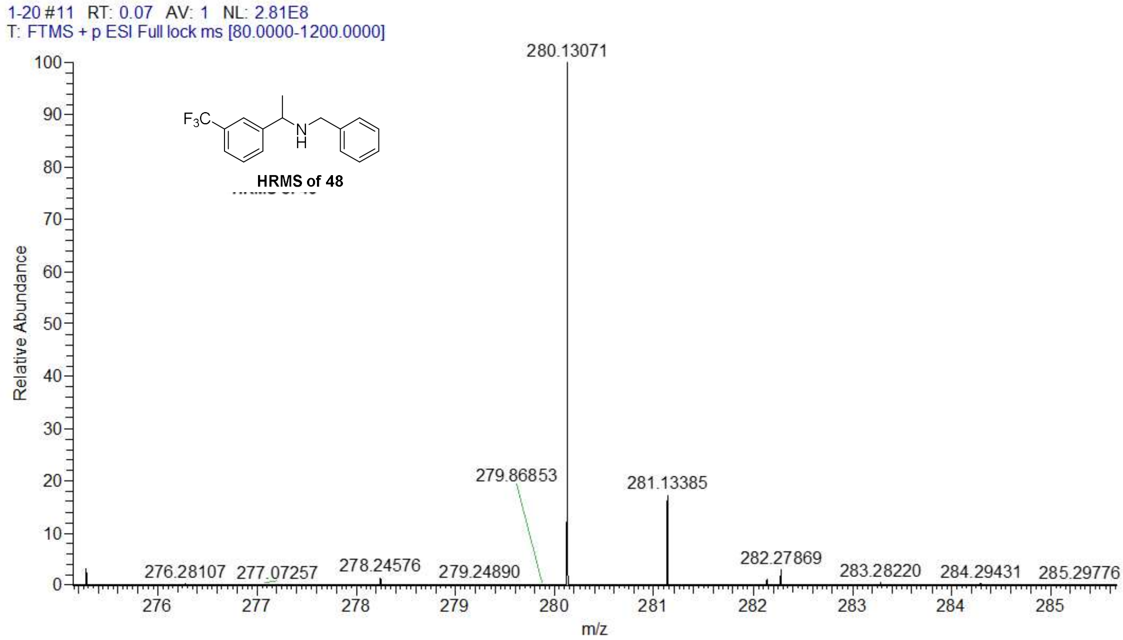

Cl
N
H
^{1}H NMR of 47
(400 MHz, Chloroform-*d*)
9.27
1.01
2.05
1.00
3.00
f1 (ppm)



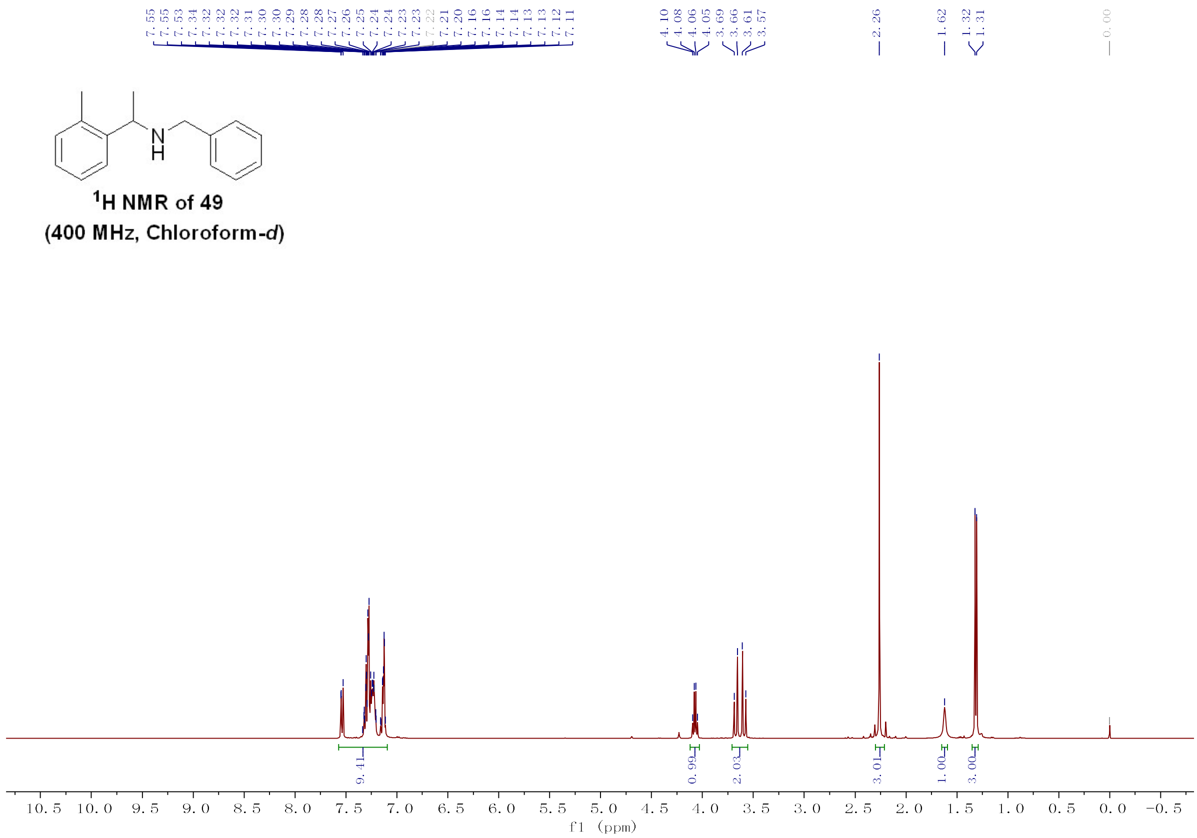
^{1}H NMR of 48
(400 MHz, Chloroform-*d*)



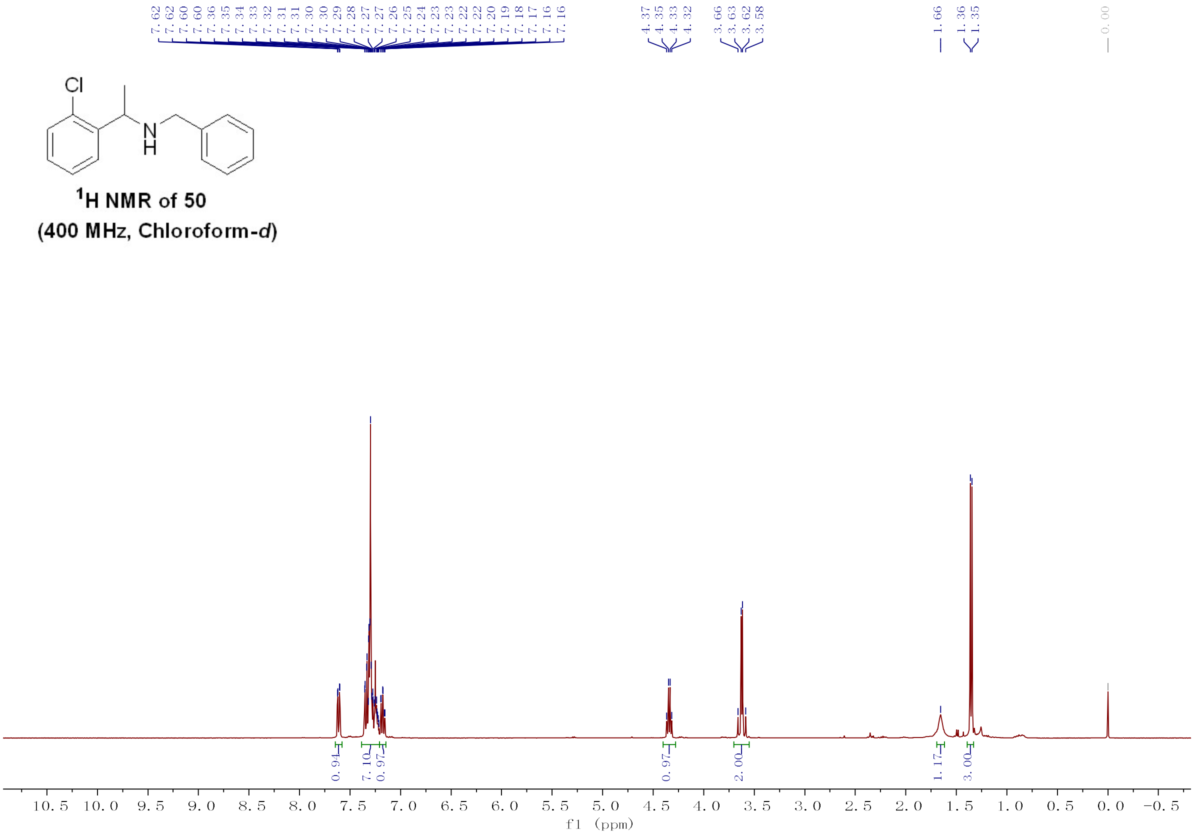
^{13}C NMR of 48
(101 MHz, Chloroform-*d*)



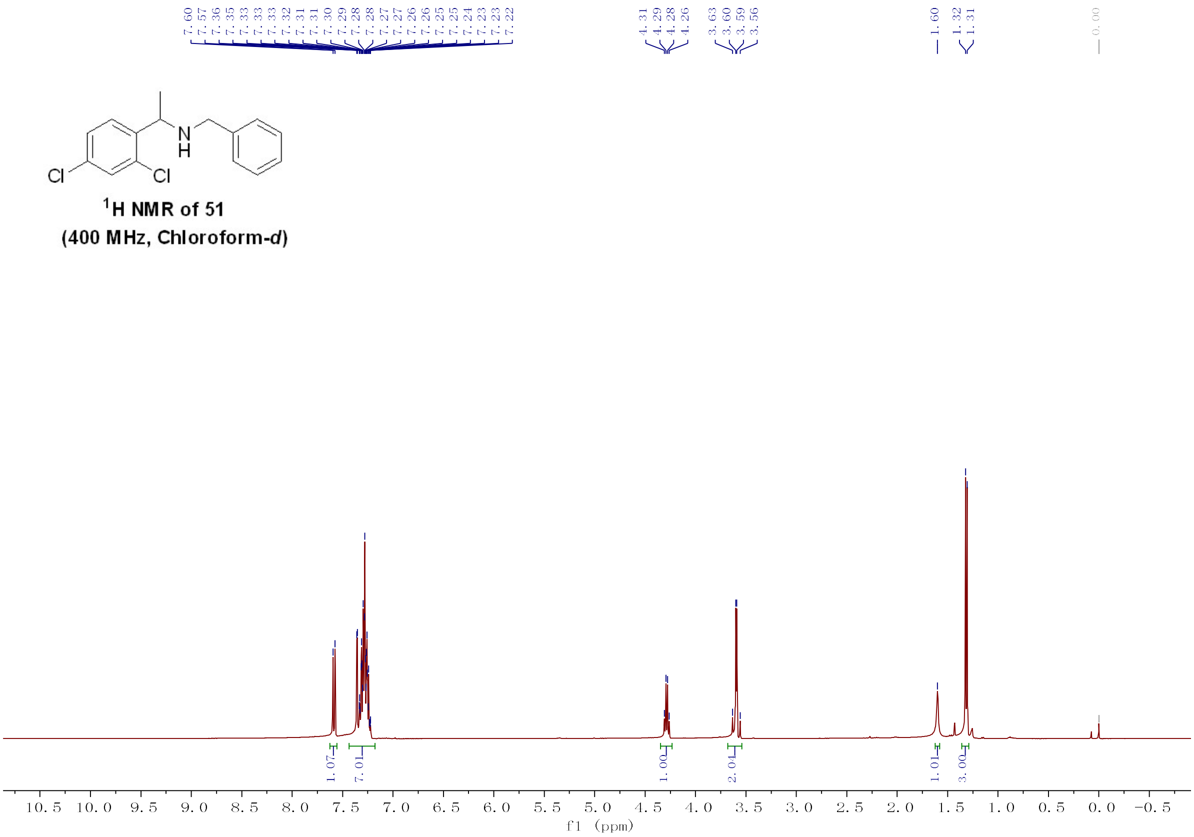
1-20 #11 RT: 0.07 AV: 1 NL: 2.81E8
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]
280.13071
279.86853
281.13385
276.28107
277.07257
278.24576
279.24890
282.27869
283.28220
284.29431
285.29776
Relative Abundance
m/z
HRMS of 48



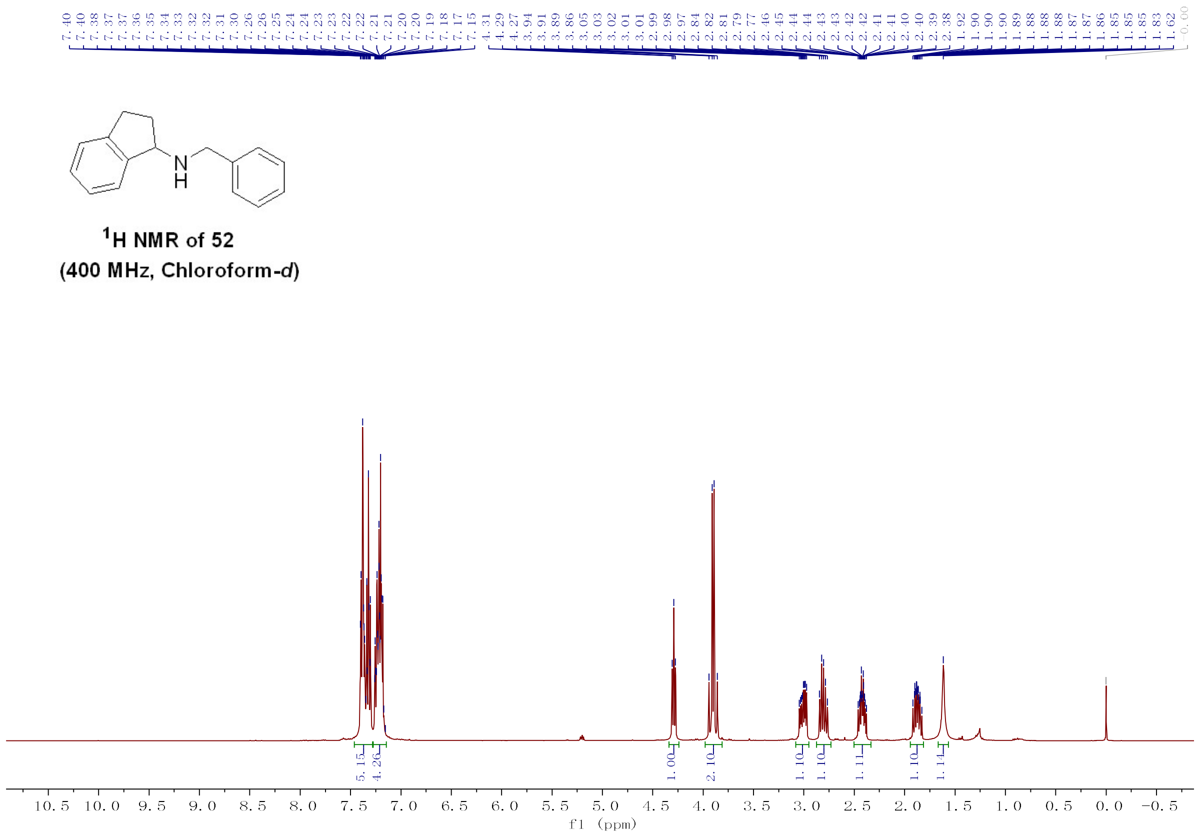
1H NMR of 49
(400 MHz, Chloroform-d)
f1 (ppm)



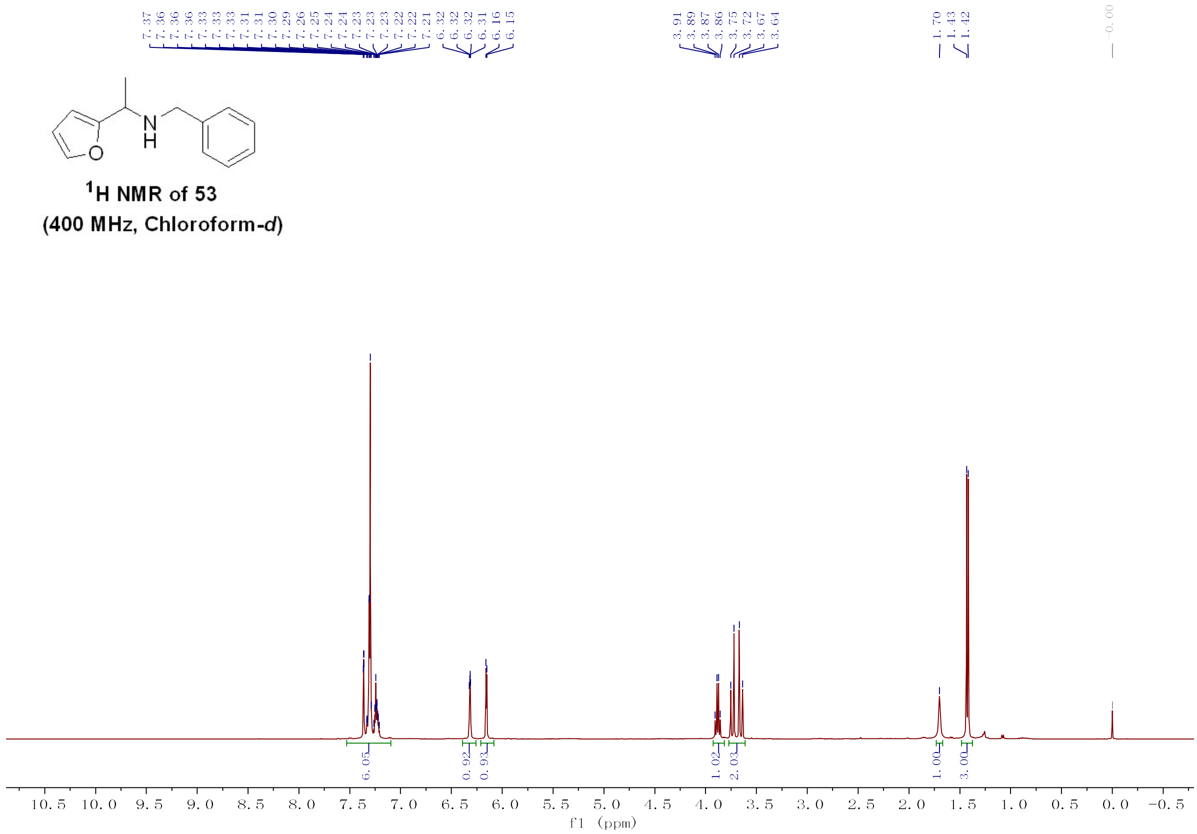
^{1}H NMR of 50
(400 MHz, Chloroform-*d*)



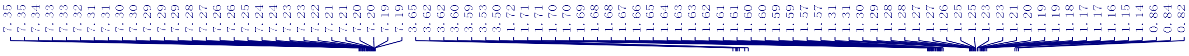
^{1}H NMR of 51
(400 MHz, Chloroform-*d*)

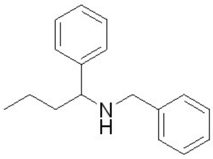


^{1}H NMR of 52
(400 MHz, Chloroform-*d*)

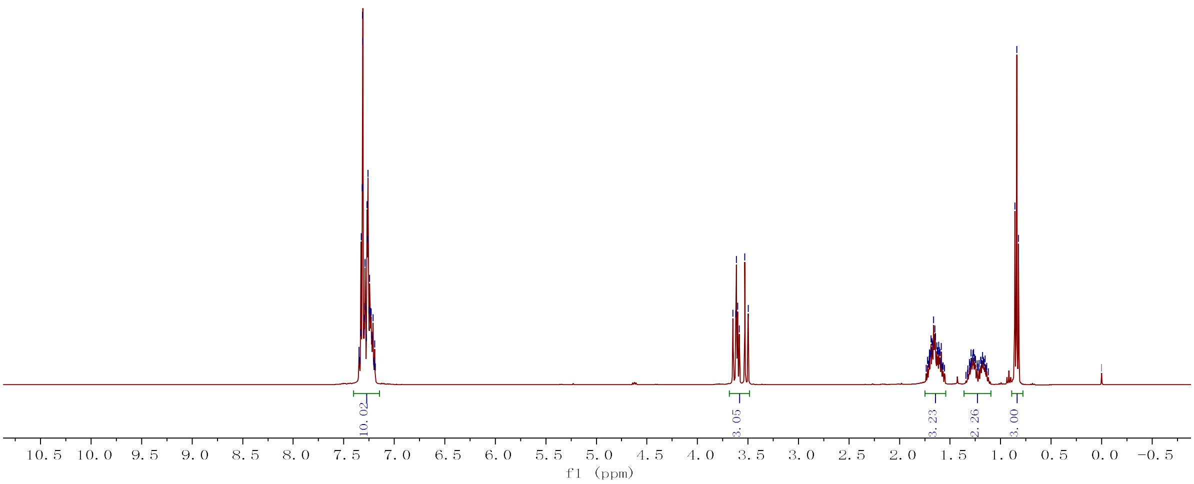


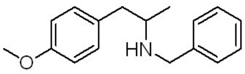
^{1}H NMR of 53
(400 MHz, Chloroform-*d*)



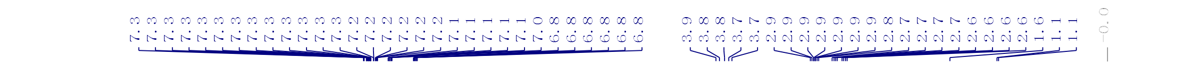


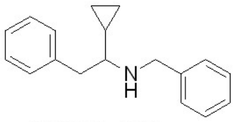
^{1}H NMR of 54
(400 MHz, Chloroform-*d*)

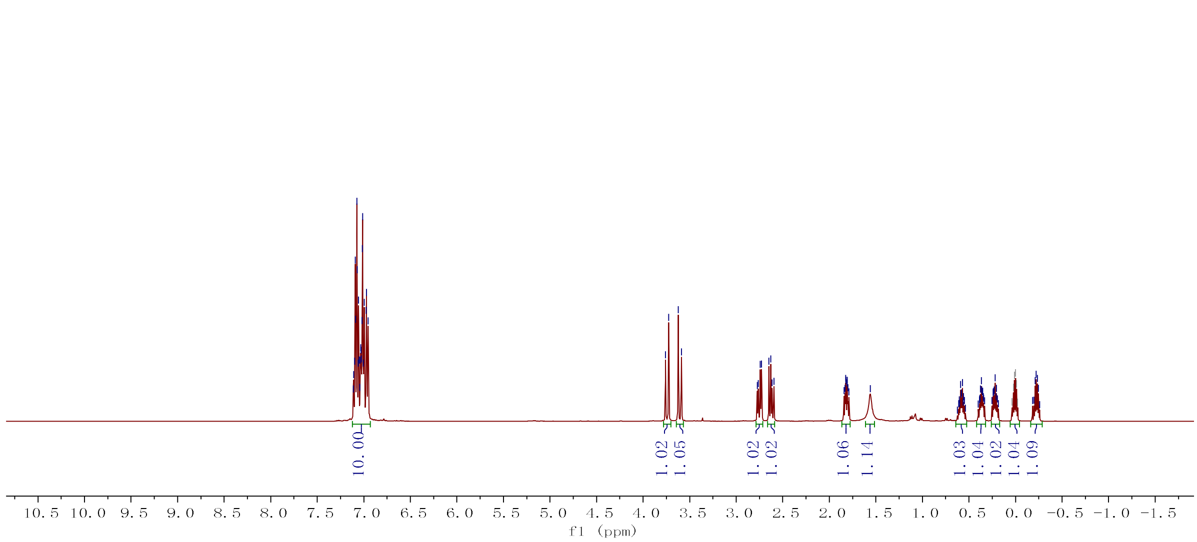




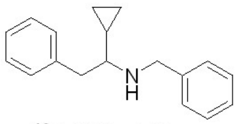
^{1}H NMR of 55
(400 MHz, Chloroform-*d*)

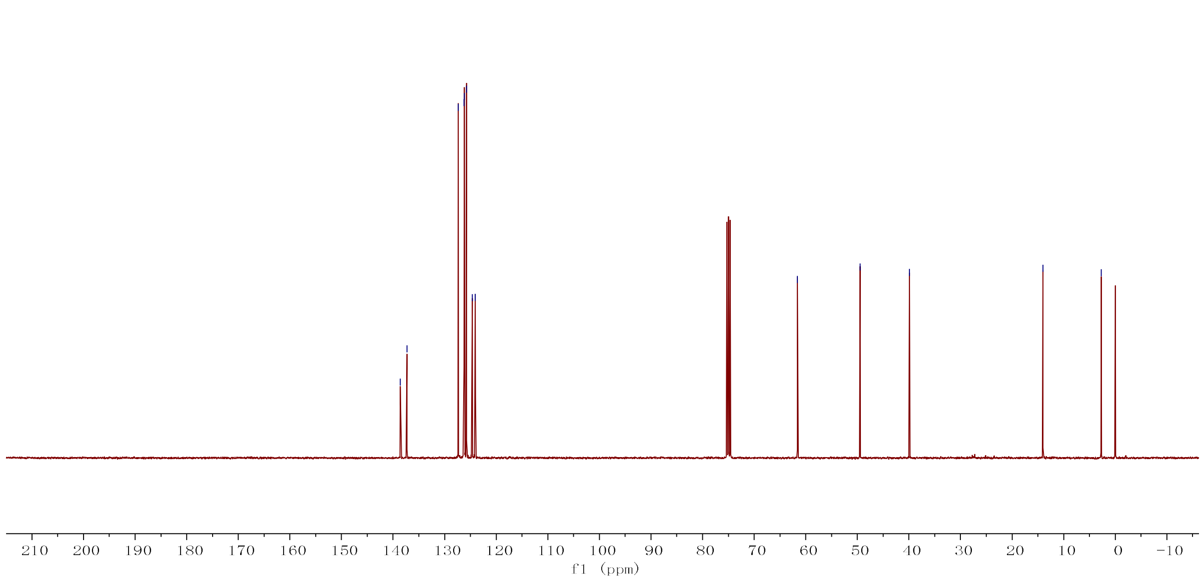




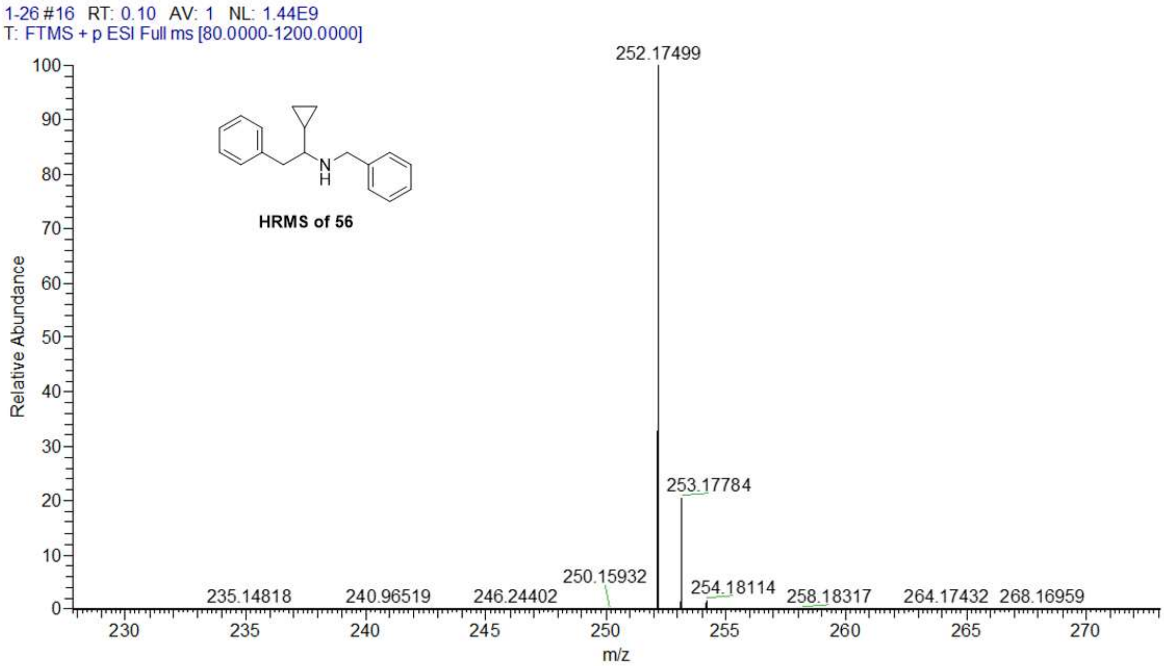


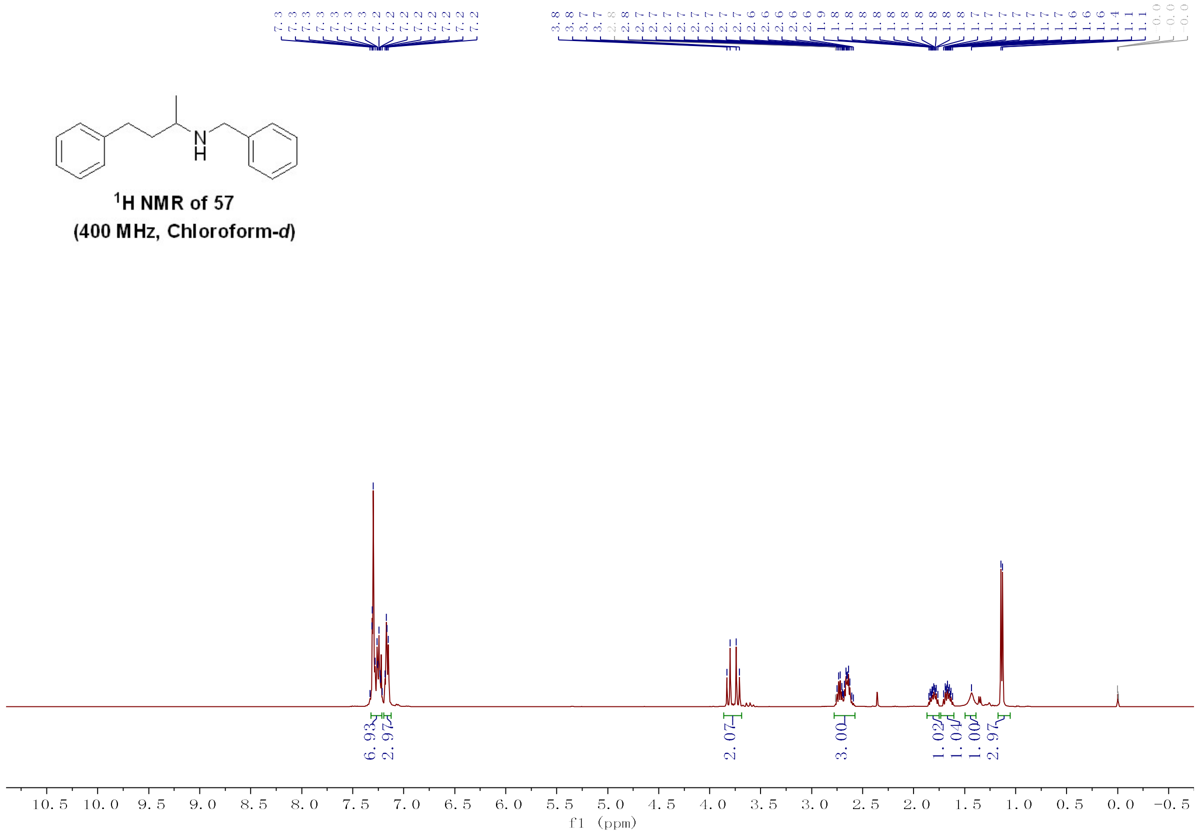
[1]H NMR of 56
(400 MHz, Chloroform-*d*)

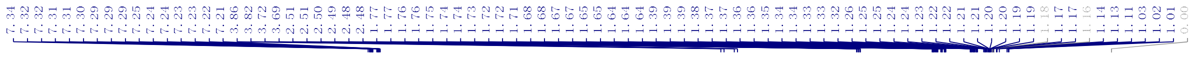


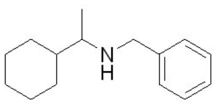


[13]C NMR of 56
(101 MHz, Chloroform-*d*)

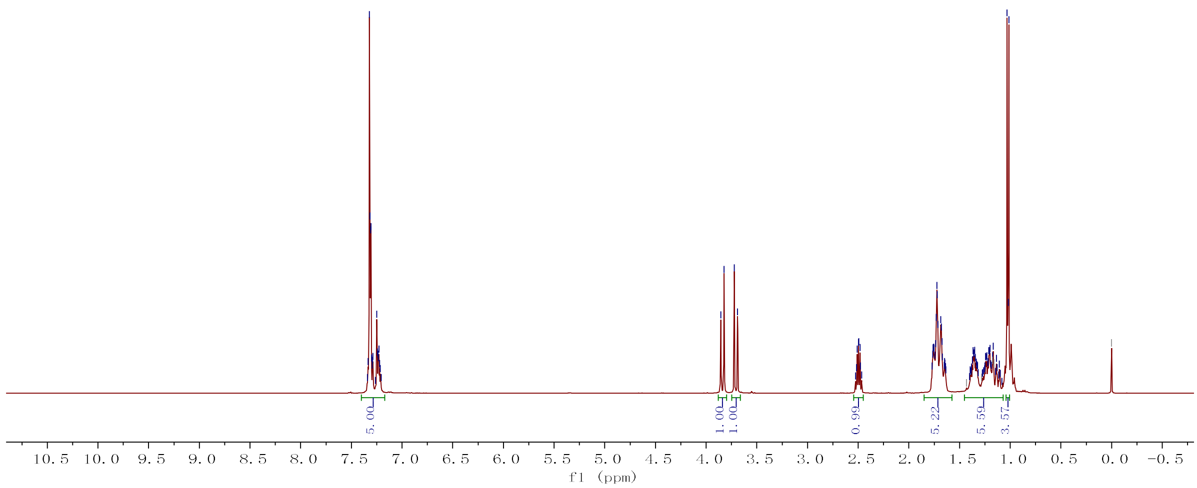

1-26 #16 RT: 0.10 AV: 1 NL: 1.44E9
T: FTMS + p ESI Full ms [80.0000-1200.0000]
252.17499
253.17784
250.15932
254.18114
235.14818
240.96519
246.24402
258.18317
264.17432
268.16959
Relative Abundance
m/z
HRMS of 56

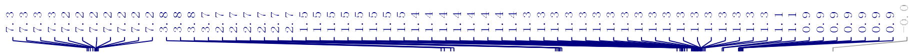

^{1}H NMR of 57
(400 MHz, Chloroform-*d*)
6.93
2.97
2.07
3.00
1.02
1.04
1.00
2.97
f1 (ppm)

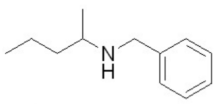




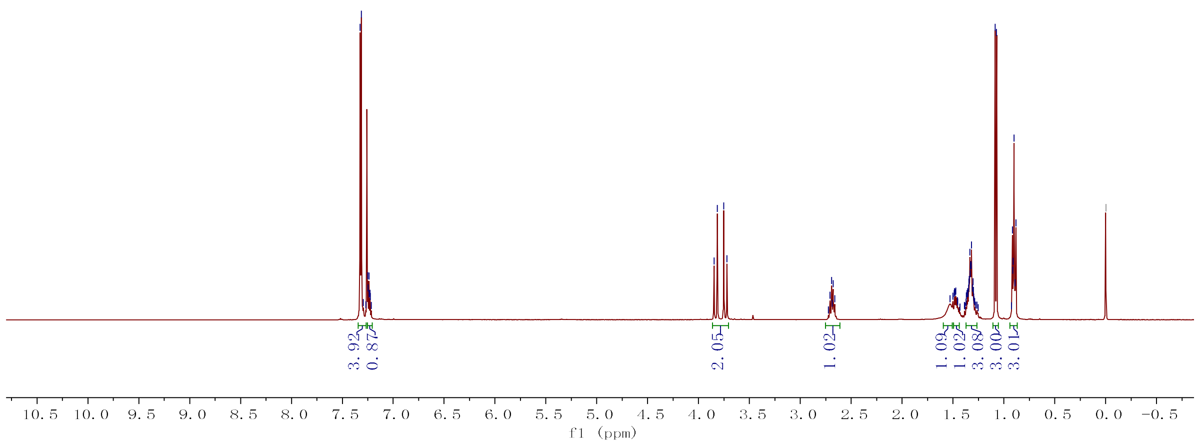
^{1}H NMR of 58
(400 MHz, Chloroform-*d*)

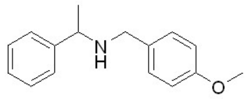




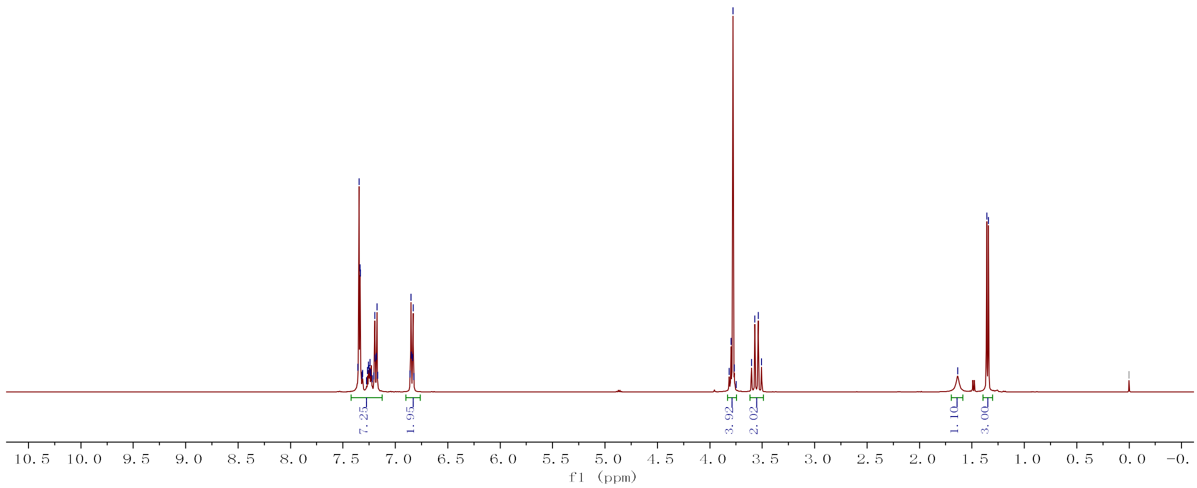


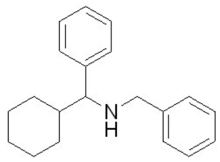
^{1}H NMR of 59
(400 MHz, Chloroform-*d*)



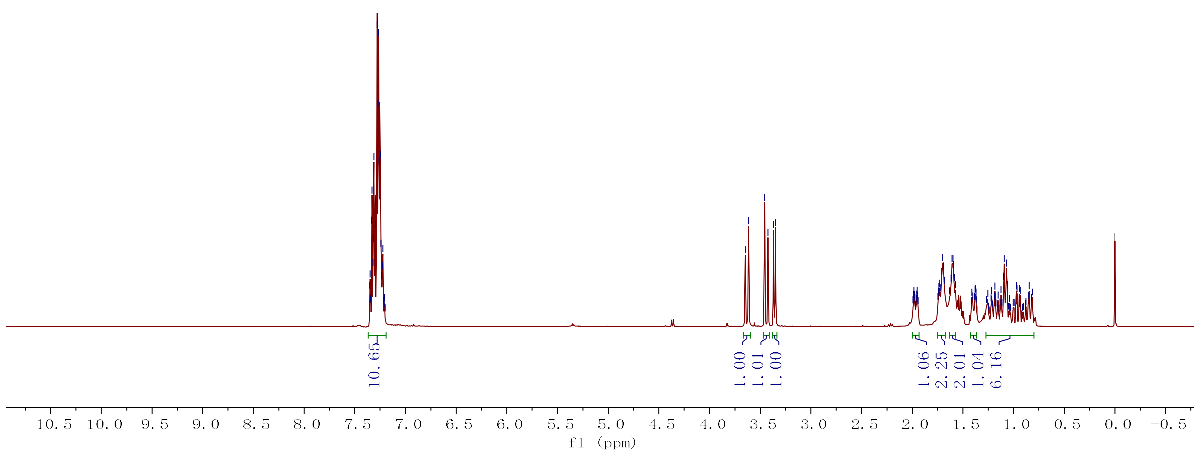


^{1}H NMR of 60
(400 MHz, Chloroform-*d*)

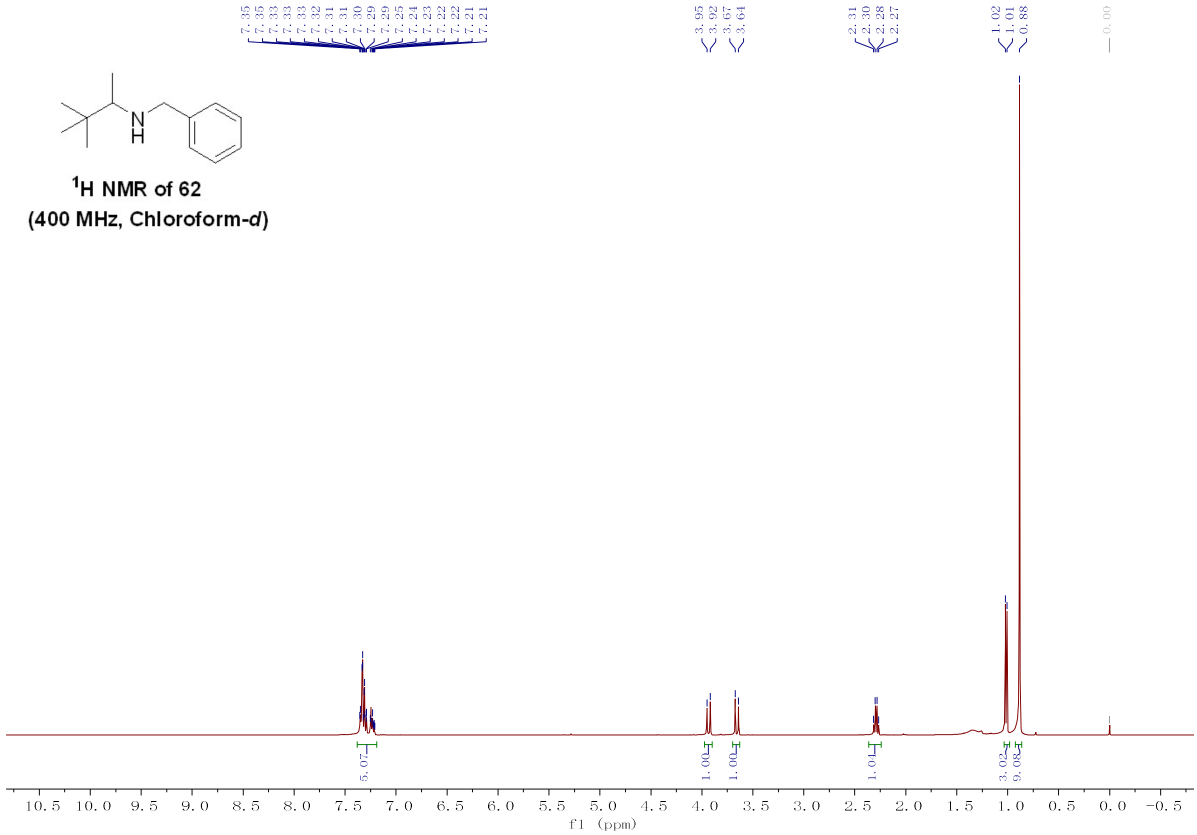




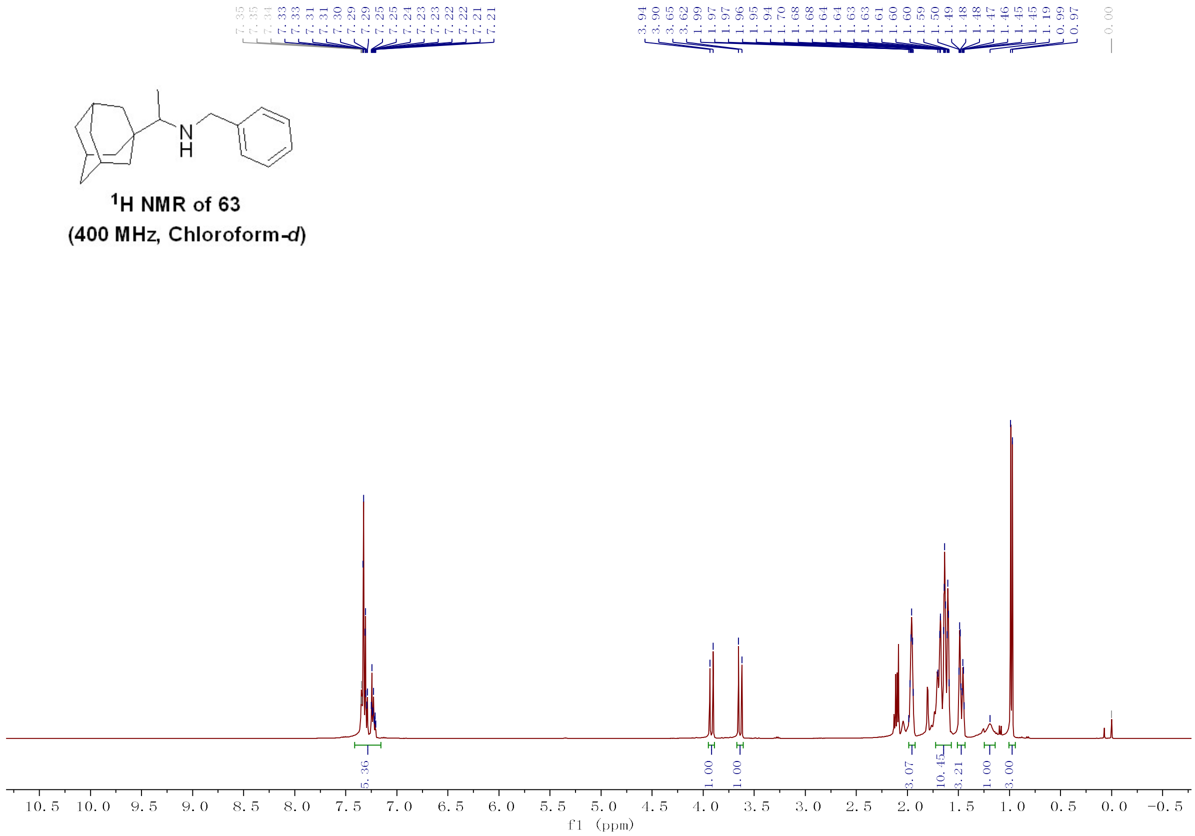
^{1}H NMR of 61
(400 MHz, Chloroform-*d*)

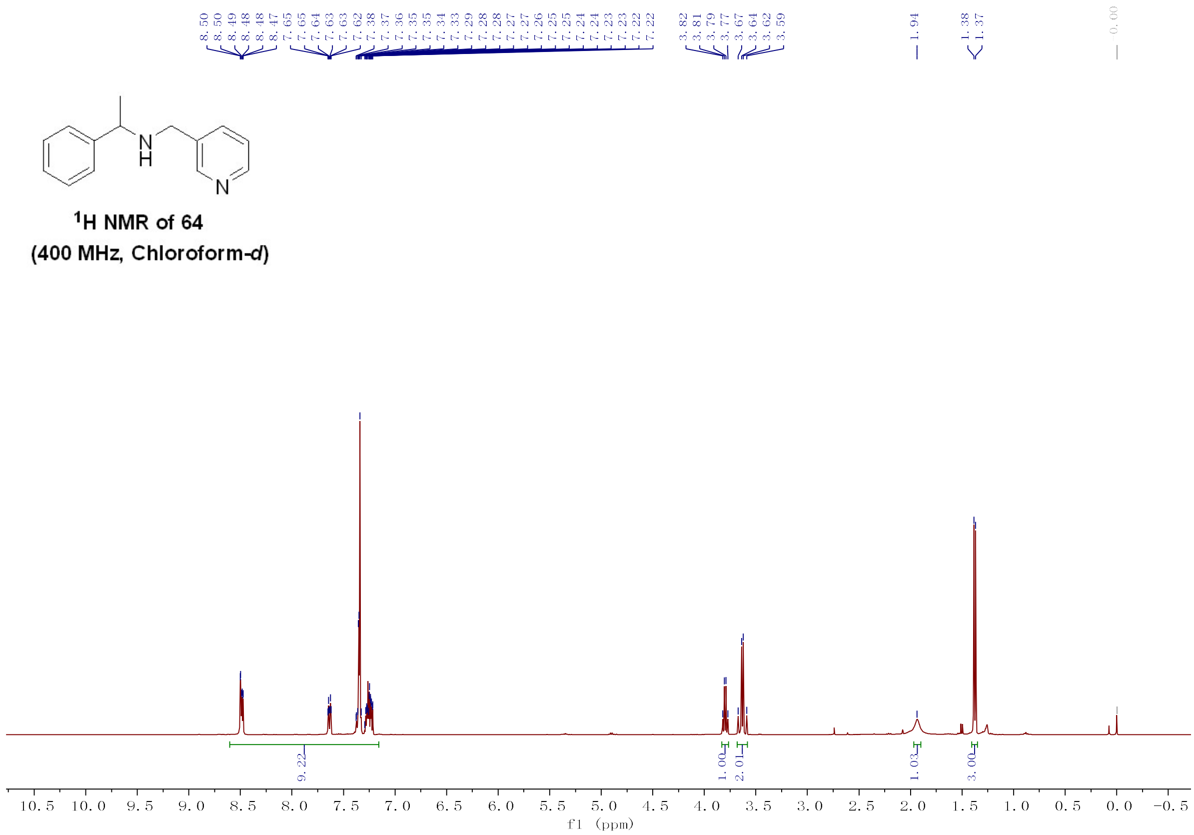


^{1}H NMR of 62
(400 MHz, Chloroform-*d*)

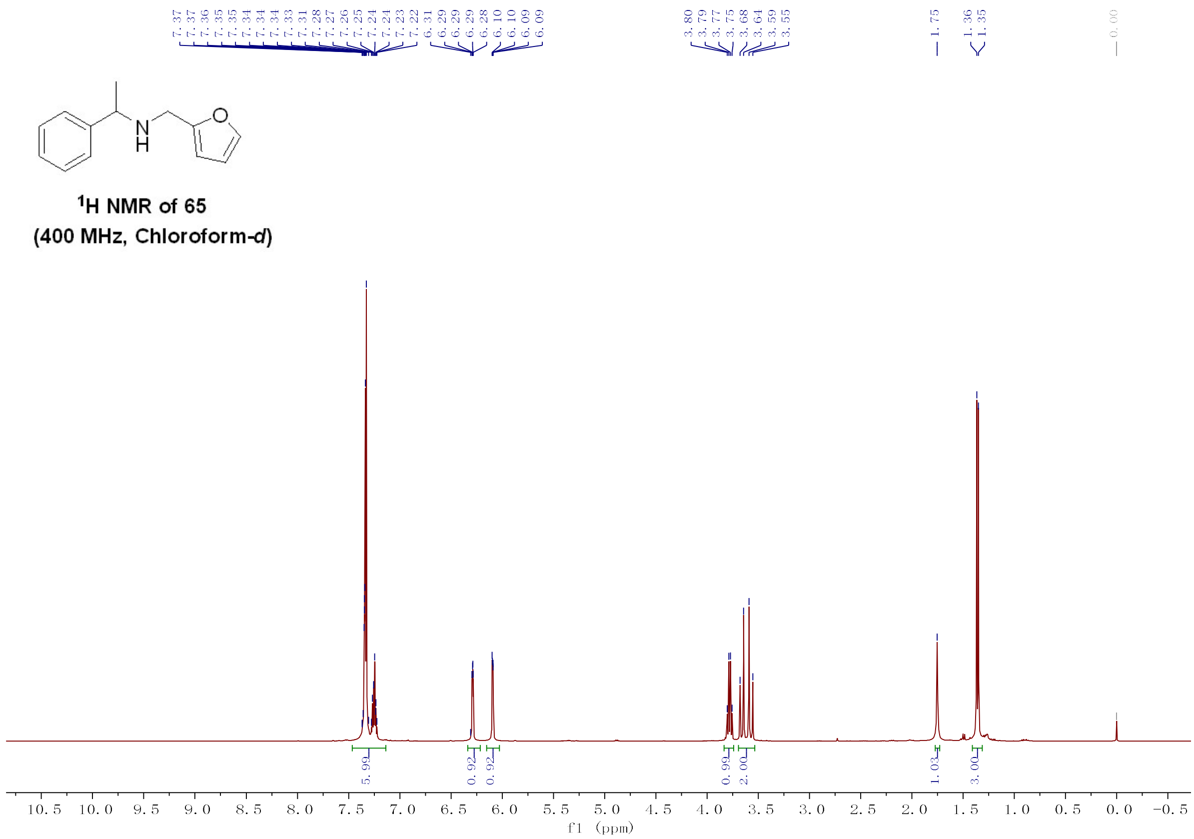


^{1}H NMR of 63
(400 MHz, Chloroform-*d*)

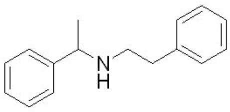


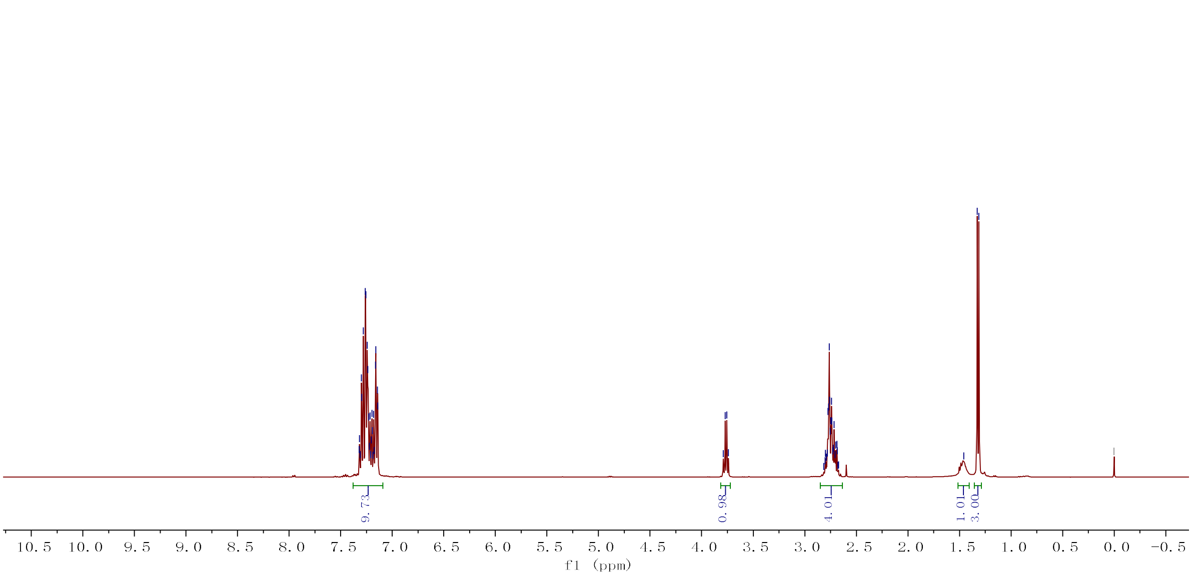


^{1}H NMR of 64
(400 MHz, Chloroform-d)

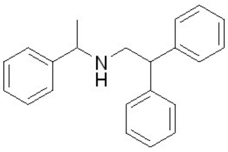


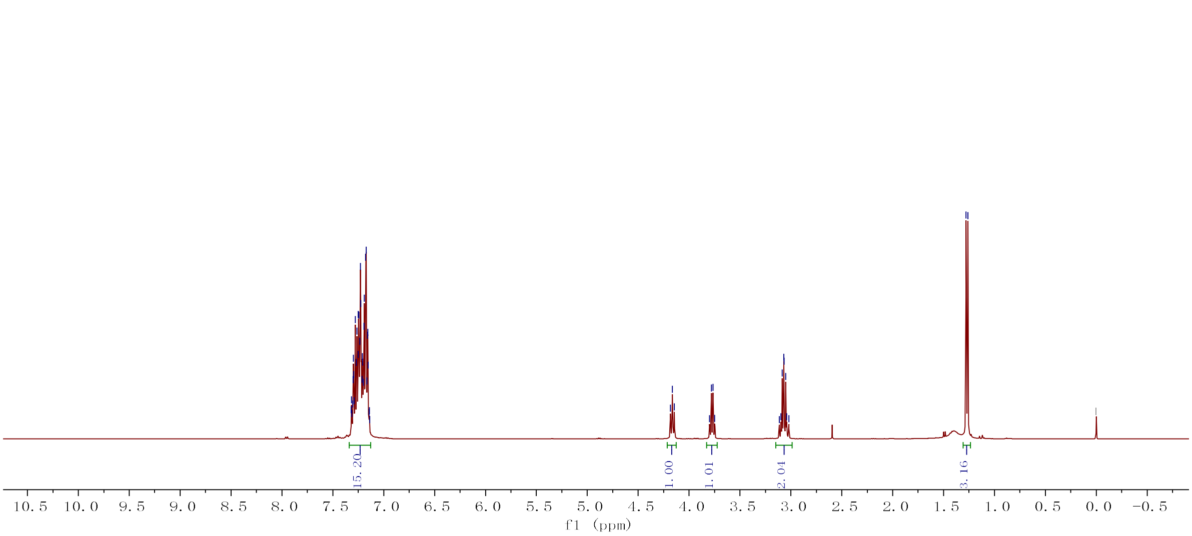
^{1}H NMR of 65
(400 MHz, Chloroform-d)



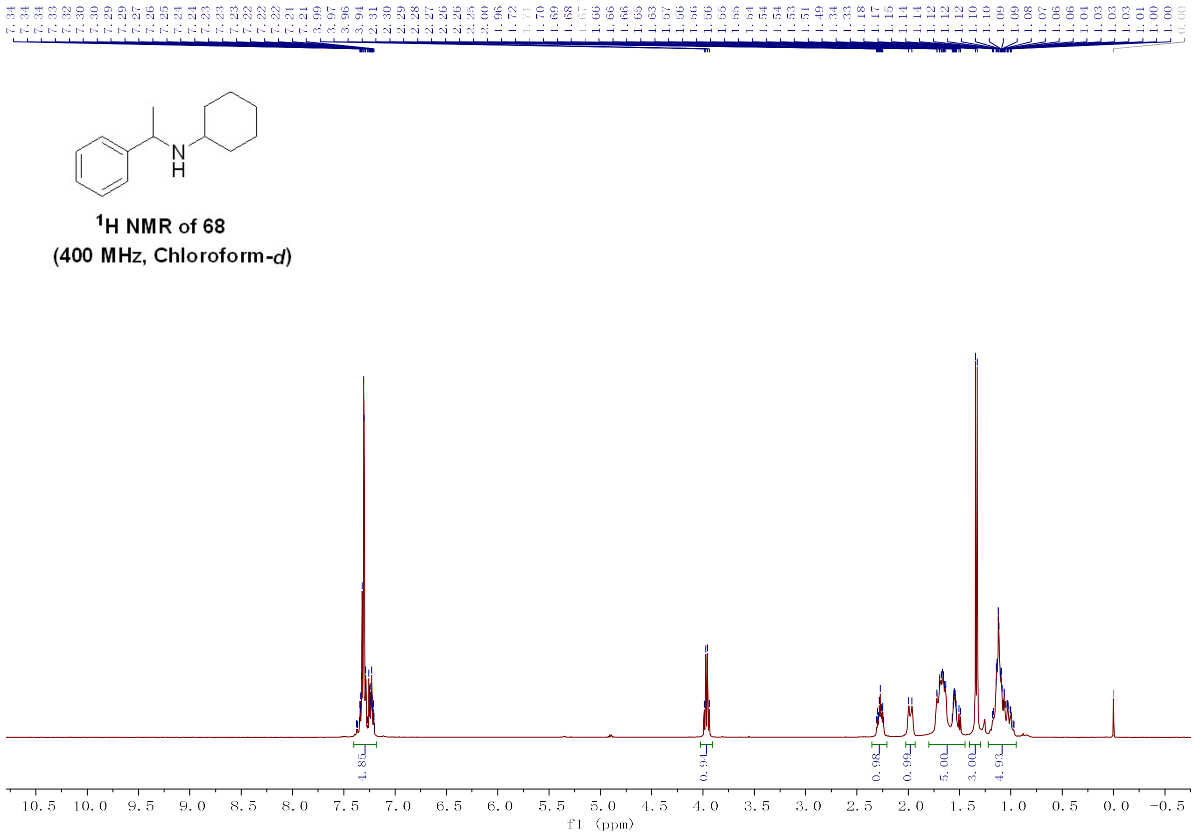


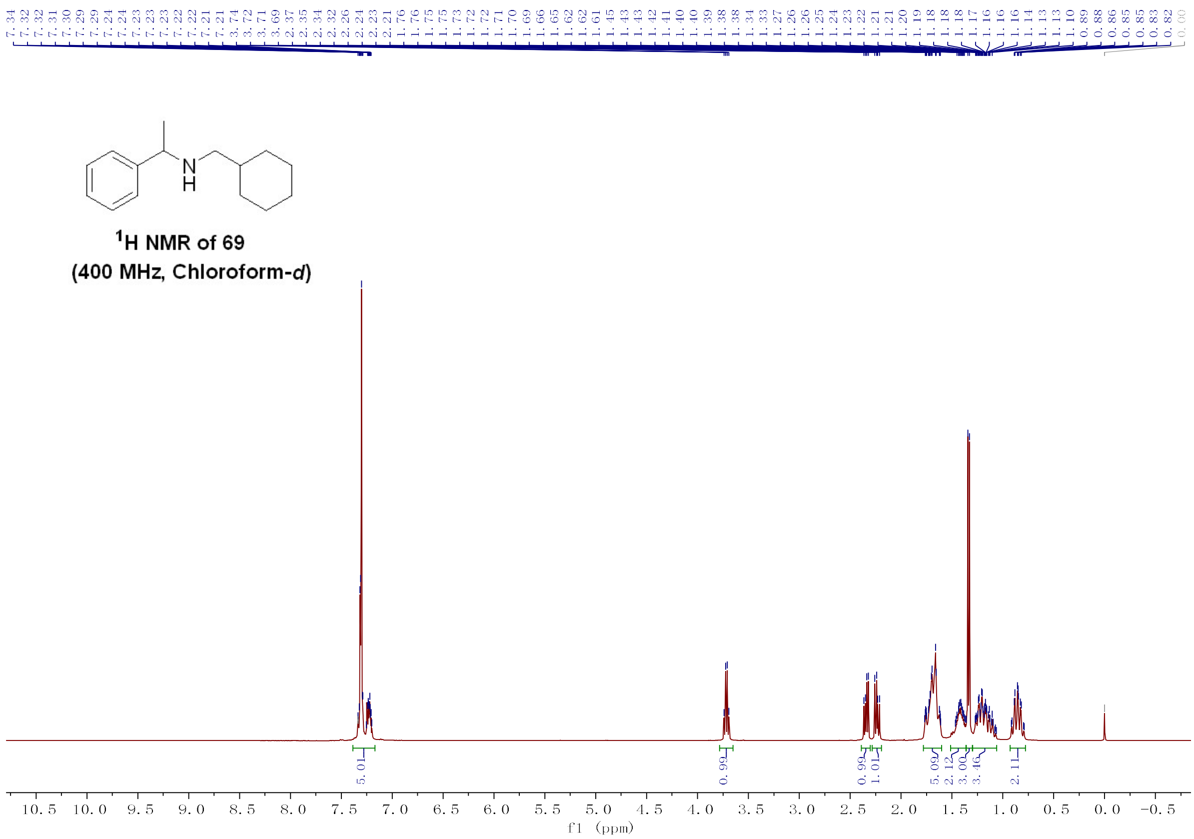
^1H NMR of 66
(400 MHz, Chloroform-*d*)

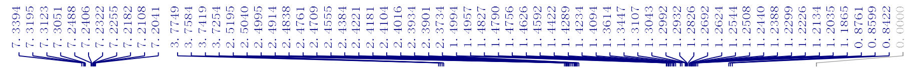


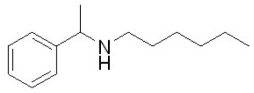


^1H NMR of 67
(400 MHz, Chloroform-*d*)

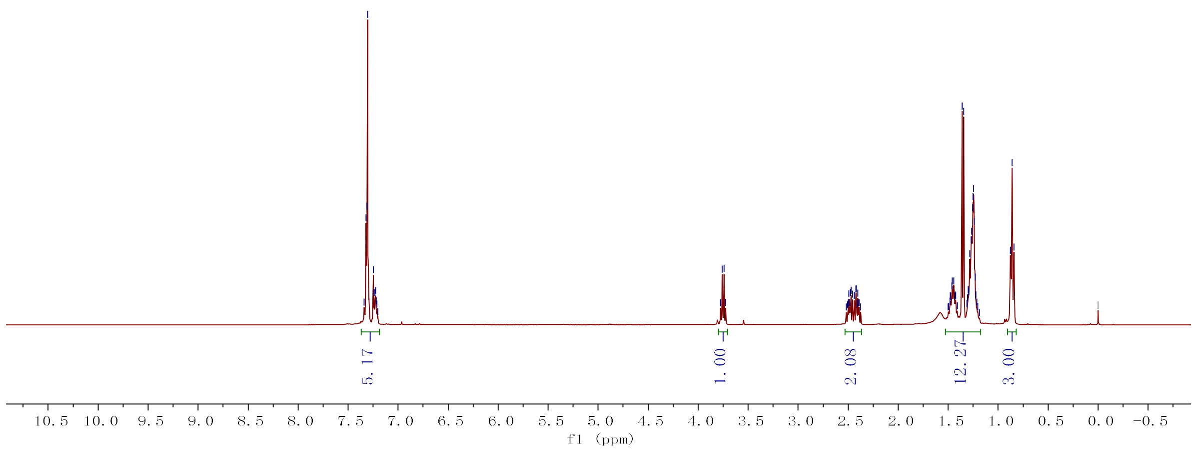

1H NMR of 68
(400 MHz, Chloroform-d)
f1 (ppm)

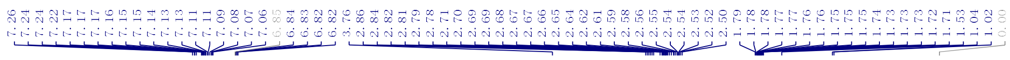

1H NMR of 69
(400 MHz, Chloroform-d)
f1 (ppm)

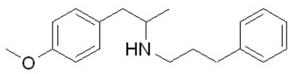




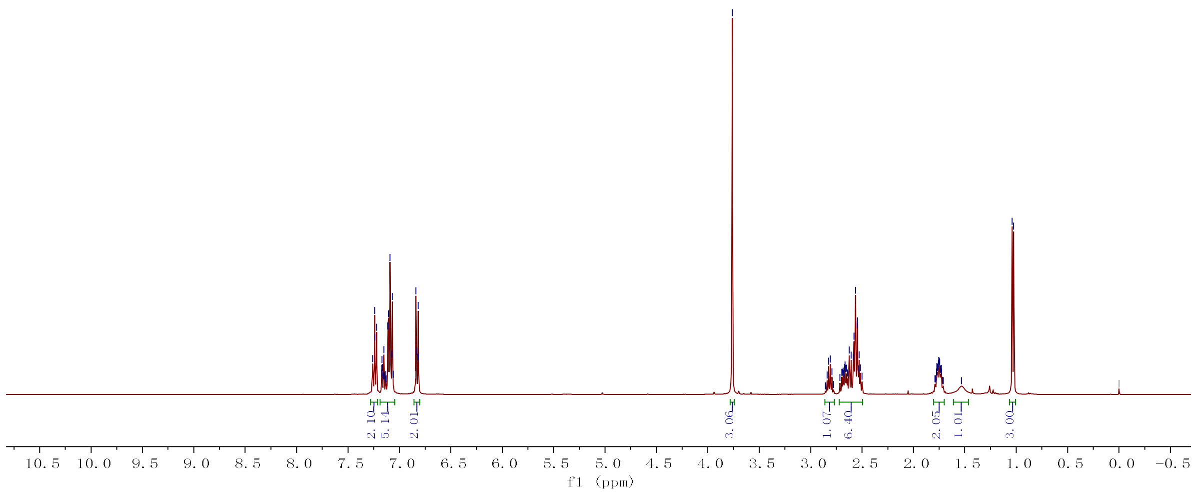
[1]H NMR of 70
(400 MHz, Chloroform-*d*)

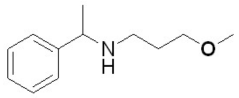




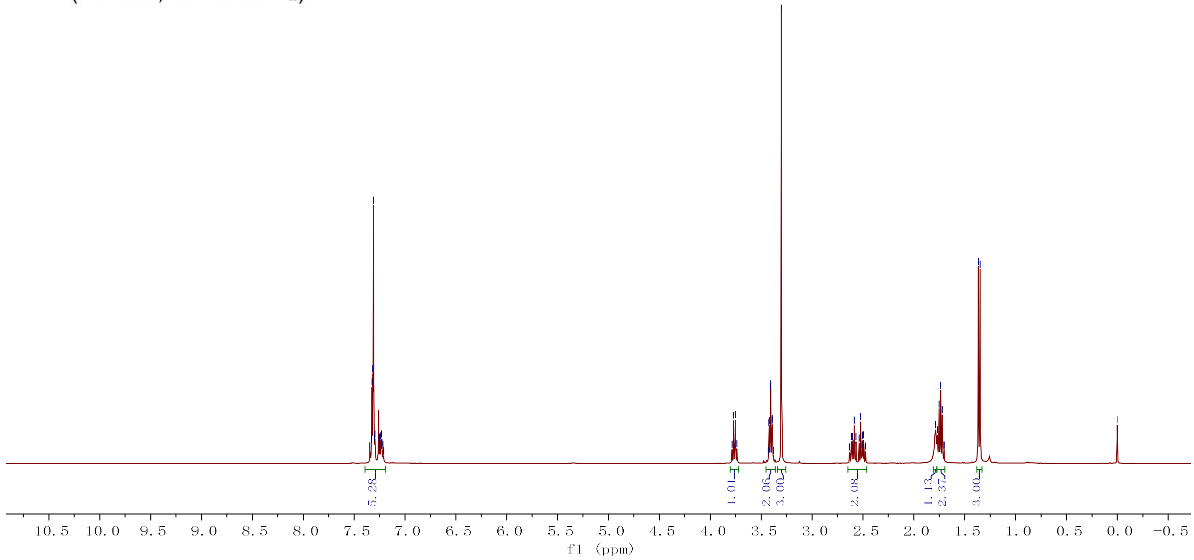


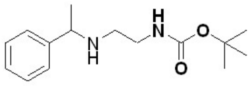
[1]H NMR of 71
(400 MHz, Chloroform-*d*)



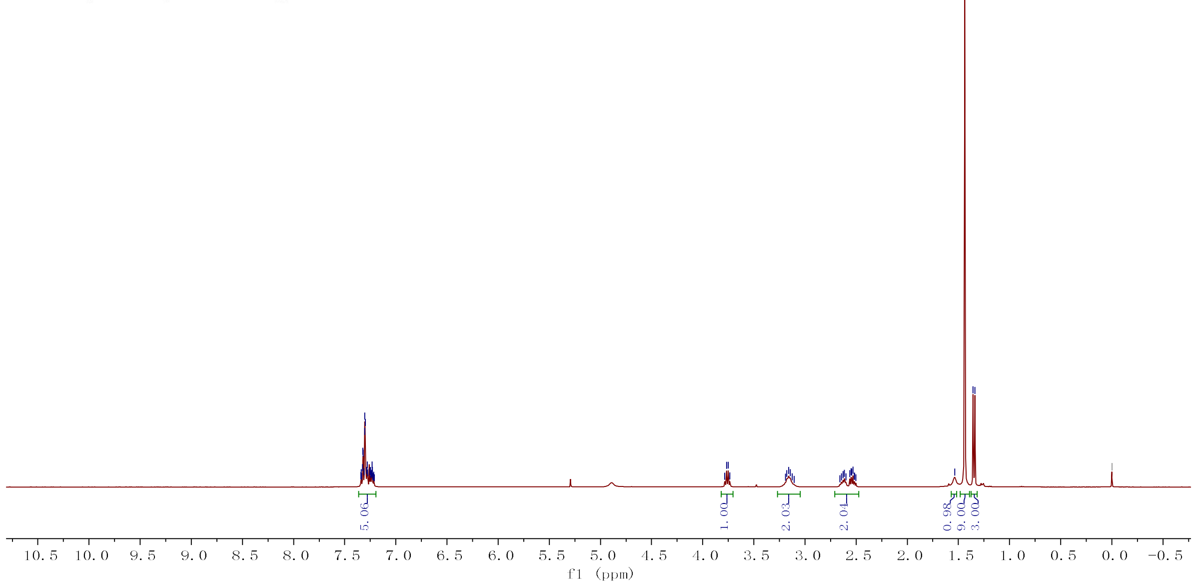


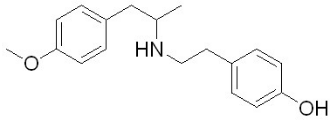
^{1}H NMR of 72
(400 MHz, Chloroform-*d*)



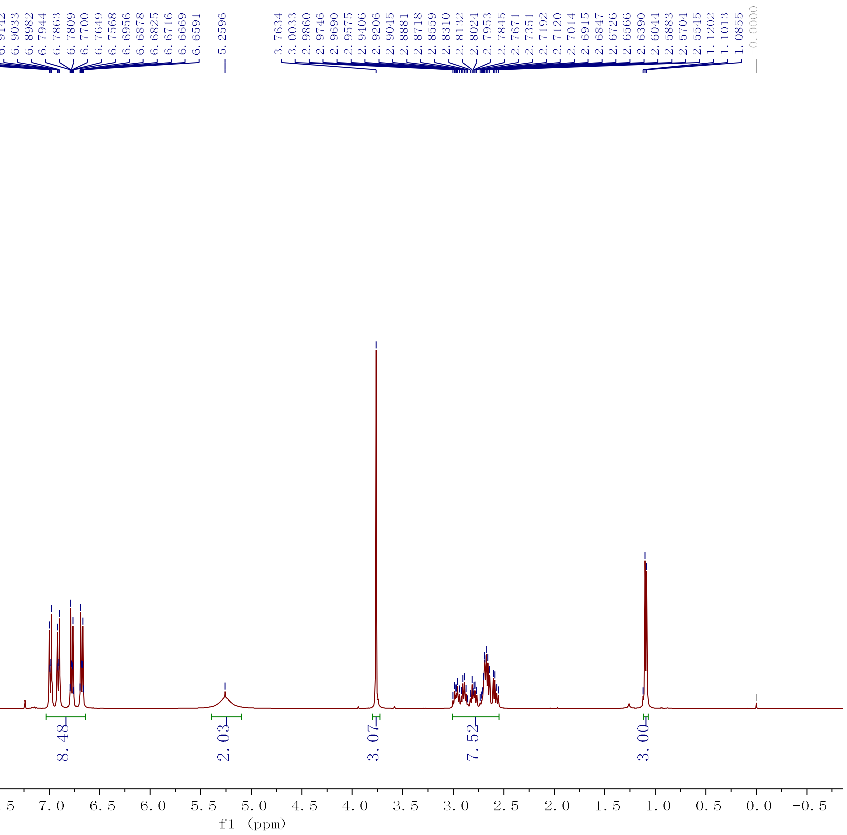


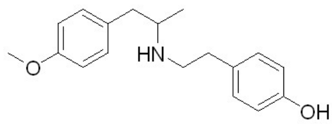
^{1}H NMR of 73
(400 MHz, Chloroform-*d*)



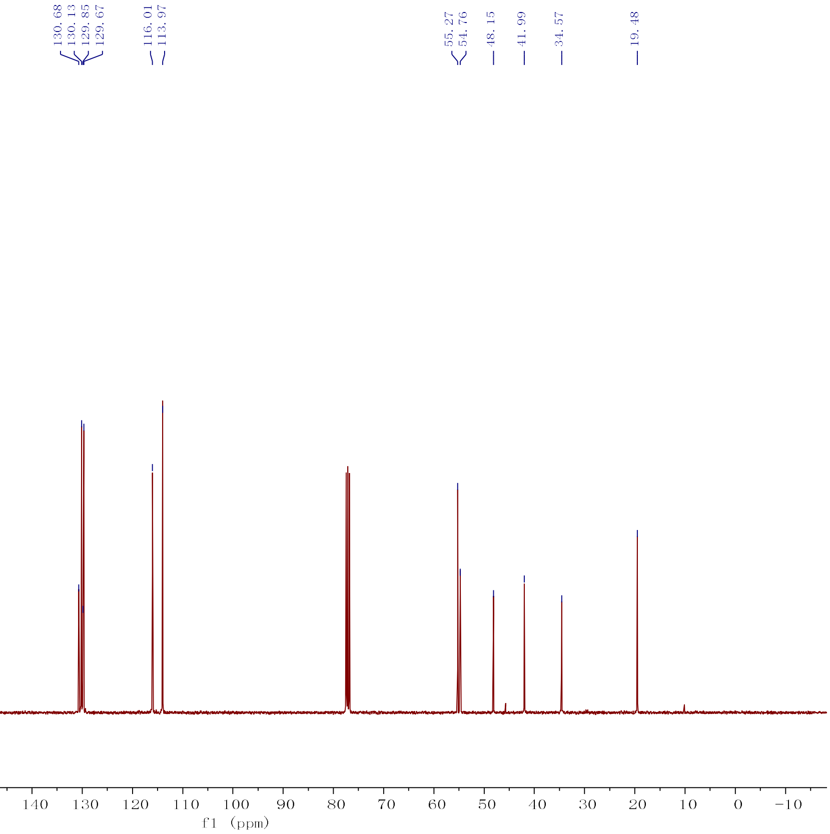


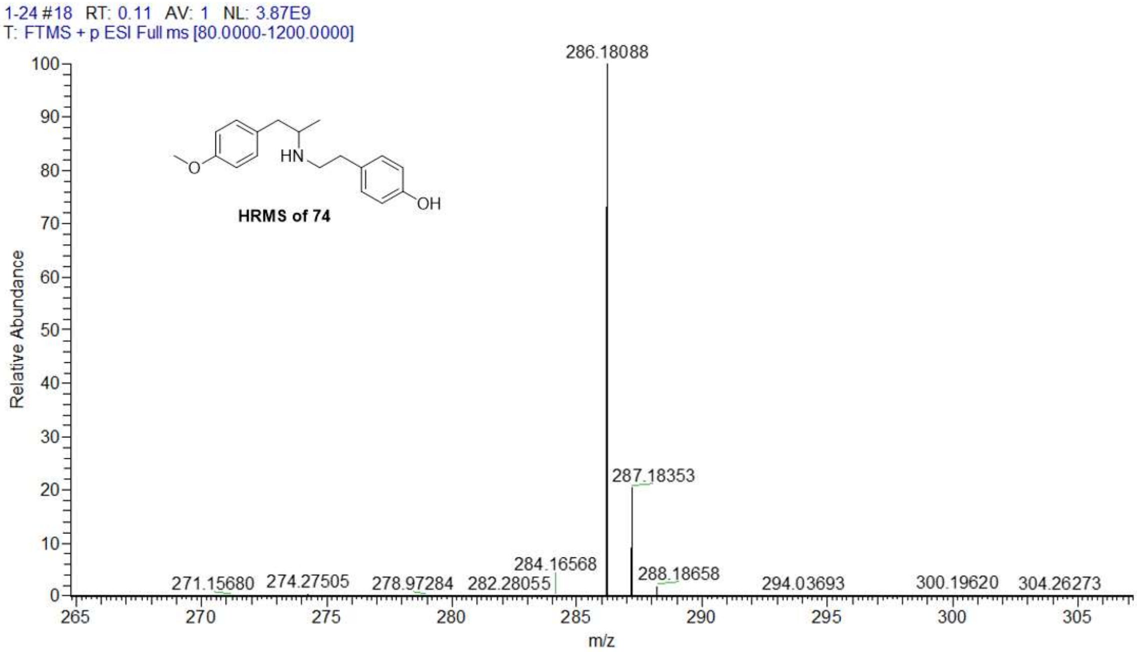
[1]H NMR of 74
(400 MHz, Chloroform-*d*)

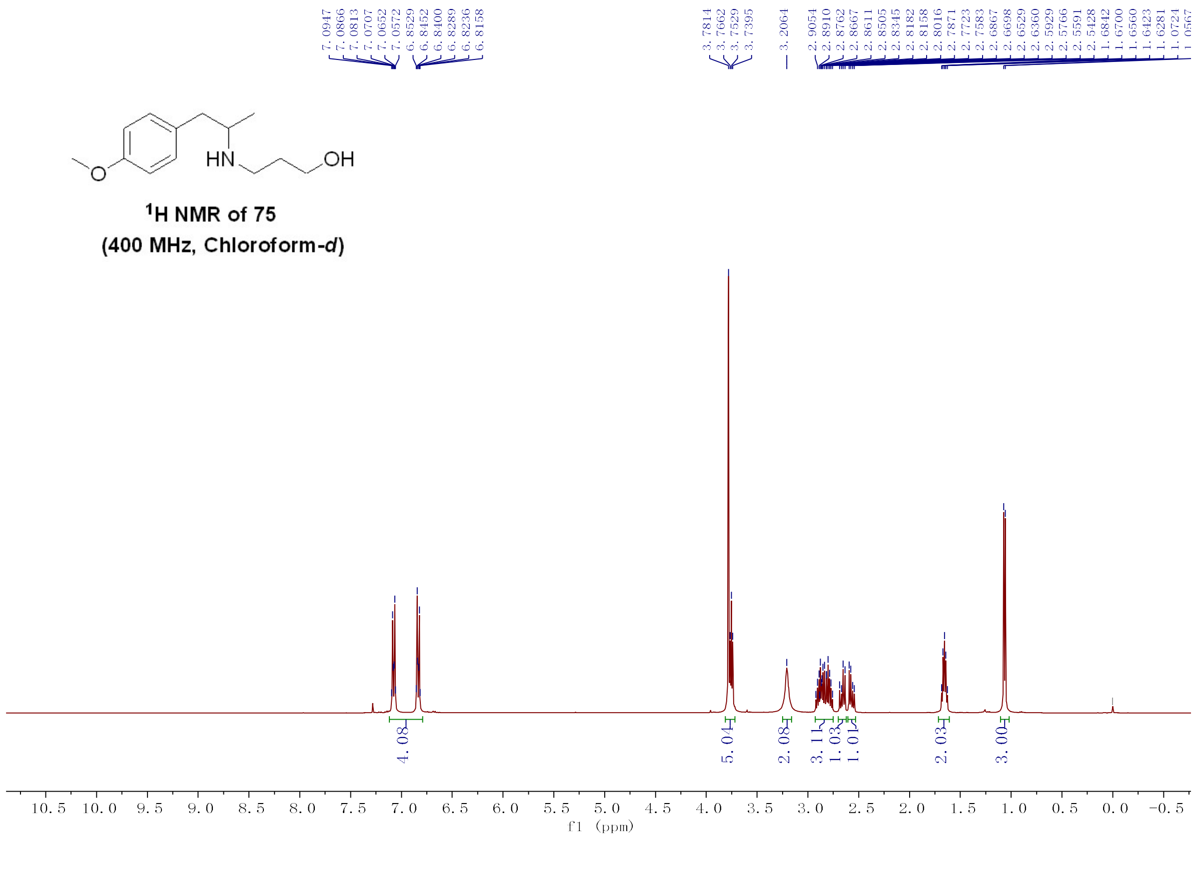


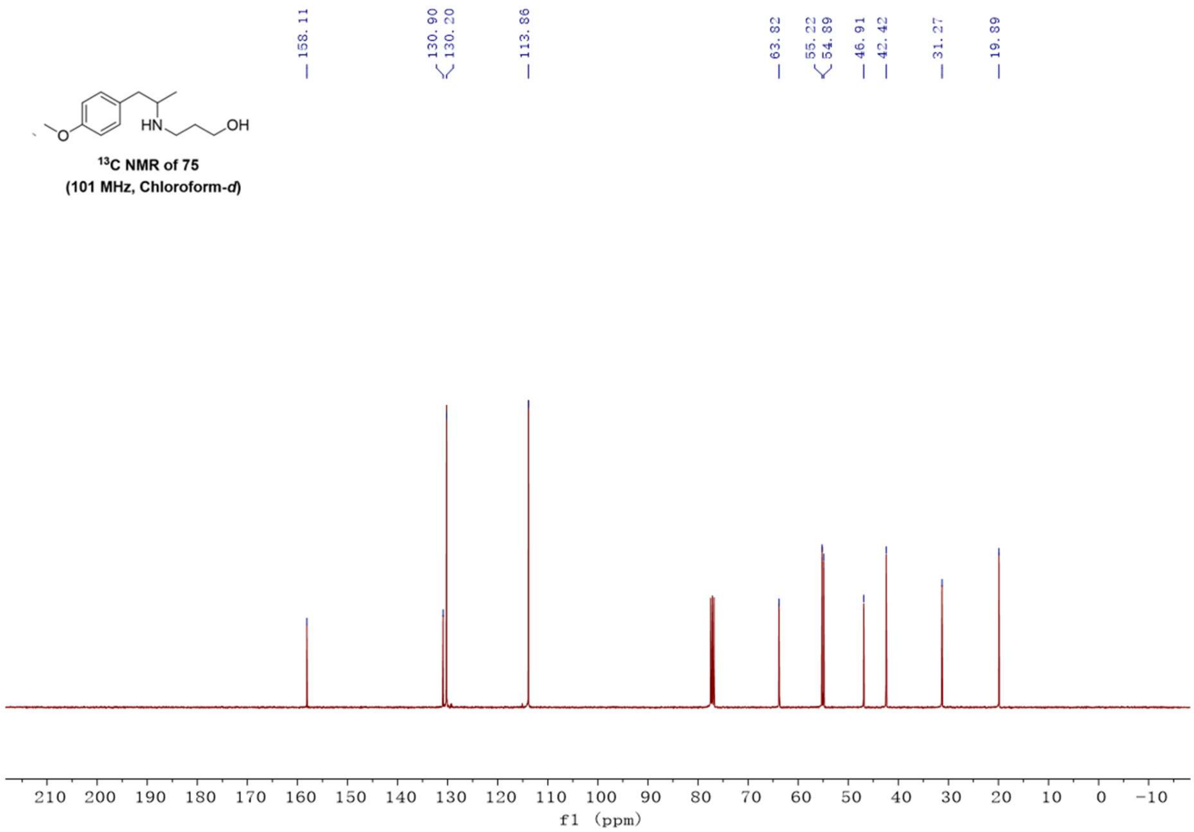


[13]C NMR of 74
(101 MHz, Chloroform-*d*)

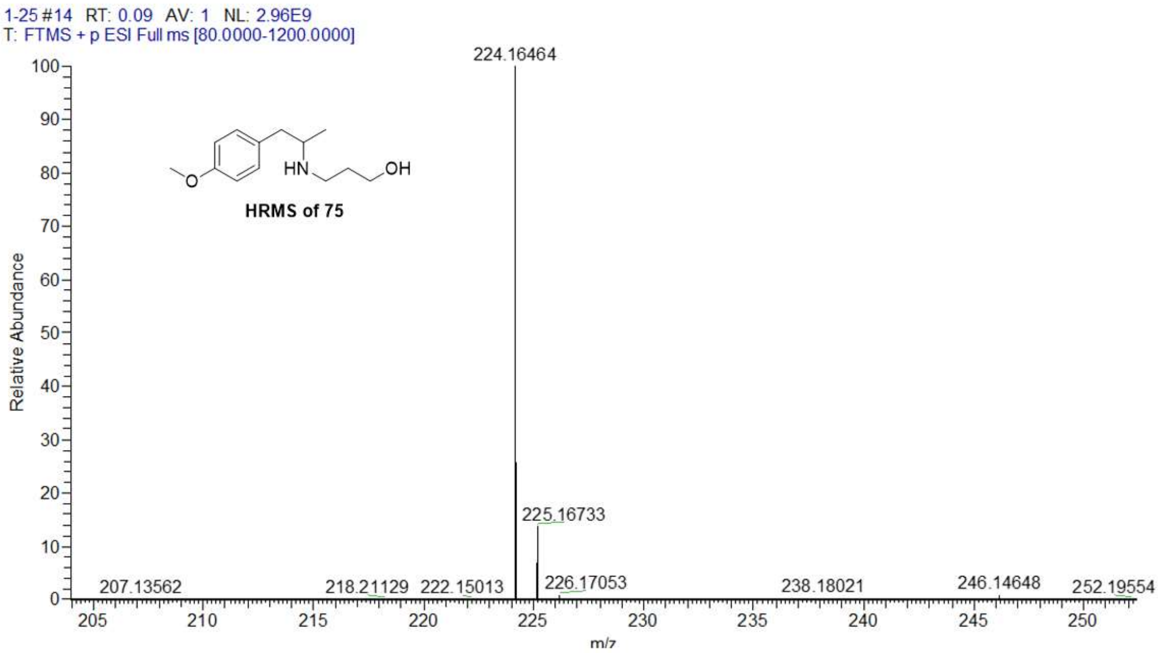



1-24 #18 RT: 0.11 AV: 1 NL: 3.87E9
T: FTMS + p ESI Full ms [80.0000-1200.0000]
HRMS of 74
286.18088
287.18353
288.18658
284.16568
271.15680
274.27505
278.97284
282.28055
294.03693
300.19620
304.26273
Relative Abundance
m/z

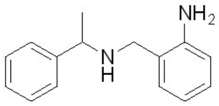

¹H NMR of 75
(400 MHz, Chloroform-d)
f1 (ppm)



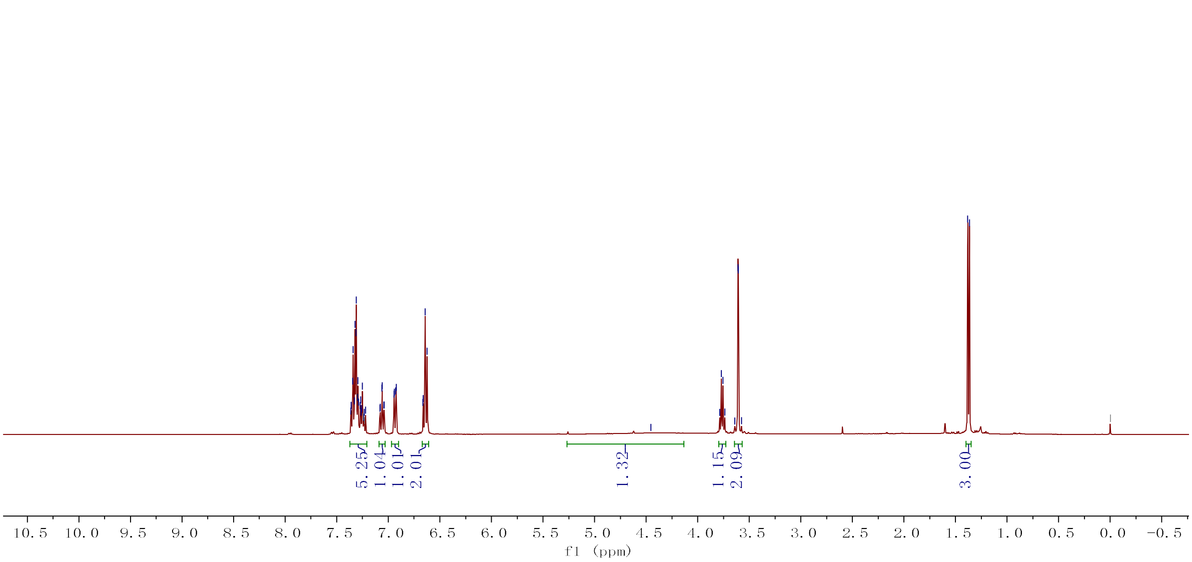
158.11
130.90
130.20
113.86
63.82
55.22
54.89
46.91
42.42
31.27
19.89
HN
OH
O
^{13}C NMR of 75
(101 MHz, Chloroform-d)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

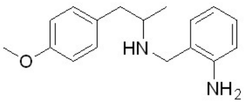


1-25 #14 RT: 0.09 AV: 1 NL: 2.96E9
T: FTMS + p ESI Full ms [80.0000-1200.0000]
224.16464
HN
OH
O
HRMS of 75
Relative Abundance
225.16733
207.13562
218.21129
222.15013
226.17053
238.18021
246.14648
252.19554
m/z

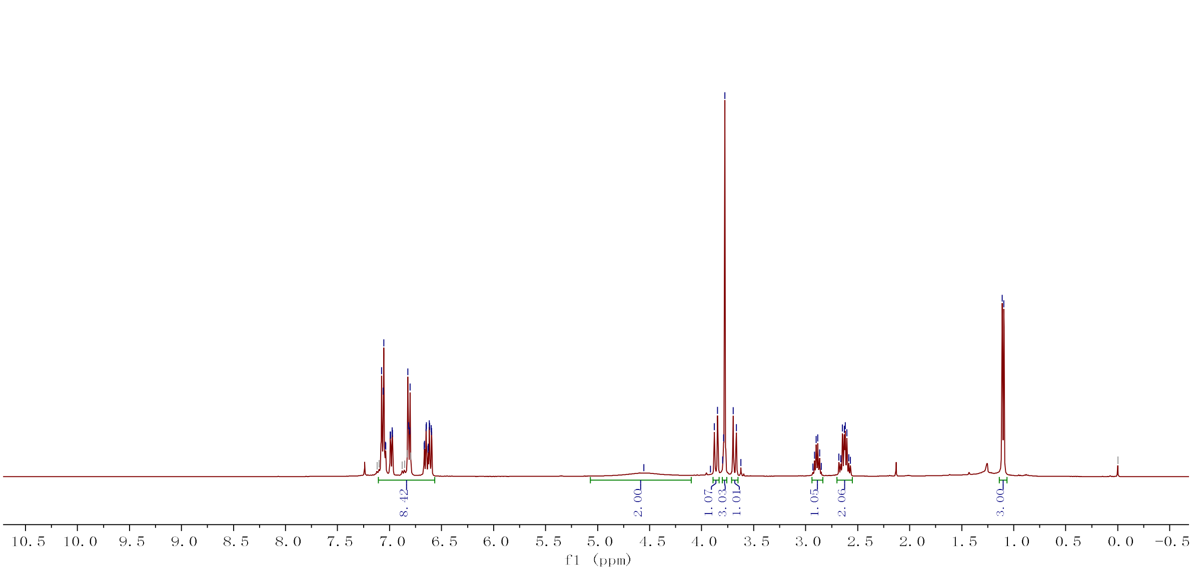


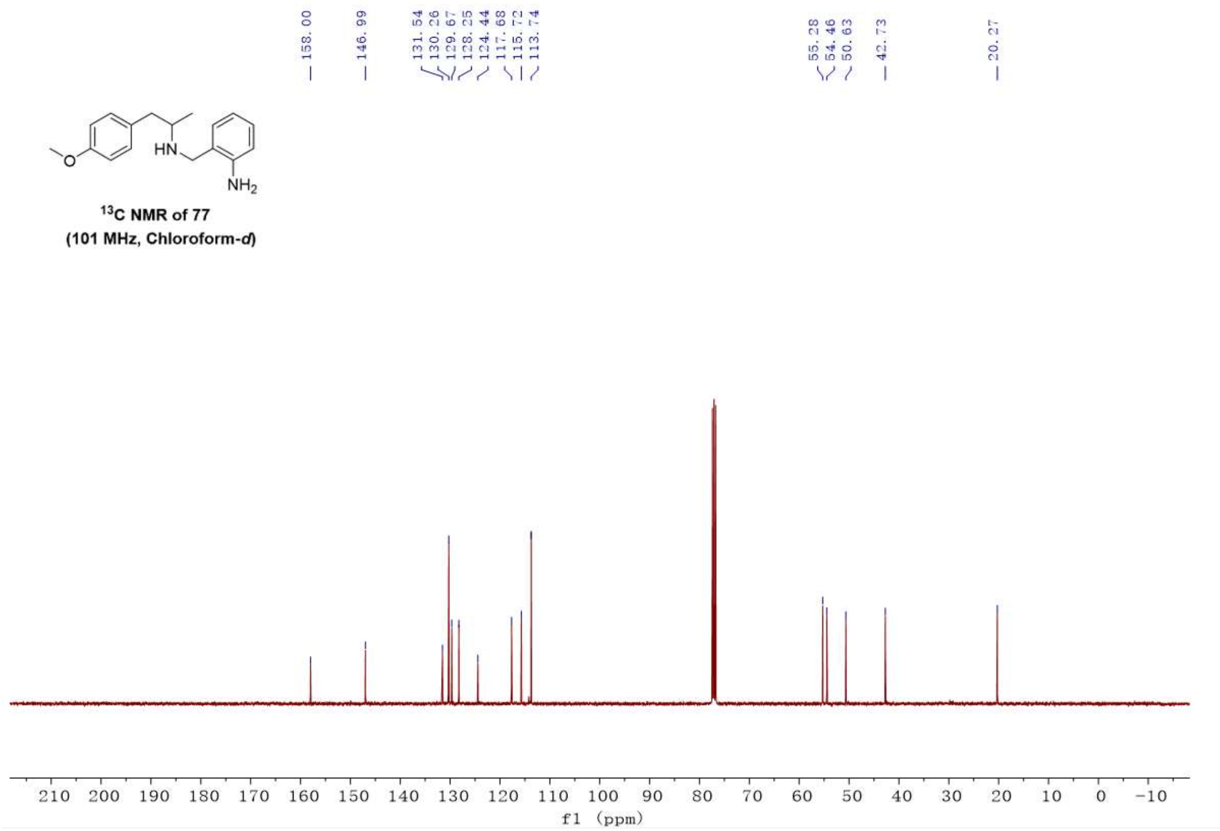
^{1}H NMR of 76
(400 MHz, Chloroform-d)

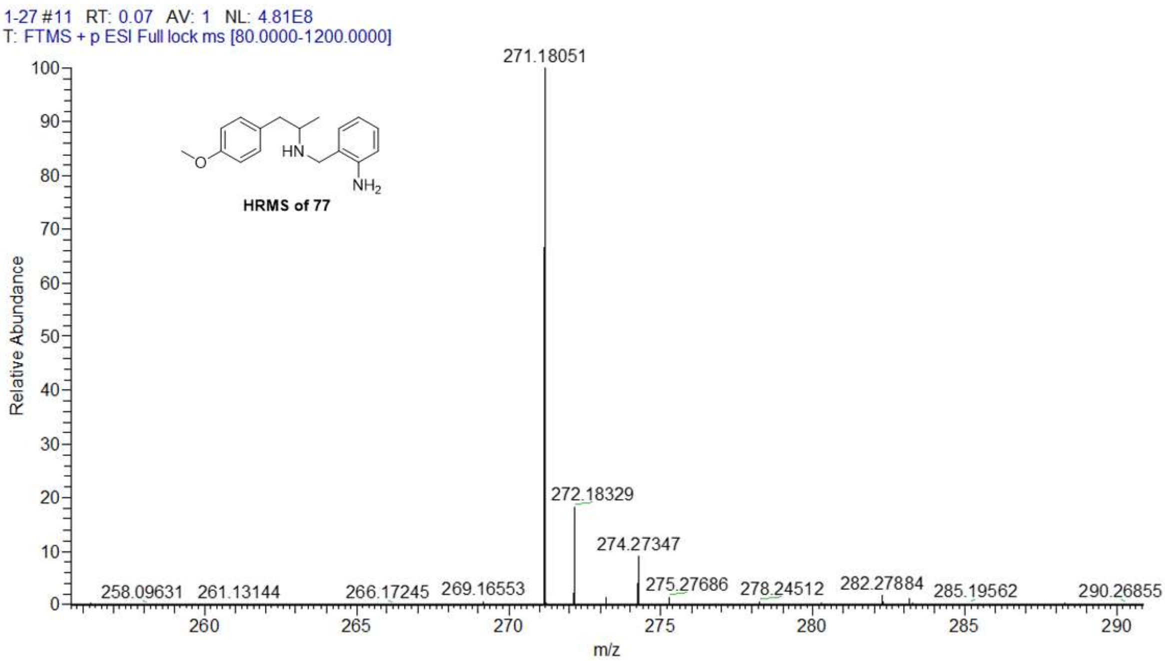


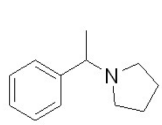


^{1}H NMR of 77
(400 MHz, Chloroform-d)

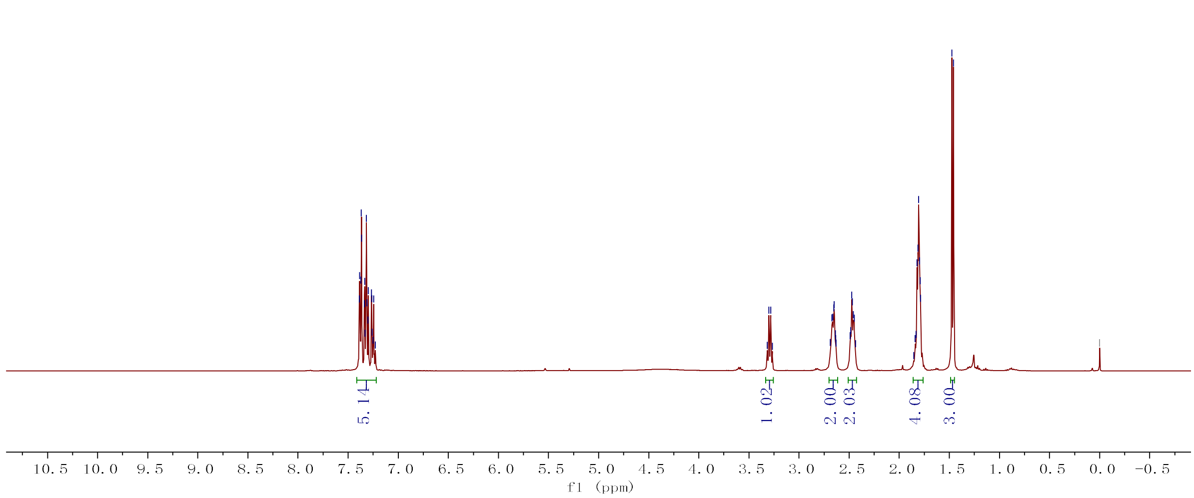


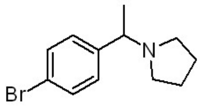

158.00
146.99
131.54
130.26
129.67
128.25
124.44
117.68
115.72
113.74
55.28
54.46
50.63
42.73
20.27
HN
NH_2
O
^{13}C NMR of 77
(101 MHz, Chloroform-*d*)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


1-27 #11 RT: 0.07 AV: 1 NL: 4.81E8
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]
271.18051
HN
NH_2
O
HRMS of 77
Relative Abundance
272.18329
274.27347
258.09631
261.13144
266.17245
269.16553
275.27686
278.24512
282.27884
285.19562
290.26855
m/z

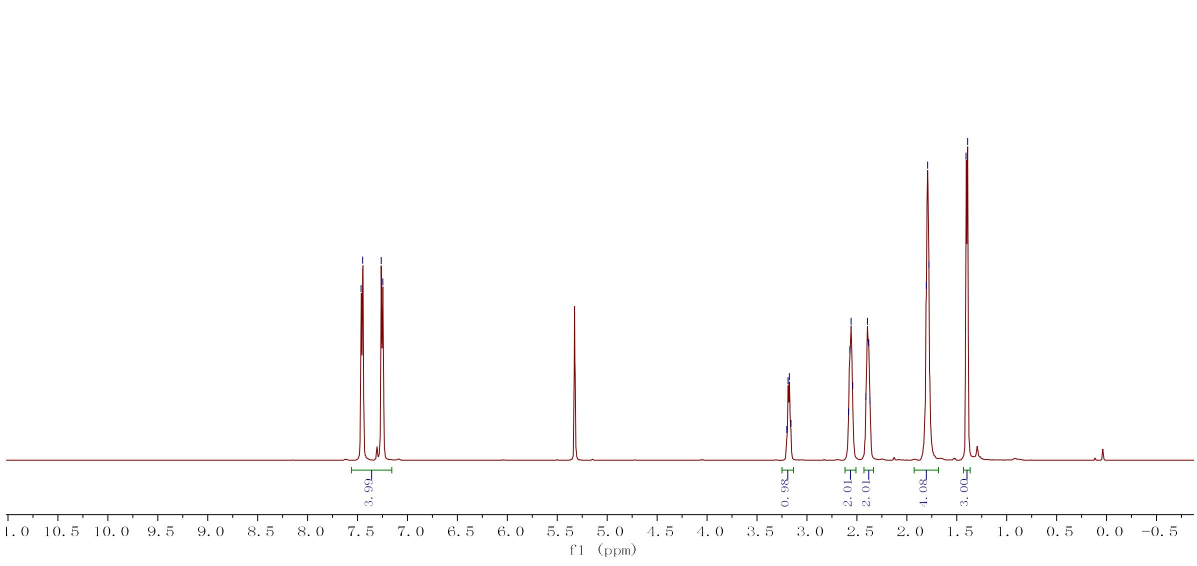


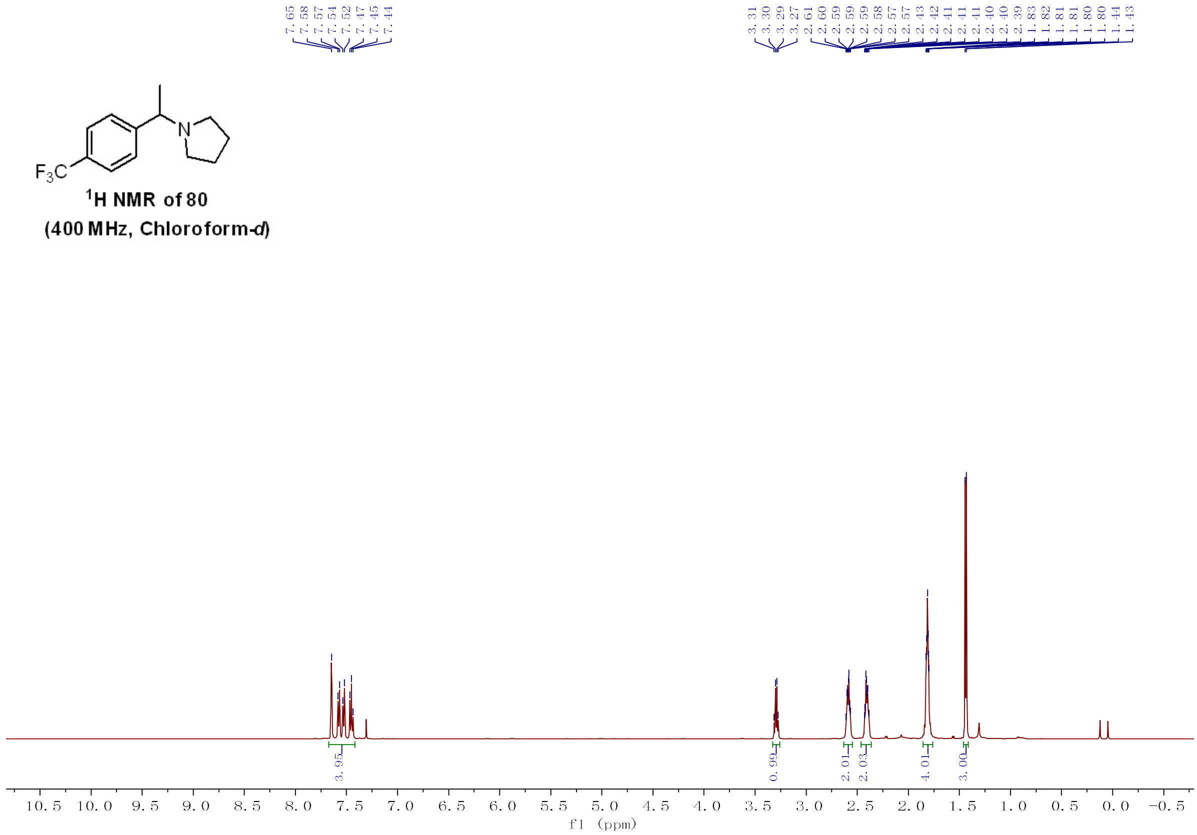
^{1}H NMR of 78
(400 MHz, Chloroform-*d*)



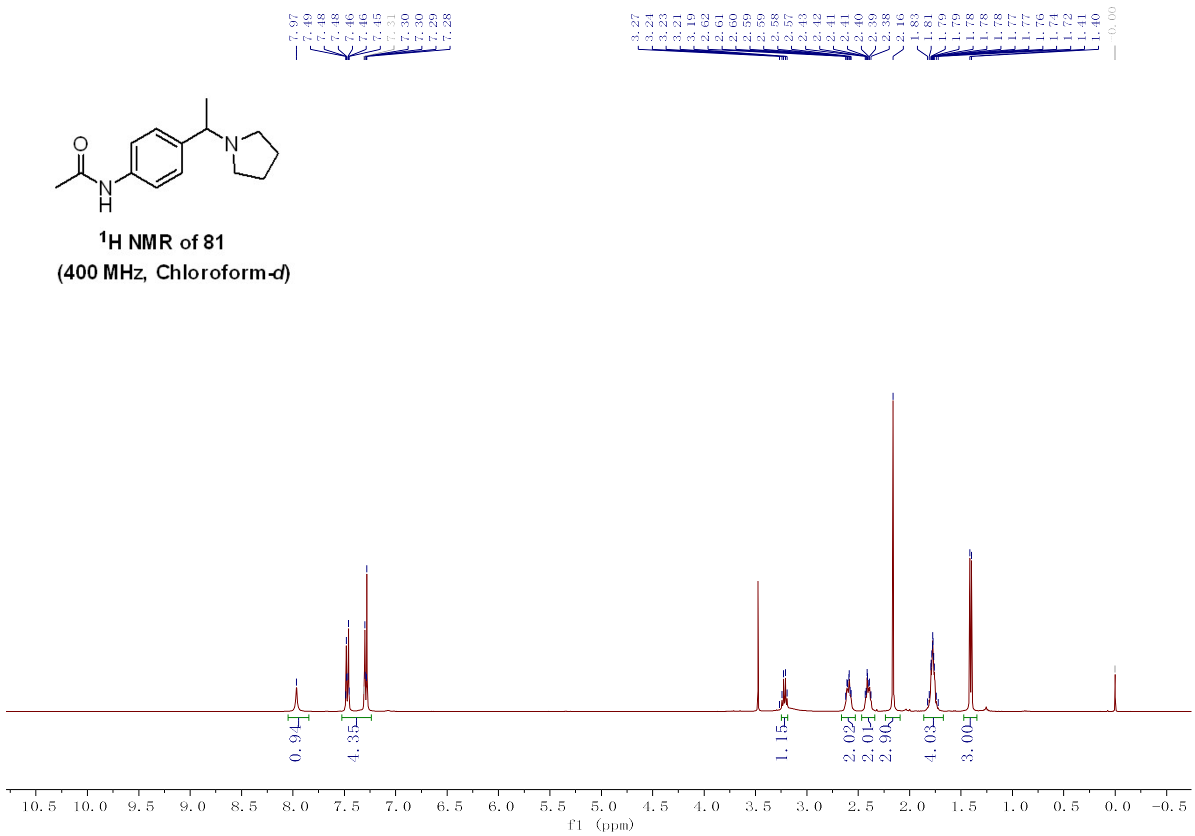


^{1}H NMR of 79
(400 MHz, Chloroform-*d*)

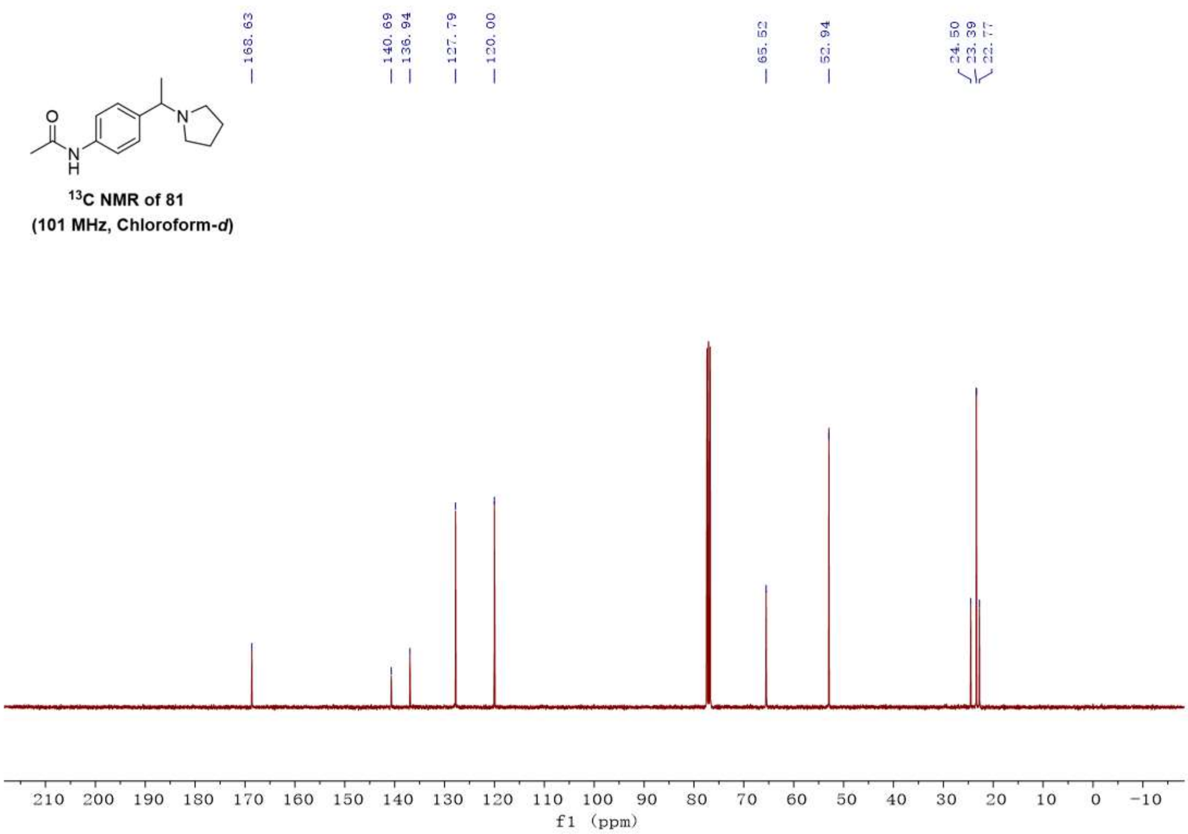




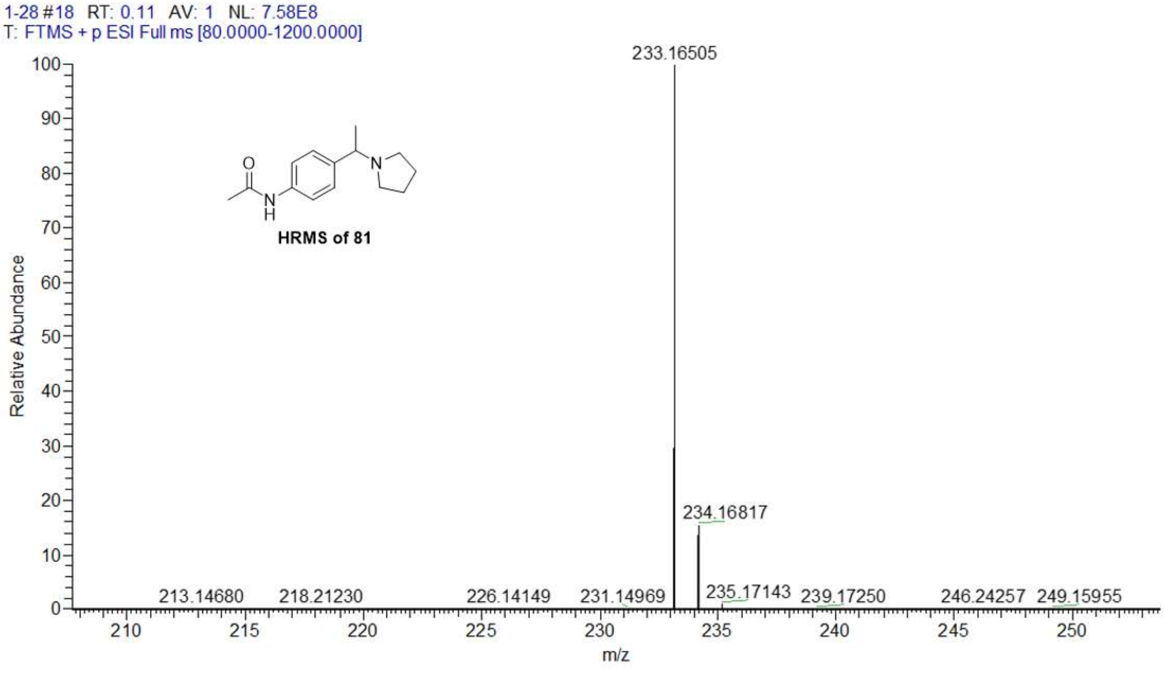
^{1}H NMR of 80
(400 MHz, Chloroform-*d*)



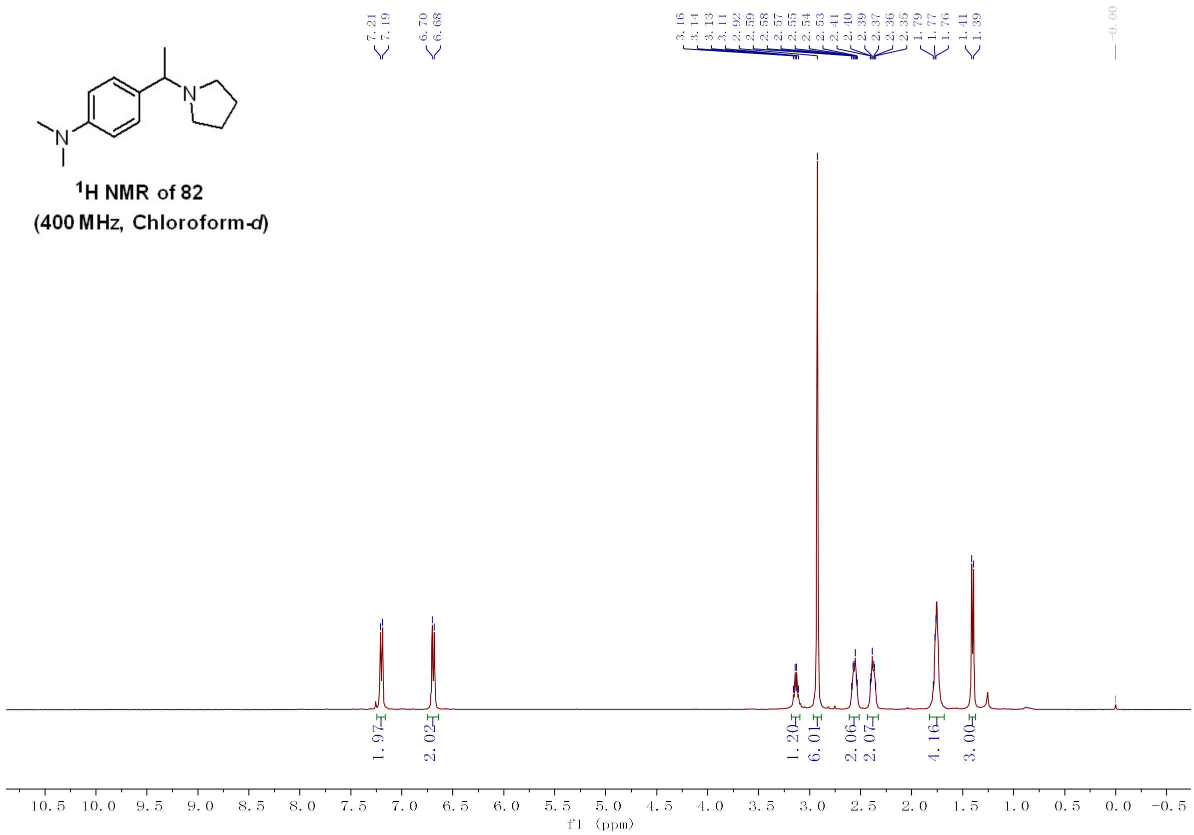
^{1}H NMR of 81
(400 MHz, Chloroform-*d*)



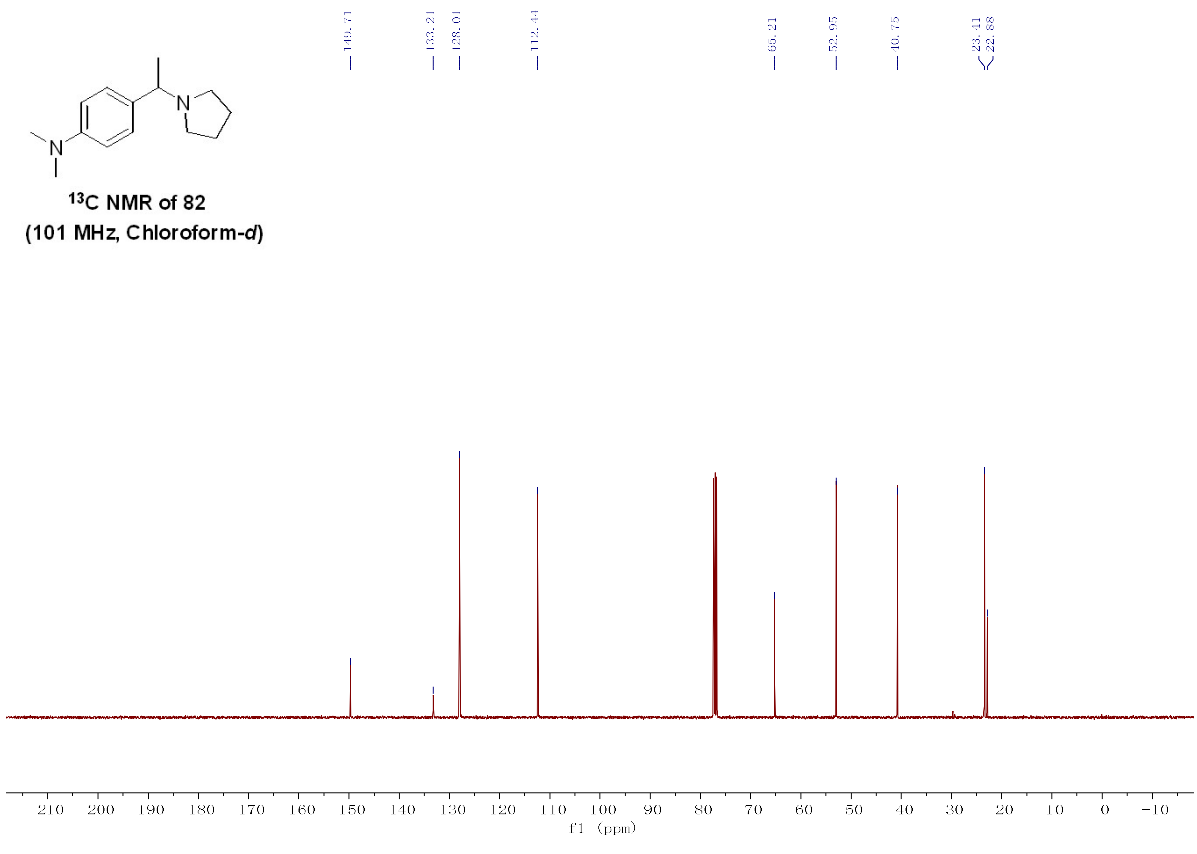
^{13}C NMR of 81
(101 MHz, Chloroform-*d*)



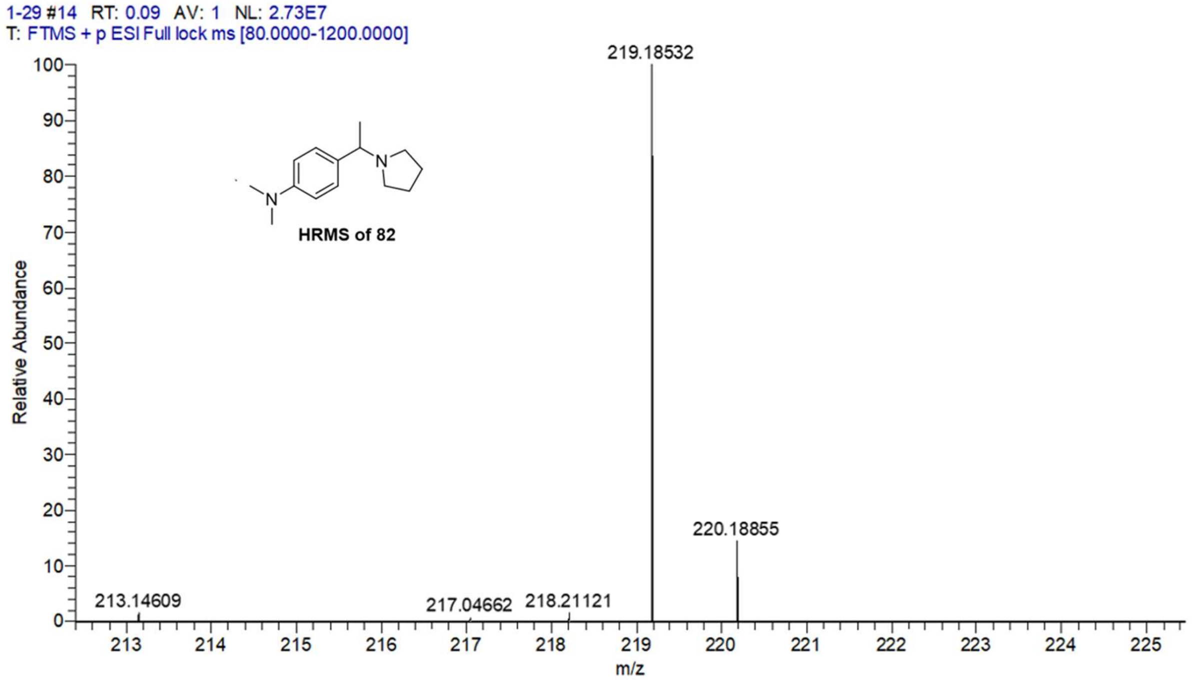
HRMS of 81



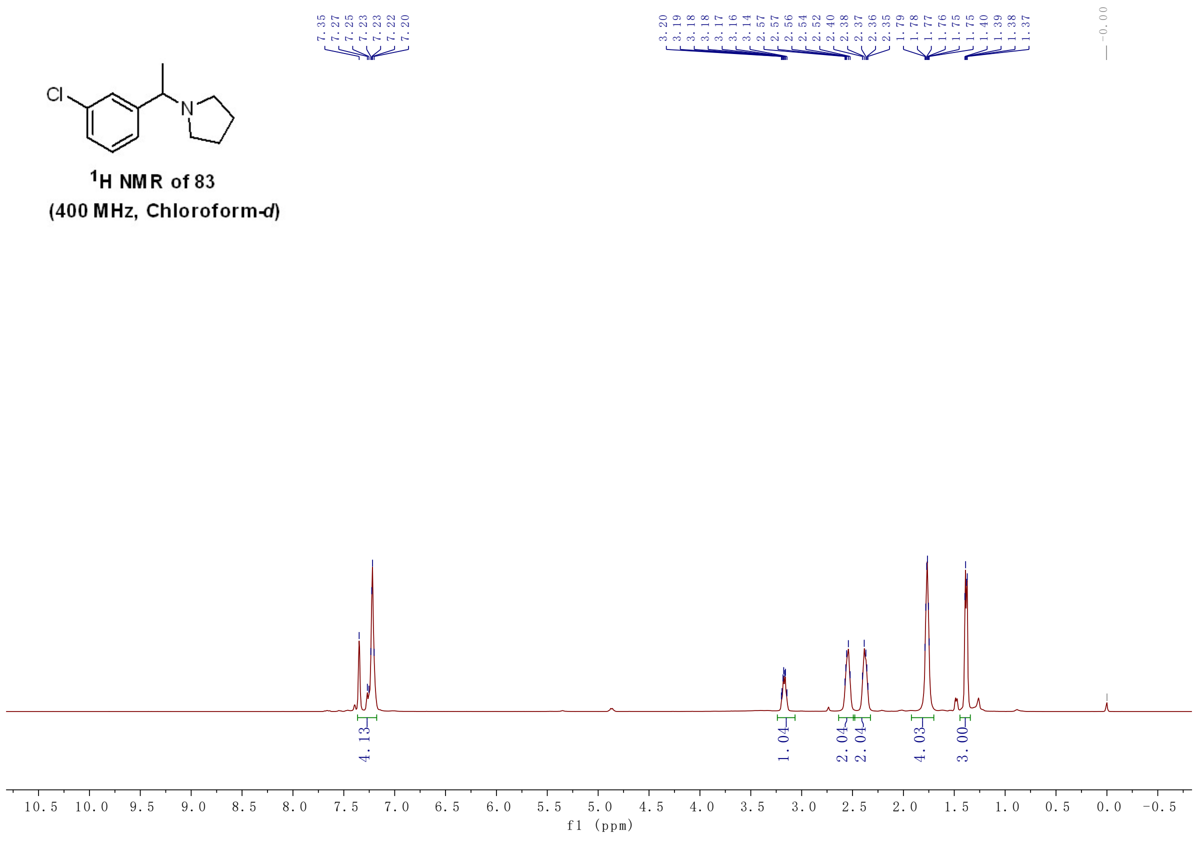
^{1}H NMR of 82
(400 MHz, Chloroform-*d*)



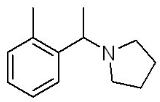
^{13}C NMR of 82
(101 MHz, Chloroform-*d*)



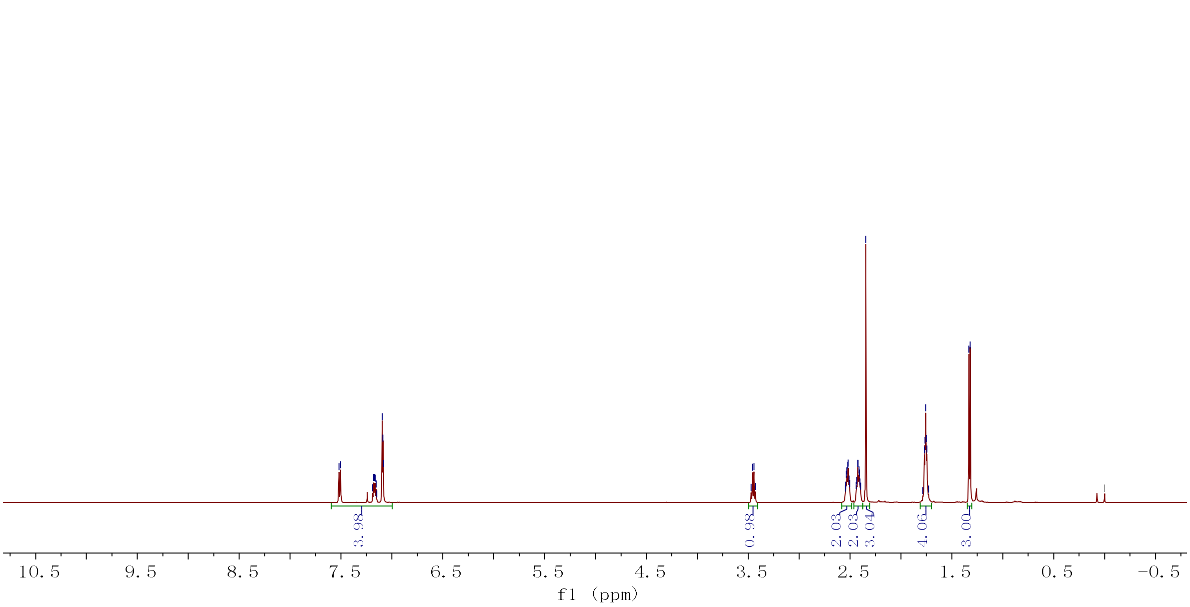
1-29 #14 RT: 0.09 AV: 1 NL: 2.73E7
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]
HRMS of 82
219.18532
220.18855
213.14609
217.04662
218.21121
Relative Abundance
m/z

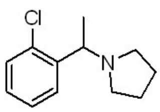


Cl
N
^{1}H NMR of 83
(400 MHz, Chloroform-*d*)
4.13
1.04
2.04
2.04
4.03
3.00
f1 (ppm)

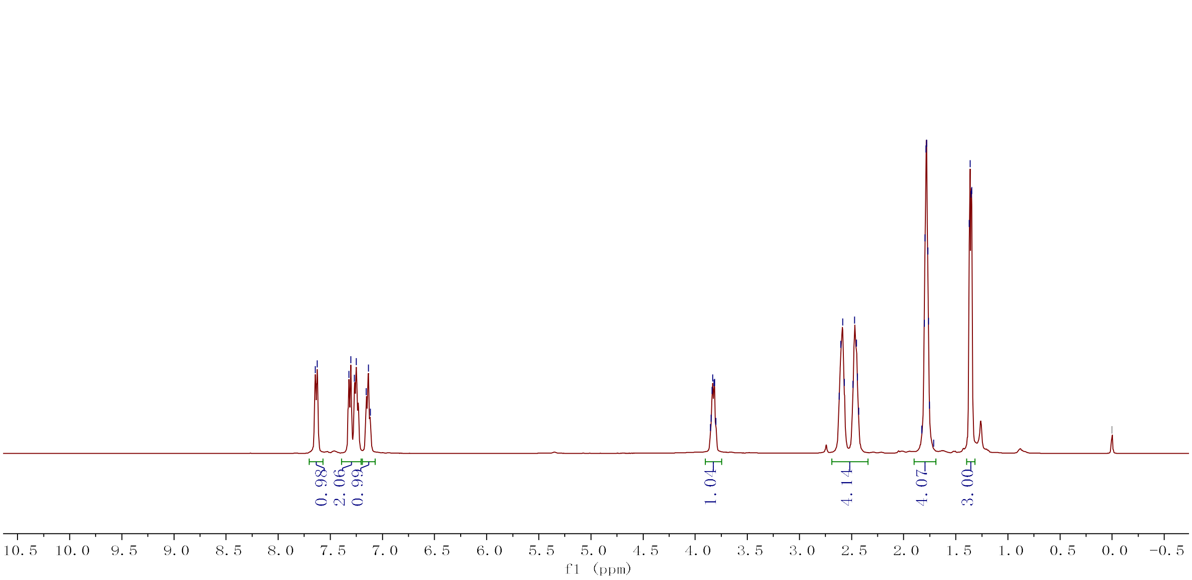


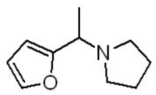
^{1}H NMR of 84
(400 MHz, Chloroform-*d*)



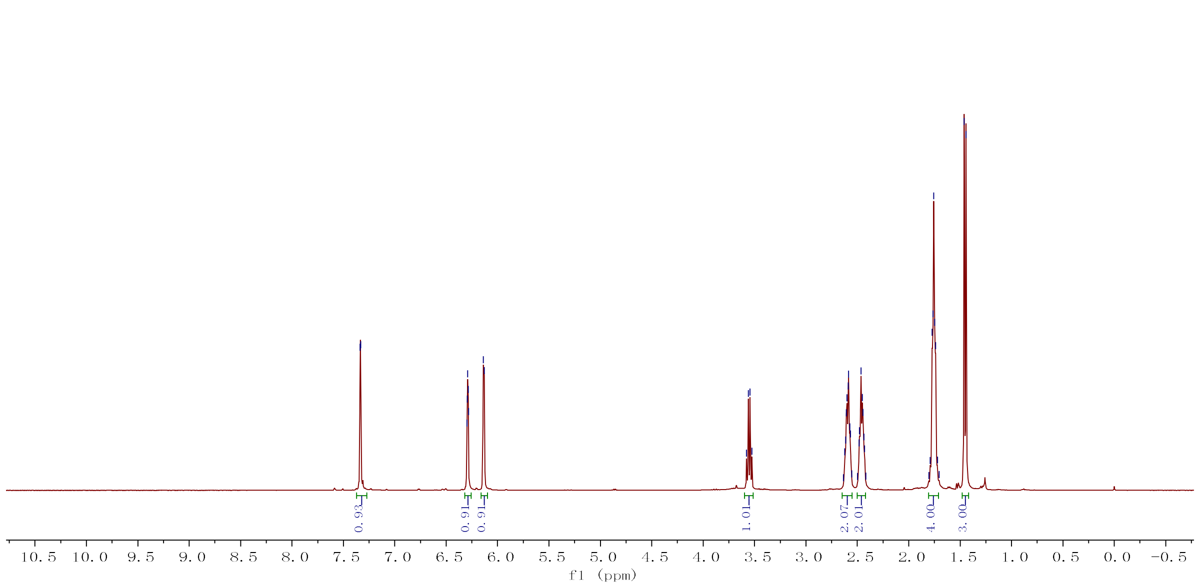


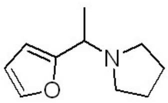
^{1}H NMR of 85
(400 MHz, Chloroform-*d*)



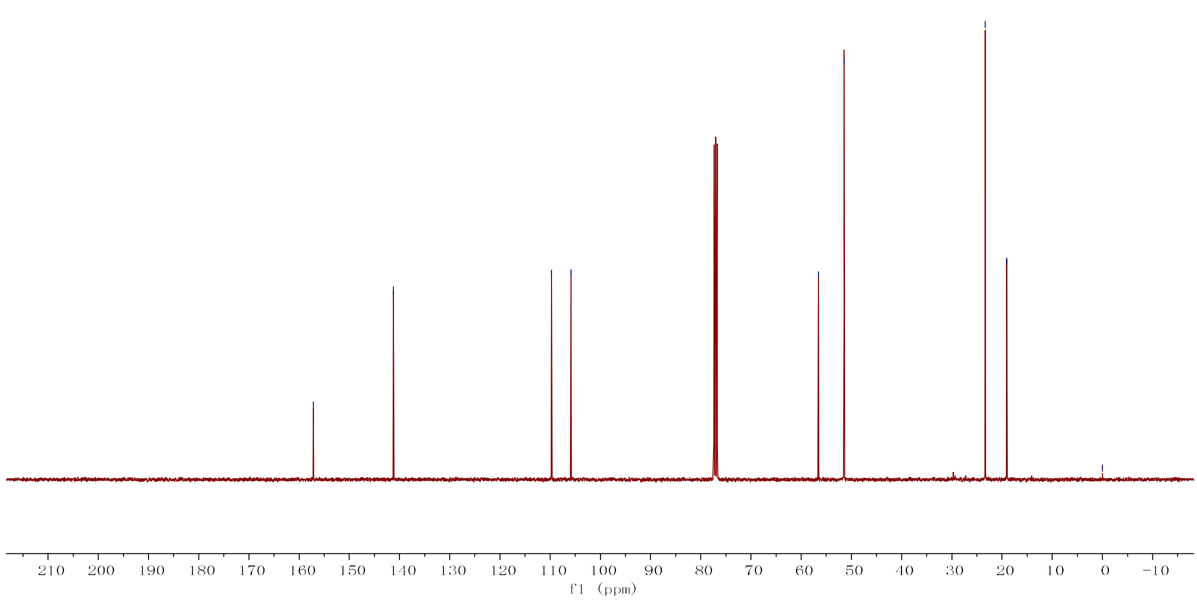


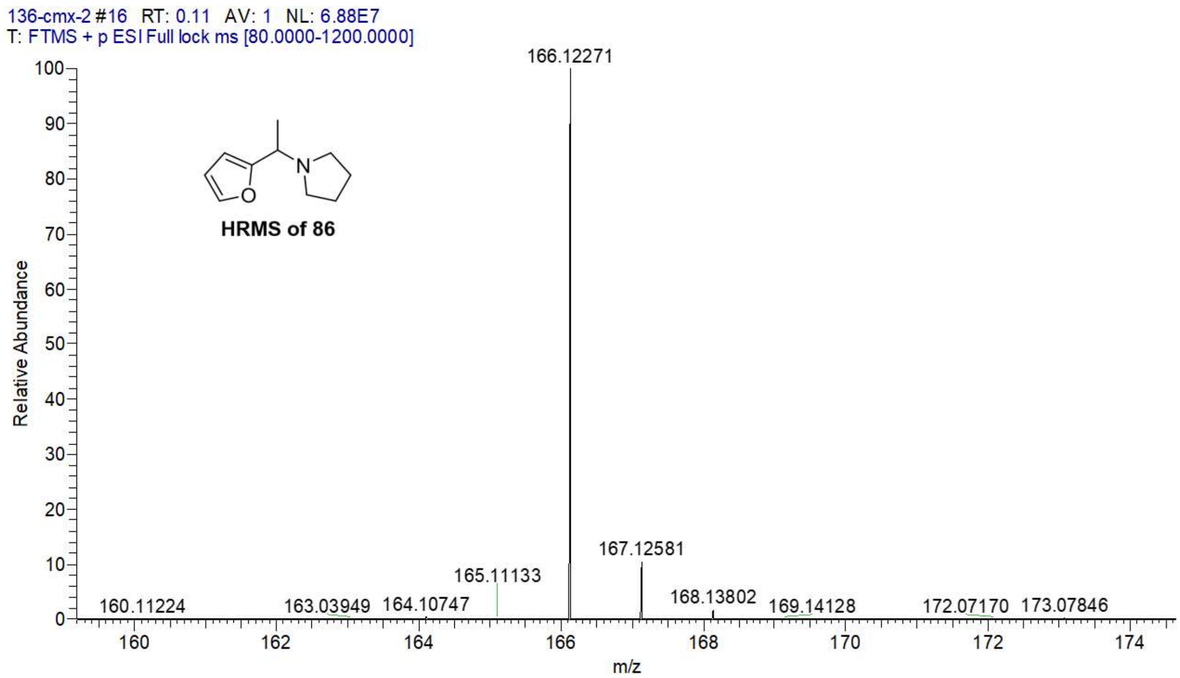
^{1}H NMR of 86
(400 MHz, Chloroform-*d*)

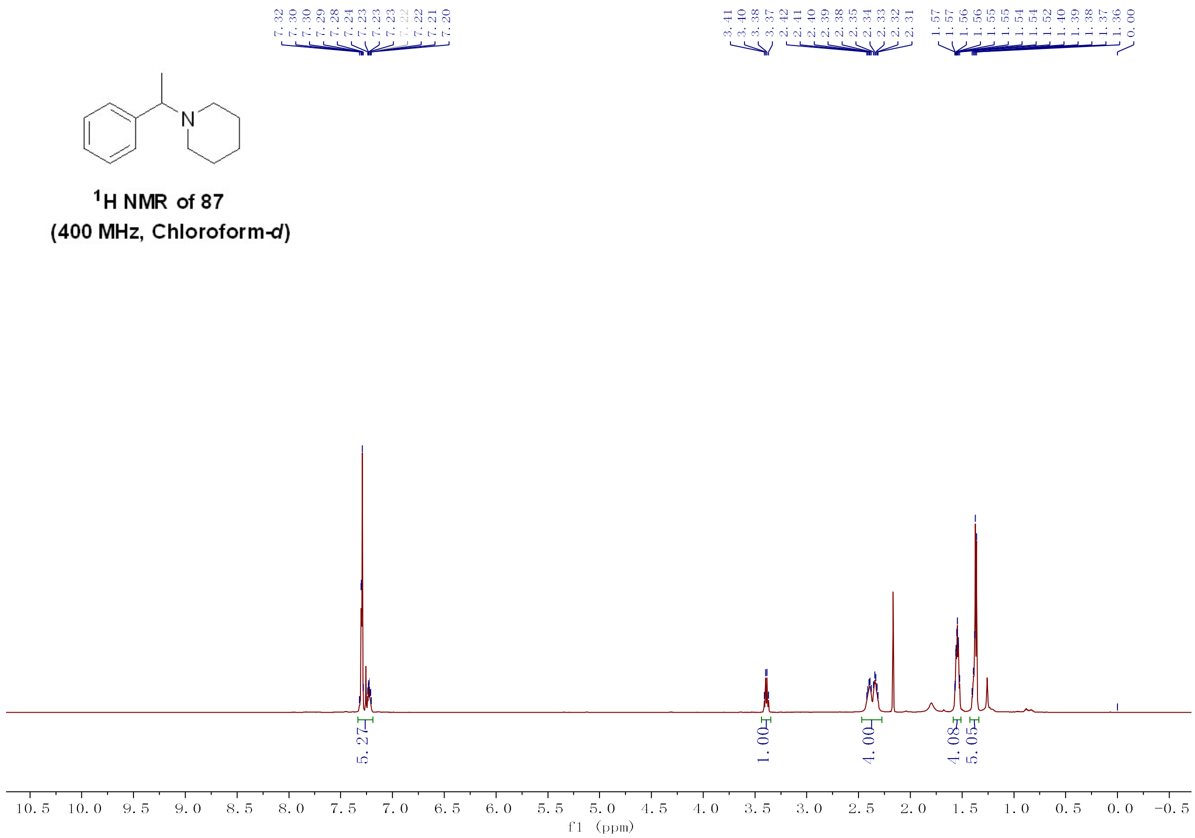


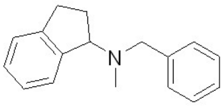


^{13}C NMR of 86
(101 MHz, Chloroform-*d*)

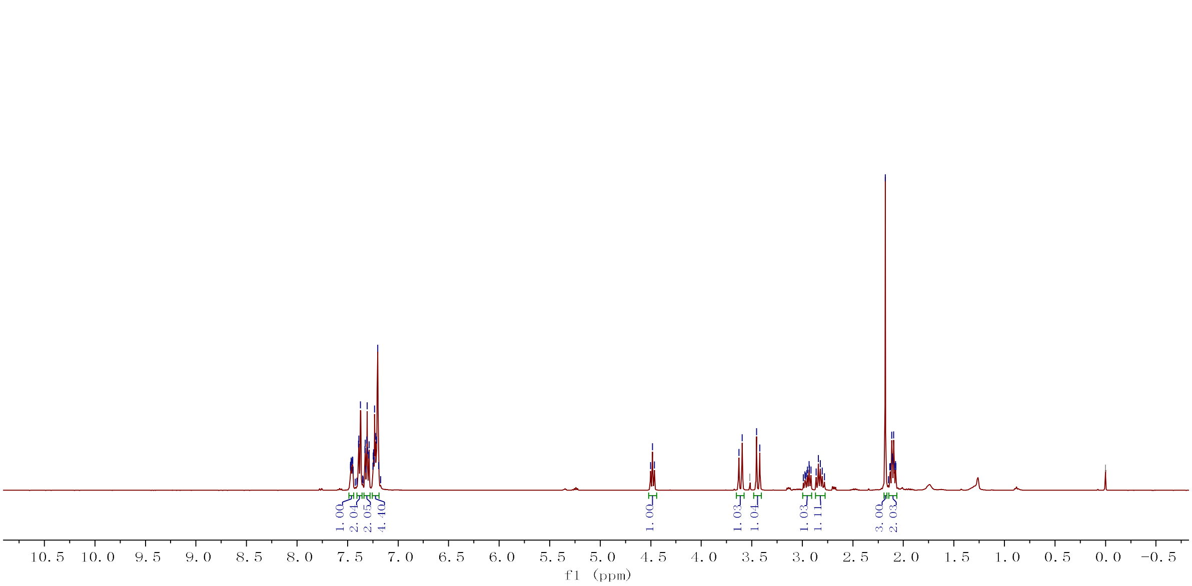


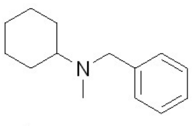

136-cmx-2 #16 RT: 0.11 AV: 1 NL: 6.88E7
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]
HRMS of 86
Relative Abundance
m/z
166.12271
167.12581
165.11133
168.13802
160.11224
163.03949
164.10747
169.14128
172.07170
173.07846


7.32 7.30 7.30 7.29 7.28 7.24 7.23 7.23 7.23 7.22 7.22 7.21 7.20
3.41 3.40 3.38 3.37 2.42 2.41 2.40 2.39 2.38 2.35 2.34 2.33 2.32 2.31 1.57 1.57 1.56 1.56 1.55 1.54 1.54 1.52 1.40 1.39 1.38 1.37 1.36 0.00
1H NMR of 87
(400 MHz, Chloroform-d)
5.27
1.00
4.00
4.08
5.05
f1 (ppm)

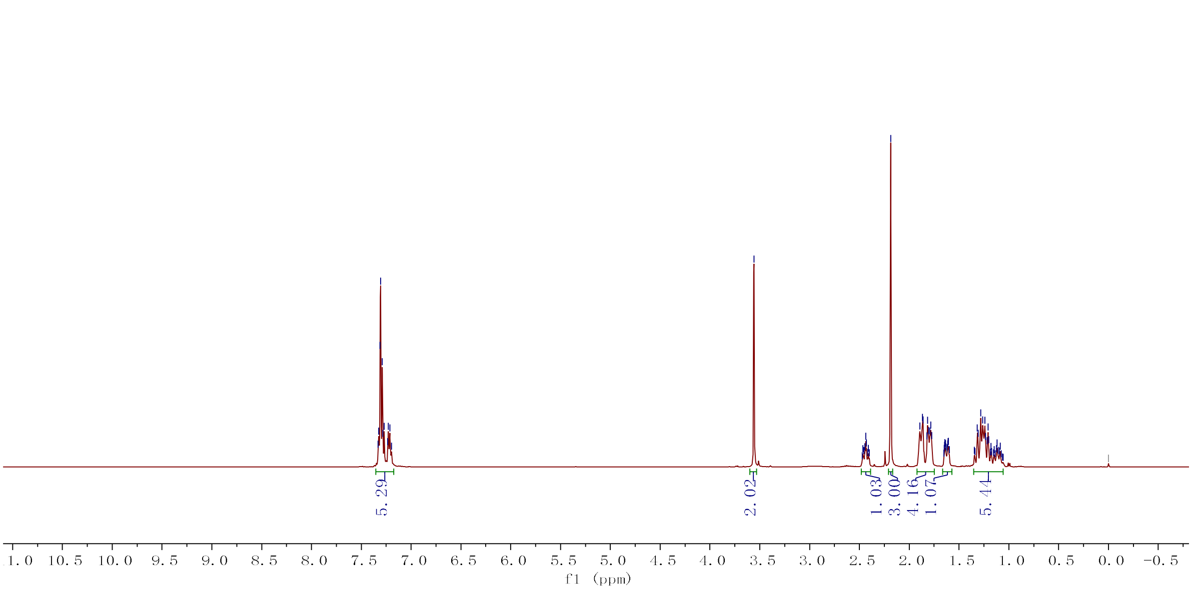


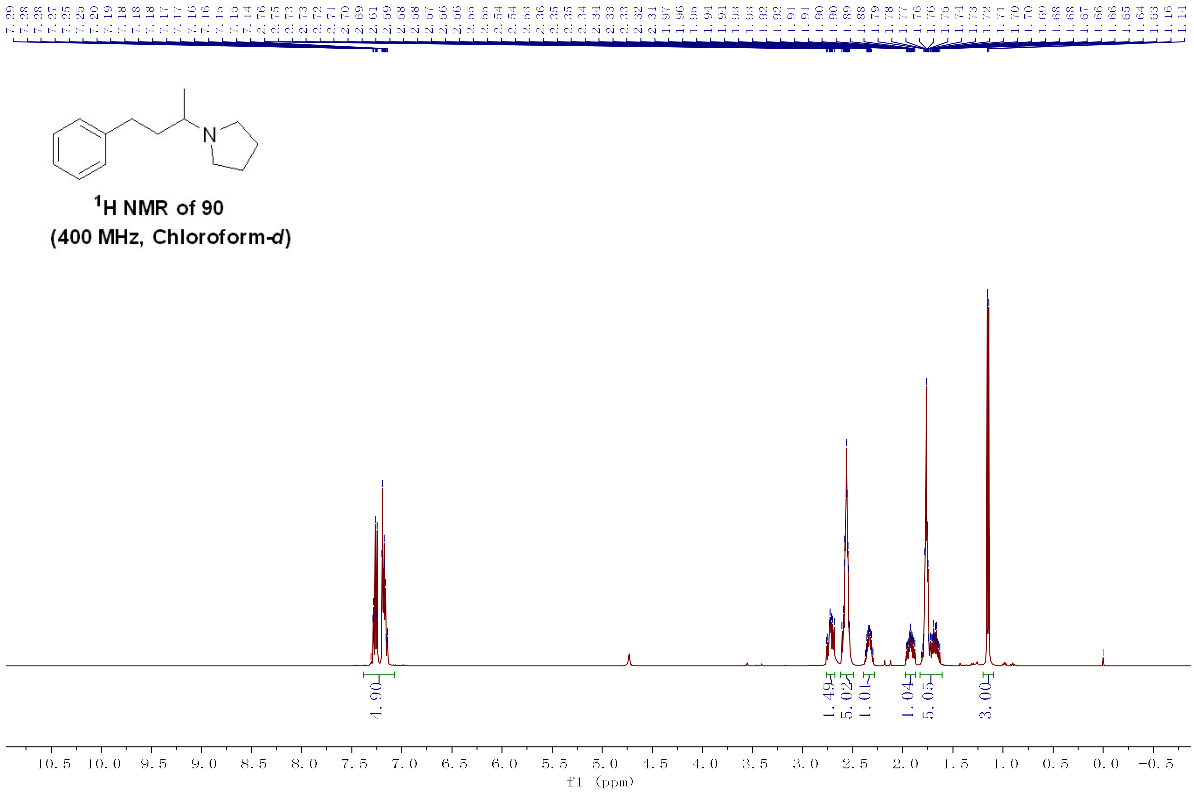
^{1}H NMR of 88
(400 MHz, Chloroform-*d*)



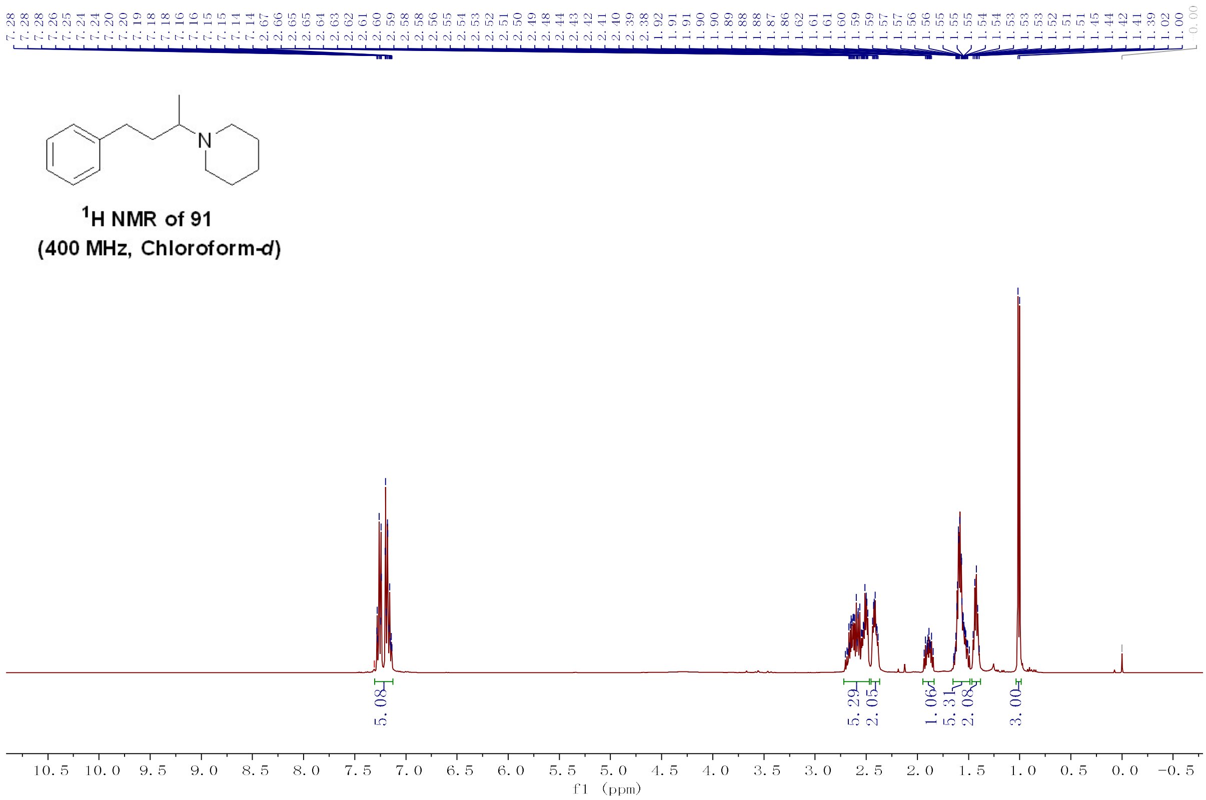


^{1}H NMR of 89
(400 MHz, Chloroform-*d*)

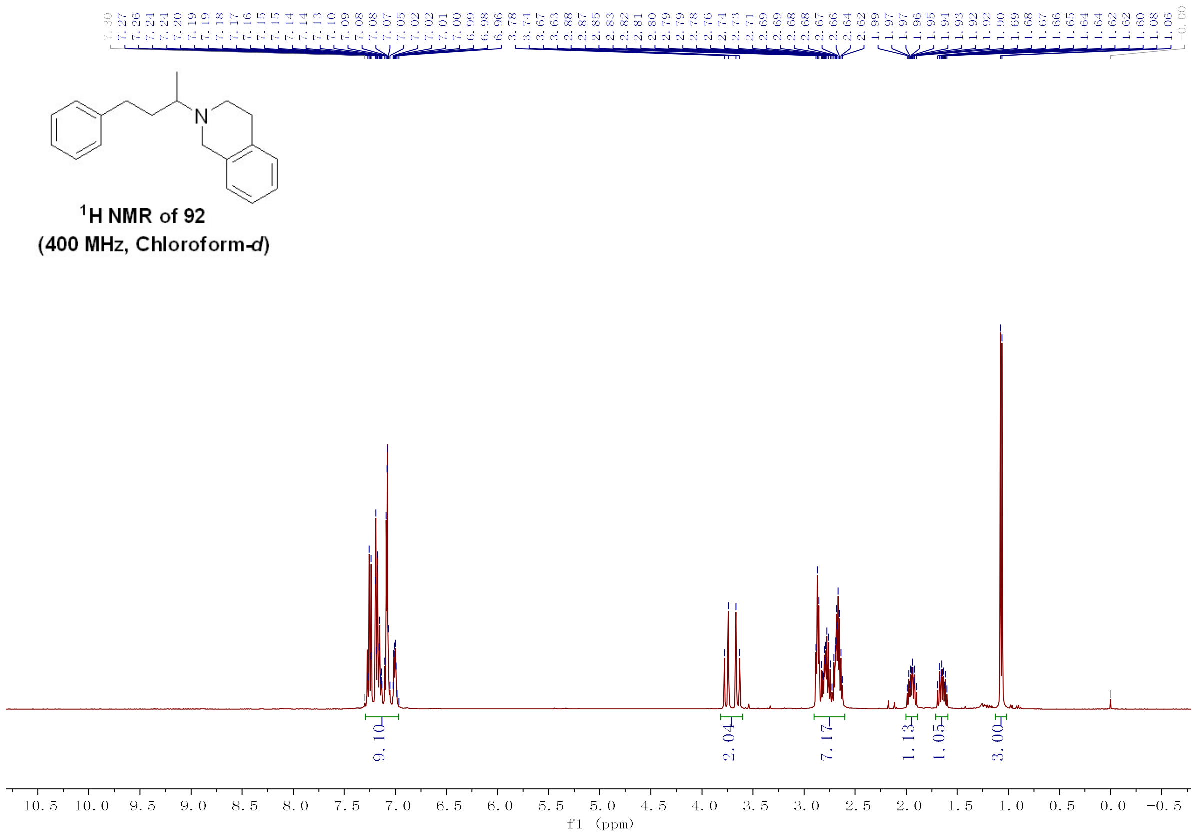




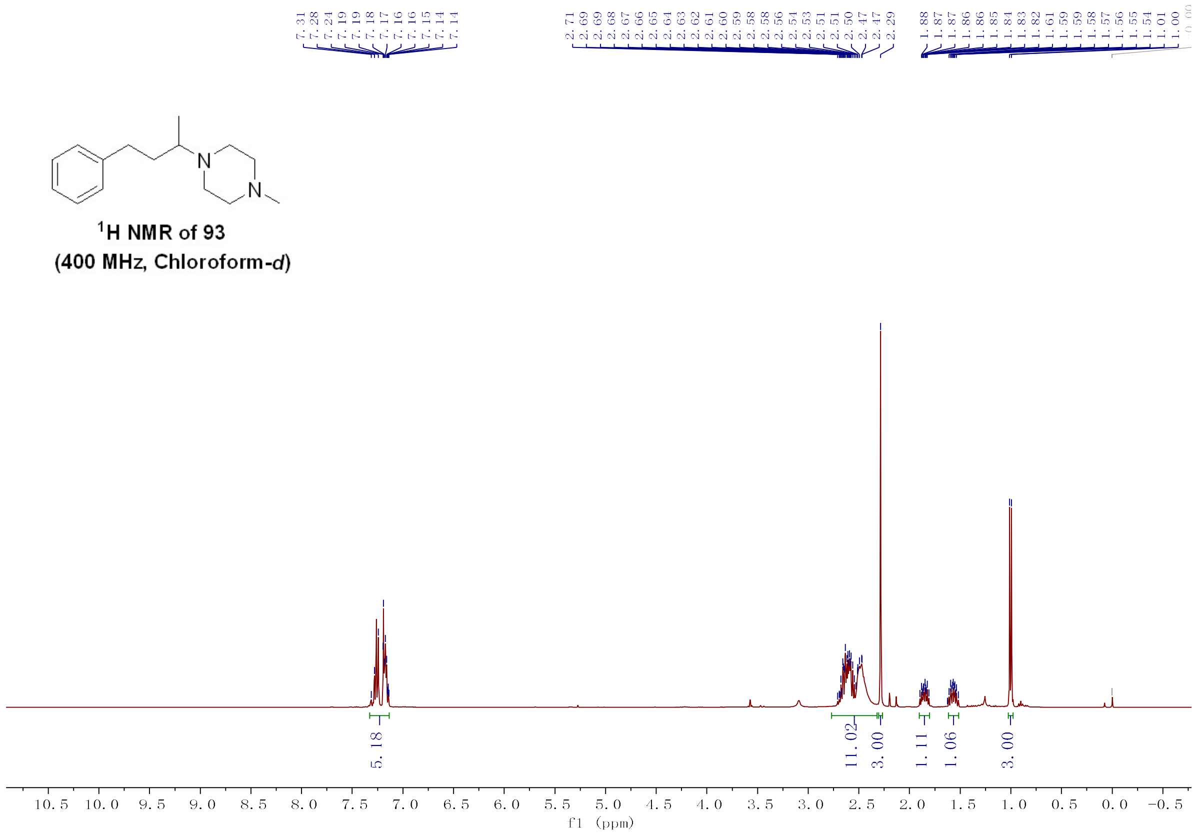
[1]H NMR of 90
(400 MHz, Chloroform-*d*)



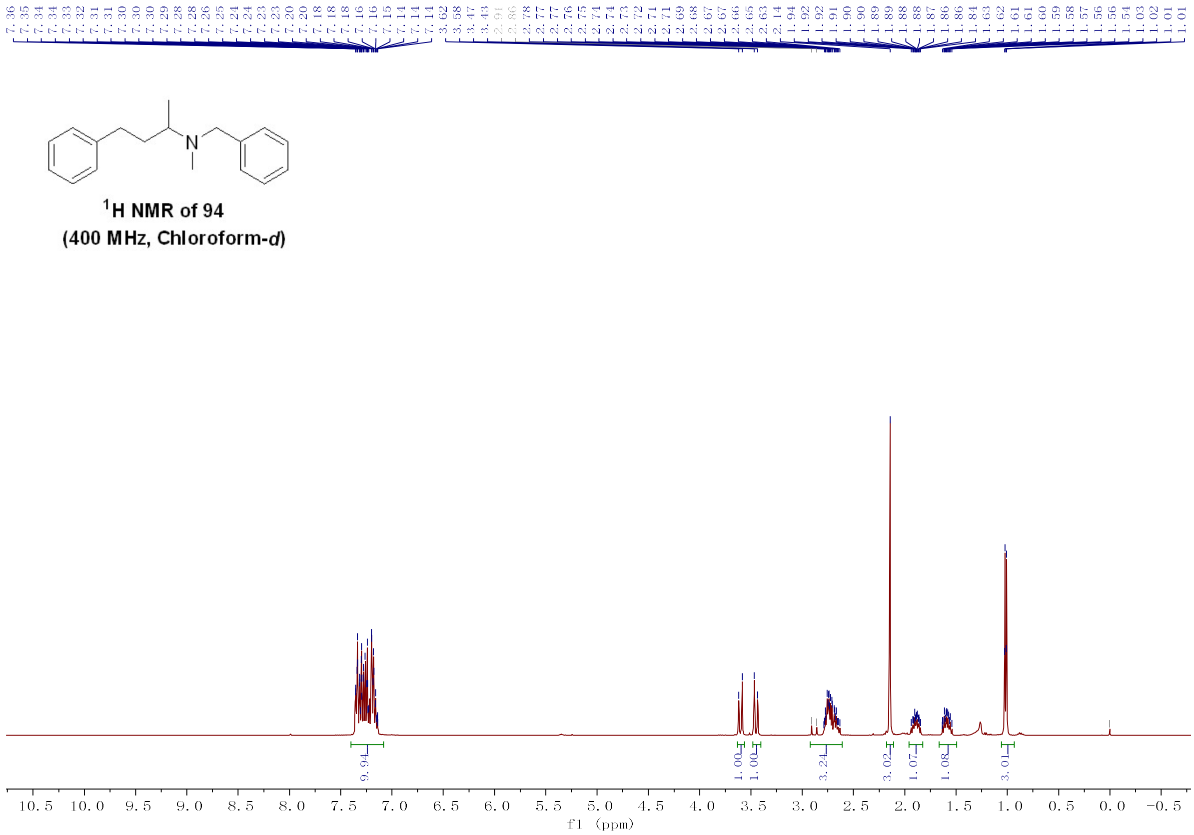
[1]H NMR of 91
(400 MHz, Chloroform-*d*)



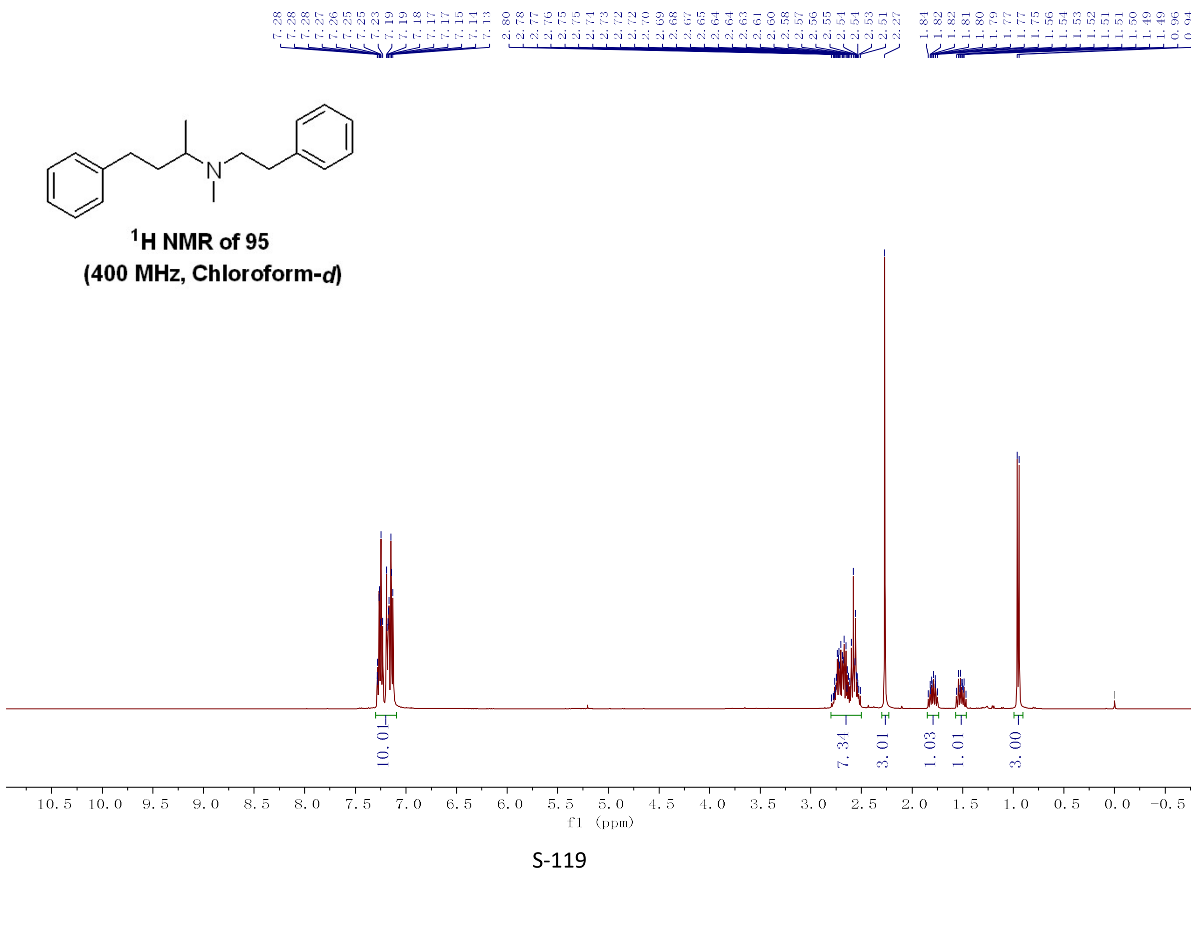
[1]H NMR of 92
(400 MHz, Chloroform-*d*)



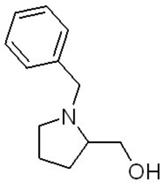
[1]H NMR of 93
(400 MHz, Chloroform-*d*)



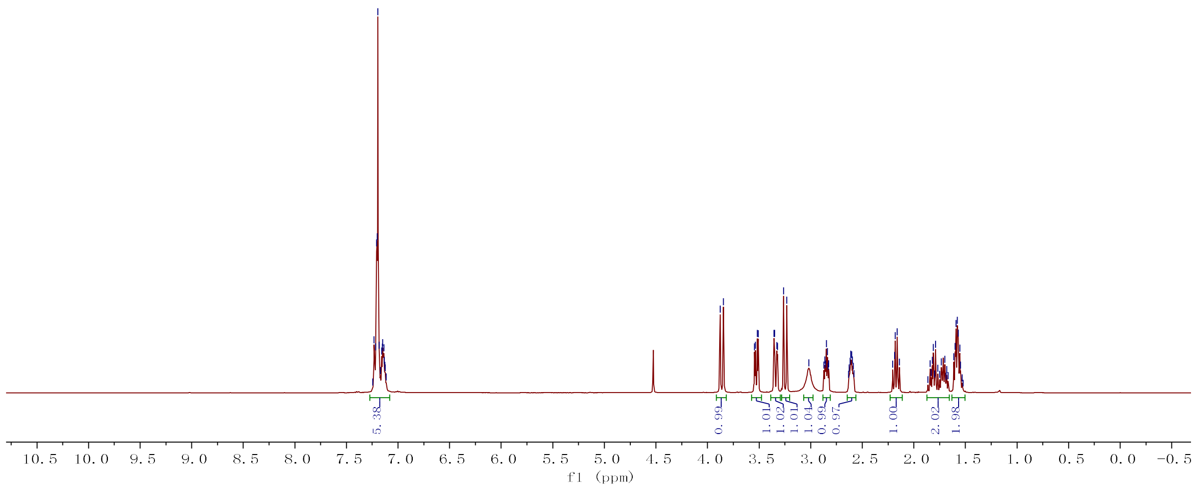
^{1}H NMR of 94
(400 MHz, Chloroform-*d*)

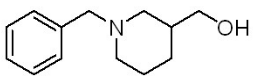


^{1}H NMR of 95
(400 MHz, Chloroform-*d*)

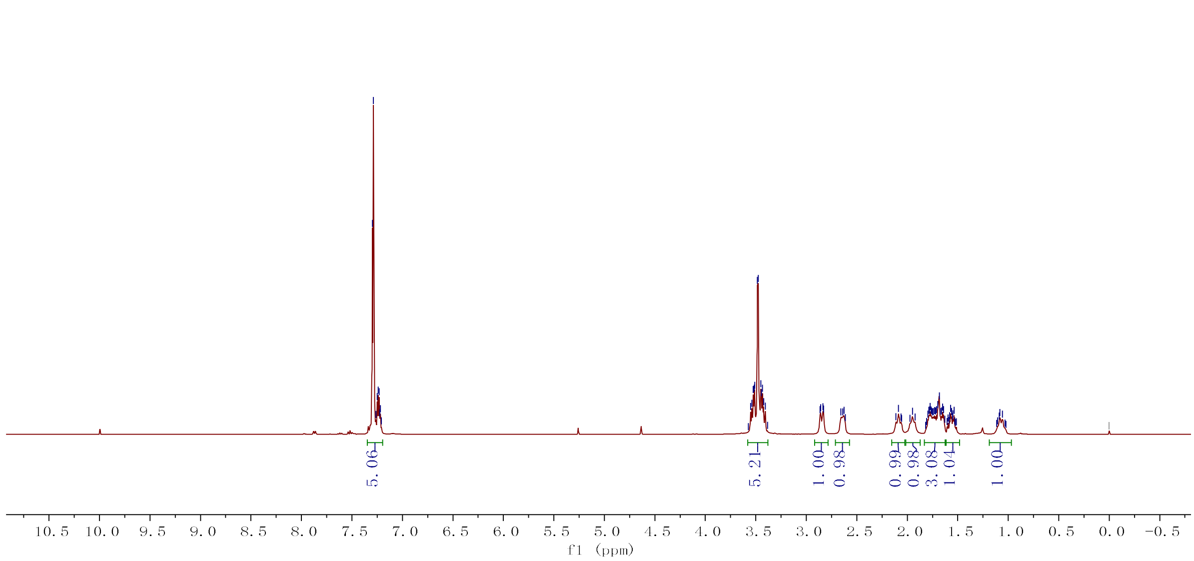


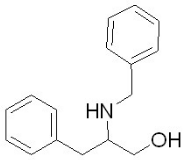
^{1}H NMR of 96
(400 MHz, Chloroform-*d*)



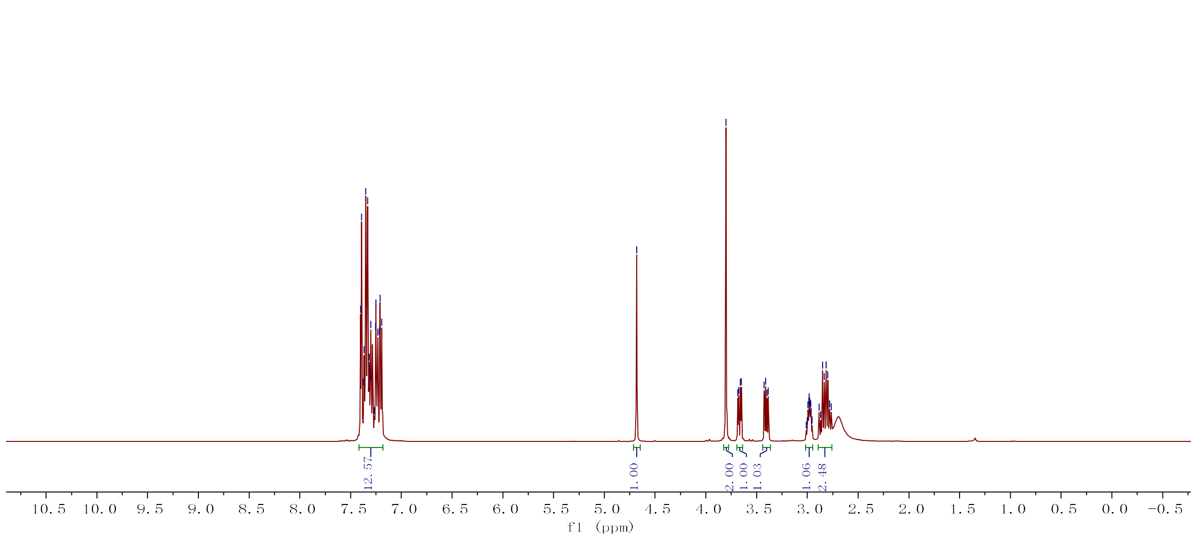


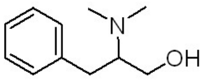
^{1}H NMR of 97
(400 MHz, Chloroform-*d*)



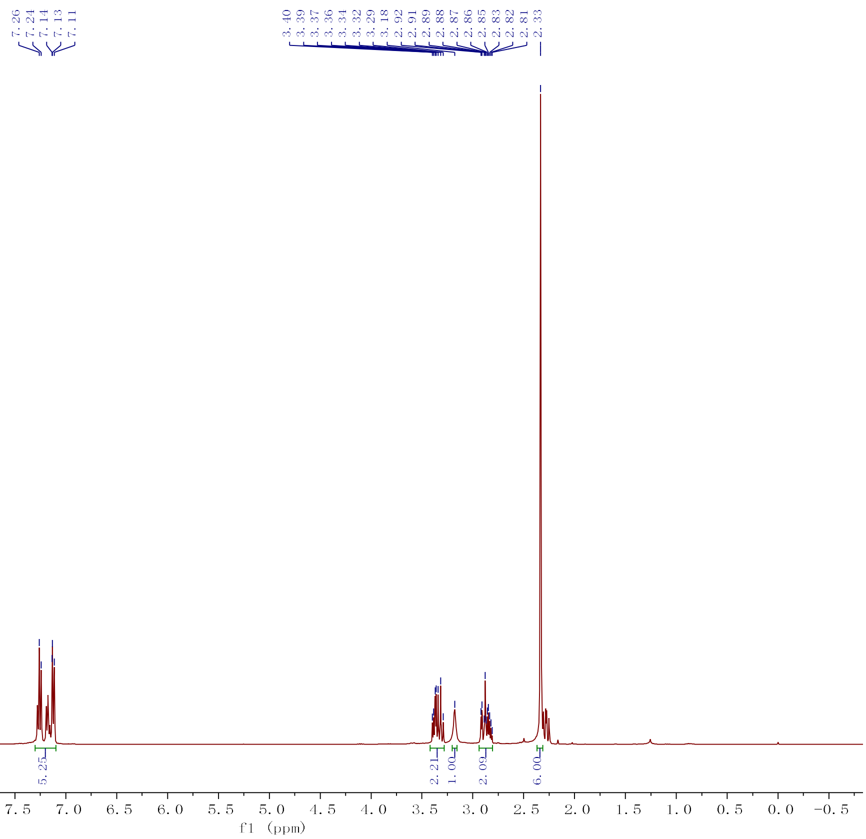


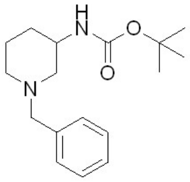
[1]H NMR of 98
(400 MHz, Chloroform-*d*)



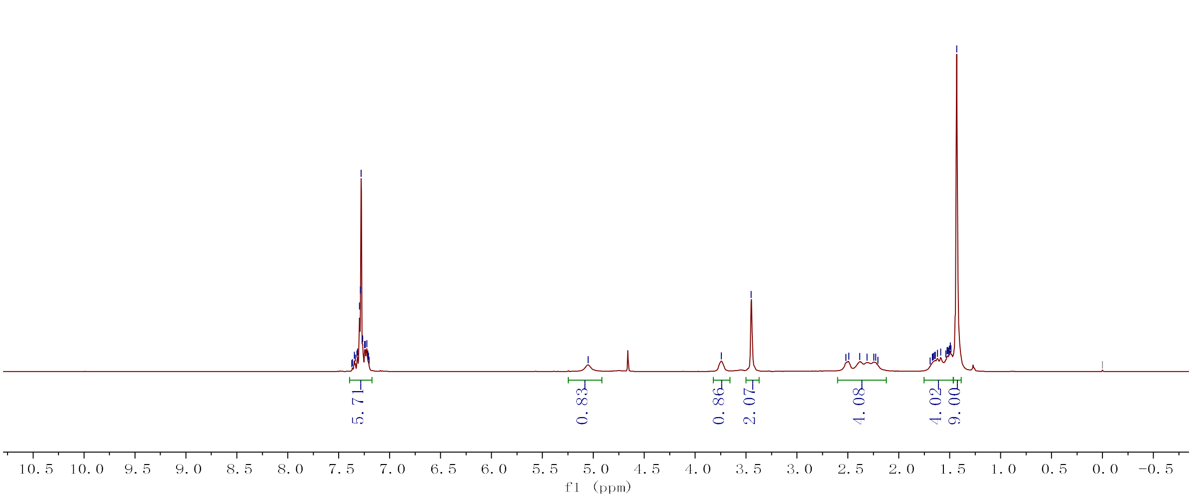


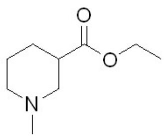
[1]H NMR of 99
(400 MHz, Chloroform-*d*)



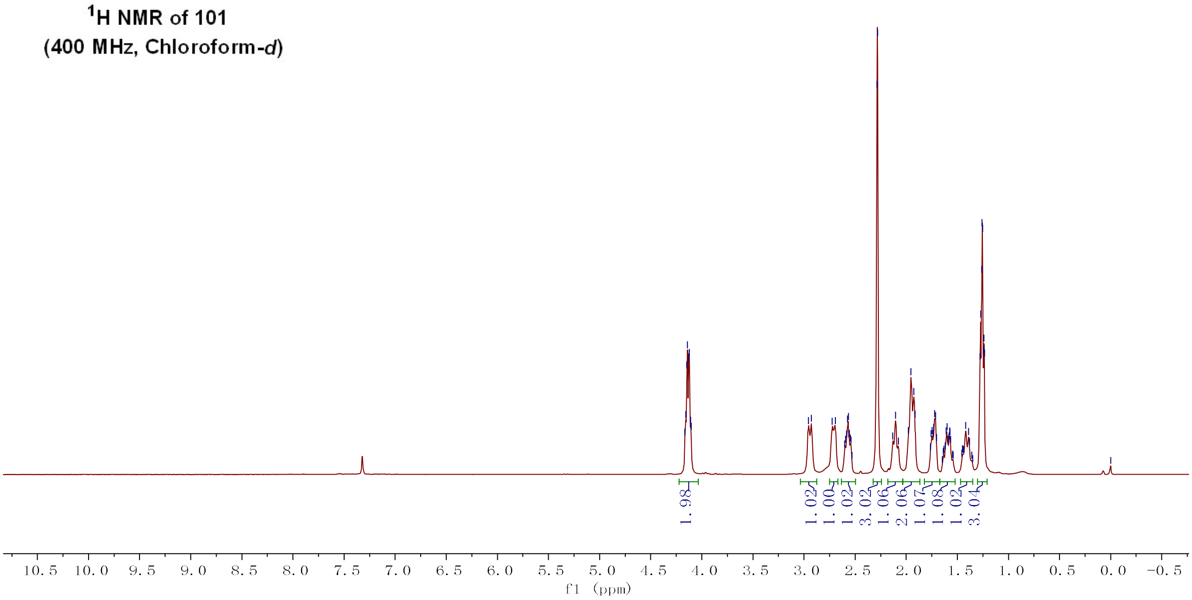


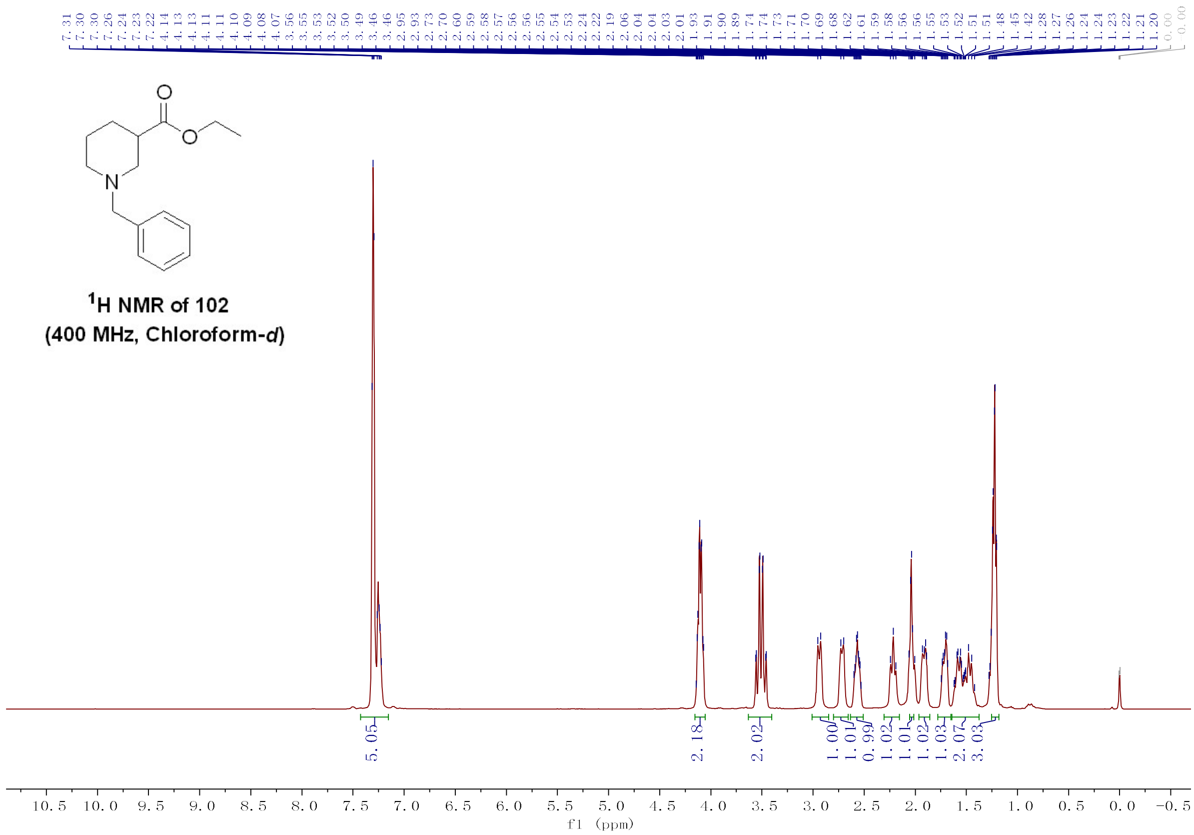
^{1}H NMR of 100
(400 MHz, Chloroform-*d*)



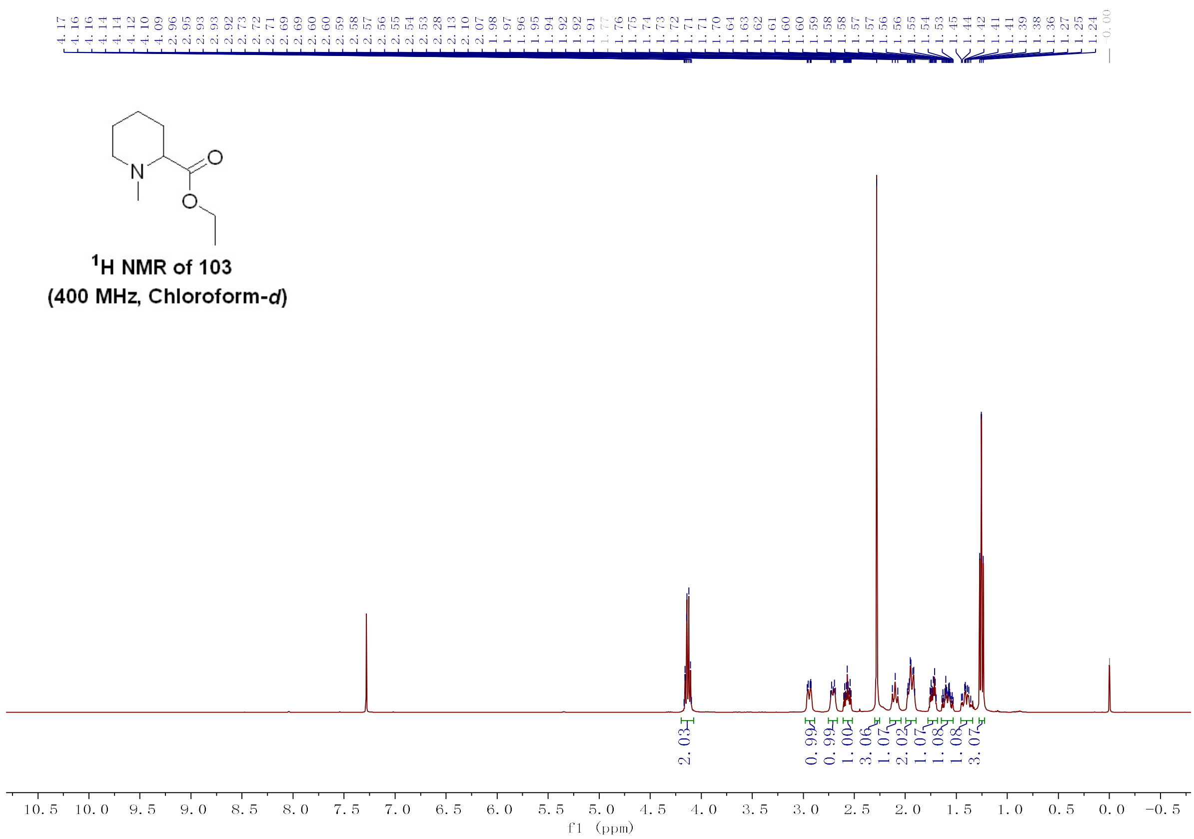


^{1}H NMR of 101
(400 MHz, Chloroform-*d*)

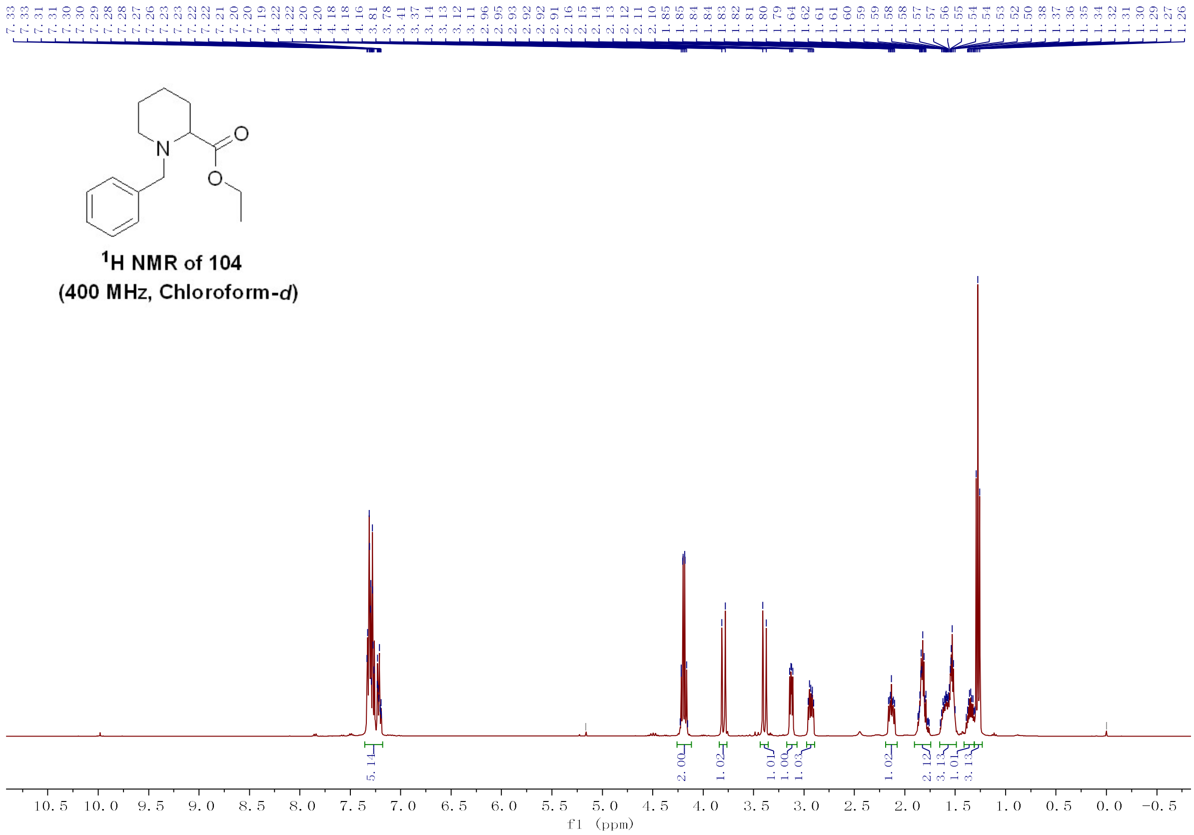




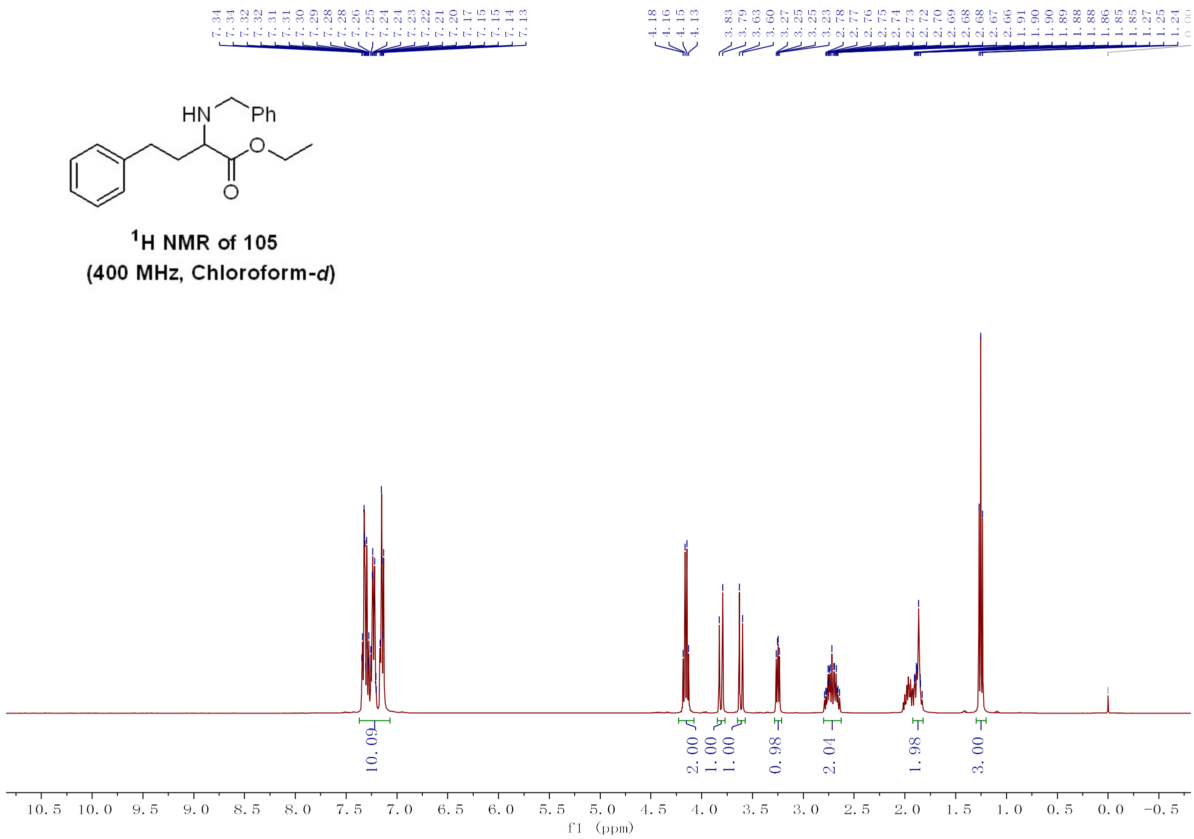
[1]H NMR of 102
(400 MHz, Chloroform-*d*)



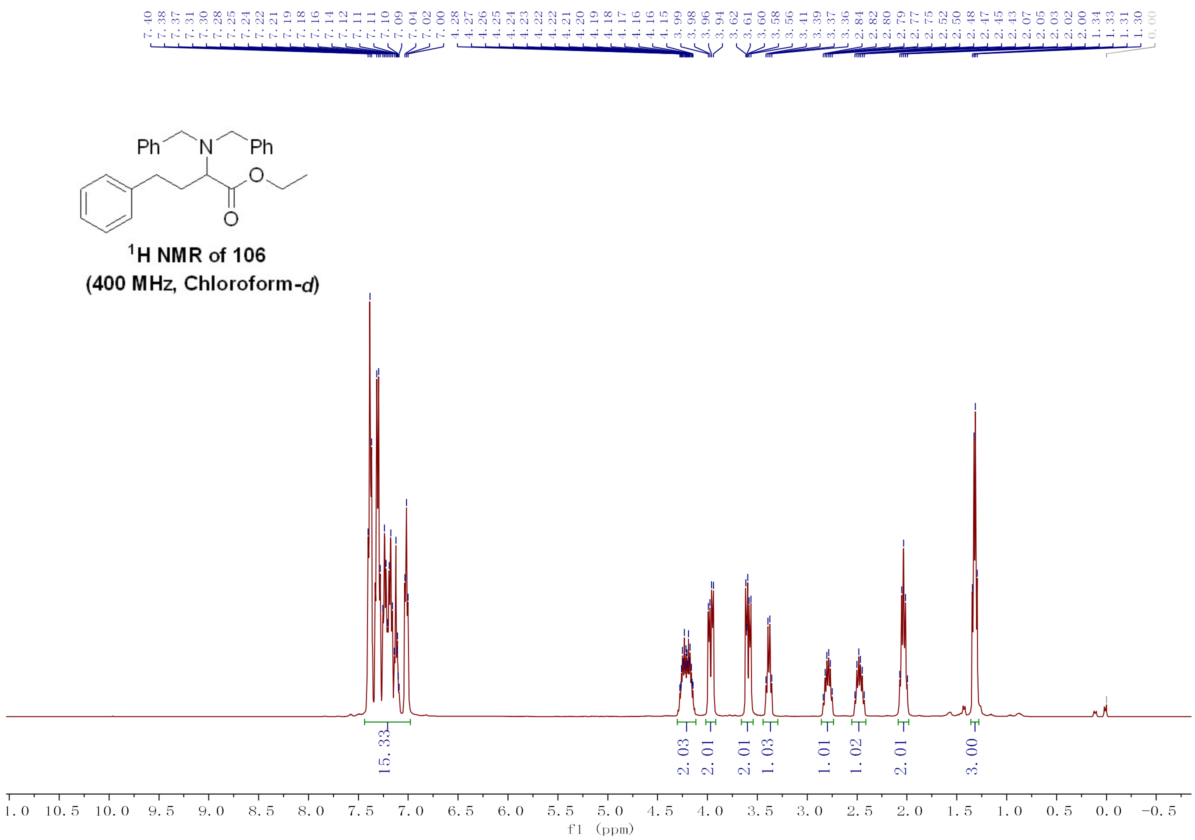
[1]H NMR of 103
(400 MHz, Chloroform-*d*)

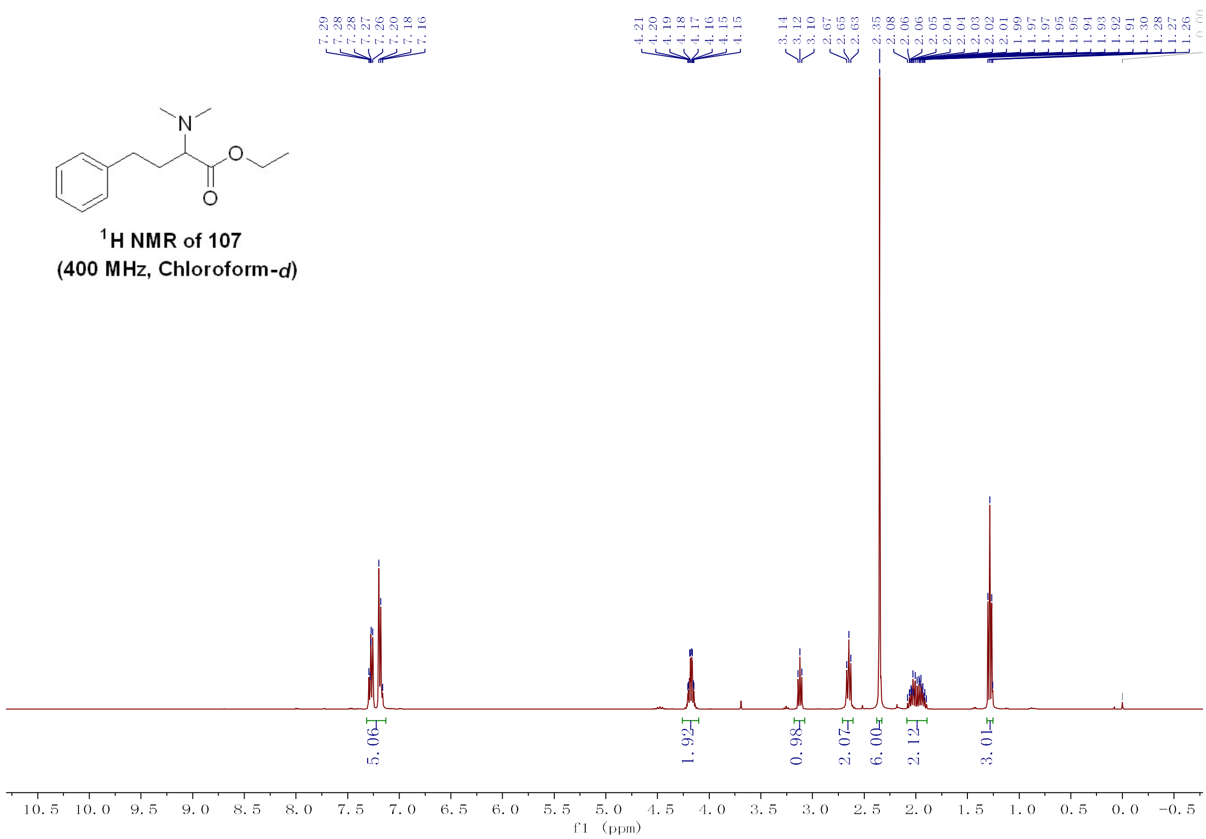


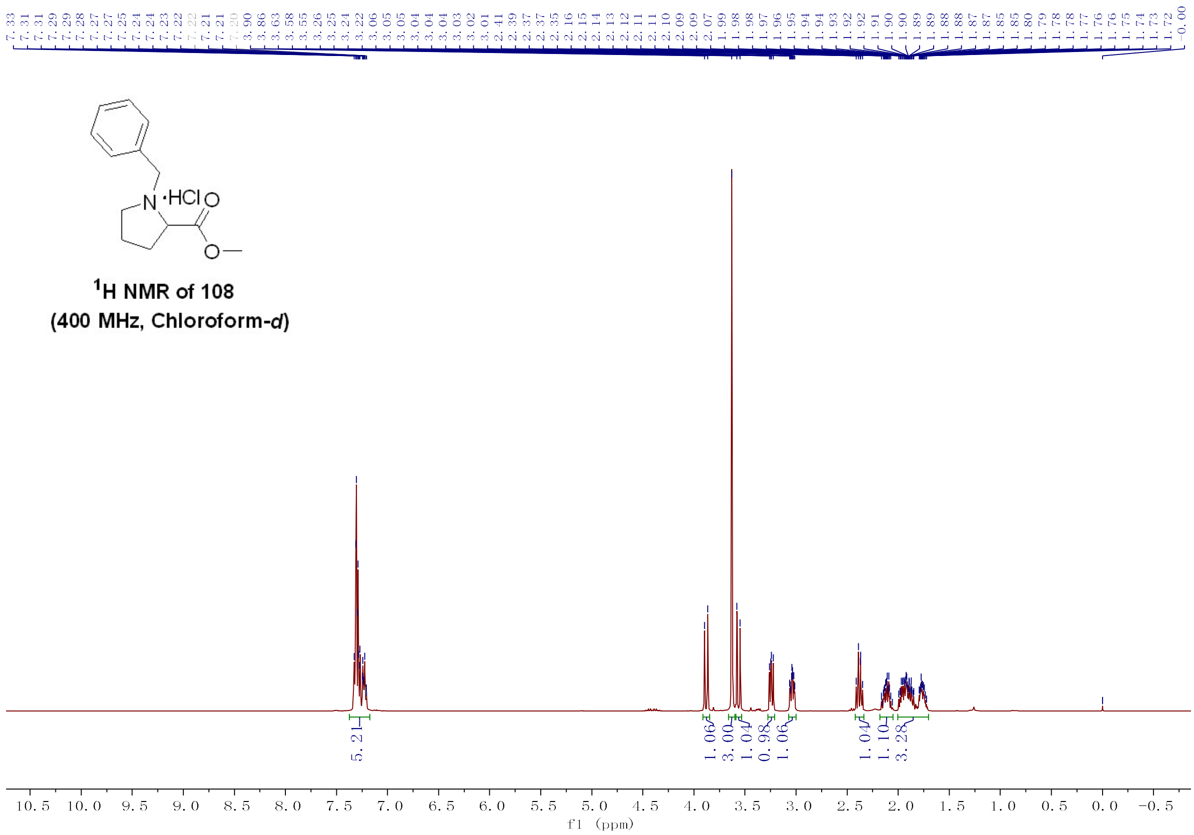
^{1}H NMR of 104
(400 MHz, Chloroform-*d*)



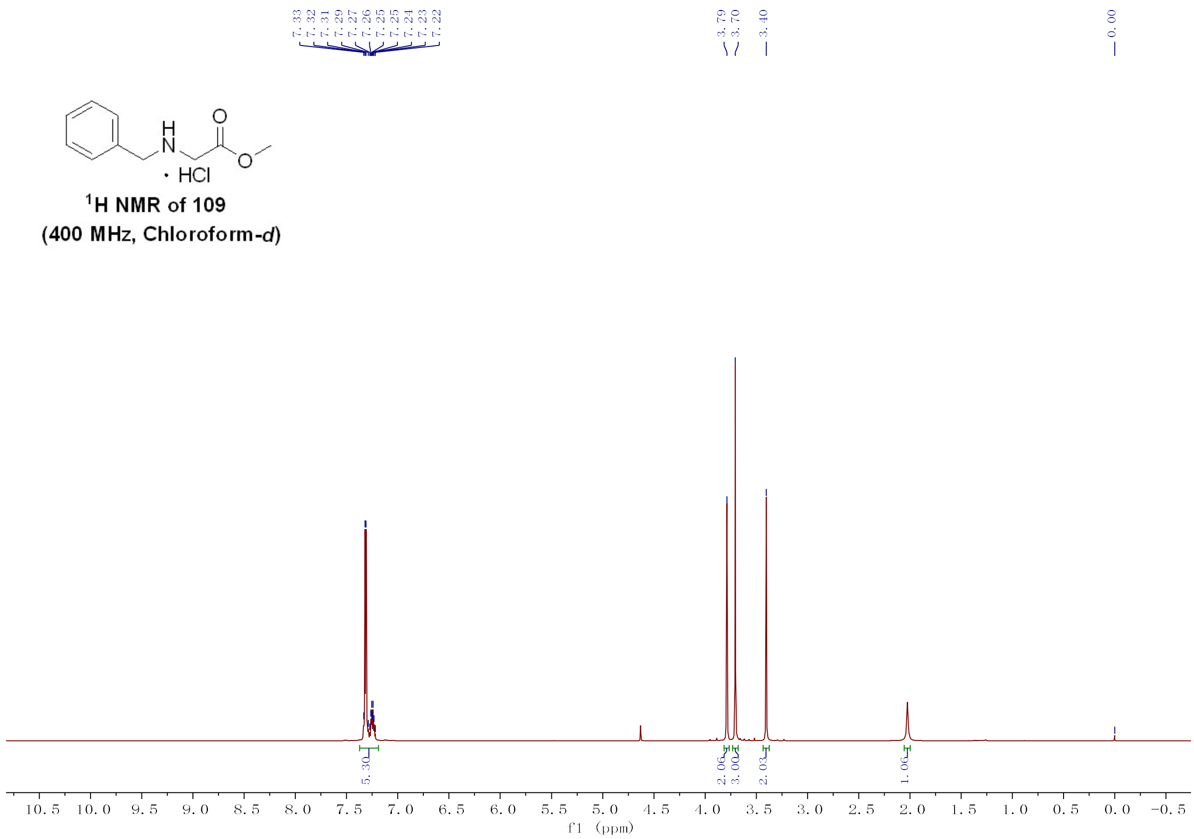
^{1}H NMR of 105
(400 MHz, Chloroform-*d*)


Ph N Ph
O
O
1H NMR of 106
(400 MHz, Chloroform-d)
15.33
2.03
2.01
2.01
1.03
1.01
1.02
2.01
3.00
f1 (ppm)

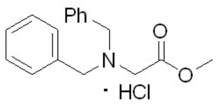

N
O
O
1H NMR of 107
(400 MHz, Chloroform-d)
5.06
1.92
0.98
2.07
6.00
2.12
3.01
f1 (ppm)



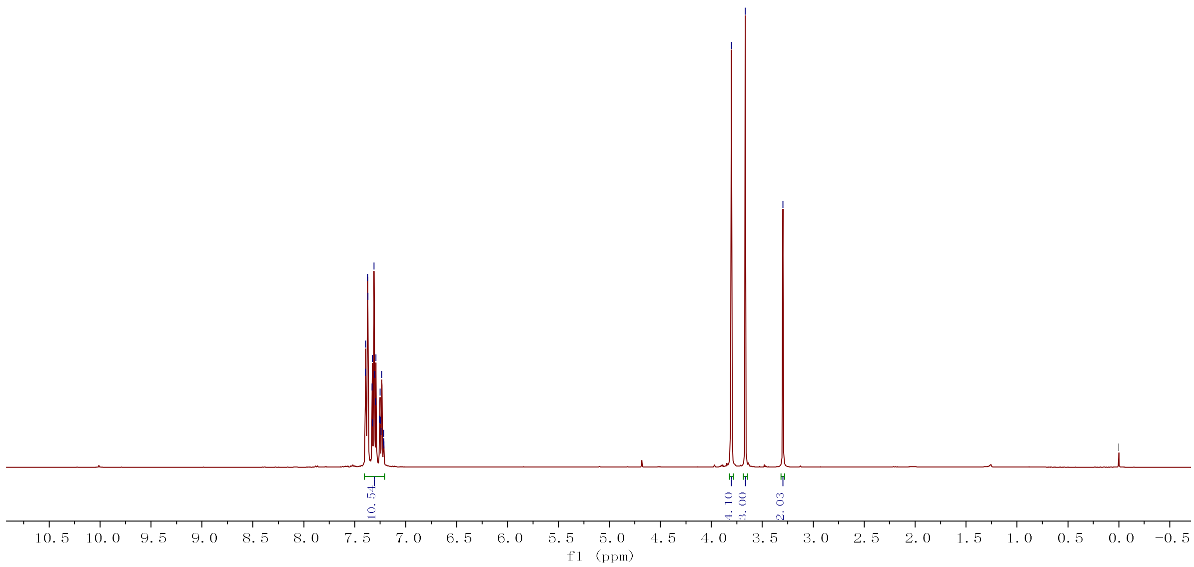
[1]H NMR of 108
(400 MHz, Chloroform-*d*)

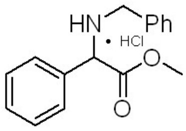


[1]H NMR of 109
(400 MHz, Chloroform-*d*)

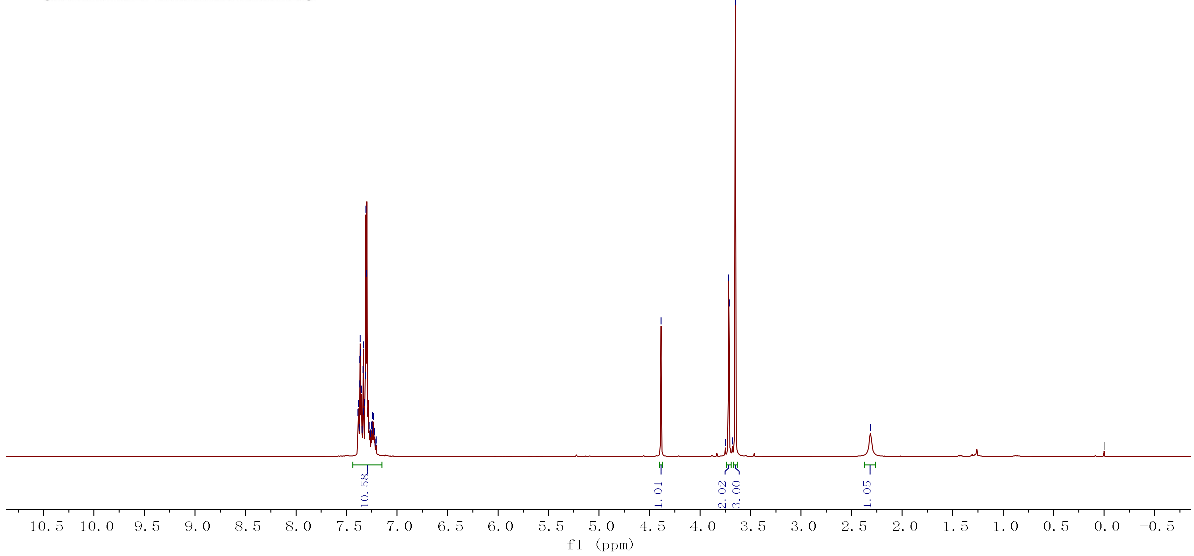


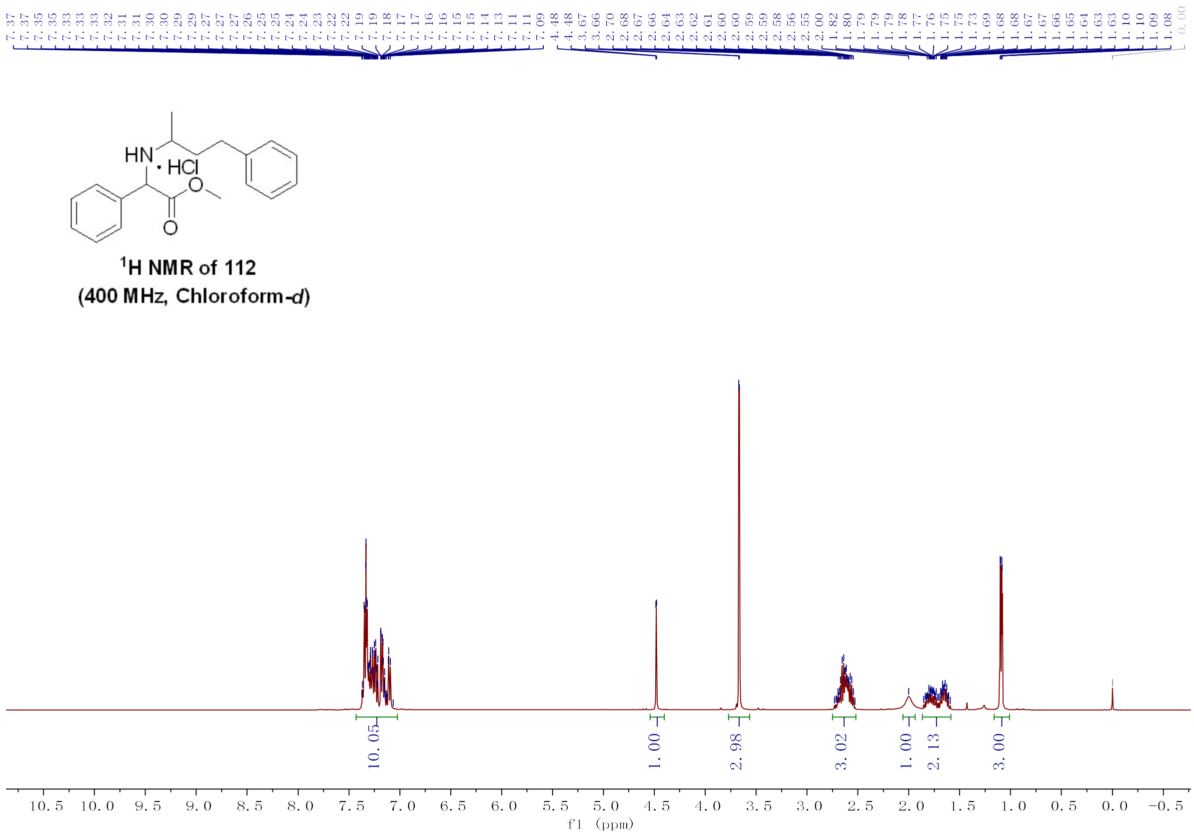
^{1}H NMR of 110
(400 MHz, Chloroform-*d*)



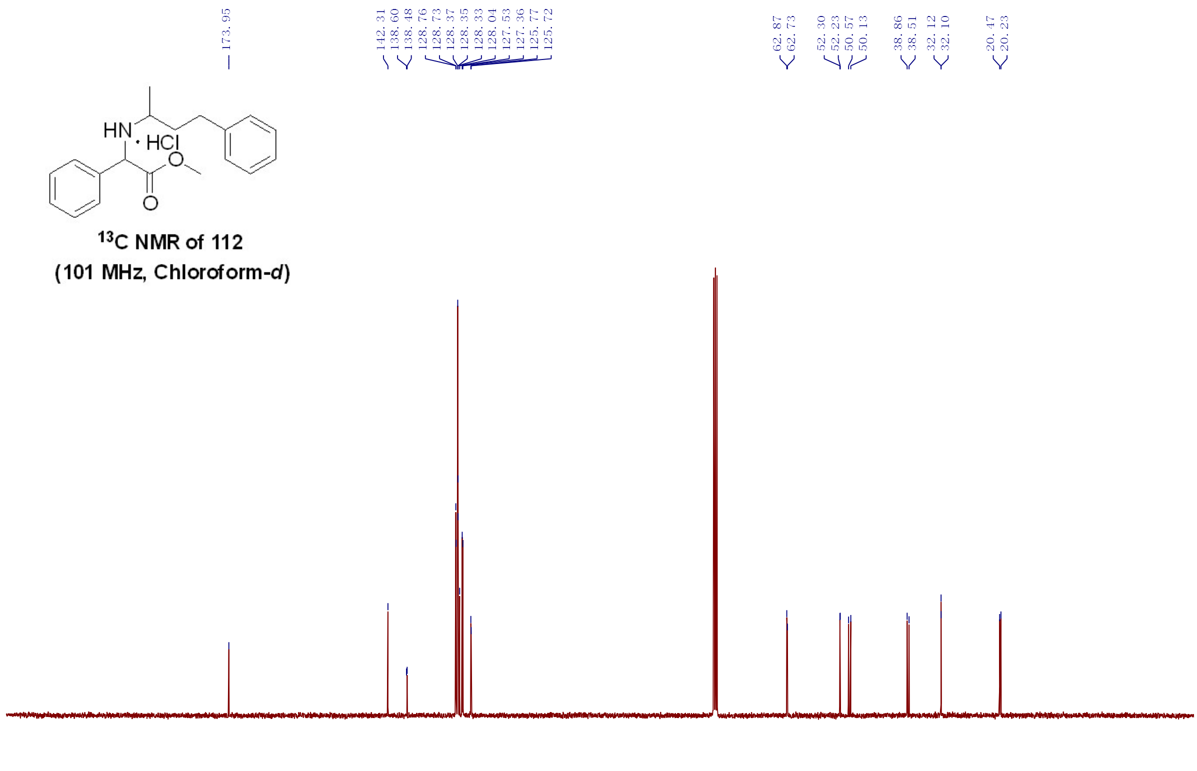


^{1}H NMR of 111
(400 MHz, Chloroform-*d*)

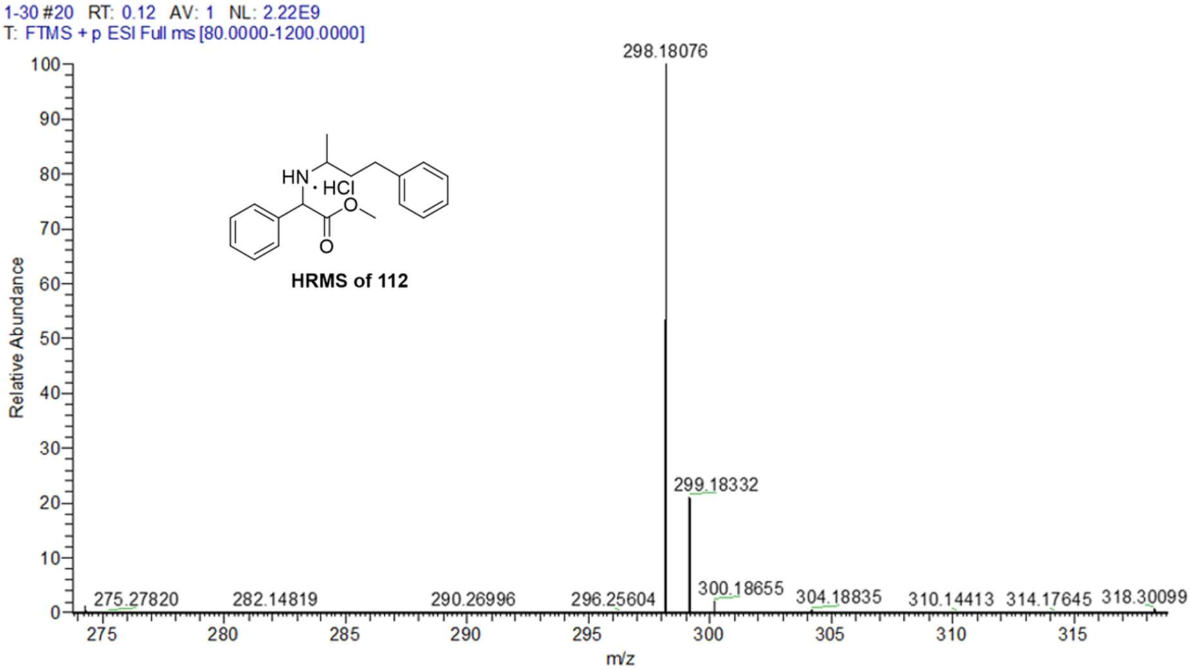


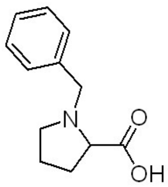


^{1}H NMR of 112
(400 MHz, Chloroform-*d*)

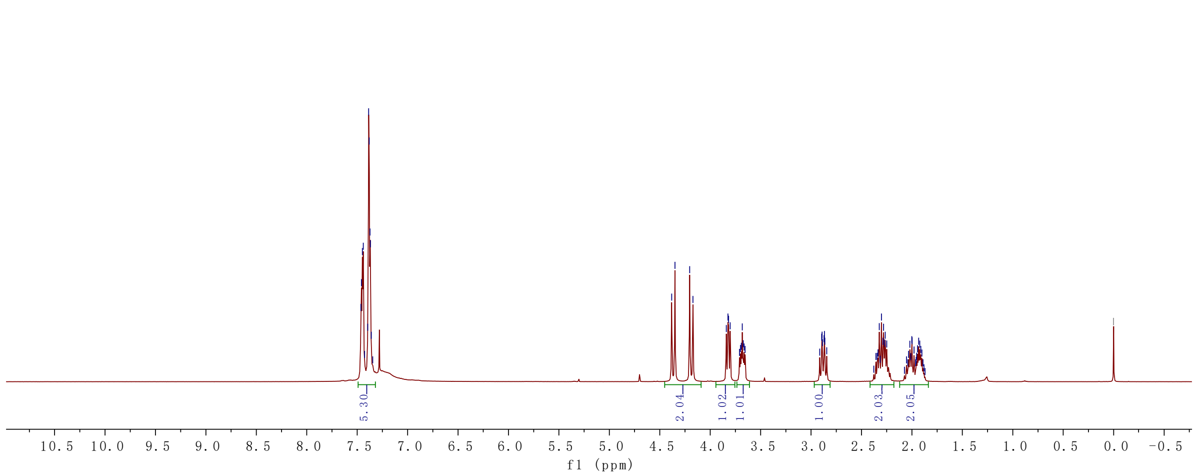


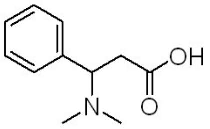
^{13}C NMR of 112
(101 MHz, Chloroform-*d*)



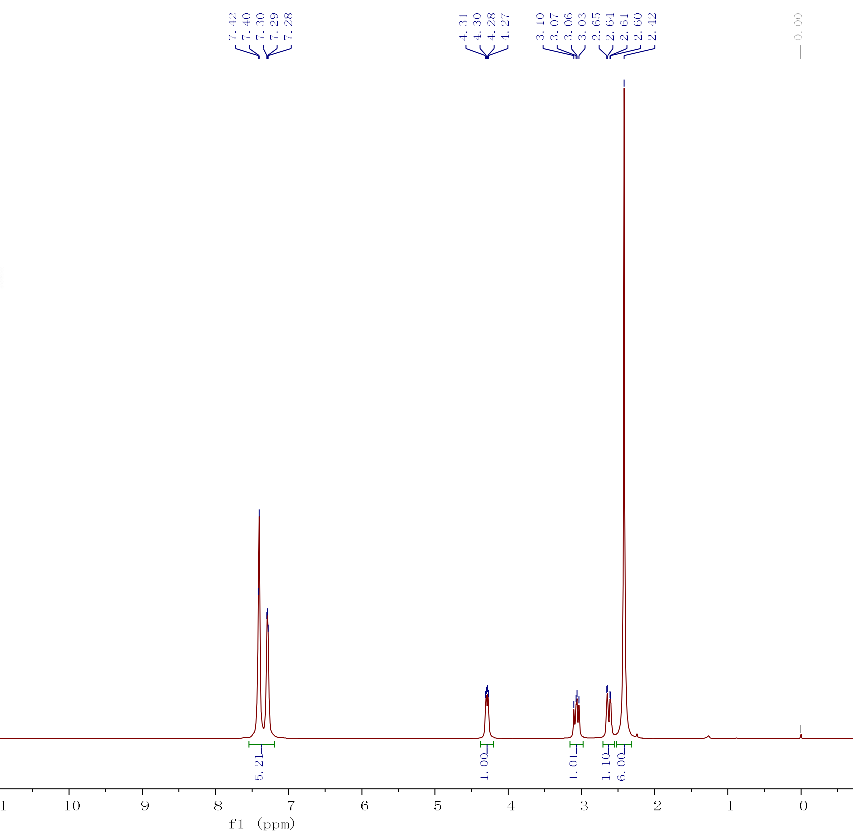


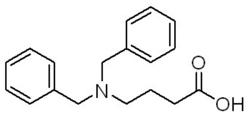
^{1}H NMR of 113
(400 MHz, Chloroform-*d*)



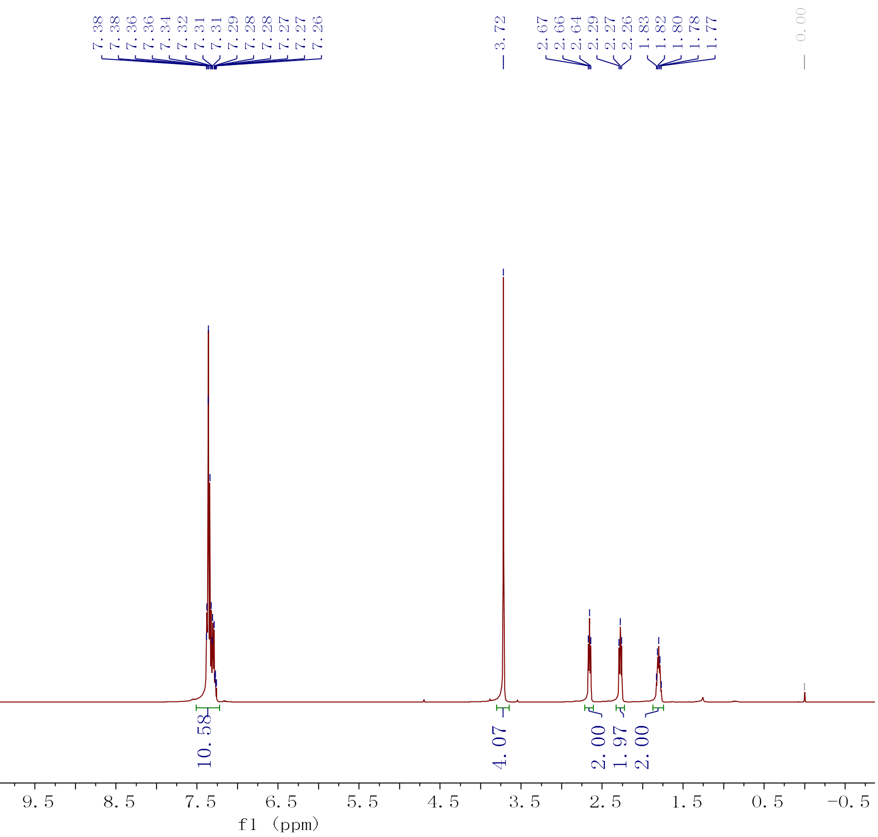


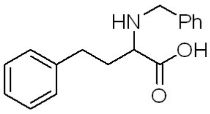
^{1}H NMR of 114
(400 MHz, Chloroform-*d*)



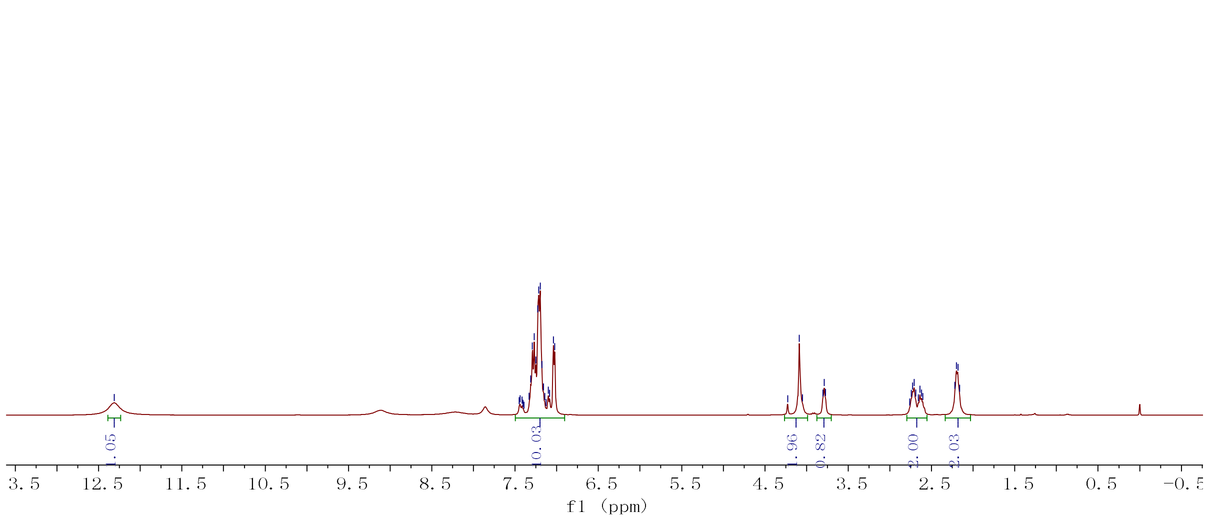


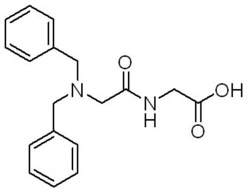
^{1}H NMR of 115
(400 MHz, Chloroform-*d*)



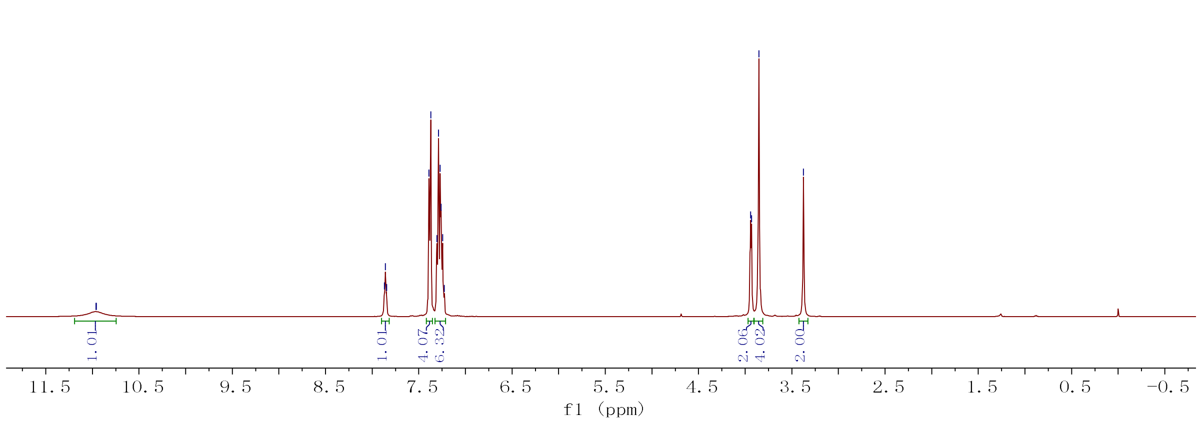


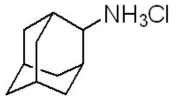
^{1}H NMR of 116
(400 MHz, Chloroform-*d*)

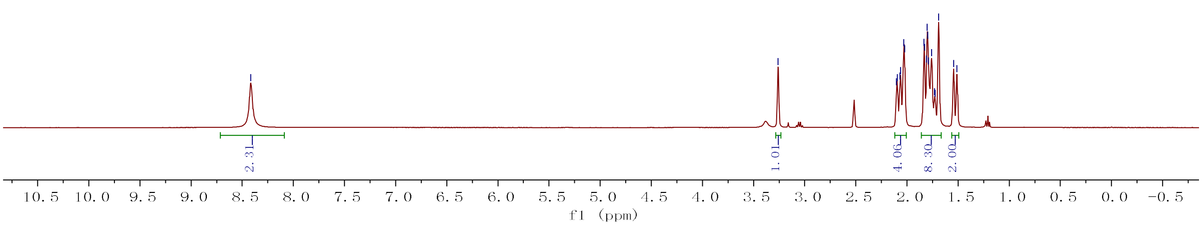




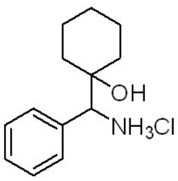
^{1}H NMR of 117
(400 MHz, Chloroform-*d*)

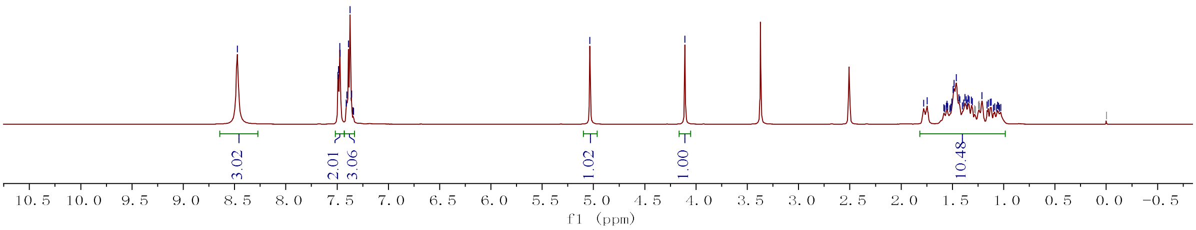




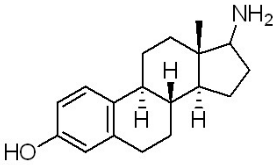


^{1}H NMR of 120
(400 MHz, DMSO-d_6)

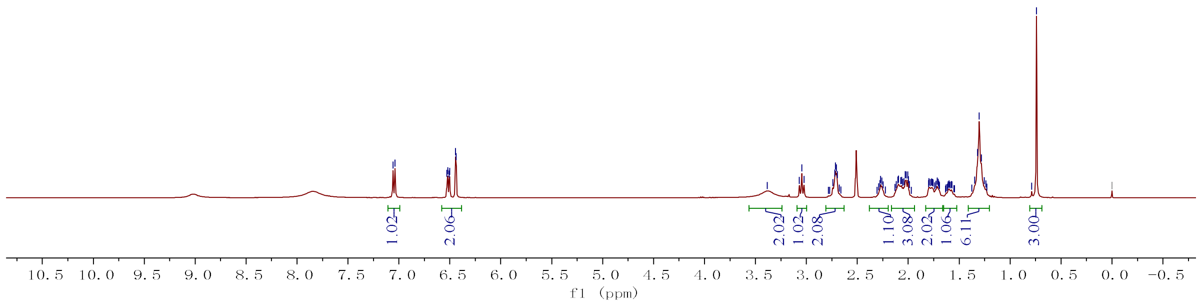


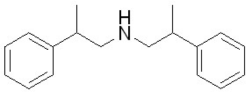


^{1}H NMR of 121
(400 MHz, DMSO-d_6)

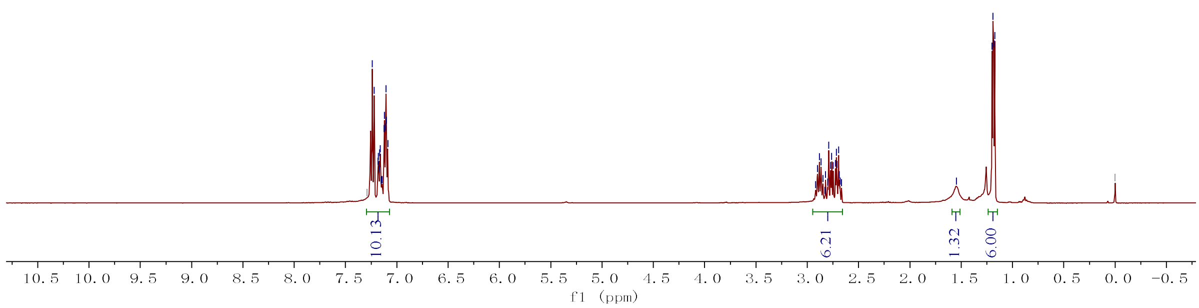


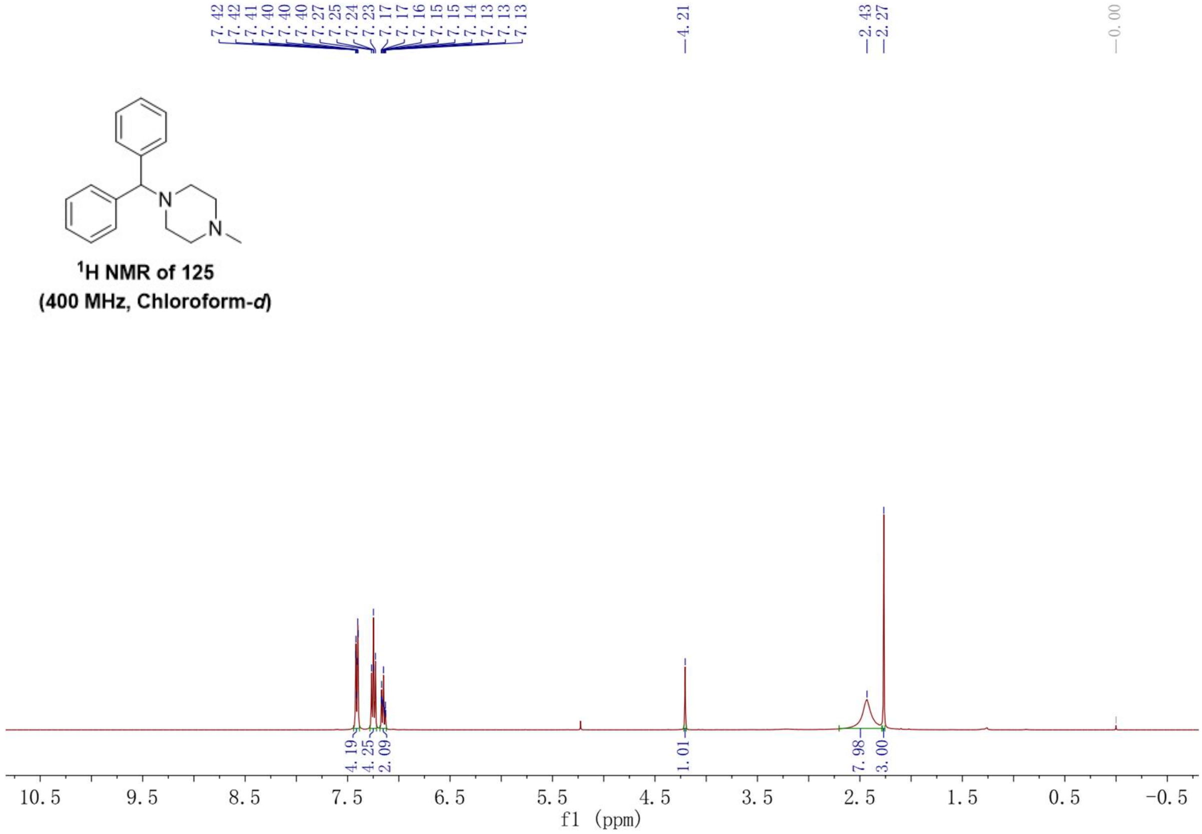
^{1}H NMR of 122
(400 MHz, DMSO-d_6)



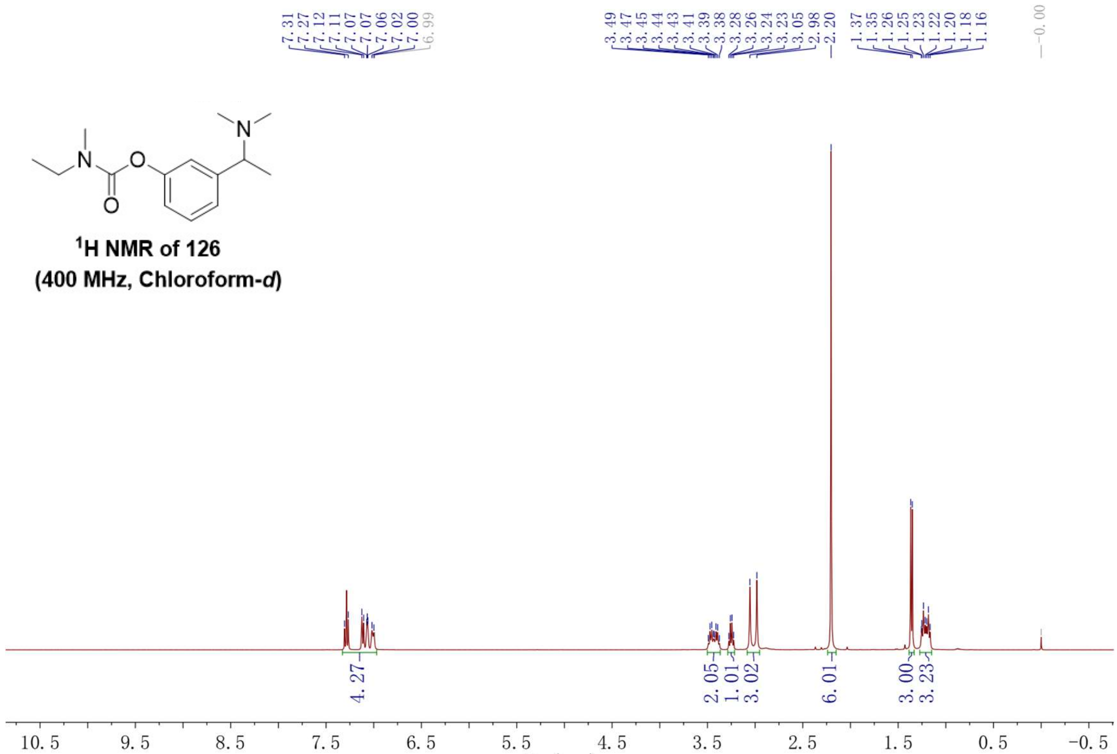


^{1}H NMR of 124
(400 MHz, Chloroform-d)

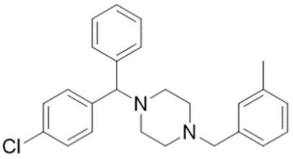




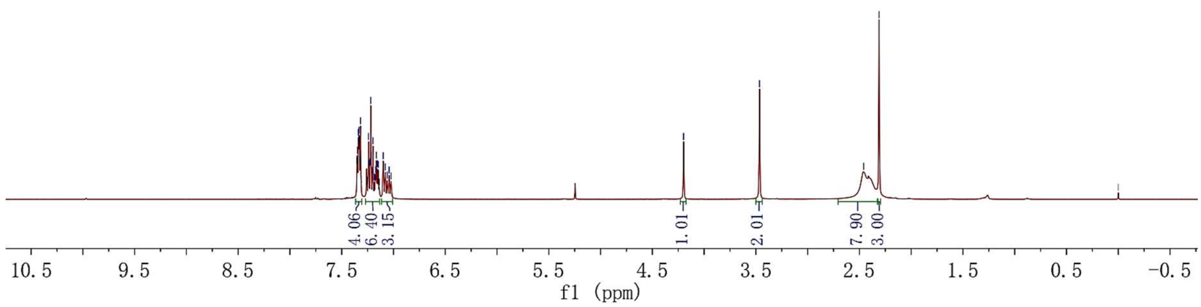
^{1}H NMR of 125
(400 MHz, Chloroform-*d*)

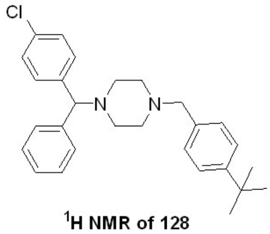


^{1}H NMR of 126
(400 MHz, Chloroform-*d*)

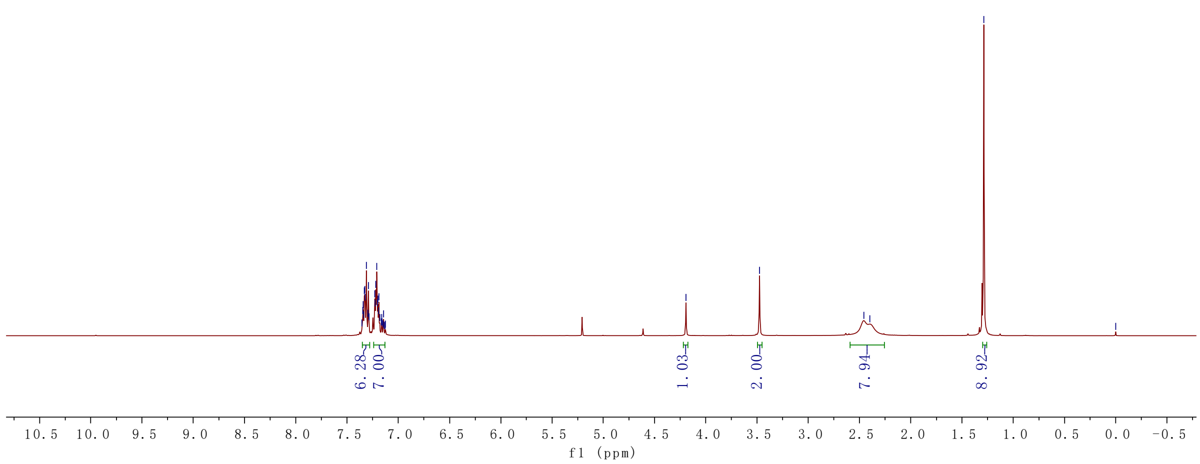


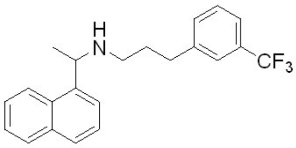
^{1}H NMR of 127
(400 MHz, Chloroform-*d*)

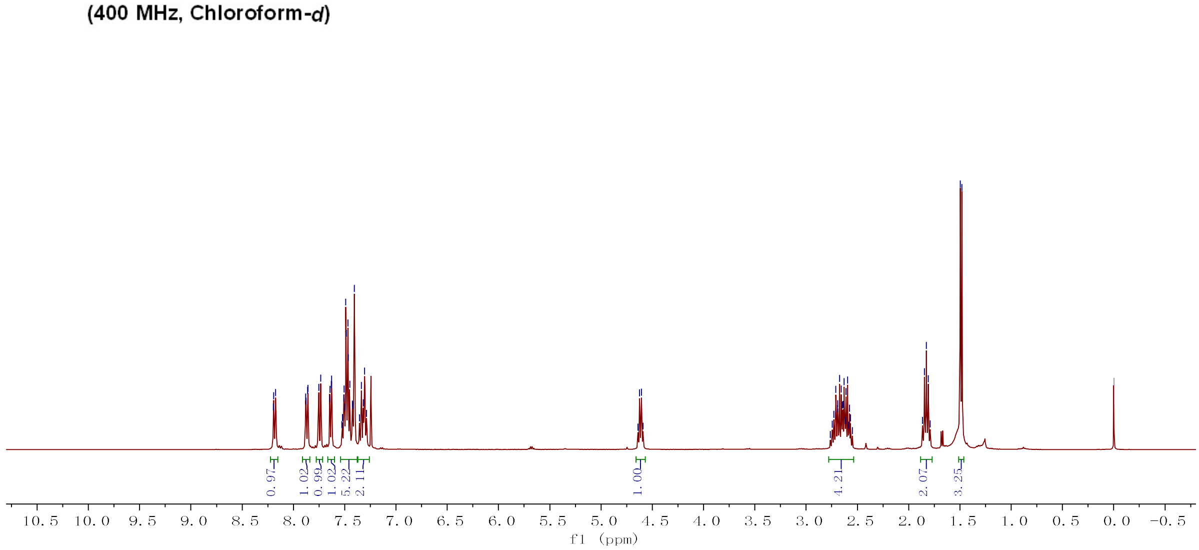




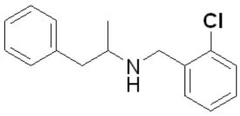
^{1}H NMR of 128
(400 MHz, Chloroform-*d*)

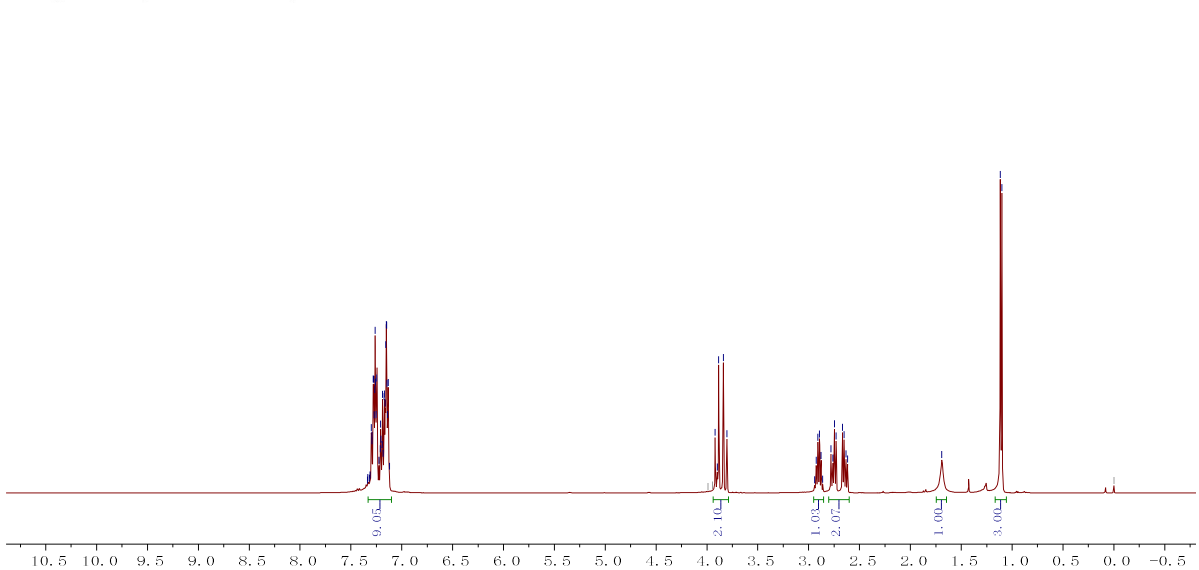




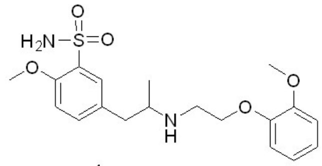


^{1}H NMR of 129
(400 MHz, Chloroform-*d*)

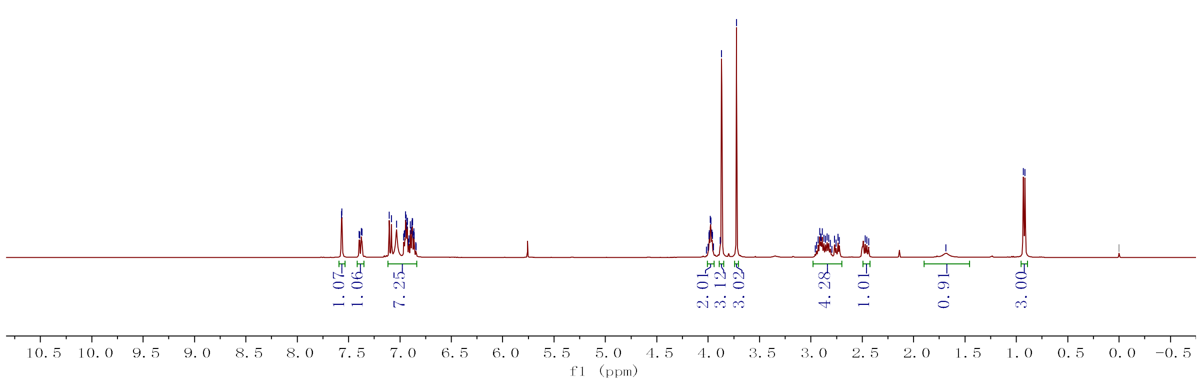


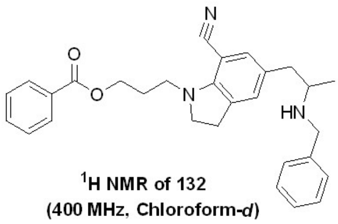


^{1}H NMR of 130
(400 MHz, Chloroform-*d*)

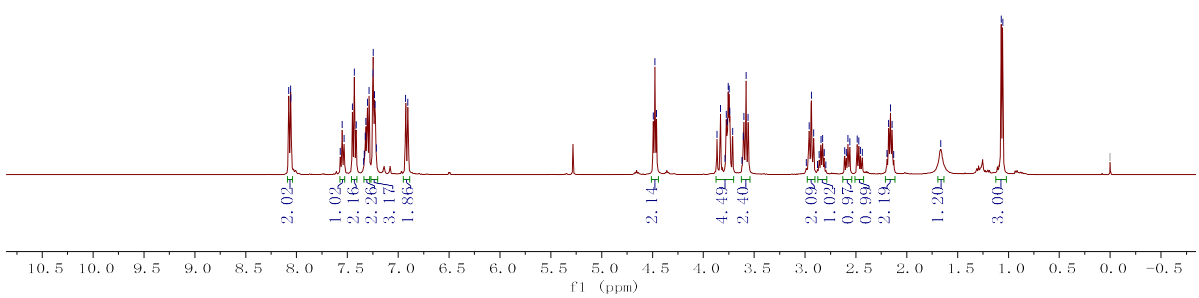


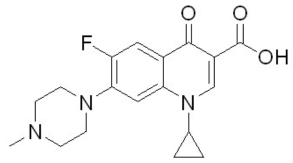
^{1}H NMR of 131
(400 MHz, DMSO-d_6)



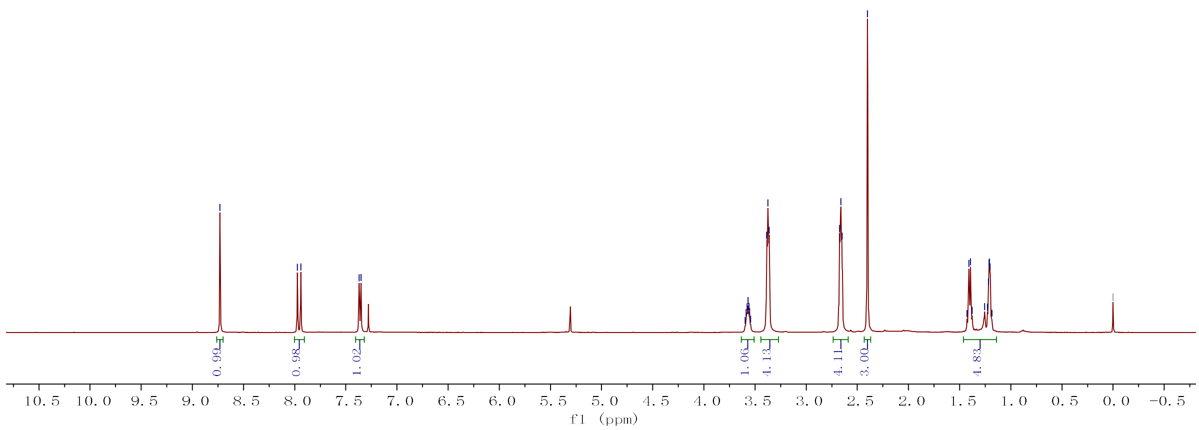


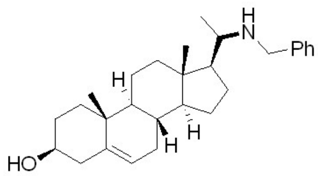
^{1}H NMR of 132
(400 MHz, Chloroform-d)



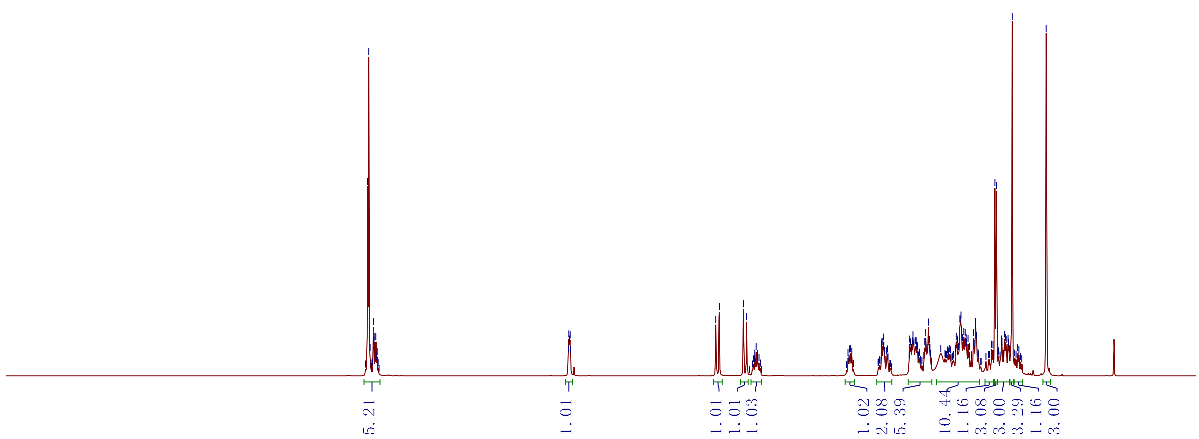


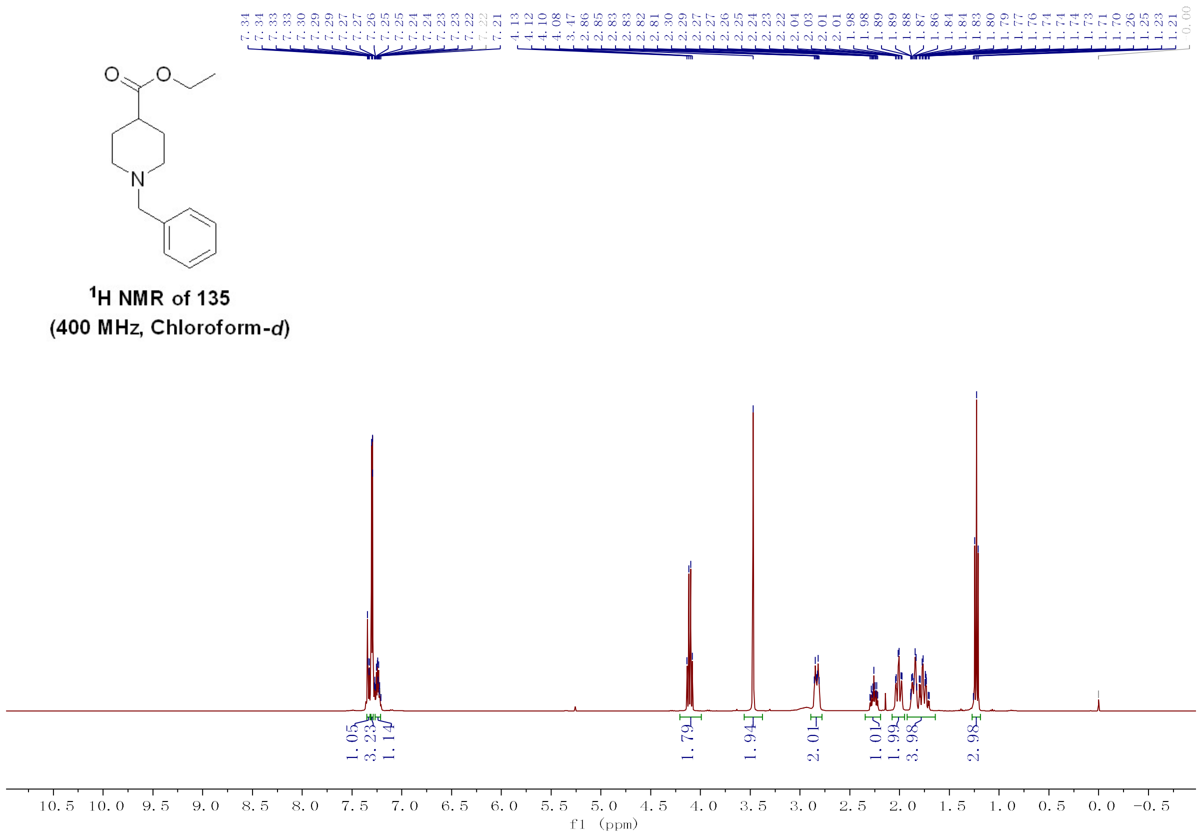
[1]H NMR of 133
(400 MHz, Chloroform-*d*)



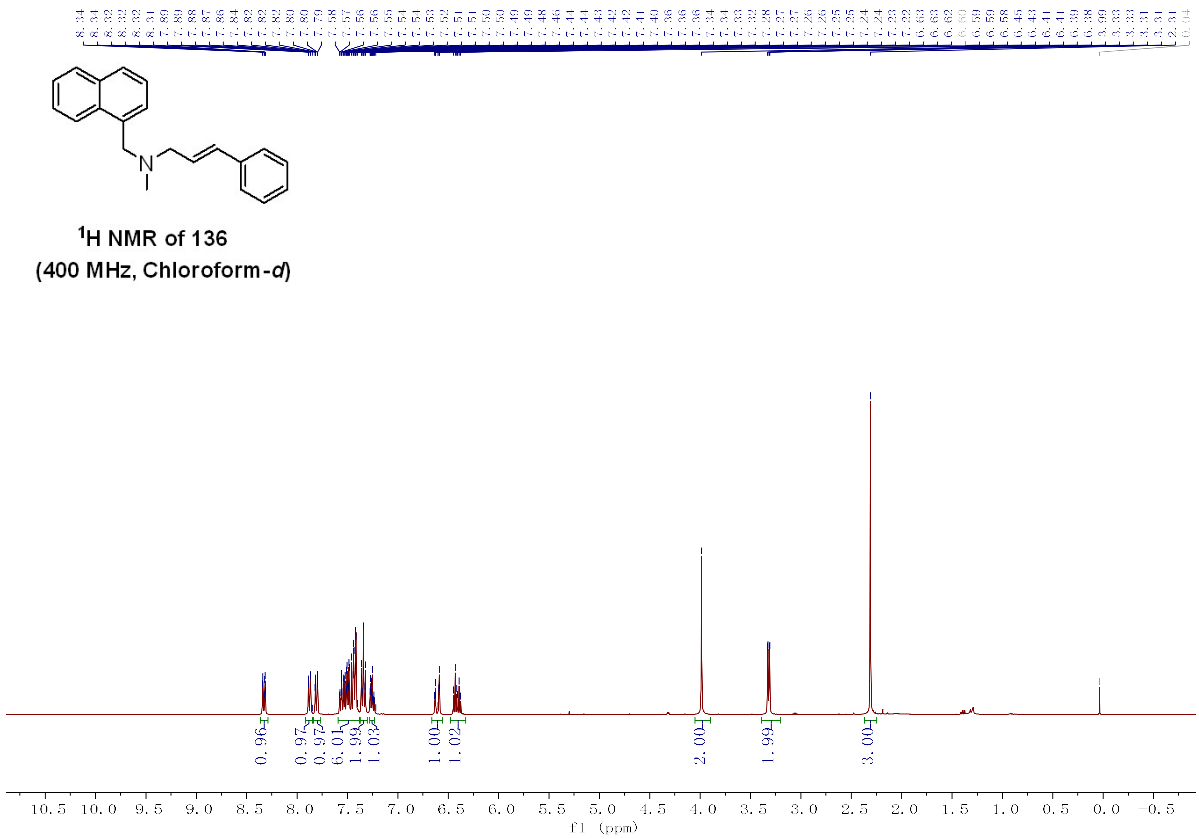


[1]H NMR of 134
(400 MHz, Chloroform-*d*)

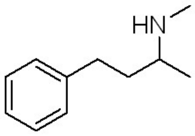




^{1}H NMR of 135
(400 MHz, Chloroform-*d*)



^{1}H NMR of 136
(400 MHz, Chloroform-*d*)



^{1}H NMR of 139
(400 MHz, Chloroform-*d*)