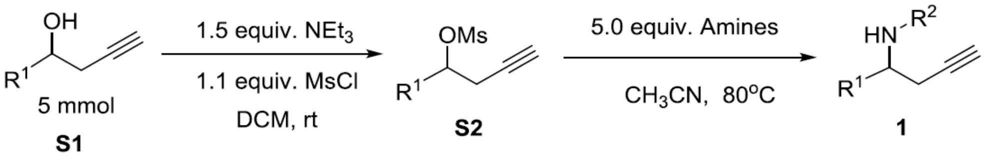
Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

1. General Information

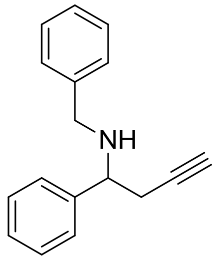
The ^{1}H NMR and ^{13}C NMR spectra were recorded at Bruker AV 400 MHz . 1H and ^{13}C NMR Chemical shifts were calibrated to tetramethylsilane as an internal reference. The data of the NMR spectra (^{1}H NMR, ^{13}C NMR and ^{19}F NMR) were recorded at 293 K on a Bruker AVANCE AV 400 (400MHz, 101MHz and 376MHz). Chemical shifts are given in (ppm) and coupling constants (*J*) in Hz. The following abbreviations are used to indicate the multiplicity: s, singlet; d, doublet: t, triplet; q, quartet; m, multiplet; Infrared spectra were recorded on an Bruker Fourier transform spectrometer (FT-IR) and are reported in wave numbers. High resolution mass spectrometric (HRMS) analyses spectrum was determined on the Varian 7.0T FTMS instrument.

2. Synthesis and characterization of the homopropargylamines 1a-1m and *N*-benzylpent-4-yn-1-amine 1q



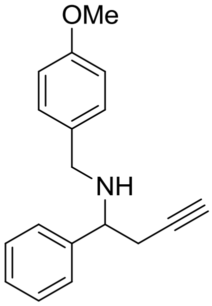
The **S1** (5.0 mmol) was dissolved in DCM (5.0 mL) in reaction tube, then the MsCl (0.92 g, 5.5 mmol, 1.1 equiv.) and Et_3N (0.76 g, 0.75 mmol, 1.5 equiv.) were added to the tube. The resulting mixture was stirred for 0.5 h at room temperature. After completion, the mixture was quenched with distilled water and extracted with CH_2Cl_2 (3 × 20 mL). The combined organic layer was washed with brine, dried over $MgSO_4$, and concentrated in vacuo. The obtained crude product **S2** was used directly for the next reaction.

To a Schlenk tube was sequentially added **S2**, amines (25 mmol, 5.0 equiv.) and CH_3CN (5 mL), the reaction mixture was stirred for overnight at 80 °C. After completion, the reaction mixture was quenched with water and extracted with CH_2Cl_2 (3 × 20 mL). The combined organic layer was washed with brine, dried over $MgSO_4$, and concentrated in vacuo. The residue was purified by flash chromatography on silica gel (gradient elution of EtOAc /petroleum ether, PE : EA = 15 : 1) to give the homopropargylic amines **1**.



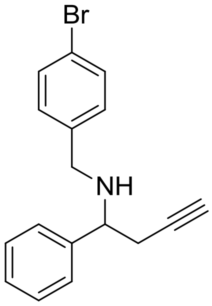
N-benzyl-1-phenylbut-3-yn-1-amine (1a)

Yellow liquid, 530 mg, yield 45%, ^{1}H NMR (400 MHz, Chloroform-d) δ 7.41 – 7.23 (m, 10 H), 3.88 – 3.85 (t, *J* = 6.8 Hz, 1H), 3.73 – 3.69 (d, *J* = 13.2 Hz, 1H), 3.60 – 3.56 (d, *J* = 13.2 Hz, 1H), 2.56 – 2.53 (m, 2H), 2.02-1.97 (t, *J* = 2.4 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.5, 140.3, 128.5, 128.4, 128.1, 127.6, 127.2, 127.0, 81.6, 70.6, 60.7, 51.4, 28.3.[1]



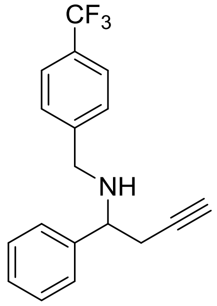
N-(4-methoxybenzyl)-1-phenylbut-3-yn-1-amine (1b)

Pale yellow oil, 463 mg, yield 35%, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40 – 7.33 (m, 4H), 7.30 -7.26 (m, 1H), 7.21 – 7.29 (d, *J* = 8.4 Hz, 2H), 6.86 – 6.84 (d, *J* = 8.4 Hz, 2H), 3.86 – 3.83 (t, *J* = 6.8 Hz, 1H), 3.79 (s, 3H), 3.65 – 3.62 (d, *J* = 12.8 Hz, 1H),3.53 – 3.49 (d, *J* = 13.2 Hz, 1H), 2.54 – 2.52 (m, 2H), 2.01-2.00 (t, *J* = 2.4 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.6, 142.5, 132.4, 129.3, 128.5, 127.6, 127.2, 113.8, 81.6, 70.5, 60.6, 55.3, 50.8, 28.2. [2]



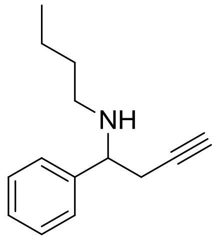
N-(4-bromobenzyl)-1-phenylbut-3-yn-1-amine (1c)

Yellow liquid, 313 mg, yield 20%, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.44 – 7.42 (d, *J* = 7.6 Hz, 2H), 7.37 -7.33 (m, 4 H), 7.30 – 7.29 (d, *J* = 5.6 Hz, 1H), 7.18 – 7.16 (d, *J* = 7.6 Hz, 2H), 3.84 – 3.81 (t, *J* = 6.8 Hz, 1H), 3.66 – 3.63 (d, *J* = 13.6 Hz, 1H), 3.54 – 3.51 (d, *J* = 13.6 Hz, 1H), 2.54 – 2.52 (m, 2H), 2.03 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.2, 139.3, 131.4, 129.8, 128.6, 127.7, 127.1, 12.7, 81.5, 70.6, 60.6, 50.7, 28.2. HRMS (ESI$^+$) calculated for $C_{17}H_{17}BrN$ (M+H$^+$) 314.0544; found 314.0544.



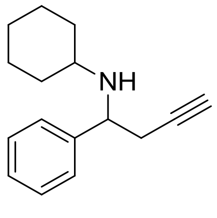
1-phenyl-*N*-(4-(trifluoromethyl)benzyl)but-3-yn-1-amine (1d)

Yellow liquid, 91 mg, yield 15%, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.57 – 7.55 (d, *J* = 8.4 Hz, 2H), 7.42 -7.34 (m, 6H), 7.31 – 7.27 (m, 1H), 3.86 – 3.83 (t, *J* = 6.0 Hz, 1H), 3.77 – 3.73 (d, *J* = 14.0 Hz, 1H), 3.66 – 3.63 (d, *J* = 15 Hz, 1H), 2.61 – 2.49 (m, 2H), 2.04 - 2.03 (t, *J* = 2.8 Hz, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 144.4, 142.1, 129.4, 129.1, 128.6, 128.3, 127.7, 127.1, 125.6, 125.4, 125.3, 125.28, 125.2, 81.4, 70.7, 60.7, 50.8, 28.2. ^{19}F NMR (376 MHz, CDCl$_3$) δ -62.2. HRMS (ESI$^+$) calculated for $C_{18}H_{17}F_3N$ (M+H$^+$) 304.1313; found 304.1313.



***N*-butyl-1-phenylbut-3-yn-1-amine (1e)**

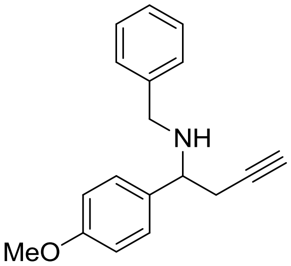
Yellow liquid, 201 mg, yield 20%, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.24 (m, 5H), 3.83 – 3.79 (q, *J* = 6.8 Hz, 1H), 2.58 – 2.39 (m, 4H), 2.03-2.02 (t, *J* = 2.1 Hz, 1H), 1.75 (s, 1H), 1.49 – 1.42 (m, 2H), 1.38 – 1.23 (m, 2H), 0.90 – 0.86 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 142.9, 128.4, 127.4, 127.0, 81.7, 70.4, 61.7, 47.4, 32.2, 28.1, 20.4, 14.0. HRMS (ESI$^+$) calculated for $C_{14}H_{20}N$ (M+H$^+$) 202.1596; found 202.1593.



***N*-(1-phenylbut-3-yn-1-yl)cyclohexanamine (1f)**

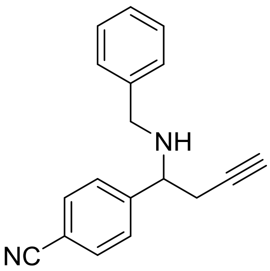
Yellow liquid, 283 mg, yield 25%, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.31

(q, *J* = 7.6 Hz, 4H), 7.28 – 7.24 (t, *J* = 7.2 Hz, 1H), 4.02 – 3.99(t, *J* = 6.4 Hz, 1H), 2.56 -2.44 (m, 2H), 2.32 – 2.26 (m, 1H), 2.01 – 1.96 (t, 2H), 1.74 – 1.54 (m, 5H), 1.15 – 0.99 (m, 5H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.4, 128.4, 127.3, 127.0, 81.7, 70.4, 58.1, 53.4, 34.6, 32.9, 28.6, 26.2, 25.2, 24.9. HRMS (ESI$^+$) calculated for $C_{16}H_{22}N$ (M+H$^+$) 228.1752; found 228.1750.



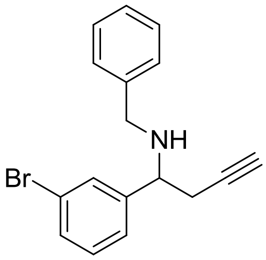
N-benzyl-1-(4-methoxyphenyl)but-3-yn-1-amine (1g)

Yellow liquid, 132 mg, yield 10%, ^{1}H NMR (400 MHz, Chloroform-*d*) 7.34 – 7.23 (m, 7H), 6.91 – 6.89 (d, *J* = 8.4 Hz, 2H), 3.84 – 3.81 (d, 4H), 3.72 – 3.68 (d, *J* = 13.2 Hz, 1H), 3.58 – 3.55 (d, *J* = 13.2 Hz, 1H), 2.53 – 2.51 (q, *J* = 2.4 Hz, 2H), 2.02 - 2.01 (t, *J* = 2.4 Hz, 1H), 1.97 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.0, 140.2, 134.3, 128.4, 128.3, 128.1, 126.9, 113.9, 81.7, 70.5, 60.1, 55.3, 51.3, 28.3. HRMS (ESI$^+$) calculated for $C_{18}H_{19}NO$ (M+H$^+$) 266.1545; found 266.1543.



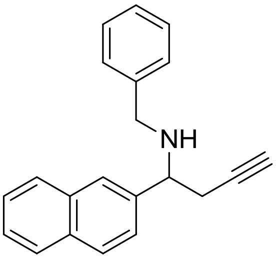
4-(1-(benzylamino)but-3-yn-1-yl)benzonitrile (1h)

Yellow liquid, 81 mg, yield 6%, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.66 – 7.64 (d, *J* = 8.0 Hz, 2H), 7.54 -7.52 (d, *J* = 8.0 Hz, 2H), 7.34 – 7.26 (m, 5H), 3.93 – 3.90 (t, *J* = 6.4 Hz, 1H), 3.69 – 3.66 (d, *J* = 13.2 Hz, 1H), 3.58 – 3.55 (d, *J* = 13.6 Hz, 1H), 2.58 – 2.46 (m, 2H), 2.04 - 2.03 (t, *J* = 2.8 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.0, 139.6, 132.4, 128.5, 128.1, 128.0, 127.2, 118.9, 111.5, 80.4, 71.2, 60.4, 51.4, 27.9. HRMS (ESI$^+$) calculated for $C_{18}H_{17}N_2$ (M+H$^+$) 261.1392; found 261.1391.



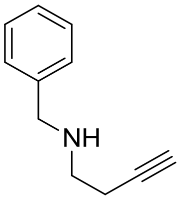
N-benzyl-1-(3-bromophenyl)but-3-yn-1-amine (1i)

Yellow liquid, 156 mg, yield 10 %, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.56 (s, 1H), 7.40 – 7.39 (d, *J* = 7.6 Hz, 1H), 7.33 – 7.17 (m, 7H), 3.82 – 3.79 (t, *J* = 6.8 Hz, 1H), 3.70 – 3.67 (d, *J* = 13.2 Hz, 1H), 3.57 – 3.53 (d, *J* = 13.2 Hz, 1H),2.50 – 2.47 (m, 2H), 2.05 (s, 1H), 2.02 – 2.01 (t, *J* = 2.4 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 145.1, 140.0, 130.8, 130.3, 130.2, 128.5, 128.1, 127.1, 126.0, 122.8, 81.1, 71.0, 60.3, 51.5, 28.2. HRMS (ESI$^+$) calculated for $C_{17}H_{17}BrN$ (M+H$^+$) 314.0544; found 314.0543.



N-benzyl-1-(naphthalen-2-yl)but-3-yn-1-amine (1j)

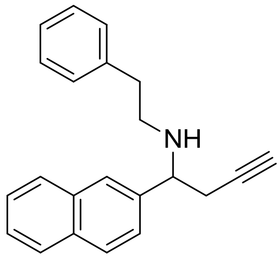
Yellow liquid, 783 mg, yield 55%, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.16 – 8.14 (d, *J* = 8 Hz, 1H), 7.86 – 7.75 (m, 3H), 7.50 – 7.44 (m, 3H), 7.29 – 7.21 (m, 5H), 4.74 – 4.71 (q, *J* = 4.4 Hz, 1H), 3.79 – 3.75 (d, *J* = 13.6 Hz, 1H), 3.64 – 3.61 (d, *J* = 13.2 Hz, 1H), 2.78 – 2.72 (m, 1H), 2.64 – 2.57 (m, 1H), 2.19 (s, 1H), 2.04 – 2.02 (t, *J* = 2.8 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 140.5, 137.7, 134.1, 131.6, 129.2, 128.5, 128.3, 128.0, 127.1, 126.1, 125.8, 125.6, 124.1, 122.9, 81.9, 71.0, 56.6, 51.7, 27.4 HRMS (ESI$^+$) calculated for $C_{21}H_{19}N$ (M+H$^+$) 286.1596; found 286.1593.



N-benzylbut-3-yn-1-amine (1k)

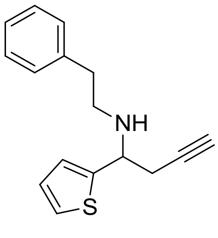
Colorless liquid, 318 mg, yield 40%, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 –

7.30 (m, 4H), 7.28 – 7.23 (m, 1H), 3.82 (s, 2H), 2.82 – 2.79 (t, *J* = 6.8 Hz, 2H), 2.44 – 2.40 (m, 2H), 2.00 – 1.99 (t, *J* = 2.8 Hz, 1H), 1.66 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.1, 128.4, 128.1, 127.0, 82.5, 69.6, 53.4, 47.3, 19.6. [3]



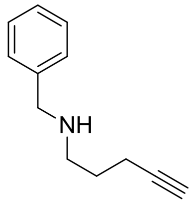
1-(naphthalen-2-yl)-*N*-phenethylbut-3-yn-1-amine (1l)

Brown liquid, 747 mg, yield 50%, ^{1}H NMR (400 MHz, Chloroform-*d*) 8.18 – 8.16 (d, *J* = 8 Hz, 1H), 7.87 – 7.85 (q, *J* = 2.4, 7.2 Hz, 1H), 7.76 – 7.74 (d, *J* = 8 Hz, 1H), 7.63 – 7.61 (d, *J* = 7.2 Hz, 1H),7.51 – 7.42 (m, 3H), 7.28 – 7.23 (m, 2H), 7.20 – 7.17 (m, 3H), 4.71 – 4.68 (q, *J* = 4.8 Hz, 1H), 2.82 (s, 4H), 2.76 – 2.70 (m, 1H), 2.59 – 2.52 (m, 1H), 1.98 – 1.95 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.0, 137.7, 134.0, 131.4, 129.1, 128.8, 128.4, 127.8, 126.1, 126.0, 125.6, 125.4, 123.8, 122.7, 81.6, 70.8, 57.2, 48.9, 36.5, 27.3. HRMS (ESI$^+$) calculated for $C_{22}H_{22}N$ (M+H$^+$) 300.1752; found 300.1750.



***N*-benzyl-1-(thiophen-2-yl)but-3-yn-1-amine (1m)**

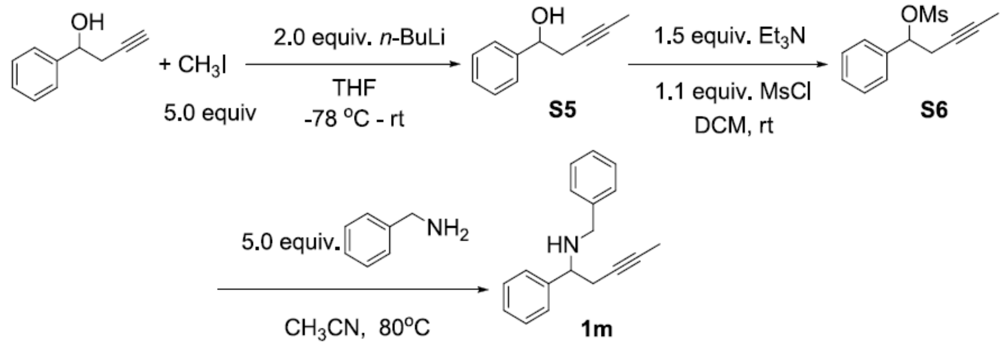
Yellow liquid, 255 mg, yield 20%, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.26 – 7.24 (t, *J* = 7.2 Hz, 2H), 7.19 – 7.17 (d, *J* = 6.4 Hz, 4H), 6.93 – 6.91 (t, *J* = 3.6 Hz, 2H), 4.14 – 4.11 (t, *J* = 6.4 Hz, 1H), 2.87 – 2.79 (m, 4H), 2.59 – 2.57 (d, *J* = 6 Hz, 2H), 1.97 (s, 1H), 1.89(s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.4, 139.9, 128.8, 128.5, 126.5, 126.2, 124.5, 124.4, 80.9, 71.1, 57.2, 48.7, 36.3, 28.6. HRMS (ESI$^+$) calculated for $C_{16}H_{18}NS$ (M+H$^+$) 256.1160; found 256.1158.



***N*-benzylpent-4-yn-1-amine (1q)**

Colorless liquid, 260 mg, yield 30%, ^{1}H NMR (400 MHz, Chloroform-*d*) 7.27 – 7.16 (m, 5H), 3.72 (s, 2H), 2.69 – 2.65 (t, *J* = 7.2 Hz, 2H), 2.22 – 2.17 (m, 2H), 1.88 – 1.86 (t, *J* = 1.8 Hz, 1H), 1.69 – 1.62 (m, 2H).[4]

3. Synthesis and characterization of the 1n

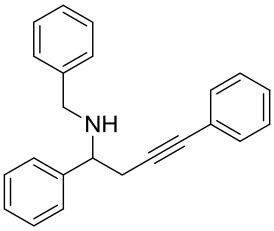


The $Pd(PPh_3)_4$ (110 mg, 0.11 mmol, 1 mol%), CuI (30 mg, 0.22 mmol, 2 mol%), piperidine (2.554 g, 30 mmol), iodobenzene (2.244 g, 11.0 mmol) and DMF (15 mL) were sequentially added to a Schlenk tube, the terminal alkynes (10 mmol) was then added, the reaction mixture is degassed by alternately freezing, evacuating and thawing. After that, the reaction mixture was stirred at 80 ℃ for 16 h at N_2 atmosphere and then quenched with saturated NaCl aqueous. The obtained reaction solution was extracted with ethyl acetate (3×20 mL) three times. The combined organic layer was washed with brine, dried over anhydrous $MgSO_4$ and filtered. The filtrate was concentrated over vacuo. The crude residue was purified by silica gel column chromatography (petrol ether/EtOAc 10:1) to afford the compound **S3** (1.89 g, yield 85%).[5]

The **S3** (1.11 g, 5.0 mmol) was dissolved in DCM (5.0 mL) in reaction tube, then the MsCl (0.92 g, 1.1 equiv.) and Et_3N (0.76 g, 1.5 equiv.) were added to the above tube. The resulting mixture was stirred for 0.5 h at room temperature. After completion, the reaction mixture was quenched with distilled water and extracted with

CH_2Cl_2 (3 × 20 mL). The combined organic layer was washed with brine, dried over $MgSO_4$ and filtered. The filtrate was concentrated over vacuo. The resulted residue (crude product **S4**) was used directly for the next reaction.

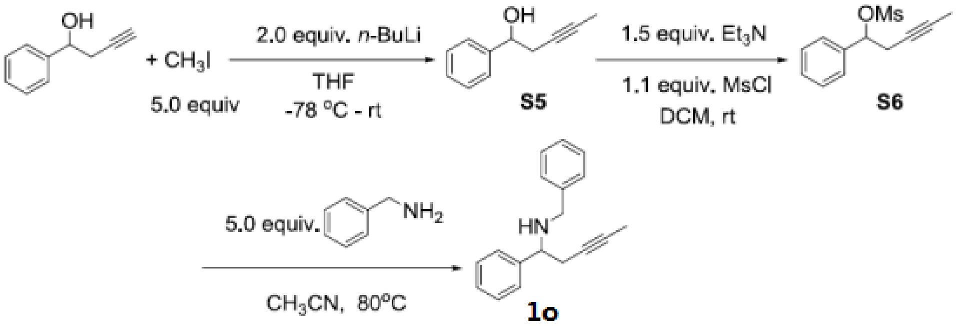
To a Schlenk tube was added the above residue S4, then the benzylamine (2.7 g, 25 mmol, 5.0 equiv.) and CH_3CN (5 mL) were sequentially added into the Schlenk tube. The reaction mixture was stirred for overnight at 80 ^oC. After completion, the reaction mixture was directly purified by flash chromatography on silica gel (gradient elution of EtOAc /petroleum ether, PE : EA = 15 : 1) to afford the compound **1n** (544 mg, total yield 35%).



***N*-benzyl-1,4-diphenylbut-3-yn-1-amine (1n)**

Colorless liquid, 544 mg, yield 35%, ^{1}H NMR (400 MHz, Chloroform-*d*) 7.45 – 7.43 (d, *J* = 7.6 Hz, 2H), 7.39 – 7.34 (m, 4H), 7.31 – 7.22 (m, 9H), 3.95 – 3.92 (t, *J* = 6.4 Hz, 1H), 3.77 – 3.74 (d, *J* = 13.2 Hz, 1H), 3.62 – 3.58 (d, *J* = 13.2 Hz, 1H), 2.75 – 2.74 (d, *J* = 6.8 Hz, 2H), 2.10 (s, 1H). ^{13}C NMR (101 MHz, CDCl3) δ142.7, 140.4, 131.6, 128.5, 128.4, 128.3, 128.2, 127.9, 127.6, 127.3, 126.9, 123.5, 87.2, 82.7, 61.0, 51.4, 29.4. HRMS (ESI$^+$) calculated for $C_{23}H_{22}N$ (M+H$^+$) 312.1752; found 312.1750.

4. Synthesis and characterization of the 1o

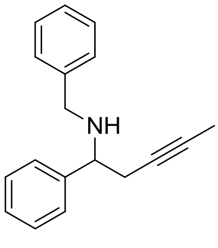


A round-bottomed flask was wrapped in aluminum foil and equipped with a dropping funnel and a thermometer. The flask was charged with

1-phenylbut-3-yn-1-ol (258 mg, 1.5 mmol, 1.0 equiv.) and tetrahydrofuran (4 mL). The resulting solution was cooled to -78 °C and a 2.5 M solution of *n*-butyllithium in hexane (1.2 mL, 3.0 mmol, 2.0 equiv.) was added dropwise. The reaction mixture was stirred at -78 ℃ for 1.5 h and the iodomethane (0.5 mL, 7.5 mmol, 5.0 equiv.) was then added dropwise. The mixture was warmed to room temperature for another 1 h and 1.0 M hydrochloric acid (10 mL) was added dropwise. The mixture was stirred for additional 30 mins at room temperature. The resulting reaction solution was separated through te separating funnel, the organic layer was collected and the aqueous layer was extracted with diethyl ether (3 × 15 mL). The combined organic layers were dried over anhydrous $MgSO_4$, filtered and concentrated in vacuo. The residue was purified by silica gel column chromatography (hexane /ethyl acetate: 10/1) to give the desired product **S5**.

The **S5** (160 mg, 1.0 mmol) was dissolved in DCM (3.0 mL) in reaction tube, then the MsCl (0.18 g, 1.0 mmol, 1.1 equiv.) and Et_3N (0.15 g, 1.5 mmol, 1.5 equiv.) were added to the above tube. The resulting mixture was stirred for 0.5 h at room temperature. After completion, the reaction mixture was quenched with distilled water and extracted with CH_2Cl_2 (3 × 10 mL). The combined organic layer was washed with brine, dried over $MgSO_4$ and filtered. The filtrate was concentrated over vacuo. The resulted residue (crude product **S6**) was used directly for the next reaction.

To a Schlenk tube was sequentially added with the **S6**, benzylamine (0.54 g, 5.0 mmol, 5.0 equiv.) and CH_3CN (5 mL). The reaction mixture was stirred for overnight at 80 °C. After completion, the reaction mixture was directly purified by flash chromatography on silica gel (gradient elution of EtOAc /petroleum ether, PE : EA = 15 : 1) to afford the compound **1o** (100 mg, total yield 40%).

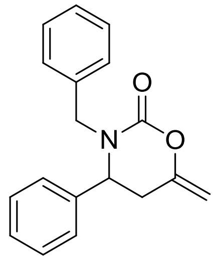


***N*-benzyl-1-phenylpent-3-yn-1-amine (1o)**

Colorless liquid, 100 mg, yield 40%, ^{1}H NMR (400 MHz, Chloroform-*d*) 7.40 – 7.23 (m, 10H), 3.82 – 3.78 (dd, *J* = 5.6, 7.6 Hz, 1H), 3.73 – 3.69 (d, *J* = 13.6 Hz, 1H), 3.58 – 3.55 (d, *J* = 13.2 Hz, 1H), 2.52 – 2.41 (m, 2H), 2.14 (s, 1H), 1.78 – 1.77 (t, *J* = 2.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.0, 140.6, 128.5, 128.4, 128.1, 127.4, 127.2, 126.9, 77.9, 76.3, 61.3, 51.5, 28.8, 3.6. HRMS (ESI$^+$) calculated for $C_{18}H_{20}N$ (M+H$^+$) 250.1596; found 250.1593.

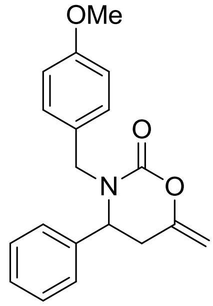
5. General procedure for the synthesis of 1, 3-oxazin-ones 2

The reactions were conducted in a 25 mL oven-dried autoclave with a glass tube inside equipped with magnetic stirring. AgOAc (3.3 mg, 0.02 mmol, 20 mol%), DBU (7.5 mg, 0.05 mmol, 50 mol%), homopropargylic amines **1** (0.1 mmol) and CO_2 (0.5 MPa, 99.999%) were successively introduced and heated at 80 °C for 6 h. After completion, the vessel was cooled to room temperature, and the pressure was released slowly to atmospheric pressure. The reaction mixture was directly purified by column chromatography on silica gel using petroleum ether/ethyl acetate (v/v,10:1–5:1) as eluents to give the desired products **2** (**2a – 2m**). The compound **2n** was obtained by flash chromatography on silica gel (gradient elution of EtOAc /petroleum ether, PE : EA = 10 : 1).



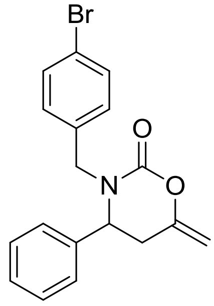
3-benzyl-6-methylene-4-phenyl-1,3-oxazinan-2-one (2a)

Colorless liquid, 28 mg, yield 99%, ^{1}H NMR (400 MHz, Chloroform-*d*) 7.39 – 7.30 (m, 6H), 7.24 – 7.23 (d, *J* = 6.8 Hz, 2H), 7.16 – 7.15 (d, *J* = 6.8 Hz, 2H), 5.33 – 5.29 (d, *J* = 15.2 Hz, 1H), 4.71 (s, 1H), 4.42 – 4.40 (dd, *J* = 2.0, 6.0 Hz, 1H), 4.05 (s, 1H), 3.69 – 3.65 (d, *J* = 15.2 Hz, 1H), 2.89 – 2.84 (dd, *J* = 6.4, 14.0 Hz, 1H), 2.51 – 2.46 (dd, *J* = 2.0, 14.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.5, 150.1, 138.7, 136.3, 128.9, 128.8, 128.4, 128.3, 127.9, 126.4, 95.0, 56.1, 50.6, 34.4. HRMS (ESI$^+$) calculated for $C_{18}H_{18}NO_2$ (M+H$^+$) 280.1338; found 280.1334.



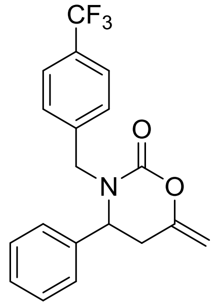
3-(4-methoxybenzyl)-6-methylene-4-phenyl-1,3-oxazinan-2-one (2b)

Colorless liquid, 31 mg, yield 99%, m.p. 135.0-136.7℃, ^{1}H NMR (400 MHz, Chloroform-*d*) 7.40 – 7.31 (m, 3H), 7.18 – 7.15 (m, 4H), 6.88 – 6.84 (m, 2H), 5.26 – 5.23 (d, *J* = 14.8 Hz, 1H), 4.70 (s, 1H), 4.42 – 4.40 (dd, *J* = 2.4, 6.0 Hz, 1H), 4.05 – 4.04 (t, *J* = 1.6 Hz, 1H),3.80 (s, 3H), 3.62 – 3.59 (d, *J* = 14.8 Hz, 1H), 2.86 – 2.80 (dt, *J* = 1.6, 6.4 Hz, 1H), 2.50 – 2.45 (dd, *J* = 2.8, 14.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.3, 151.5, 150.1, 138.8, 129.8, 128.9, 128.34, 128.26, 126.4, 114.1, 94.9, 55.8, 55.3, 50.0, 34.4.



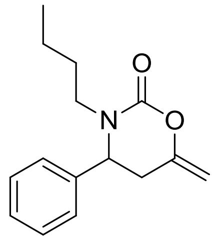
3-(4-bromobenzyl)-6-methylene-4-phenyl-1,3-oxazinan-2-one (2c)

Colorless liquid, 36 mg, yield 99%, ^{1}H NMR (400 MHz, Chloroform-*d*) 7.46 – 7.44 (d, *J* = 8.4 Hz, 2H), 7.40 – 7.33 (m, 3H), 7.16 – 7.10 (m, 4H), 5.21 – 5.18 (d, *J* = 15.2 Hz, 1H), 4.72 (s, 1H), 4.40 – 4.38 (dd, *J* = 2.8, 6.4 Hz, 1H), 4.08 (s, 1H), 3.68 – 3.65 (d, *J* = 14.8 Hz, 1H), 2.89 – 2.84 (dd, *J* = 6.0 Hz, 1H), 2.53 – 2.49 (dd, *J* = 2.8, 14.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.5, 149.9, 138.5, 135.3, 131.9, 130.0, 129.0, 128.5, 126.4, 121.9, 95.3, 56.4, 50.1, 34.4. HRMS (ESI$^+$) calculated for $C_{18}H_{16}BrNO_2Na$ (M+Na$^+$) 380.0262; found 380.0260.



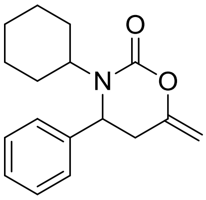
6-methylene-4-phenyl-3-(4-(trifluoromethyl)benzyl)-1,3-oxazinan-2-one (2d)

Colorless viscous liquid, 34 mg, yield 98%, ^{1}H NMR (400 MHz, Chloroform-*d*) 7.59 – 7.57 (d, *J* = 8.4 Hz, 2H), 7.40 – 7.34 (m, 5H), 7.16 – 7.14 (dd, *J* = 2.0, 8.0 Hz, 2H), 5.28 – 5.24 (d, *J* = 15.6 Hz, 1H), 4.74 (s, 1H), 4.41 – 4.39 (dd, *J* = 2.8, 6.0 Hz, 1H), 4.10 – 4.09 (t, *J* = 1.2 Hz, 1H), 3.84 – 3.80 (d, *J* = 15.6 Hz, 1H), 2.93 – 2.88 (m, 1H), 2.56 – 2.51 (dd, *J* = 2.8, 14.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.5, 149.9, 140.4, 138.4, 130.3, 130.0, 129.1, 128.6, 128.4, 126.4, 125.8, 125.74, 125.7, 125.67, 125.4, 122.7, 95.4, 56.8, 50.4, 34.4. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.4. HRMS (ESI$^+$) calculated for $C_{19}H_{16}F_3NNaO_2$ (M+Na$^+$) 370.1031; found 370.1030.



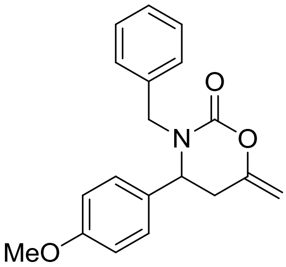
3-butyl-6-methylene-4-phenyl-1,3-oxazinan-2-one (2e)

Colorless liquid, 22 mg, yield 87%, ^{1}H NMR (400 MHz, Chloroform-*d*) 7.39 – 7.27 (m, 3H), 7.18 – 7.17 (d, *J* = 7.2 Hz, 2H), 4.66 (s, 1H), 4.56 – 4.54 (q, *J* = 2.8, 6.0 Hz, 1H), 4.03 (s, 1H), 3.74 – 3.67 (m, 1H), 3.00 – 2.95 (dd, *J* = 6.0, 14.0 Hz, 1H), 2.85 – 2.78 (m, 1H), 2.56 – 2.52 (dd, *J* = 2.4, 14.0 Hz, 1H), 1.59 – 1.51 (m, 2H), 1.32 – 1.23 (m, 2H), 0.90 – 0.86 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.0, 150.1, 139.3, 128.8, 128.2, 126.2, 94.6, 57.7, 48.4, 34.5, 29.5, 20.0, 13.8. HRMS (ESI$^+$) calculated for $C_{15}H_{19}NNaO_2$ (M+Na$^+$) 268.1313; found 268.1313.



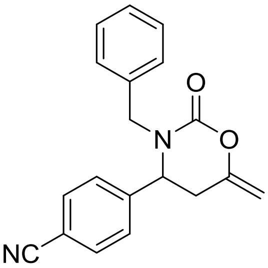
3-cyclohexyl-6-methylene-4-phenyl-1,3-oxazinan-2-one (2f)

Colorless liquid, 22 mg, yield 81%, ^{1}H NMR (400 MHz, Chloroform-*d*) 7.35 – 7.27 (m, 3H), 7.18 – 7.16 (d, *J* = 7.2 Hz, 2H), 4.68 – 4.66 (d, *J* = 4.8 Hz, 1H), 4.60 (s, 1H), 4.13 – 4.07 (m, 1H), 3.92 (s, 1H), 2.89 – 2.84 (dd, *J* = 5.6, 14.4 Hz, 1H), 2.51 – 2.48 (d, *J* = 14.0 Hz, 1H), 1.80 – 1.78 (d, *J* = 9.6 Hz, 2H), 1.64 – 1.49 (m, 4H), 1.41 – 1.16 (m, 2H), 1.12 – 0.95 (m, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 150.7, 149.9, 140.9, 128.5, 127.8, 126.0, 94.0, 57.8, 53.8, 35.3, 30.8, 30.0, 25.8, 25.6, 25.3 HRMS (ESI$^+$) calculated for $C_{17}H_{21}NNaO_2$ (M+Na$^+$) 294.1470; found 294.1469.



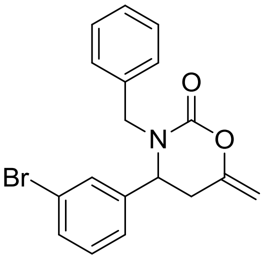
3-benzyl-4-(4-methoxyphenyl)-6-methylene-1,3-oxazinan-2-one (2g)

Colorless liquid, 31 mg, yield 99%, ^{1}H NMR (400 MHz, Chloroform-*d*) 7.36 – 7.83 (m, 3H), 7.24 – 7.22 (t, *J* = 1.2 Hz, 2H), 7.09 – 7.07 (d, *J* = 8.8 Hz, 2H), 6.91 – 6.88 (d, *J* = 8.8 Hz, 2H), 5.30 – 5.27 (d, *J* = 15.2 Hz, 1H), 4.72 (s, 1H), 4.37 – 4.35 (dd, *J* = 2.1, 6.0 Hz, 1H), 4.08 (s, 1H), 3.82 (s, 3H), 3.68 – 3.65 (d, *J* = 14.8 Hz, 1H), 2.86 – 2.81 (dd, *J* = 6.0, 14.0 Hz, 1H), 2.48 – 2.44 (dd, *J* = 2.4, 14.0 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 159.6, 151.5, 150.3, 136.3, 130.7, 128.8, 128.2, 127.9, 127.6, 114.3, 95.0, 55.5, 55.3, 50.4, 34.5. HRMS (ESI$^+$) calculated for $C_{19}H_{19}NNaO_3$ (M+Na$^+$) 332.1263; found 332.1262.



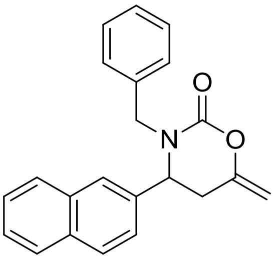
4-(3-benzyl-6-methylene-2-oxo-1,3-oxazinan-4-yl)benzonitrile (2h)

Colorless viscous liquid, 30 mg, yield 99%, ^{1}H NMR (400 MHz, Chloroform-*d*) 7.68 – 7.66 (d, *J* = 8.0 Hz, 2H), 7.33 – 7.32 (d, *J* = 6.0 Hz, 3H), 7.28 – 7.26 (d, *J* = 8.0 Hz, 2H), 7.22 – 7.20 (t, *J* = 2.0, 7.6 Hz, 2H), 5.28 – 5.25 (d, *J* = 14.8 Hz, 1H), 4.73 (s, 1H), 4.51 – 4.49 (dd, *J* = 1.6, 6.0 Hz, 1H), 4.06 (s, 1H), 3.74 – 3.71 (d, *J* = 14.8 Hz, 1H), 2.94 – 2.89 (dd, *J* = 6.0, 14.0 Hz, 1H), 2.48 – 2.44 (dd, *J* = 2.0, 14.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.1, 149.2, 144.2, 135.6, 132.7, 128.9, 128.3, 127.1, 118.2, 112.4, 95.7, 56.0, 51.2, 34.0. HRMS (ESI$^+$) calculated for $C_{19}H_{16}N_2NaO_2$ (M+Na$^+$) 327.1109; found 327.1106.



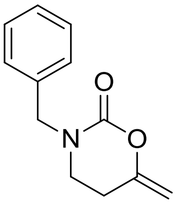
3-benzyl-4-(3-bromophenyl)-6-methylene-1,3-oxazinan-2-one (2i)

Colorless liquid, 36 mg, yield 99%, ^{1}H NMR (400 MHz, Chloroform-*d*) 7.47 – 7.45 (d, 1H), 7.36 – 7.22 (m, 7H), 7.10 – 7.08 (d, *J* = 7.6 Hz, 1H), 5.31 – 5.27 (d, *J* = 15.2 Hz, 1H), 4.74 (s, 1H), 4.40 – 4.38 (dd, *J* = 2.4, 6.0 Hz, 1H), 4.07 – 4.06 (t, *J* = 2 Hz, 1H), 3.71 – 3.67 (d, *J* = 15.2 Hz, 1H), 2.89 – 2.84 (dd, *J* = 6.4, 14.4 Hz, 1H), 2.49 – 2.44 (dd, *J* = 2.4, 14.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.3, 149.5, 141.1, 135.9, 131.6, 130.5, 129.5, 128.9, 128.2, 128.1, 124.9, 123.1, 95.5, 55.6, 50.9, 34.2. HRMS (ESI$^+$) calculated for $C_{18}H_{16}BrNNaO_2$ (M+Na$^+$) 380.0262; found 380.0260.



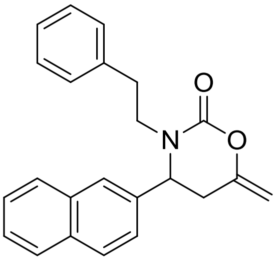
3-benzyl-6-methylene-4-(naphthalen-2-yl)-1,3-oxazinan-2-one (2j)

Colorless liquid, 31 mg, yield 93%, ^{1}H NMR (400 MHz, Chloroform-*d*) 7.91 – 7.89 (q, 1H), 7.83 – 7.81 (d, *J* = 8.4 Hz, 1H), 7.69 – 7.67 (q, 1H), 7.51 – 7.47 (m, 3H), 7.34 –7.28 (m, 4H), 7.22 – 7.20 (q, *J* = 3.2, 2.0 Hz, 2H), 5.42 – 5.38 (d, *J* = 15.2 Hz, 1H), 5.27 – 5.26 (d, *J* = 4.8 Hz, 1H), 4.62 (s, 1H), 3.83 (s, 1H), 3.68– 3.64 (d, *J* = 15.2 Hz, 1H), 2.98 – 2.93 (m, 1H), 2.67 – 2.63 (dd, *J* = 1.2, 14.0 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 152.0, 150.1, 136.4, 134.1, 133.0, 130.0, 129.5, 128.9, 128.9, 128.3, 128.0, 126.8, 125.9, 125.4, 123.7, 121.5, 95.4, 52.7, 51.0, 33.1. HRMS (ESI$^+$) calculated for $C_{22}H_{20}NO_2$ (M+H$^+$) 330.1494; found 330.1493.



3-benzyl-6-methylene-1,3-oxazinan-2-one (2k)

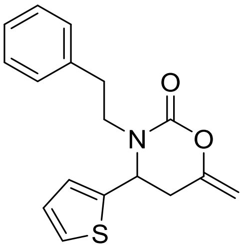
Colorless liquid, 20 mg, yield 99%, ^{1}H NMR (400 MHz, Chloroform-*d*) 7.37 – 7.27 (m, 5H), 4.67 (s, 1H), 4.59 (s, 2H), 4.24 (s, 1H), 3.23 – 3.20 (t, *J* = 6.4 Hz, 2H), 2.56 – 2.53 (t, *J* = 6.0 Hz, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 152.7, 151.2, 136.2, 128.8, 128.1, 127.9, 92.9, 52.7, 43.2, 26.2.[6]



6-methylene-4-(naphthalen-2-yl)-3-phenethyl-1,3-oxazinan-2-one (2l)

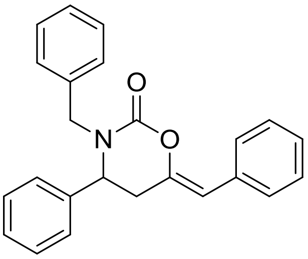
Colorless liquid, 31 mg, yield 91%, ^{1}H NMR (400 MHz, Chloroform-*d*) 7.91 – 7.88 (q, 1H), 7.80 – 7.78 (d, *J* = 8.4 Hz, 1H), 7.52 – 7.50 (q, 2H), 7.47 – 7.41 (m, 2H), 7.35

–7.29 (m, 3H), 7.22 – 7.19 (q, 3H), 4.80 – 4.79 (d, *J* = 4.8 Hz, 1H), 4.58 (s, 1H), 4.16 – 4.10 (m, 1H), 3.80 (s, 1H), 3.14 – 3.06 (m, 1H), 2.94 – 2.79 (m, 3H), 2.50 – 2.47 (d, *J* = 14.0 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 152.0, 150.1, 136.4, 134.1, 133.0, 130.0, 129.5, 128.9, 128.9, 128.3, 128.0, 126.8, 125.9, 125.4, 123.7, 121.5, 95.4, 55.3, 50.9, 34.1, 32.7. HRMS (ESI$^+$) calculated for $C_{23}H_{21}NNaO_2$ (M+Na$^+$) 366.1470; found 366.1469.



6-methylene-3-phenethyl-4-(thiophen-2-yl)-1,3-oxazinan-2-one (2m)

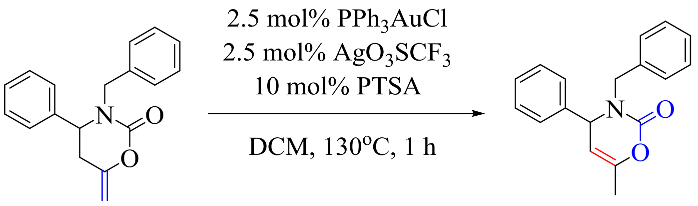
Colorless liquid, 27 mg, yield 90%, m.p. 136.9-137.9℃, ^{1}H NMR (400 MHz, Chloroform-*d*) 7.32 – 7.19 (m, 6H), 6.96 – 6.94 (t, *J* = 3.6 Hz, 1H), 6.86 – 6.85 (d, *J* = 3.2 Hz, 1H), 4.73 (s, 1H), 4.33 – 4.31 (q, *J* = 2.8, 6.0 Hz, 1H), 4.16 (s, 1H), 4.00 – 3.93 (m, 1H), 3.16 – 3.09 (m, 1H), 3.05 – 2.98 (m, 1H), 2.85 – 2.79 (m, 1H), 2.76 – 2.71 (q, *J* = 5.6 Hz, 1H), 2.50 – 2.46 (dd, *J* = 2.8, 14.4 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 150.1, 142.5, 138.7, 128.9, 128.7, 126.9, 126.7, 125.5, 125.4, 95.3, 54.7, 50.5, 34.3, 33.9. HRMS (ESI$^+$) calculated for $C_{17}H_{17}NNaO_2S$ (M+Na$^+$) 322.0878; found 322.0876.



(*Z*)-3-benzyl-6-benzylidene-4-phenyl-1,3-oxazinan-2-one (2n)

Colorless liquid, 15 mg, yield 43%, ^{1}H NMR (400 MHz, Chloroform-*d*) 7.64 – 7.62 (d, *J* = 7.6 Hz, 2H), 7.37 – 7.15 (m, 13H), 5.35 – 5.31 (d, *J* = 15.2 Hz, 1H), 5.22 (s, 1H), 4.47 – 4.45 (q, *J* = 2.4, 6.0 Hz, 1H), 3.73 – 3.69 (d, *J* = 14.8 Hz, 1H), 3.07 – 3.02 (q, *J* = 6.0, 14.0 Hz, 1H), 2.55 – 2.51 (dd, *J* = 2.4, 14.0 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 151.1, 143.2, 138.8, 136.2, 133.7, 129.0, 128.8, 128.4, 128.4 128.3, 127.9, 127.0, 126.5, 126.2, 109.8, 56.5, 50.8, 35.7 . HRMS (ESI$^+$) calculated for $C_{24}H_{21}NNaO_2$ (M+Na$^+$) 378.1470; found 378.1468.

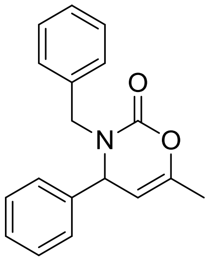
6. The transformation of the 1, 3-oxazin-ones 2a



2a
0.2 mmol

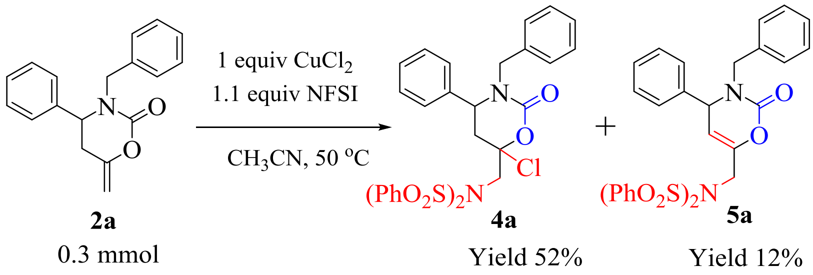
3a
Yield 95%

The Ph_3PAuCl (2.5 mg, 0.005 mmol, 2.5 mol%), AgOTf (1.3 mg, 0.005 mmol, 2.5 mol%), and *p*-toluenesulfonic acid (3.4 mg, 0.02 mmol, 10 mol%) were sequentially added to a stirred solution of the corresponding **2a** (56 mg, 0.2 mmol) in dichloromethane (2 mL). The resulting mixture was heated in a sealed tube at 130 ℃ until disappearance of the starting material (TLC, for about 45 mins). The reaction mixture was cooled to room temperature and filtered through a pack of celite. The filtrate was extracted with dichloromethane (3 × 5 mL), and the combined extracts were washed twice with saturated brine. The organic layer was dried over $MgSO_4$ and concentrated under reduced pressure. Column chromatography isolation of the residue gave the analytically pure adduct **3a** (53 mg, yield 95%).[7]

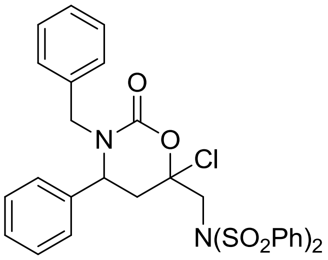


3-benzyl-6-methyl-4-phenyl-3,4-dihydro-2H-1,3-oxazin-2-one (3a)

Colorless liquid, 53 mg, yield 95%, ^{1}H NMR (400 MHz, Chloroform-*d*) 7.32 – 7.21 (m, 6H), 7.16 – 7.13 (t, *J* = 7.2 Hz, 4H), 5.19 – 5.16 (d, *J* = 14.8 Hz, 1H), 4.73 – 4.72 (d, *J* = 3.6 Hz, 1H), 4.58 – 4.57 (d, *J* = 2.8 Hz, 1H), 3.52 – 3.48 (d, *J* = 15.2 Hz, 1H), 1.81 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.0, 146.3, 140.3, 135.7, 129.1, 128.7, 128.6, 128.4, 127.9, 127.1, 100.3, 58.3, 48.8, 18.4. HRMS (ESI$^+$) calculated for $C_{18}H_{18}NO_2$ (M+H$^+$) 280.1338; found 280.1335.

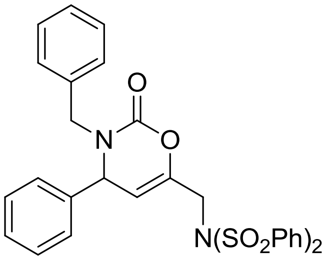


To a Schlenk tube was added NFSI (142 mg, 0.45 mmol, 1.5 equiv), CuCl (3 mg, 0.03 mmol, 0.1 equiv) and $CuCl_2$ (40 mg, 0.3 mmol, 1.0 equiv) under N_2 atmosphere. Then **2a** (0.3 mmol, 84mg, 1.0 equiv) and CH_3CN (1.5 mL) were sequentially added into a Schlenk tube. The reaction mixture was stirred at 60 °C for about 1 h until complete disappearance of **2a** (monitored by TLC). The mixture was passed through a short Al_2O_3 column by using CH_2Cl_2 as elution and concentrated in vacuo, and purified by flash chromatography on silica gel (gradient elution of EtOAc/petroleum ether, PE/EA=10:1).[8]



N-((3-benzyl-6-chloro-2-oxo-4-phenyl-1,3-oxazinan-6-yl)methyl)-N-(phenylsulfonyl)benzenesulfonamide (4a)

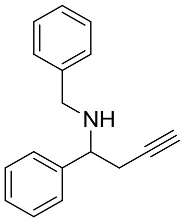
Colorless liquid, 95 mg, yield 52%, ^{1}H NMR (400 MHz, Chloroform-*d*) 8.17 – 8.16 (d, *J* = 4.4 Hz, 4H), 7.75 – 7.71 (t, *J* = 7.2 Hz, 2H), 7.64 – 7.60 (t, *J* = 7.6 Hz,4H), 7.33 – 7.25 (m, 6H), 7.02 (s, 2H), 6.64 – 6.62 (d, *J* = 6.8 Hz, 2H), 5.08 – 5.04 (d, *J* = 14.8 Hz, 1H), 4.82 – 4.78 (d, *J* = 16 Hz, 1H), 4.46 – 4.42 (dd, *J* = 5.6, 11.2 Hz, 1H), 4.37 – 4.33 (d, *J* = 16 Hz, 1H), 3.45 – 3.42 (d, *J* = 10.8 Hz, 1H), 2.59 – 2.54 (dd, *J* = 5.6, 14.8 Hz, 1H), 1.98 – 1.92 (dd, *J* = 11.6, 14.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.2, 139.8, 137.6, 135.2, 134.1, 129.2, 129.1, 128.8, 128.5, 128.4, 127.8, 127.3, 127.2, 98.0, 58.0, 55.7, 49.1, 40.1. HRMS (ESI^+) calculated for $C_{30}H_{27}ClN_2NaO_6S_2$ ($M+Na^+$) 633.0897; found 633.0895.



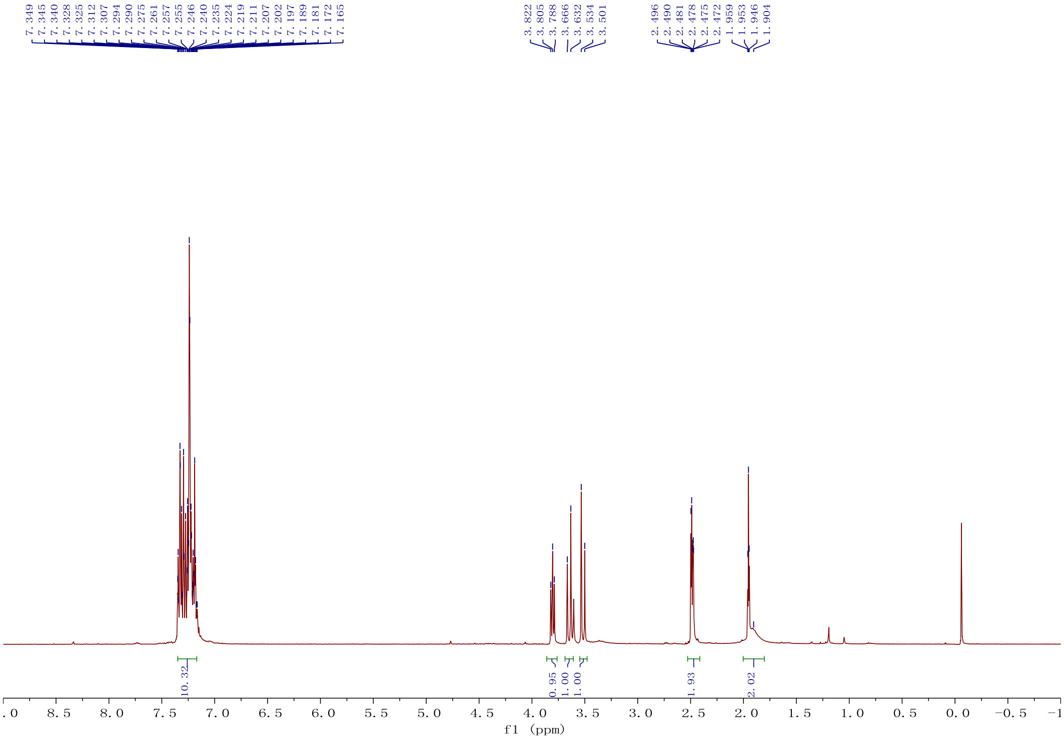
N-((3-benzyl-2-oxo-4-phenyl-3,4-dihydro-2*H*-1,3-oxazin-6-yl)methyl)-*N*-(phenylsulfonyl)benzenesulfonamide (5a)

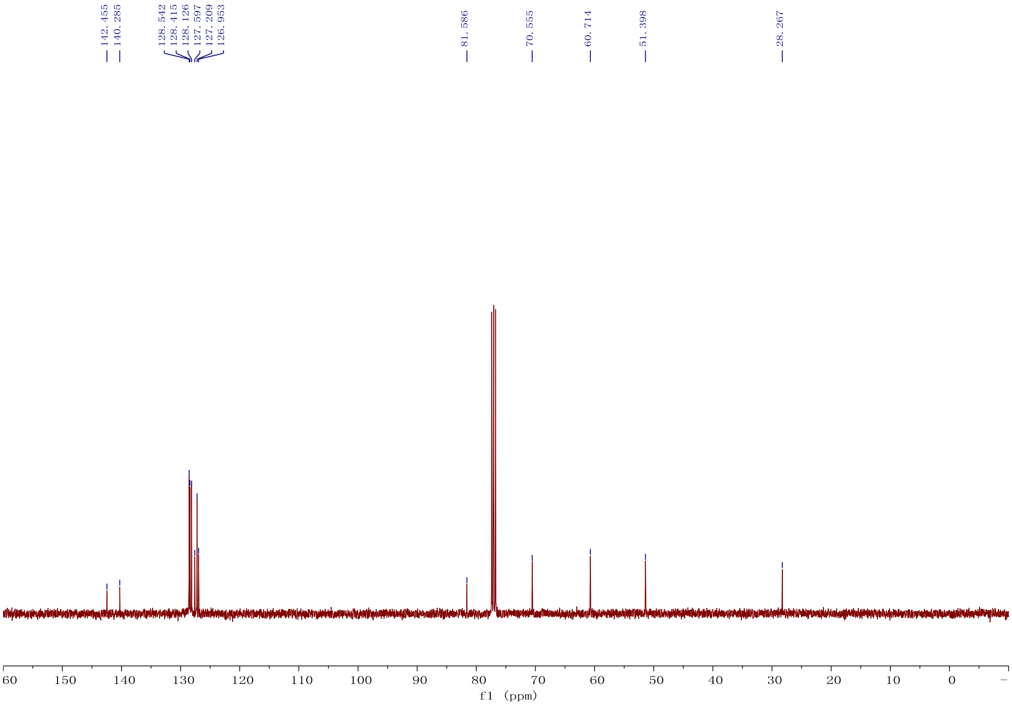
Colorless liquid, 21 mg, yield 12%, ^{1}H NMR (400 MHz, Chloroform-*d*) 7.98 – 7.96 (d, *J* = 8.0 Hz, 4H), 7.57 – 7.53 (t, *J* = 7.6 Hz, 2H), 7.43 – 7.34 (m, 10H), 7.21 – 7.15 (m, 4H), 5.20 – 5.16 (d, *J* = 15.2 Hz, 1H), 4.87 – 4.86 (d, *J* = 4 Hz, 1H), 4.60 – 4.59 (d, *J* = 4 Hz, 1H), 4.52 – 4.47 (d, *J* = 18.0 Hz, 1H), 4.37 – 4.32 (d, *J* = 18 Hz, 1H), 3.56 – 3.52 (d, *J* = 13.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.7, 143.8, 139.2, 138.9, 135.2, 134.1, 129.3, 129.0, 128.9, 128.8, 128.55, 128.54, 128.1, 127.3, 102.3, 58.3, 48.9, 47.5 . HRMS (ESI^{+}) calculated for $C_{30}H_{26}N_2NaO_6S_2$ (M+Na^{+}) 597.1130; found 597.1128.

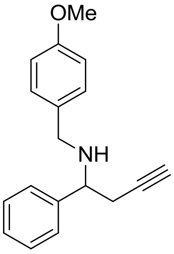
7. The spectra of homopropargylamines 1 and 1n



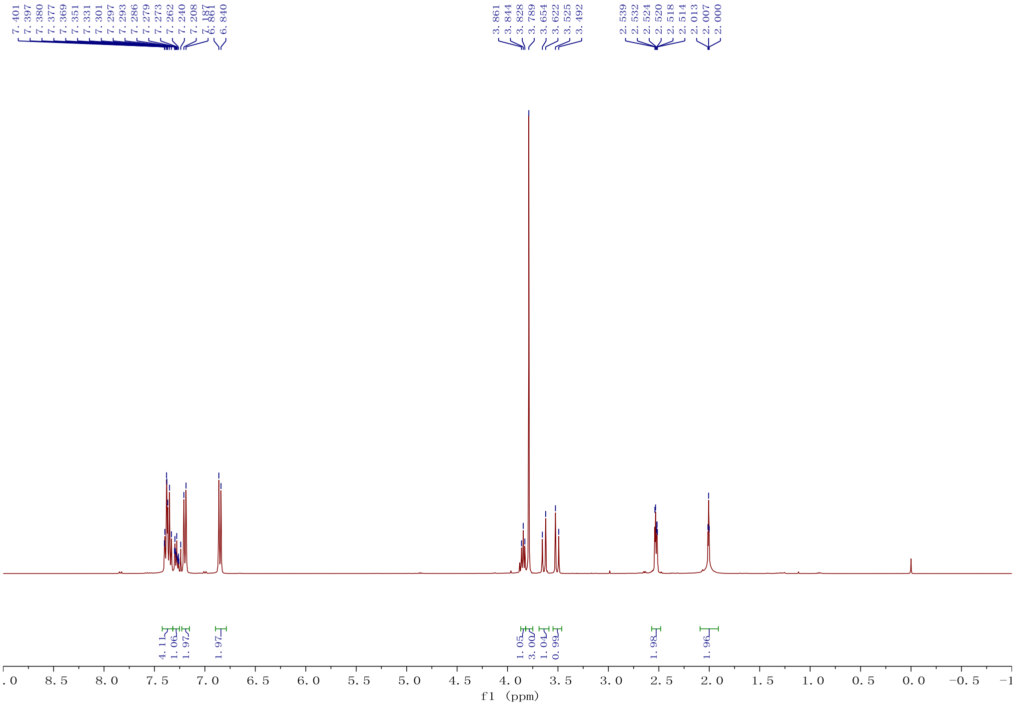
1a






OMe
NH

1b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7.240
7.208
7.187
6.861
6.840
3.861
3.844
3.828
3.789
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3.622
3.525
3.492
2.539
2.532
2.524
2.520
2.518
2.514
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2.007
2.000
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1.97
1.97
1.05
3.00
1.04
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1.98
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6.0
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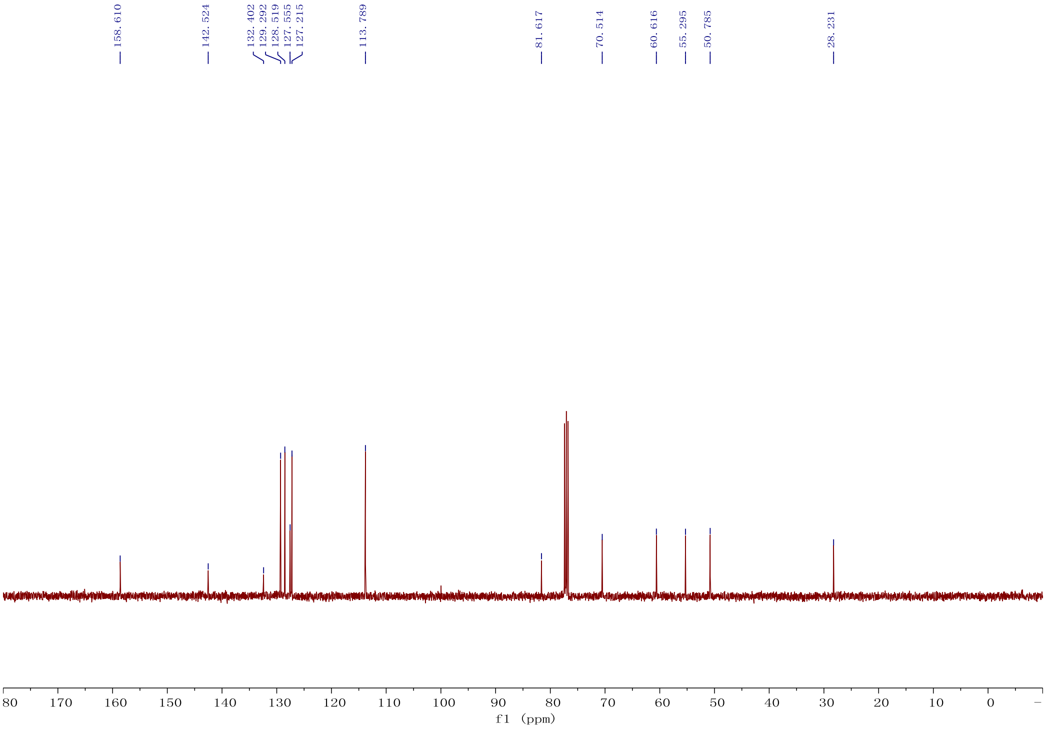
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28.231
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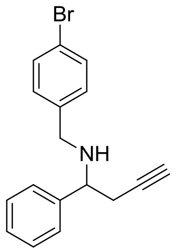
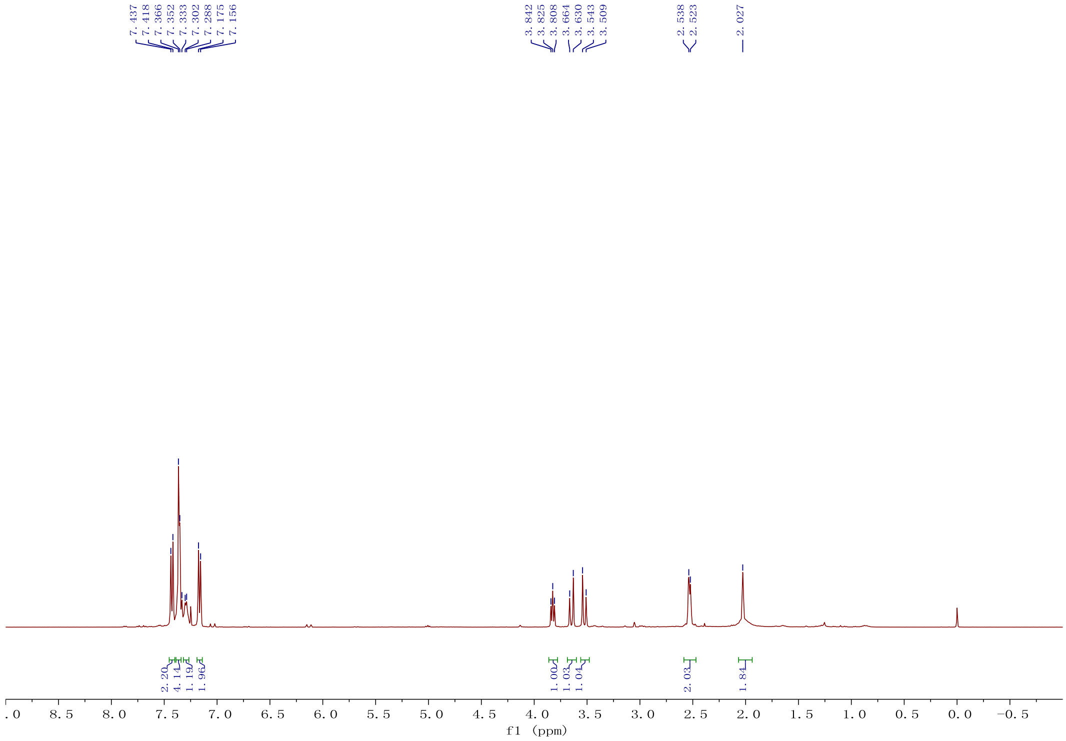
f1 (ppm)


Br
NH

1c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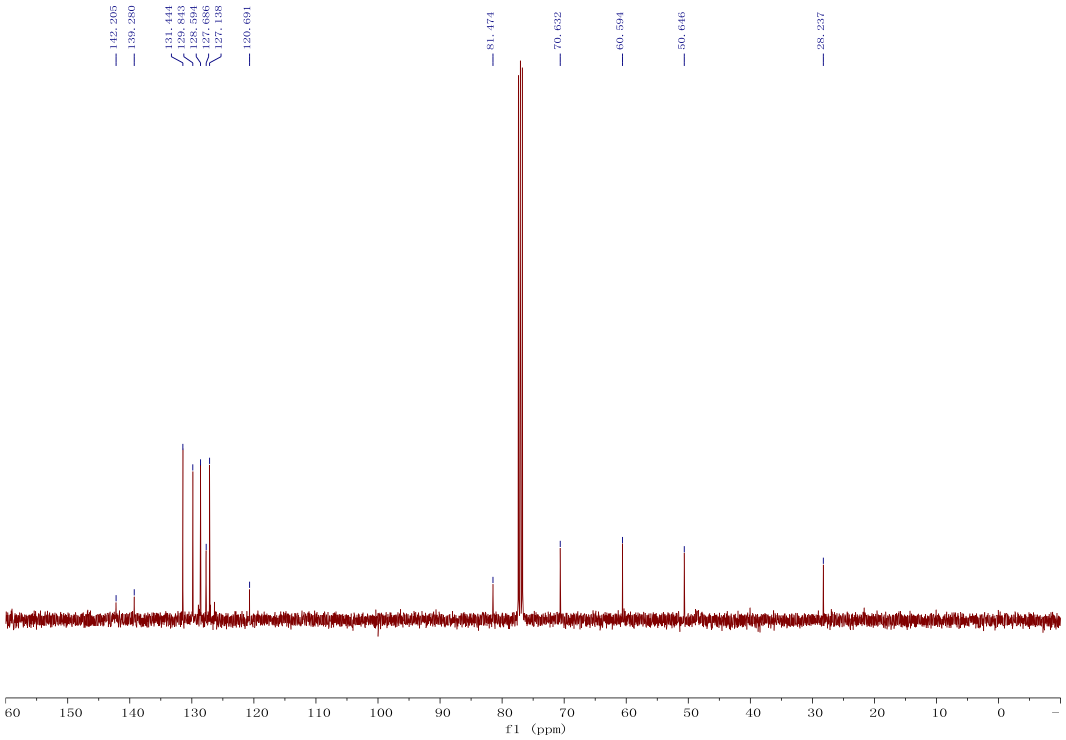
f1 (ppm)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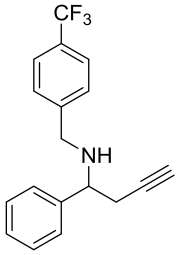
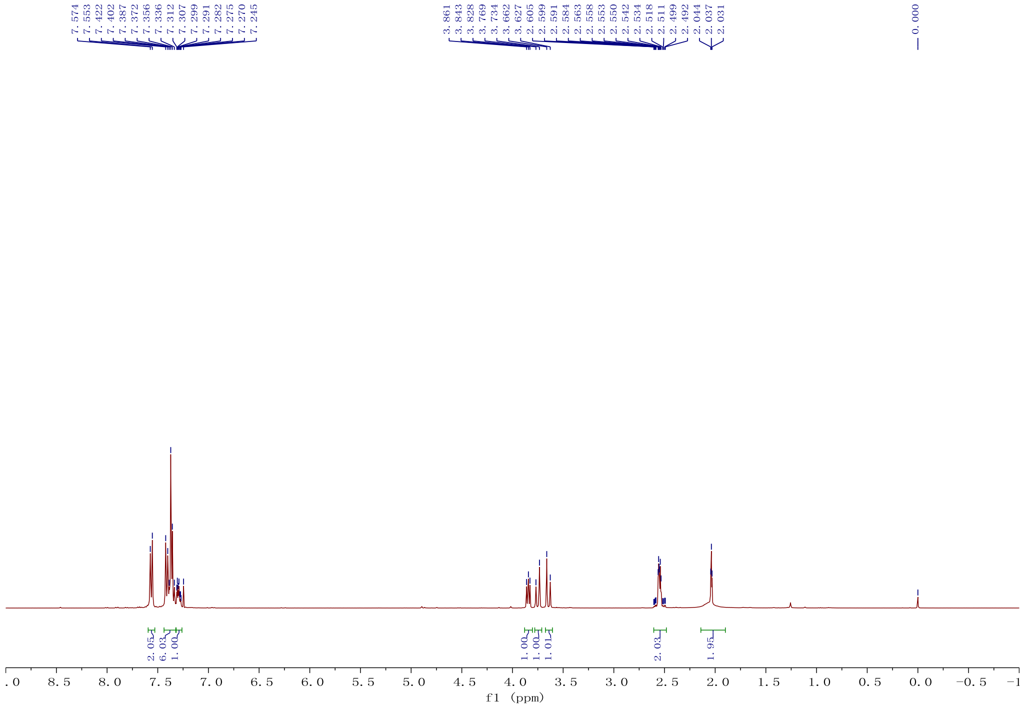
f1 (ppm)


CF3
NH

1d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7.270
7.245
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3.843
3.828
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3.734
3.662
3.627
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2.599
2.591
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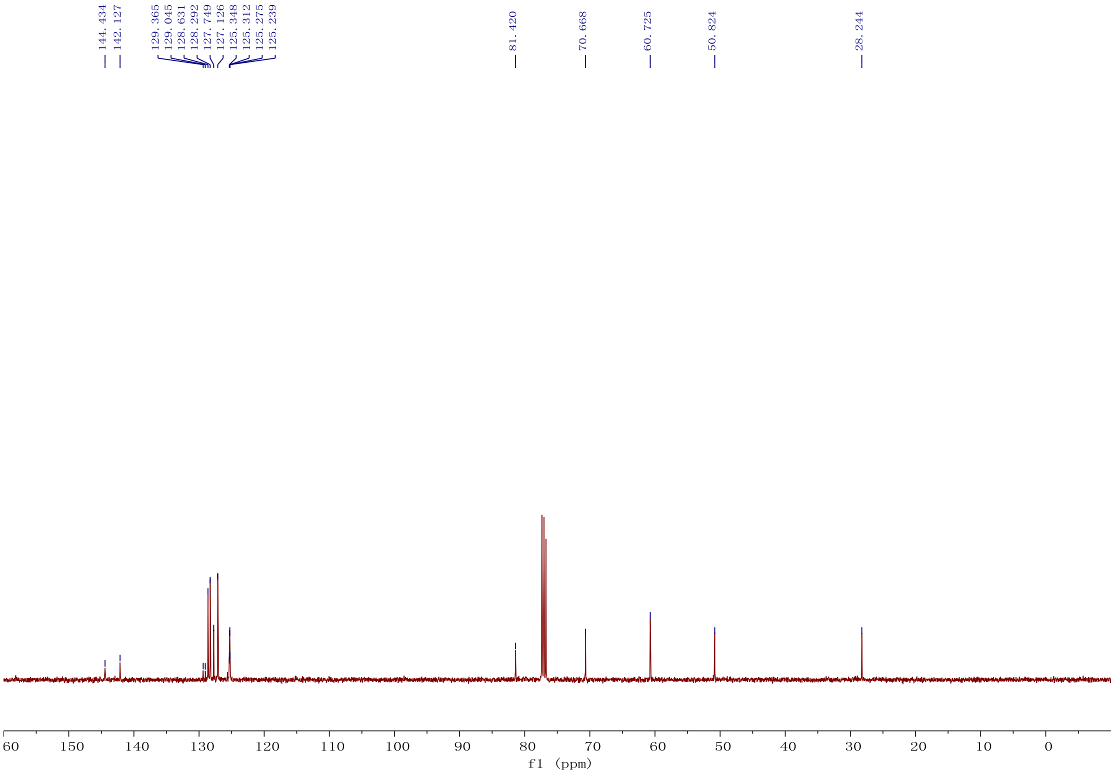
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70.668
60.725
50.824
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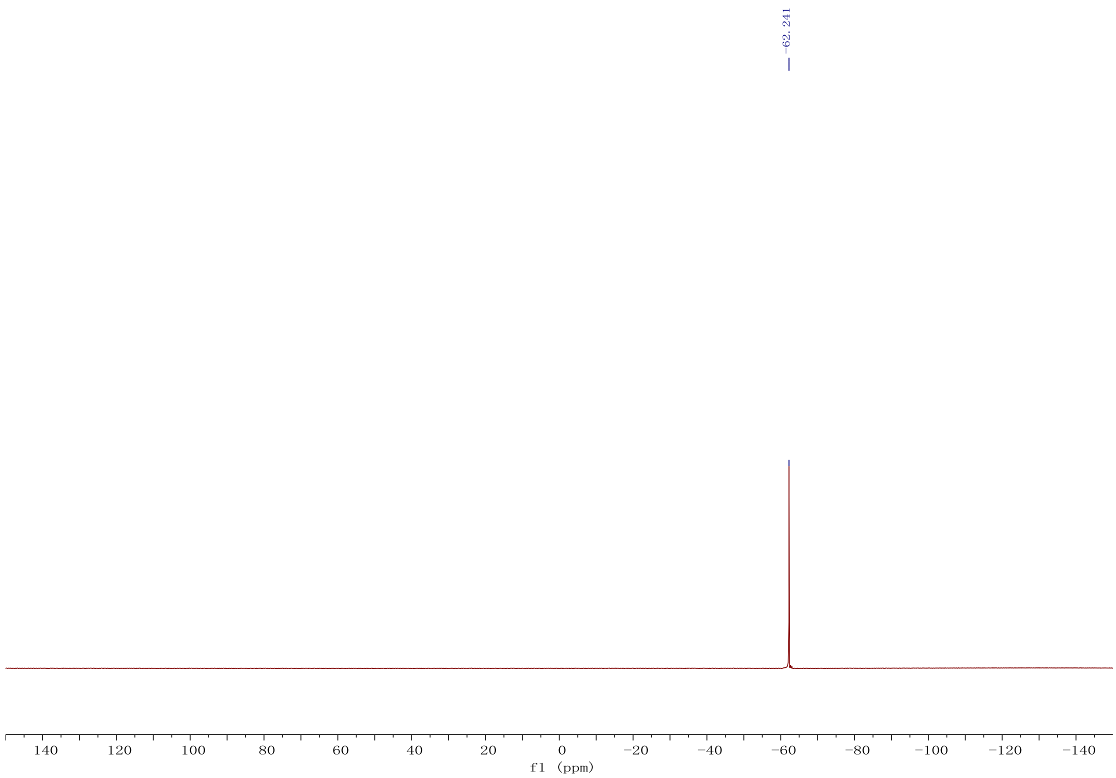
f1 (ppm)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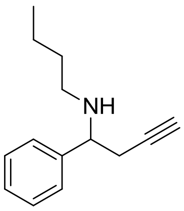
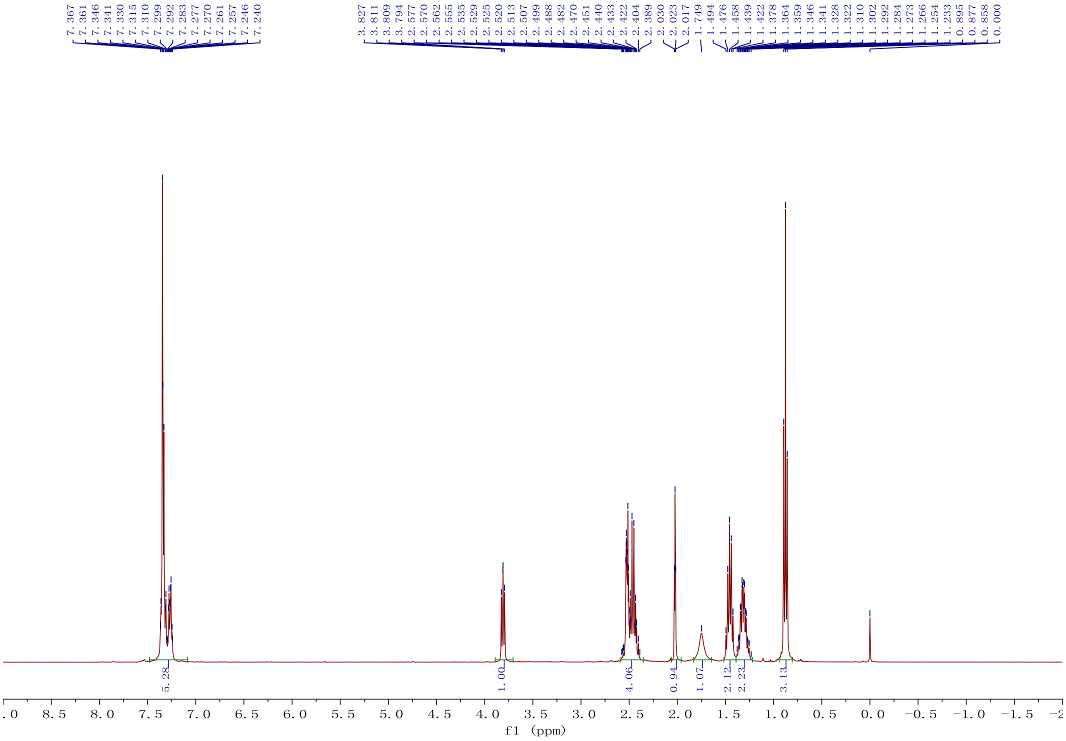
f1 (ppm)


NH

1e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2.513
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2.422
2.404
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2.023
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1.458
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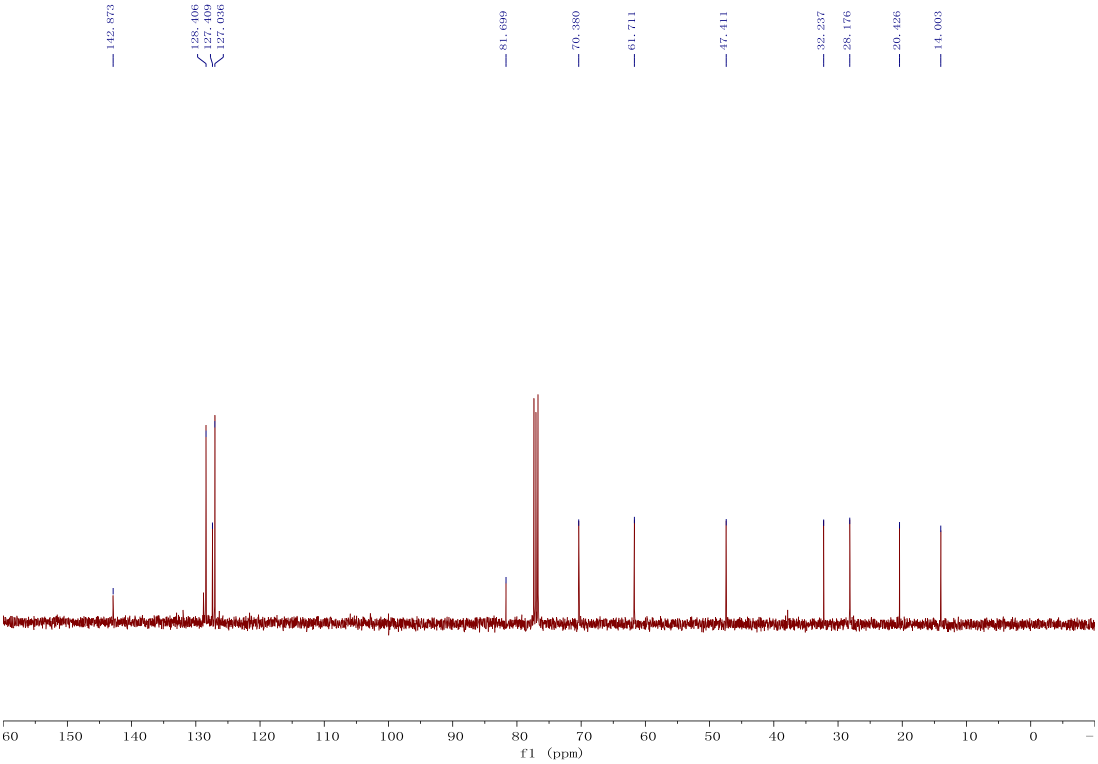
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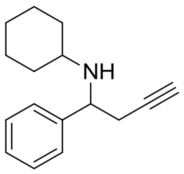
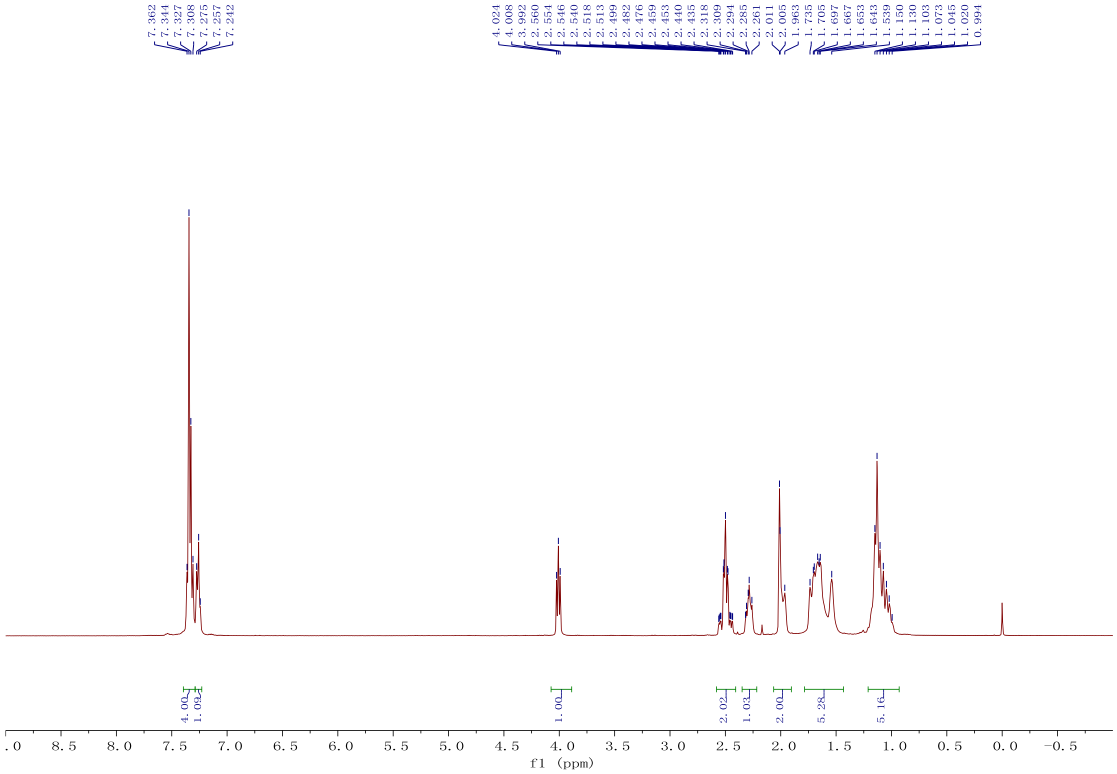
f1 (ppm)


NH

1f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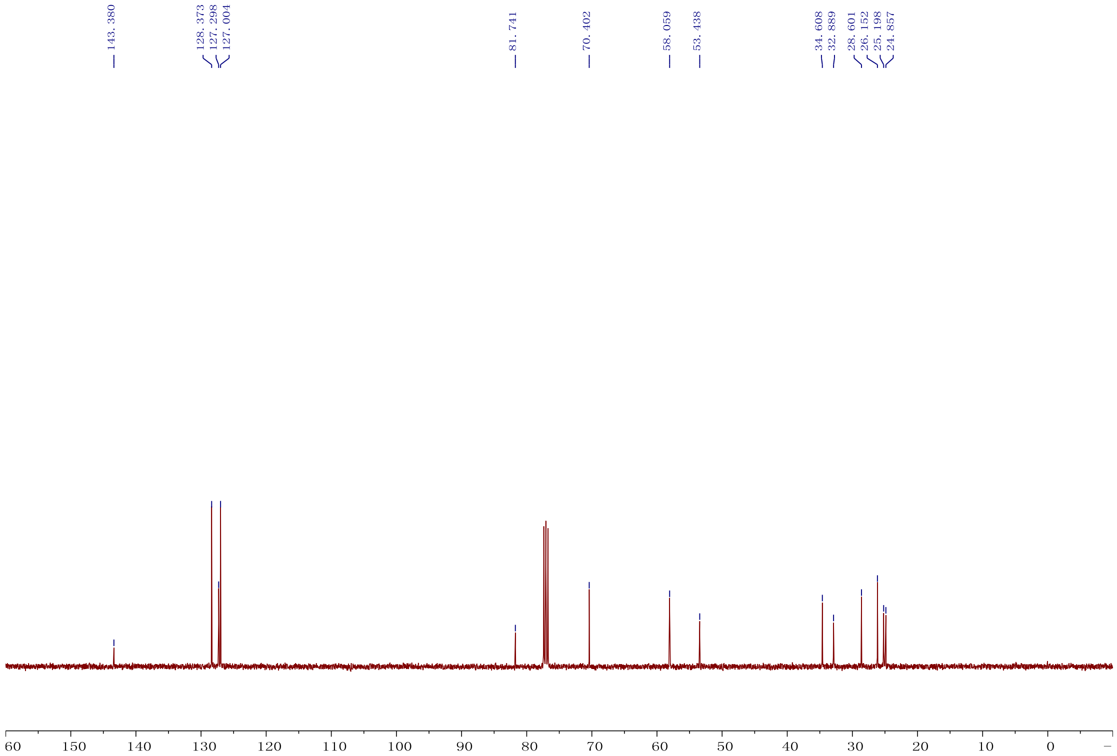
f1 (ppm)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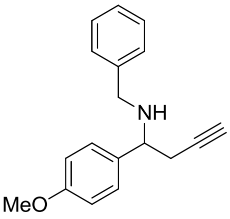
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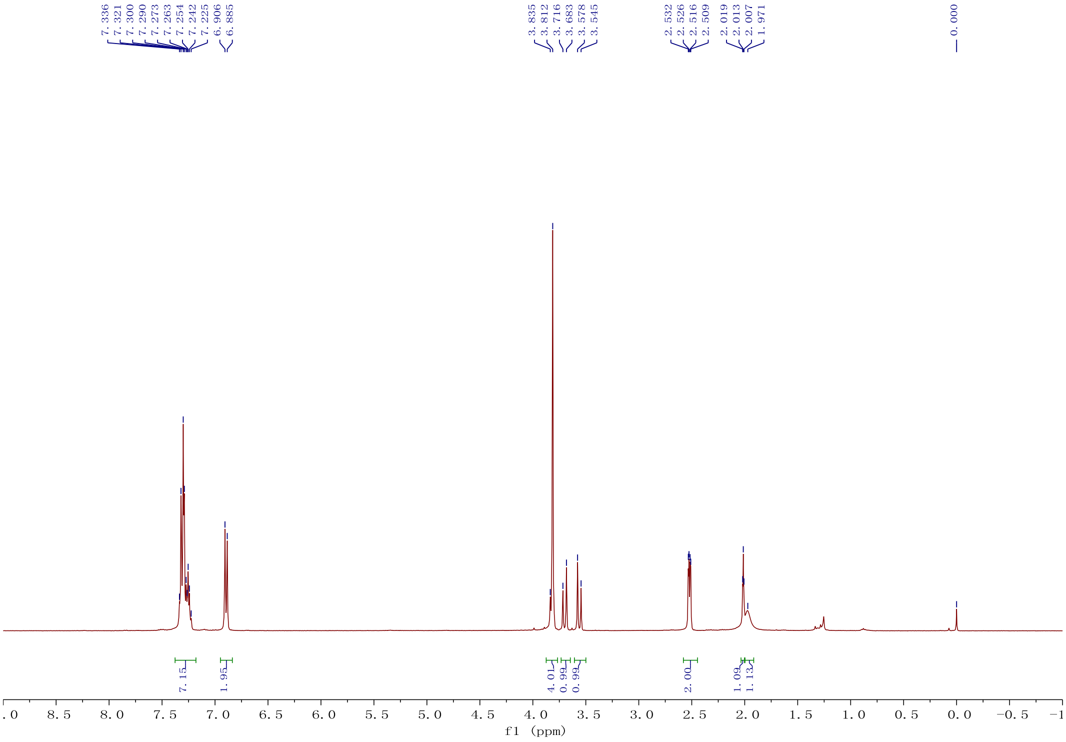
MeO

1g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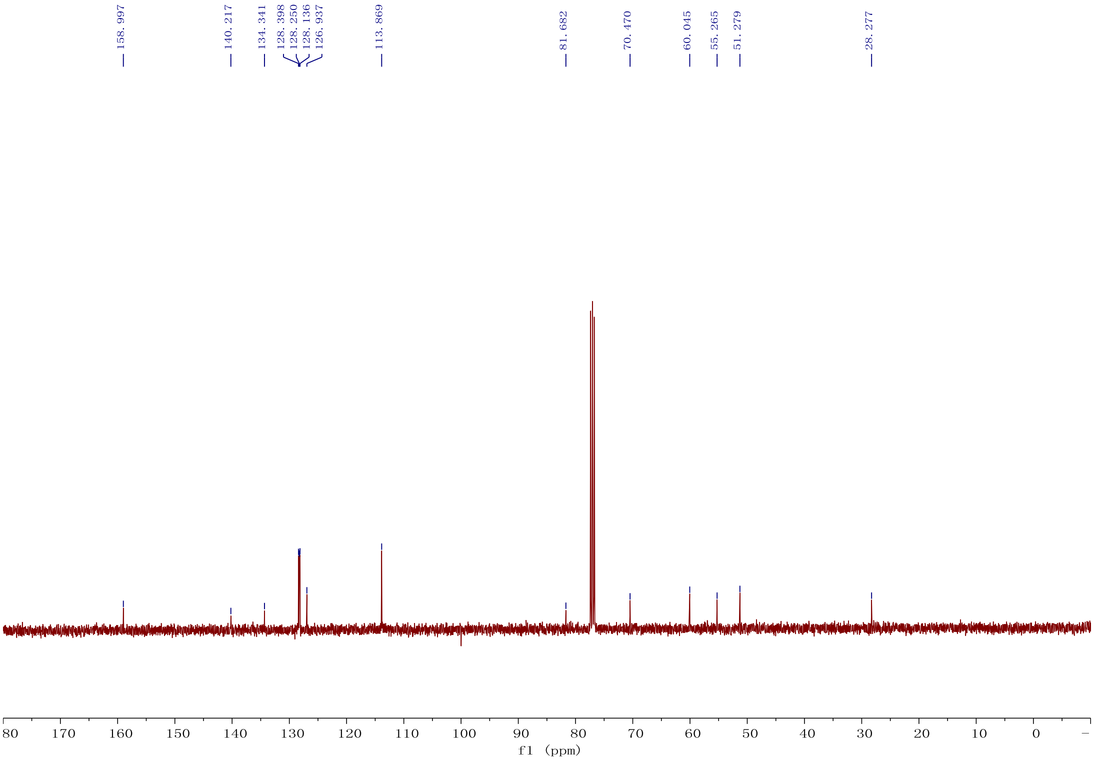
f1 (ppm)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170
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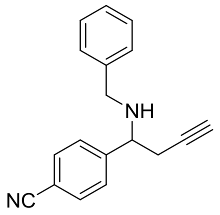
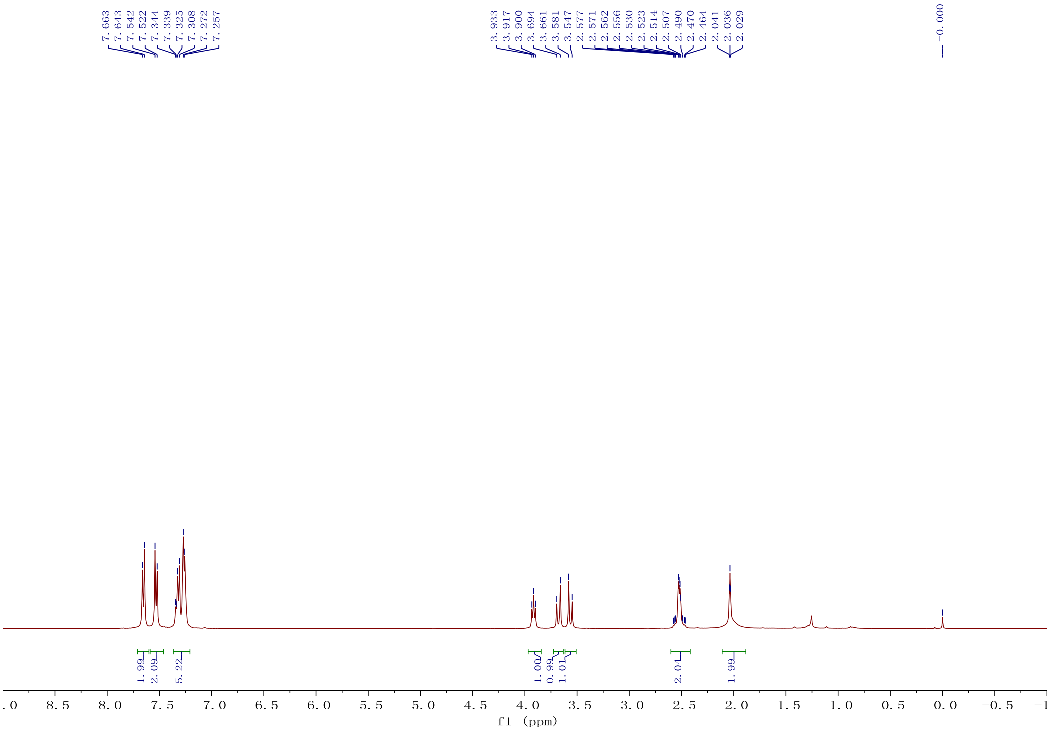
f1 (ppm)


NH
NC

1h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0.99
1.01
2.04
1.99
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4.5
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1.5
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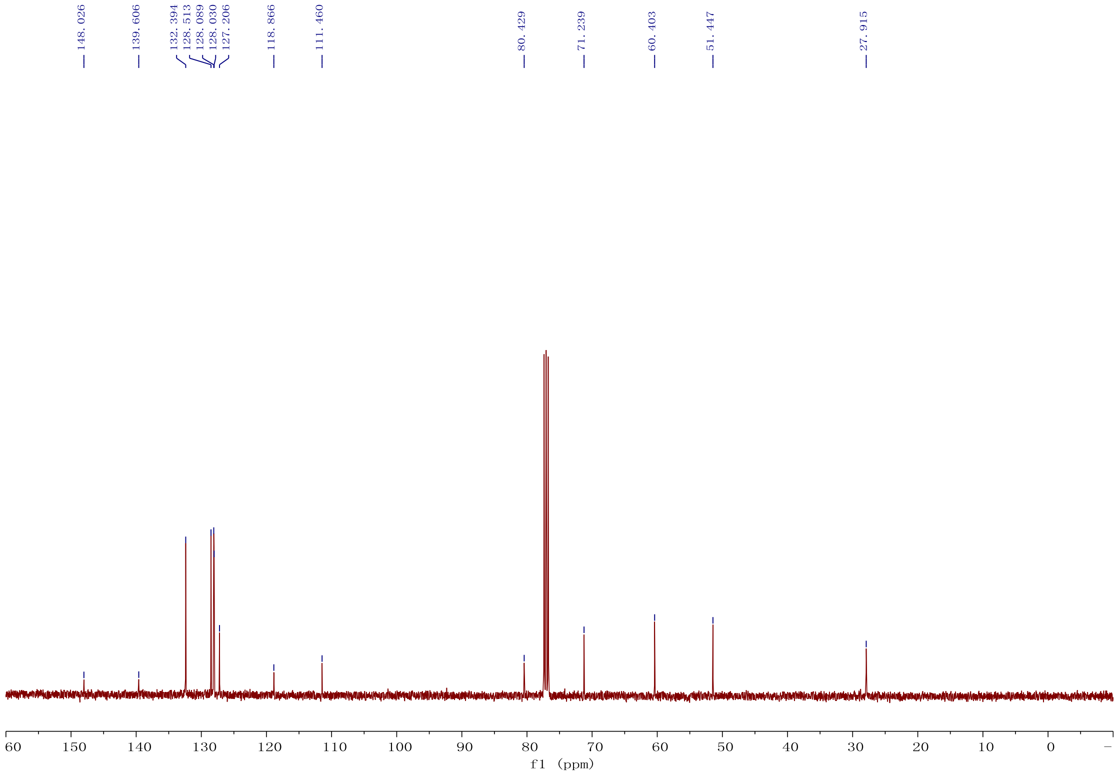
f1 (ppm)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20
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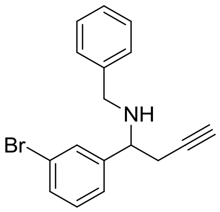
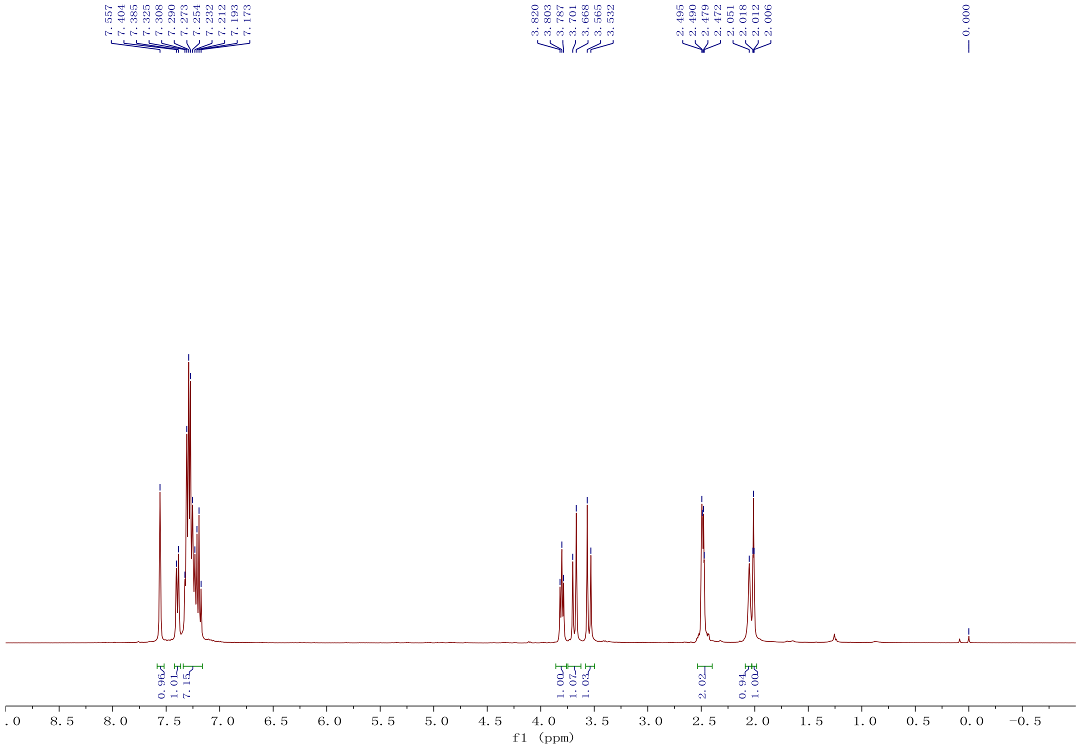
-
f1 (ppm)


NH
Br

1i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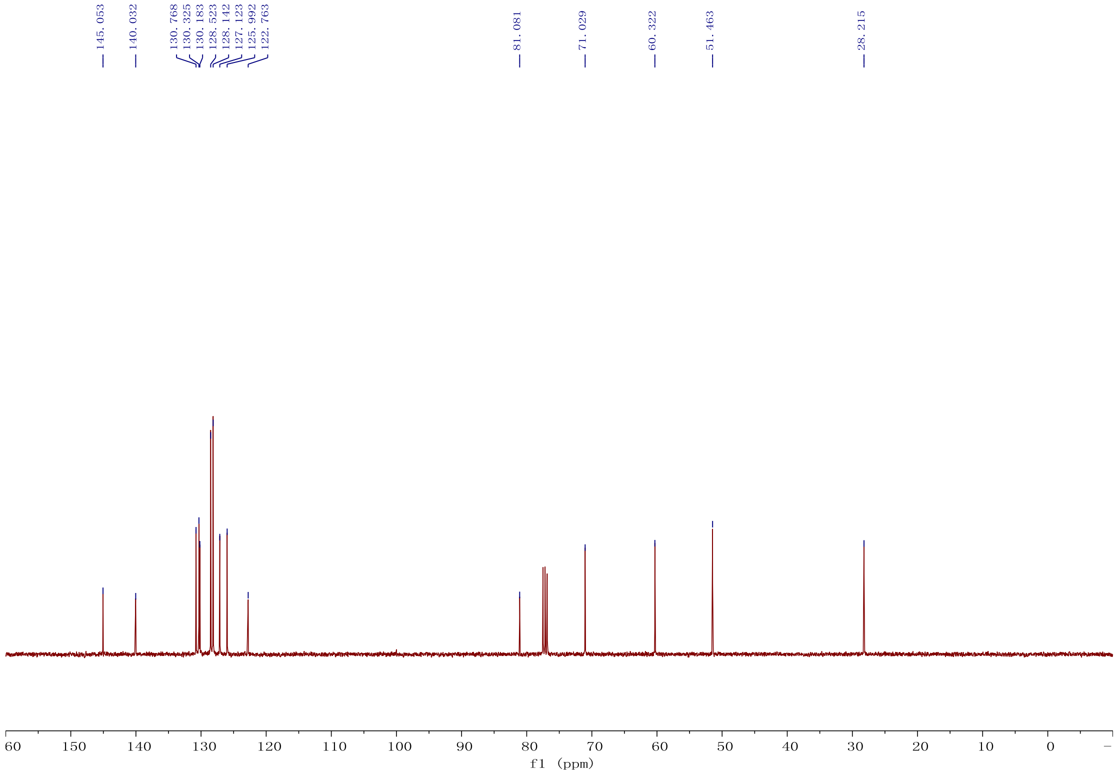
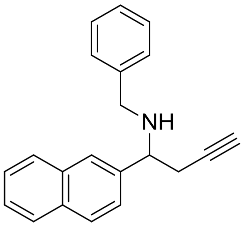
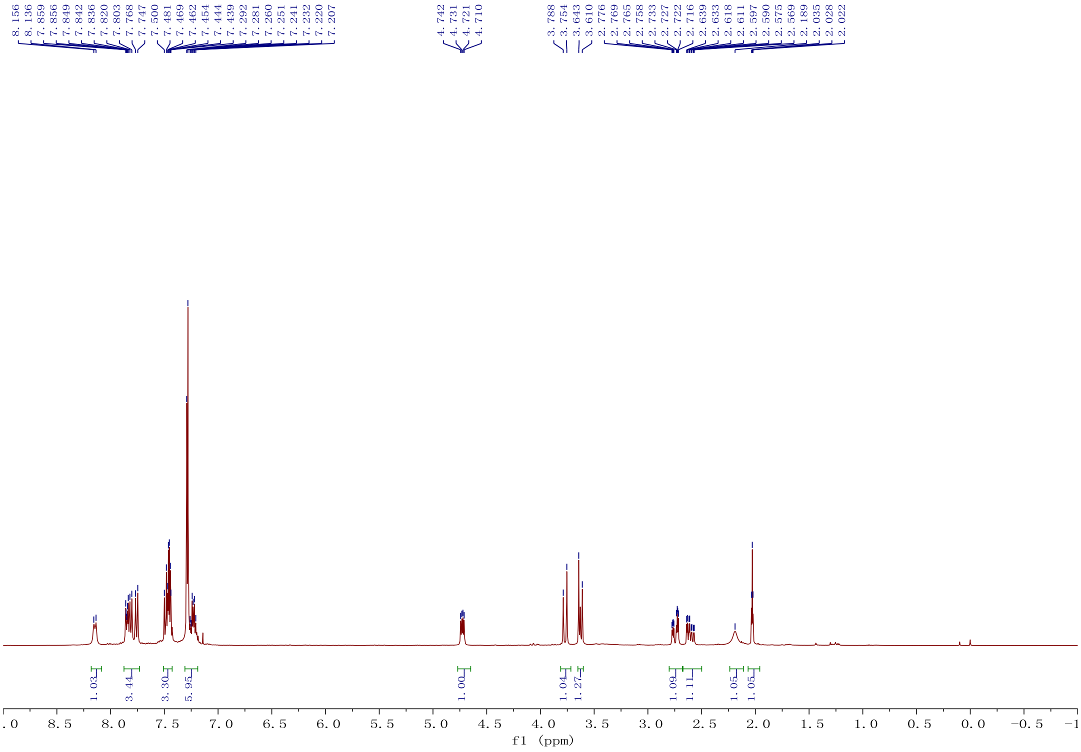
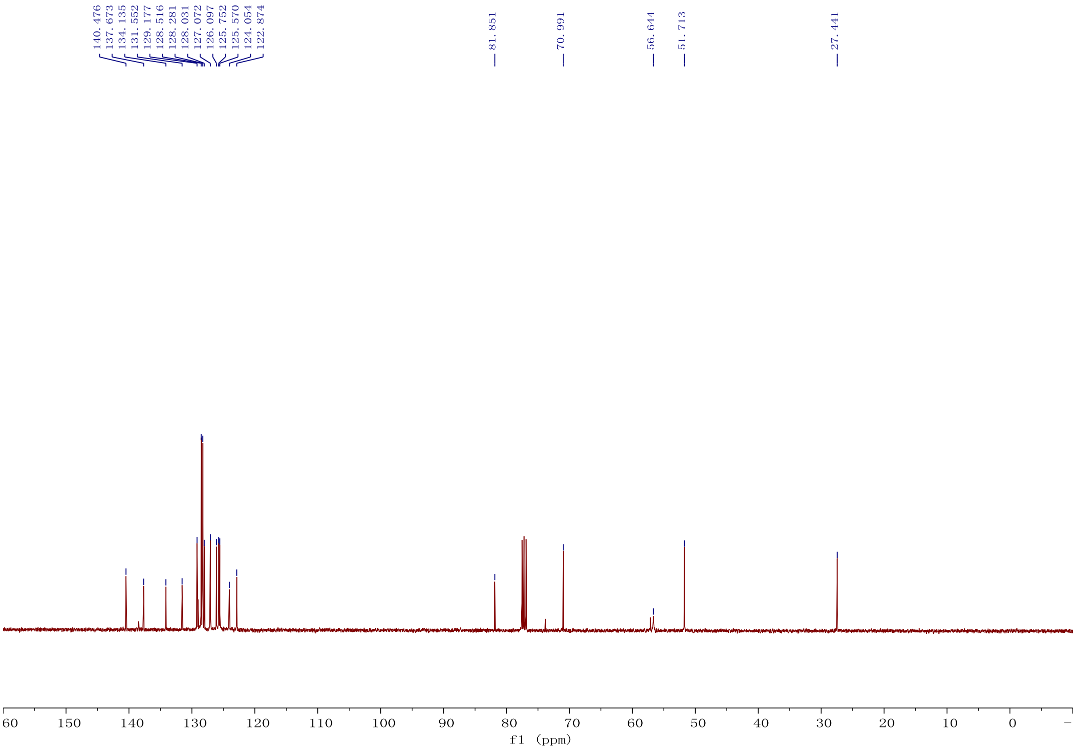
7.404
7.385
7.325
7.308
7.290
7.273
7.254
7.232
7.212
7.193
7.173
3.820
3.803
3.787
3.701
3.668
3.565
3.532
2.495
2.490
2.479
2.472
2.051
2.018
2.012
2.006
0.000
0.96
1.01
7.15
1.00
1.07
1.03
2.02
0.94
1.00
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

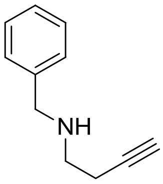

145.053
140.032
130.768
130.325
130.183
128.523
128.142
127.123
125.992
122.763
81.081
71.029
60.322
51.463
28.215
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



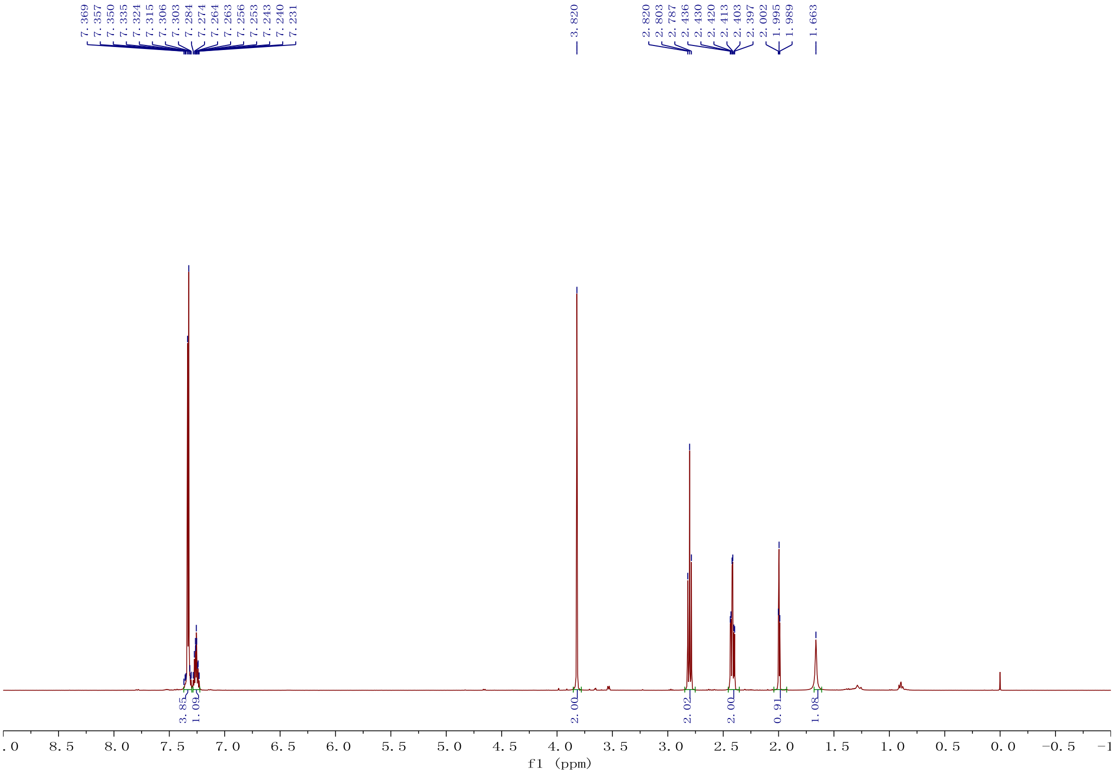
1j

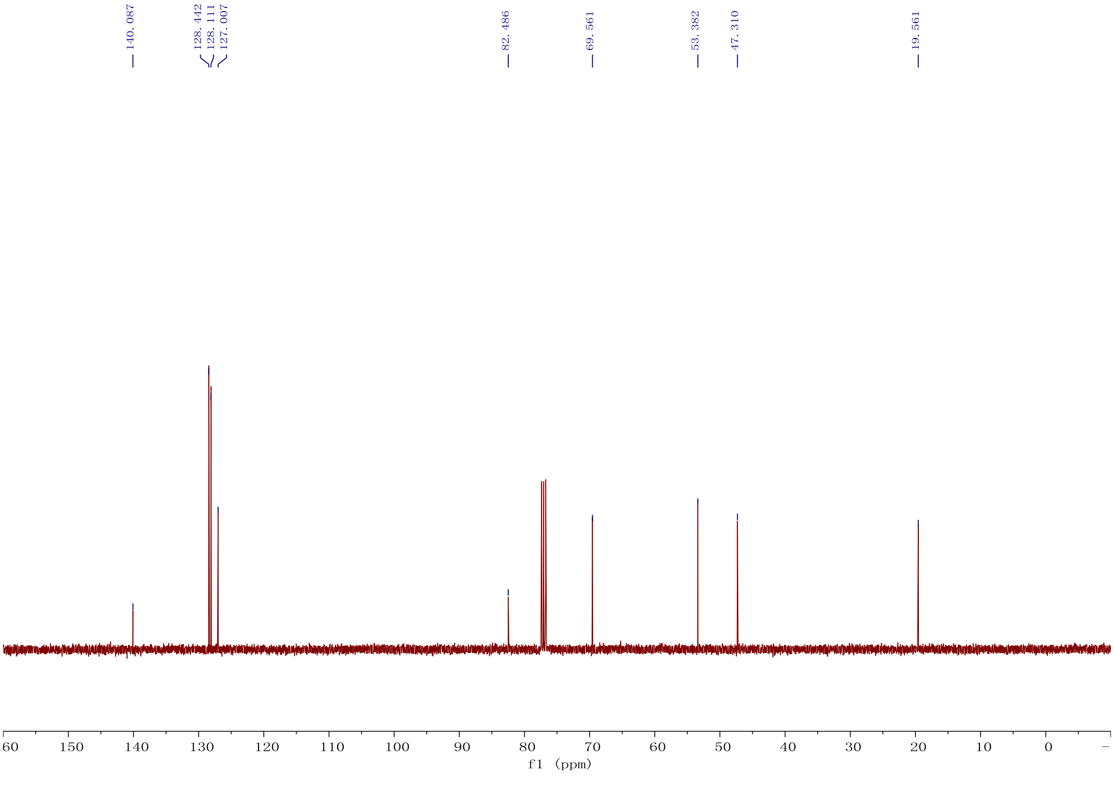

8.156
8.136
7.859
7.856
7.849
7.842
7.836
7.820
7.803
7.768
7.747
7.500
7.481
7.469
7.462
7.454
7.444
7.439
7.292
7.281
7.260
7.251
7.241
7.232
7.220
7.207
4.742
4.731
4.721
4.710
3.788
3.754
3.643
3.610
2.776
2.769
2.765
2.758
2.733
2.727
2.722
2.716
2.639
2.633
2.618
2.611
2.597
2.590
2.575
2.569
2.189
2.035
2.028
2.022
1.03
3.44
3.30
5.95
1.00
1.04
1.27
1.09
1.11
1.05
1.05
.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
−1
f1 (ppm)

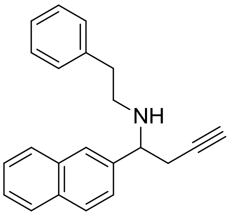

140.476
137.673
134.135
131.552
129.177
128.516
128.281
128.031
127.072
126.097
125.752
125.570
124.054
122.874
81.851
70.991
56.644
51.713
27.441
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


NH

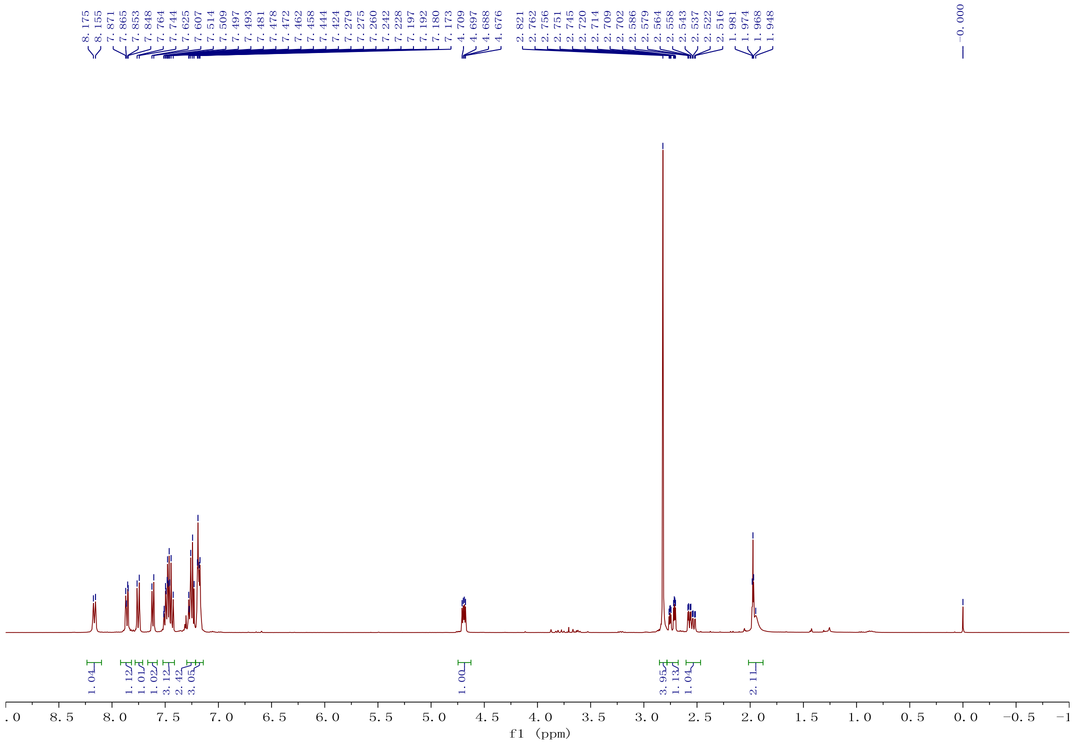
1k

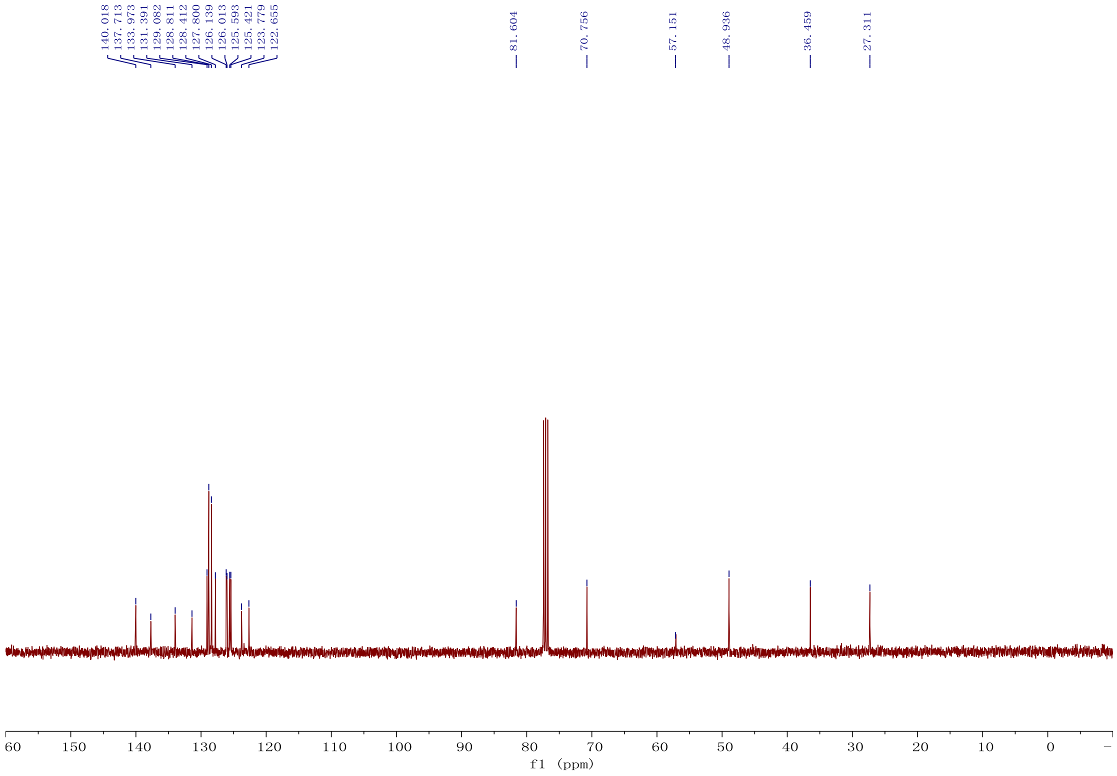

7.369
7.357
7.350
7.335
7.324
7.315
7.306
7.303
7.284
7.274
7.264
7.263
7.256
7.253
7.243
7.240
7.231
3.820
2.820
2.803
2.787
2.436
2.430
2.420
2.413
2.403
2.397
2.002
1.995
1.989
1.663
3.85
1.09
2.00
2.02
2.00
0.91
1.08
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1
f1 (ppm)

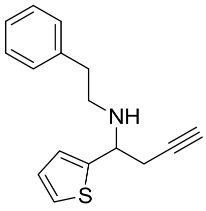

140.087
128.442
128.111
127.007
82.486
69.561
53.382
47.310
19.561
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



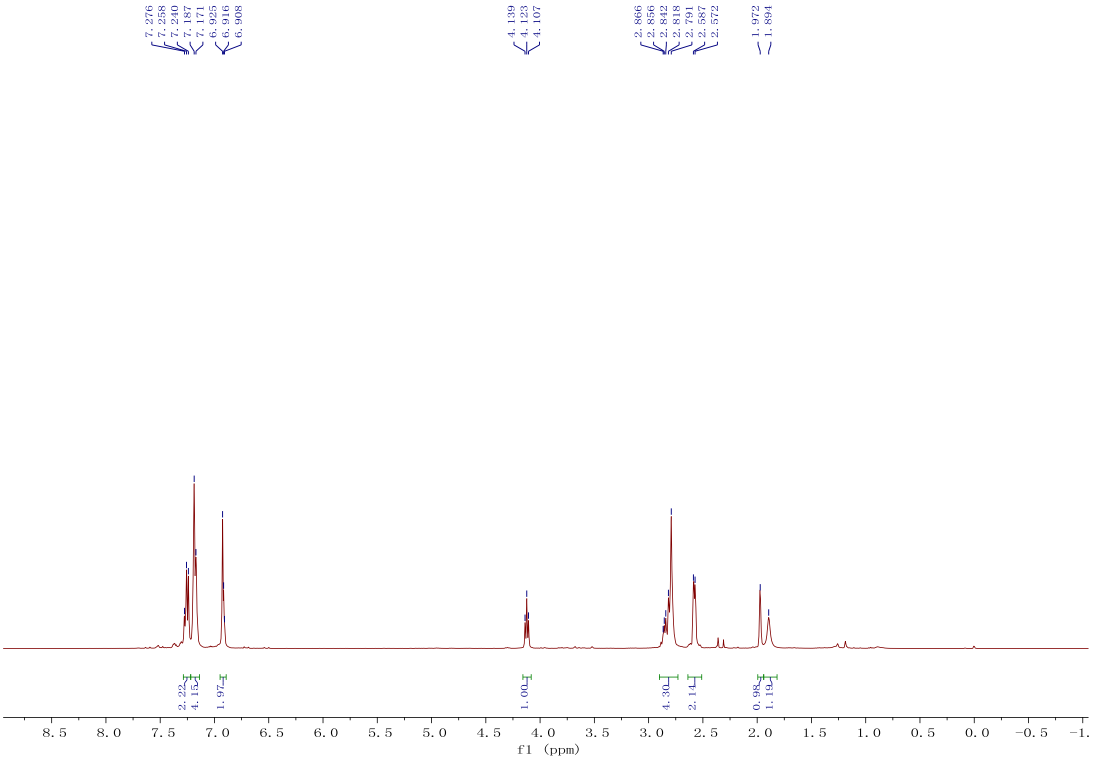
1l

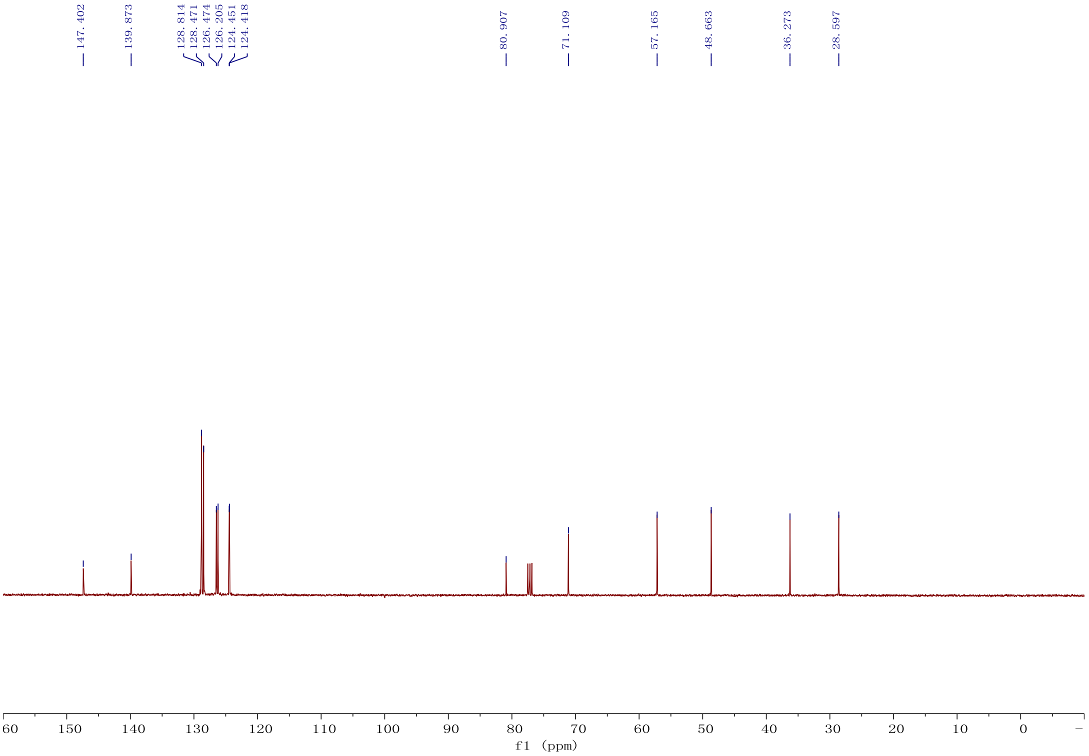

8.175
8.155
7.871
7.865
7.853
7.848
7.764
7.744
7.625
7.607
7.514
7.509
7.497
7.493
7.481
7.478
7.472
7.462
7.458
7.444
7.424
7.279
7.275
7.260
7.242
7.228
7.197
7.192
7.180
7.173
4.709
4.697
4.688
4.676
2.821
2.762
2.756
2.751
2.745
2.720
2.714
2.709
2.702
2.586
2.579
2.564
2.558
2.543
2.537
2.522
2.516
1.981
1.974
1.968
1.948
-0.000
1.04
1.12
1.01
1.02
3.12
2.42
3.05
1.00
3.95
1.13
1.04
2.11
.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
-1
f1 (ppm)

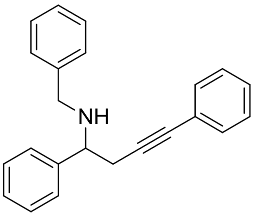

140.018
137.713
133.973
131.391
129.082
128.811
128.412
127.800
126.139
126.013
125.593
125.421
123.779
122.655
81.604
70.756
57.151
48.936
36.459
27.311
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



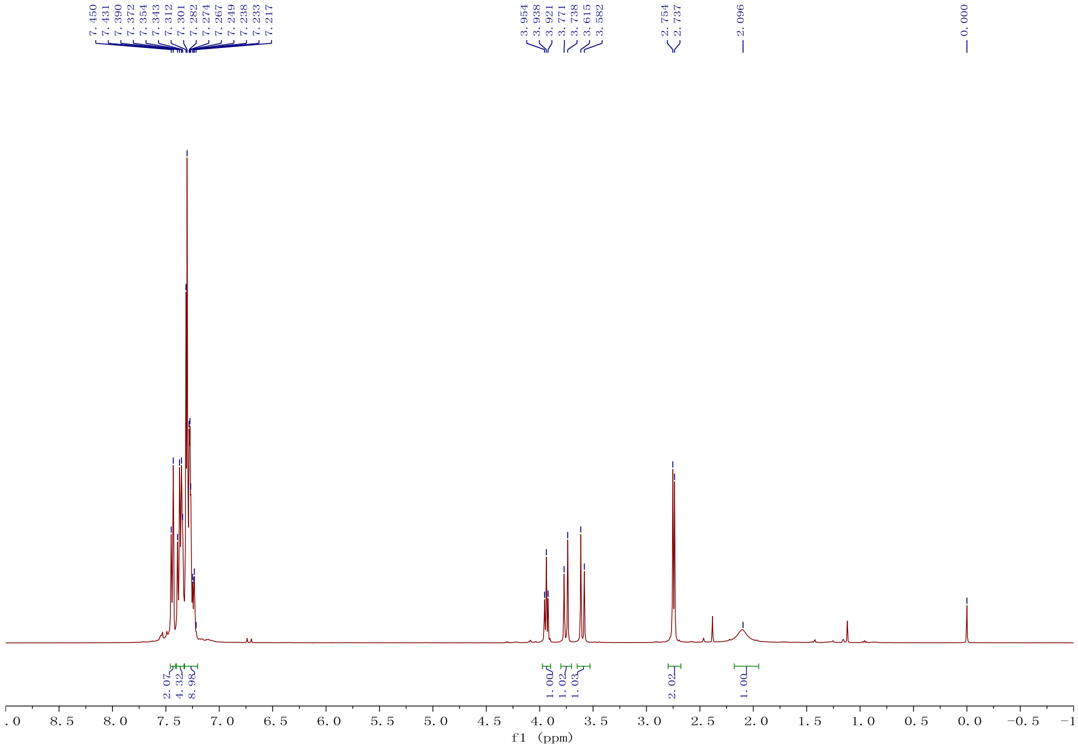
1m

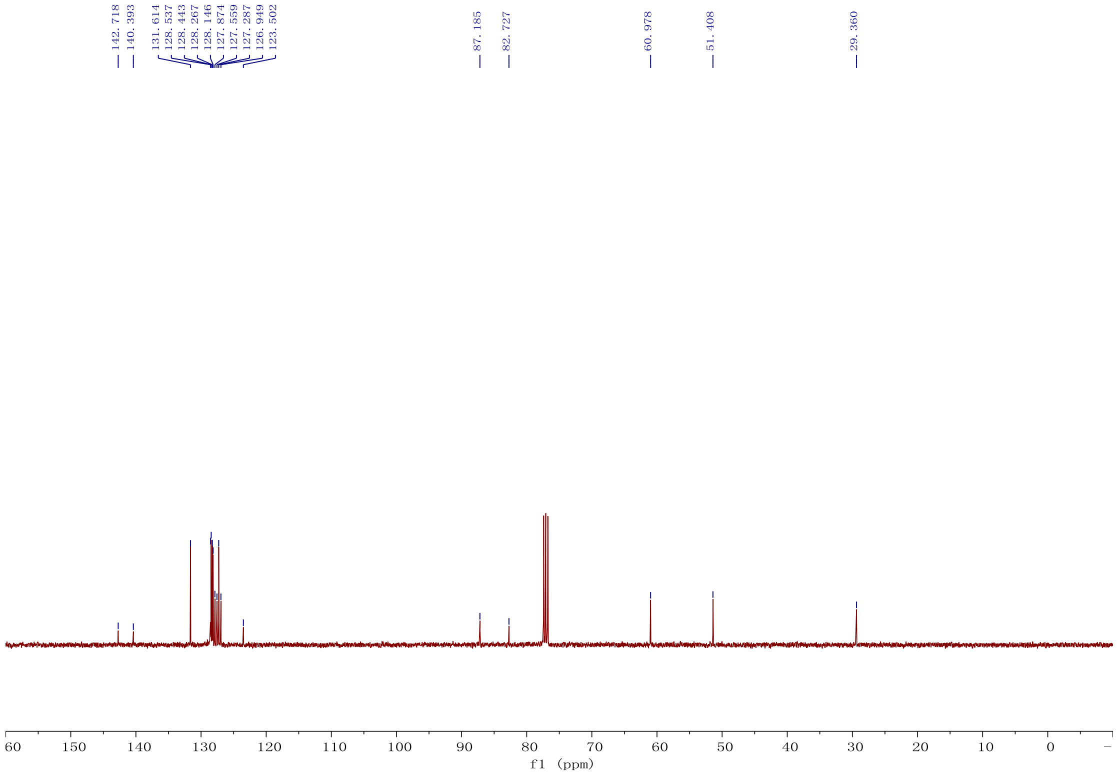

7.276
7.258
7.240
7.187
7.171
6.925
6.916
6.908
4.139
4.123
4.107
2.866
2.856
2.842
2.818
2.791
2.587
2.572
1.972
1.894
2.22
4.15
1.97
1.00
4.30
2.14
0.98
1.19
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.
f1 (ppm)

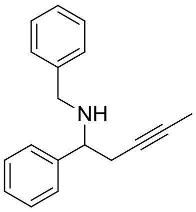

147.402
139.873
128.814
128.471
126.474
126.205
124.451
124.418
80.907
71.109
57.165
48.663
36.273
28.597
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



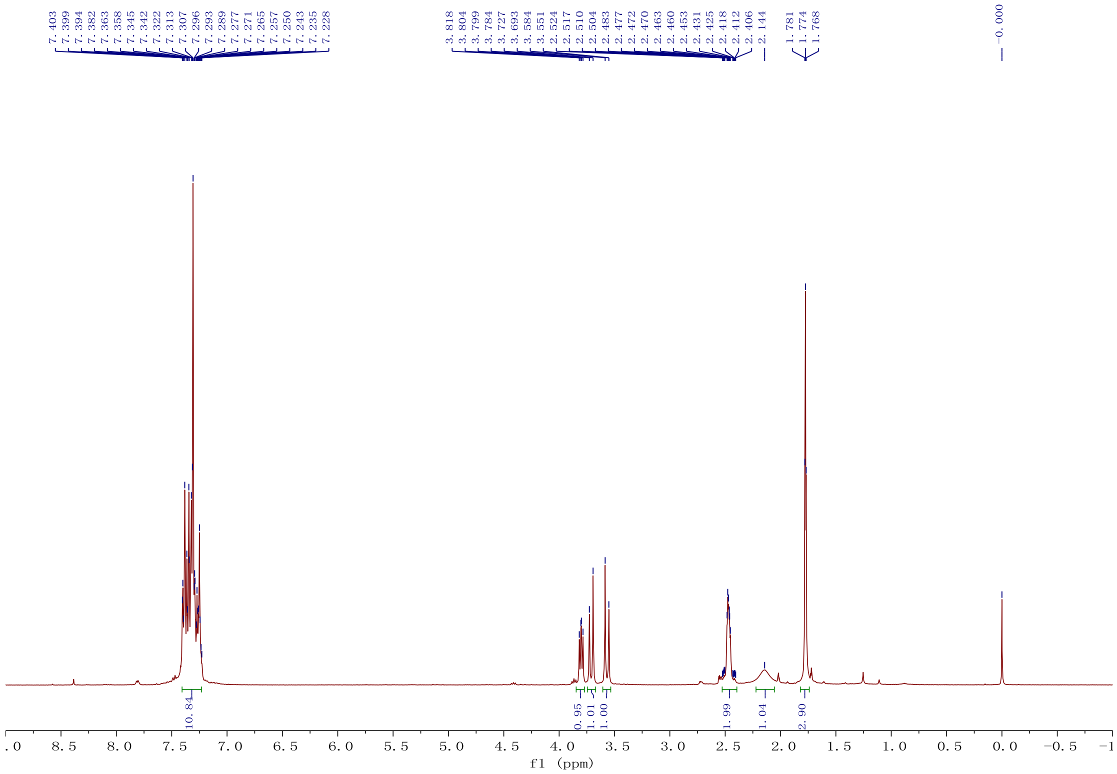
1n


7.450
7.431
7.390
7.372
7.354
7.343
7.312
7.301
7.282
7.274
7.267
7.249
7.238
7.233
7.217
3.954
3.938
3.921
3.771
3.738
3.615
3.582
2.754
2.737
2.096
0.000
2.07
4.32
8.98
1.00
1.02
1.03
2.02
1.00
.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
−1
f1 (ppm)

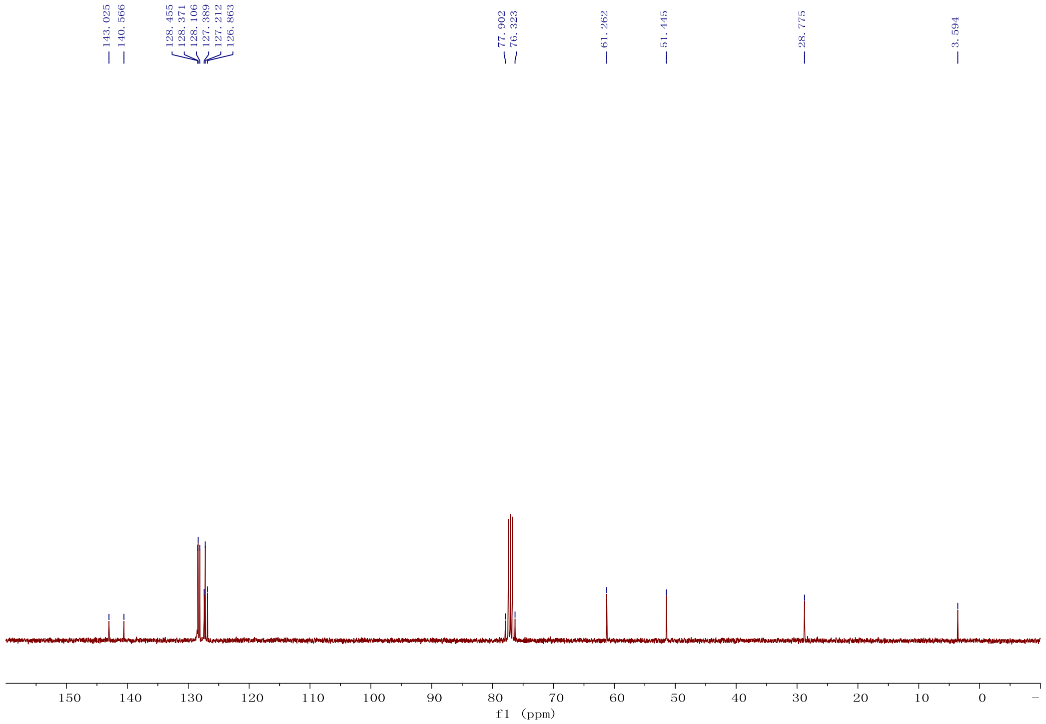

142.718
140.393
131.614
128.537
128.443
128.267
128.146
127.874
127.559
127.287
126.949
123.502
87.185
82.727
60.978
51.408
29.360
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−
f1 (ppm)



1o

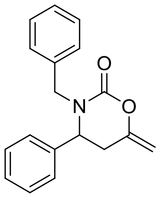


7.403
7.399
7.394
7.382
7.363
7.358
7.345
7.342
7.322
7.313
7.307
7.296
7.293
7.289
7.277
7.271
7.265
7.257
7.250
7.243
7.235
7.228
3.818
3.804
3.799
3.784
3.727
3.693
3.584
3.551
2.524
2.517
2.510
2.504
2.483
2.477
2.472
2.470
2.463
2.460
2.453
2.431
2.425
2.418
2.412
2.406
2.144
1.781
1.774
1.768
−0.000
10.84
0.95
1.01
1.00
1.99
1.04
2.90
.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
−1
f1 (ppm)

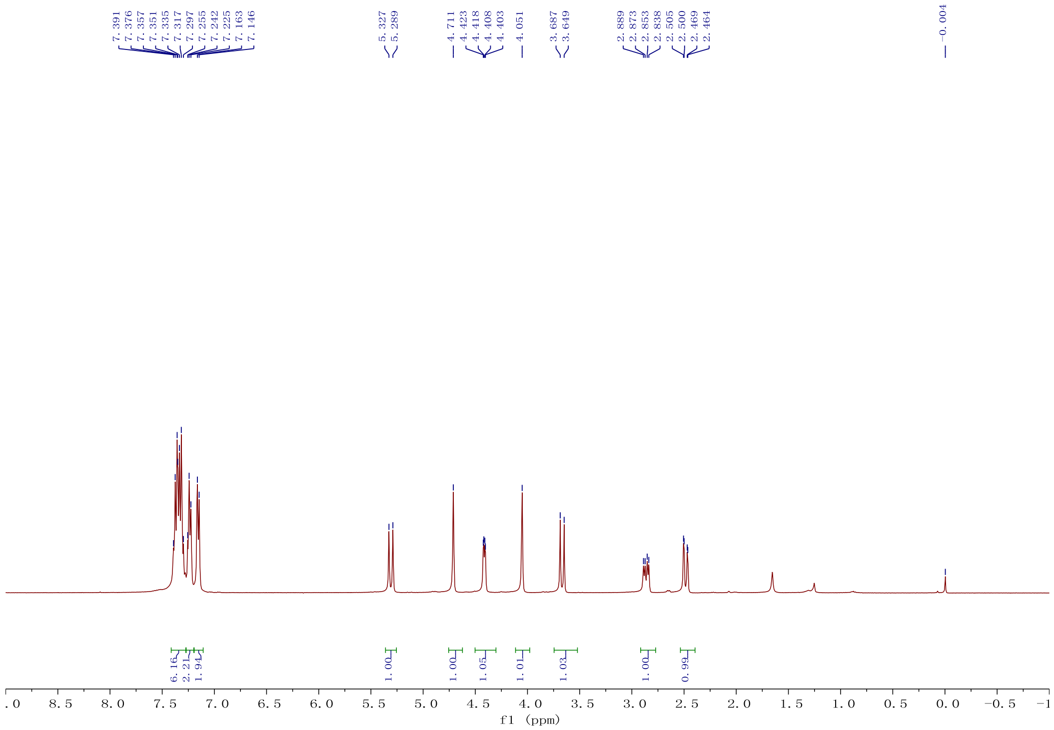


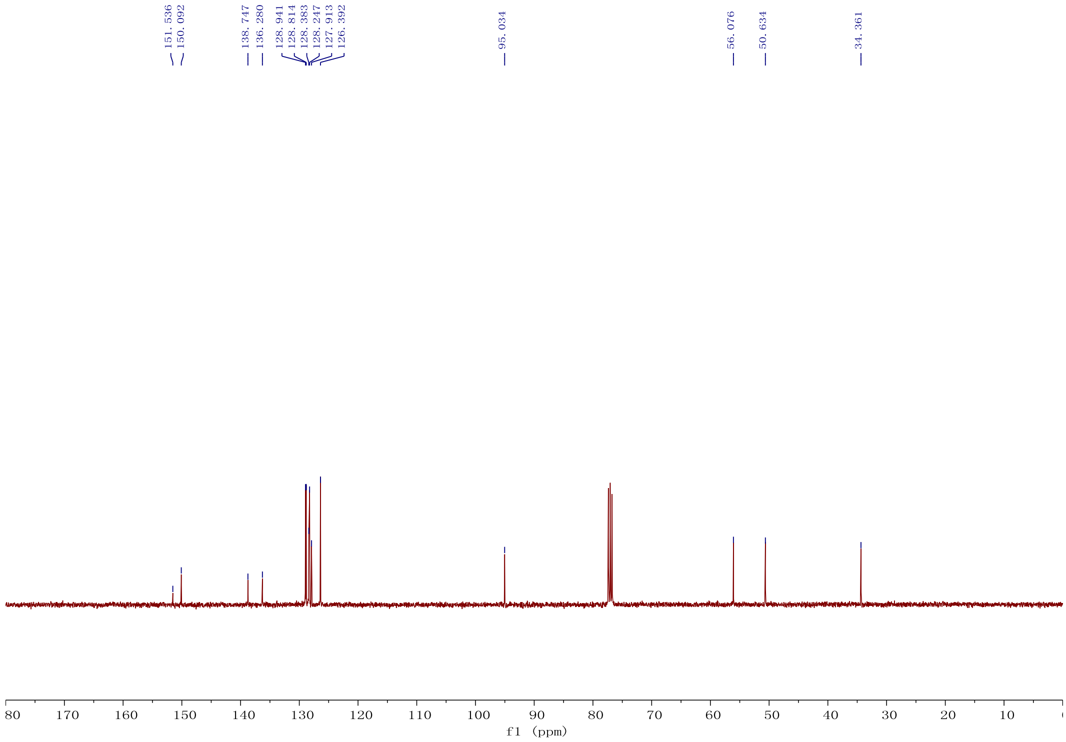
143.025
140.566
128.455
128.371
128.106
127.389
127.212
126.863
77.902
76.323
61.262
51.445
28.775
3.594
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−
f1 (ppm)

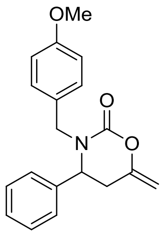
8. The spectra of 1, 3-oxazin-2-ones 2a



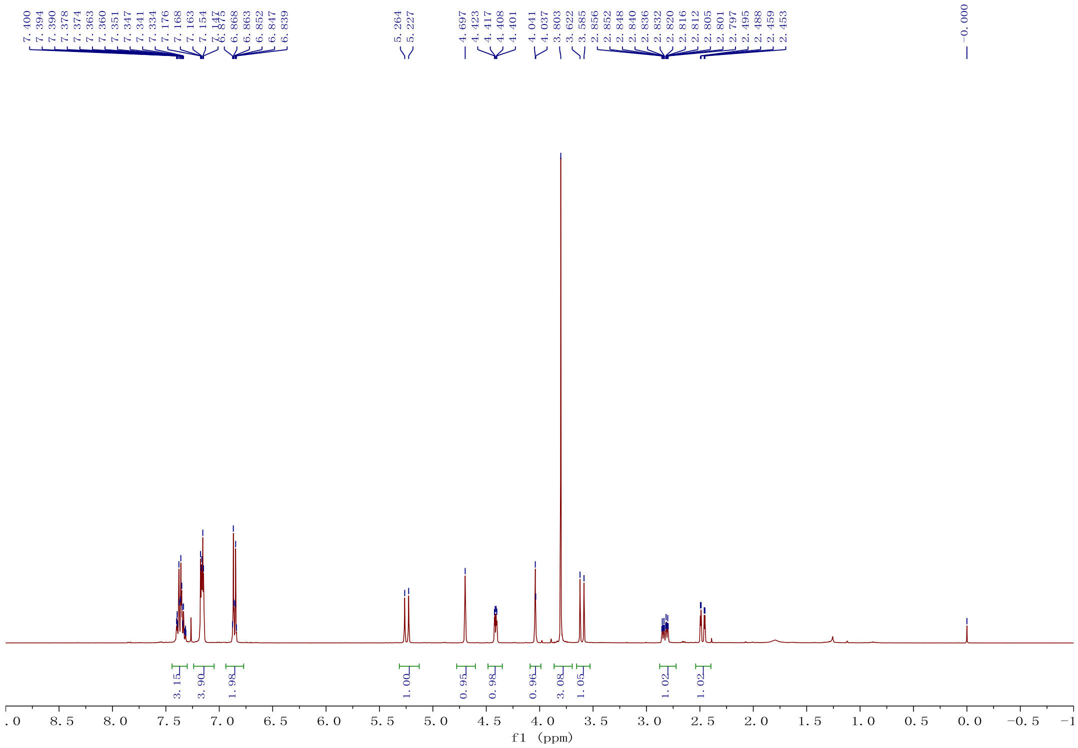
2a

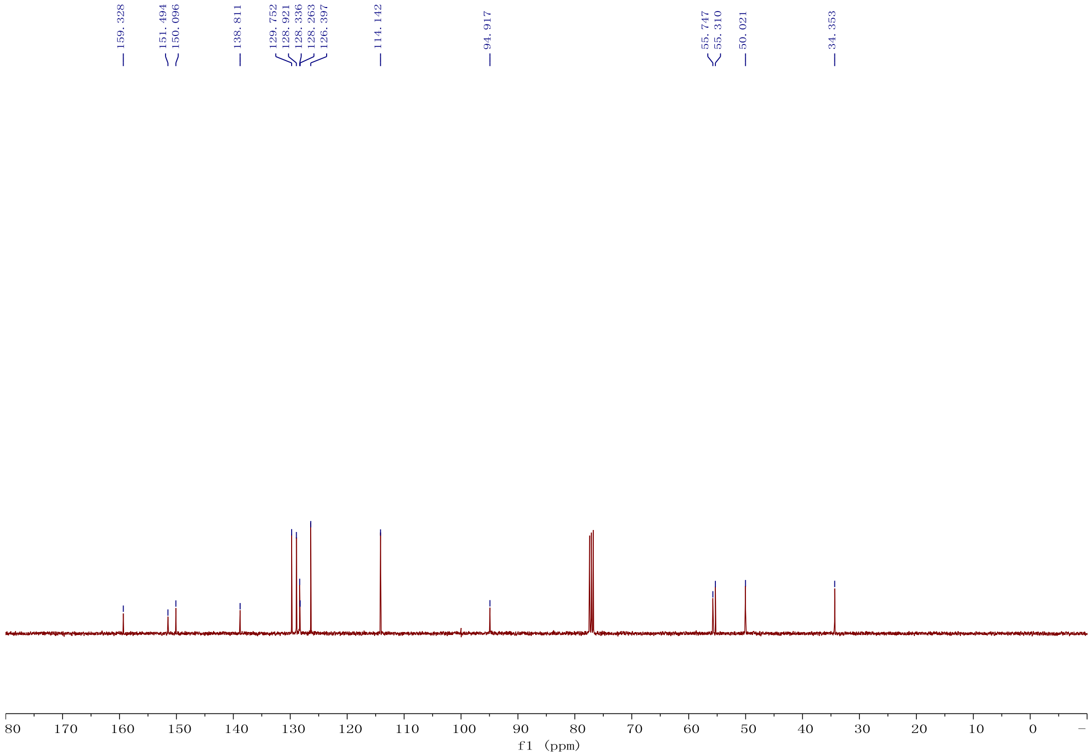


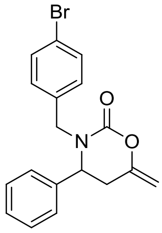



OMe
O
N
O

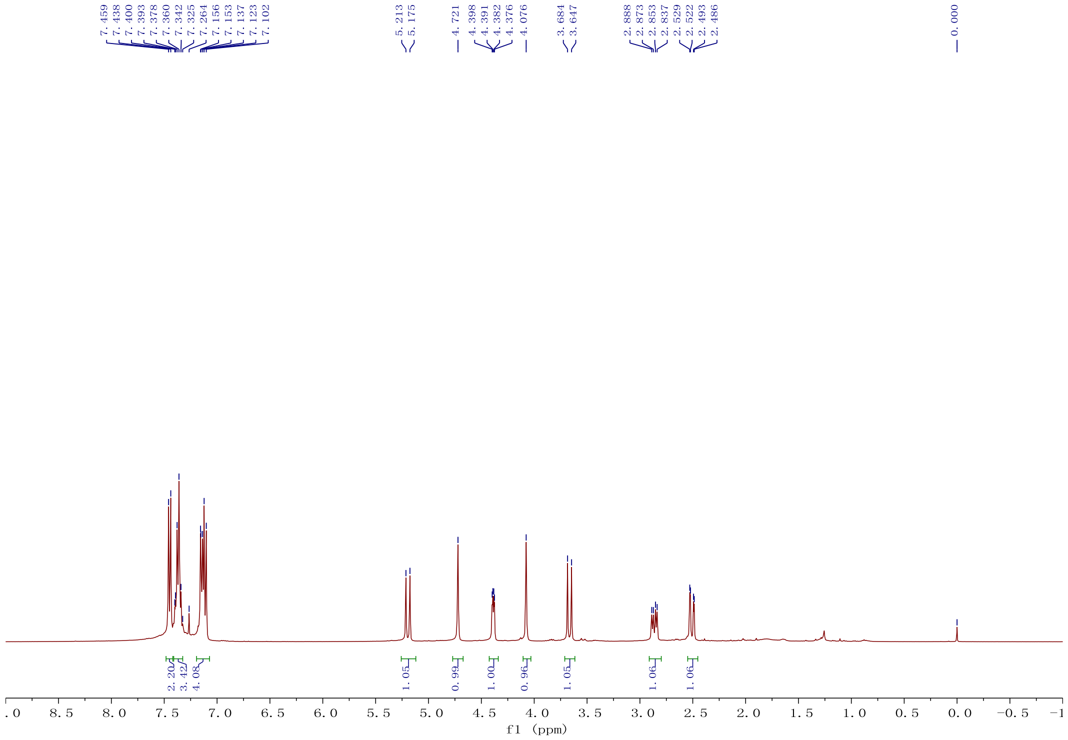
2b

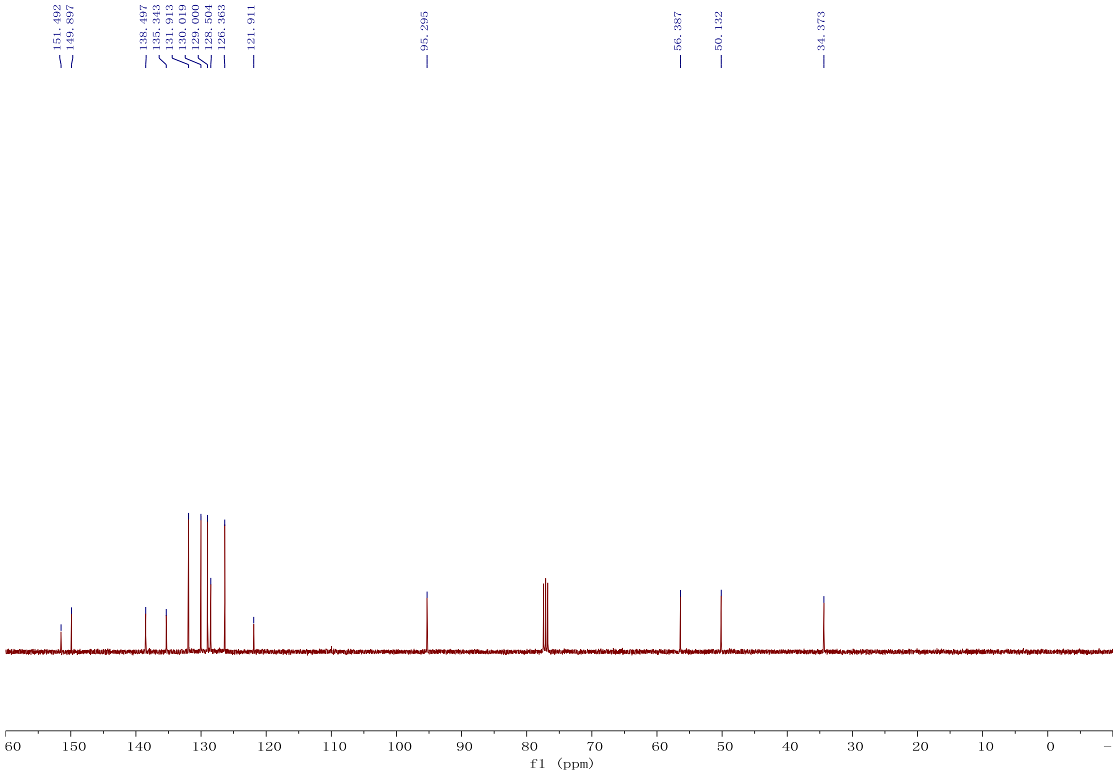

7.400
7.394
7.390
7.378
7.374
7.363
7.360
7.351
7.347
7.341
7.334
7.176
7.168
7.163
7.154
7.147
6.875
6.868
6.863
6.852
6.847
6.839
5.264
5.227
4.697
4.423
4.417
4.408
4.401
4.041
4.037
3.803
3.622
3.585
2.856
2.852
2.848
2.840
2.836
2.832
2.820
2.816
2.812
2.805
2.801
2.797
2.495
2.488
2.459
2.453
−0.000
3.15
3.90
1.98
1.00
0.95
0.98
0.96
3.08
1.05
1.02
1.02
.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
−1
f1 (ppm)

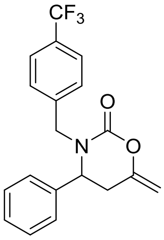

159.328
151.494
150.096
138.811
129.752
128.921
128.336
128.263
126.397
114.142
94.917
55.747
55.310
50.021
34.353
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Br
O
N
O

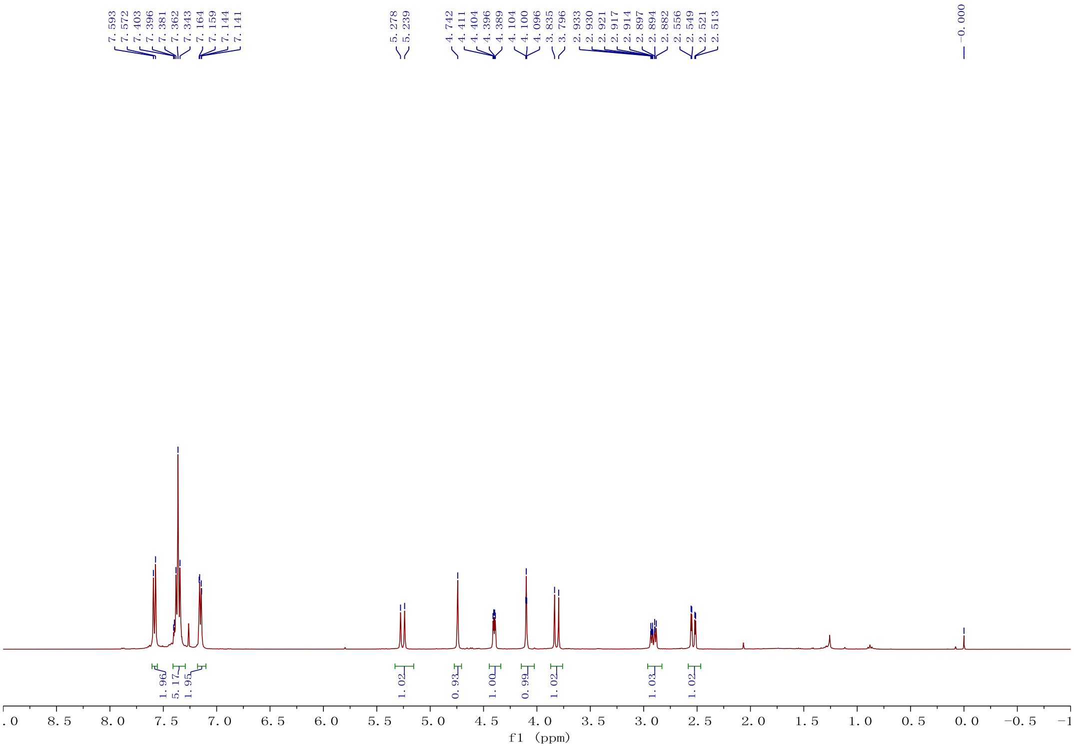
2c

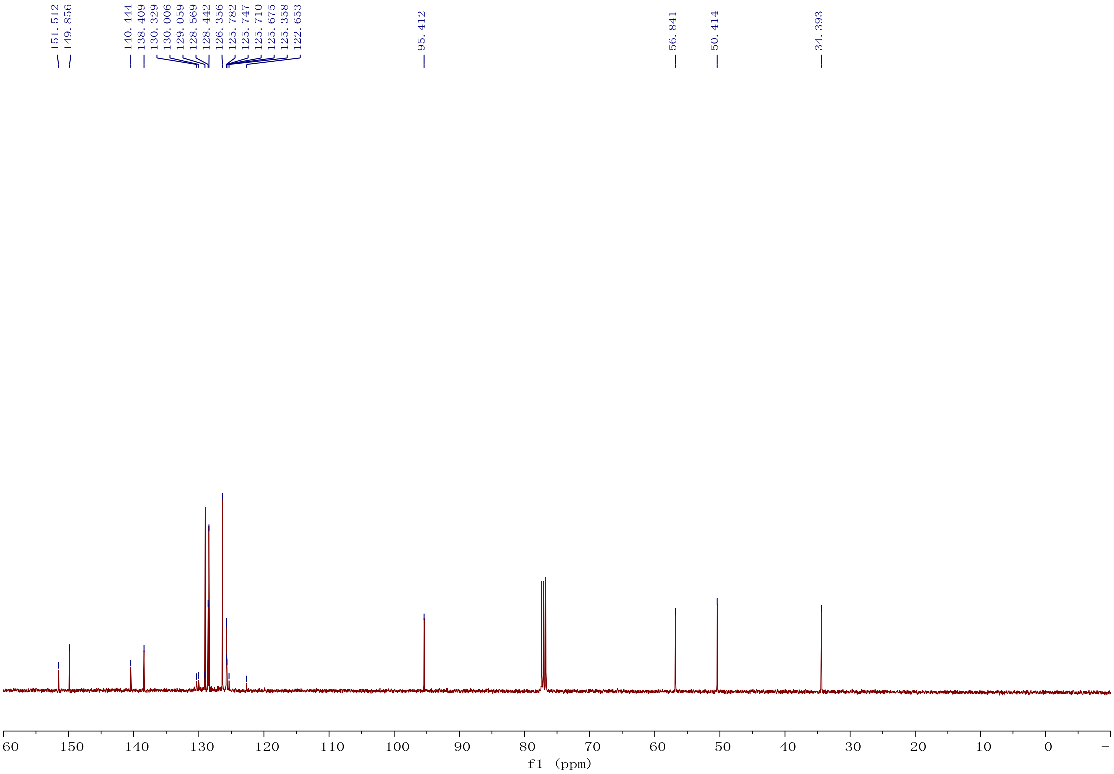

7.459
7.438
7.400
7.393
7.378
7.360
7.342
7.325
7.264
7.156
7.153
7.137
7.123
7.102
5.213
5.175
4.721
4.398
4.391
4.382
4.376
4.076
3.684
3.647
2.888
2.873
2.853
2.837
2.529
2.522
2.493
2.486
0.000
2.20
3.42
4.08
1.05
0.99
1.00
0.96
1.05
1.06
1.06
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1
f1 (ppm)


151.492
149.897
138.497
135.343
131.913
130.019
129.000
128.504
126.363
121.911
95.295
56.387
50.132
34.373
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


CF3
O
N
O

2d


7.593
7.572
7.403
7.396
7.381
7.362
7.343
7.164
7.159
7.144
7.141
5.278
5.239
4.742
4.411
4.404
4.396
4.389
4.104
4.100
4.096
3.835
3.796
2.933
2.930
2.921
2.917
2.914
2.897
2.894
2.882
2.556
2.549
2.521
2.513
0.000
1.96
5.17
1.95
1.02
0.93
1.00
0.99
1.02
1.03
1.02
.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
−1
f1 (ppm)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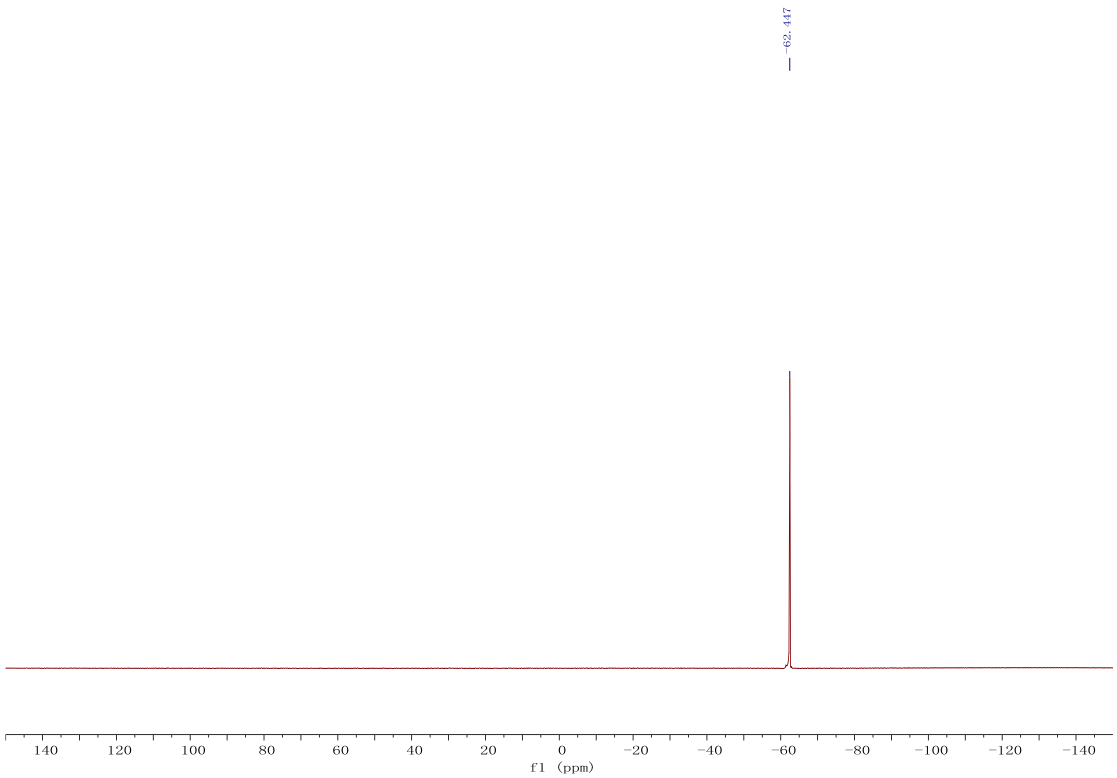
140.444
138.409
130.329
130.006
129.059
128.569
128.442
126.356
125.782
125.747
125.710
125.675
125.358
122.653
95.412
56.841
50.414
34.393
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



−62.447
140
120
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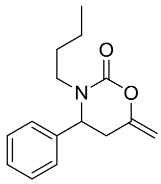
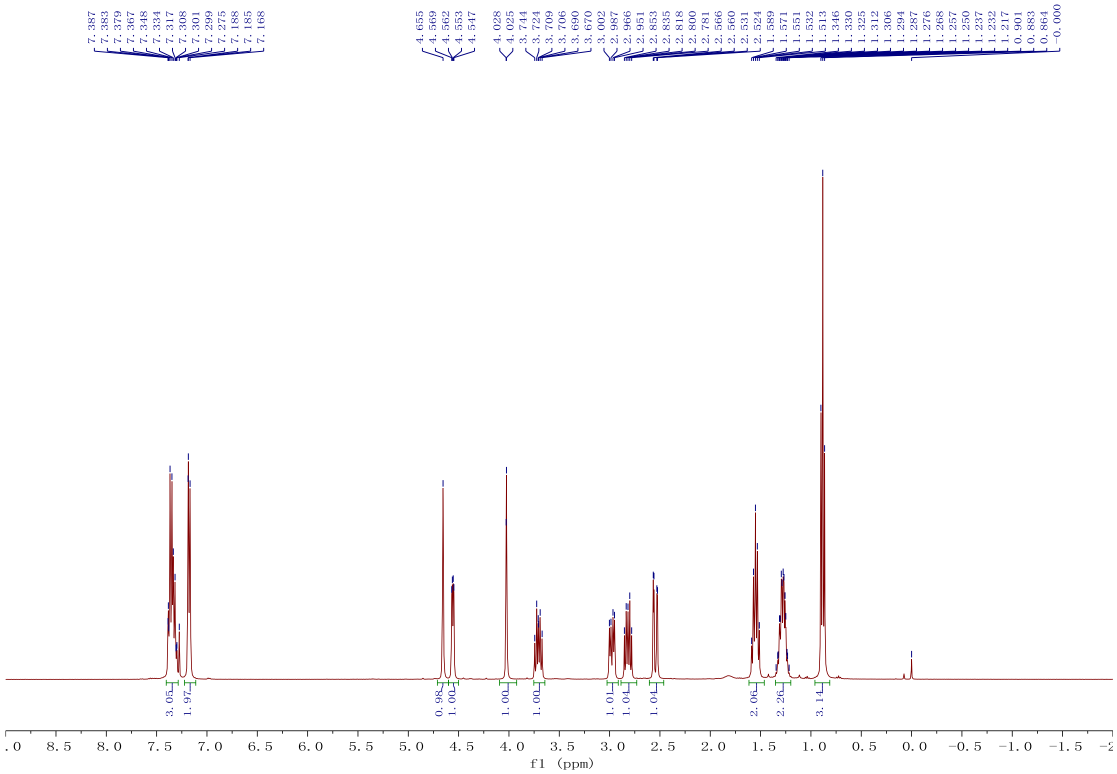
80
60
40
20
0
−20
−40
−60
−80
−100
−120
−140
f1 (ppm)


O
N
O

2e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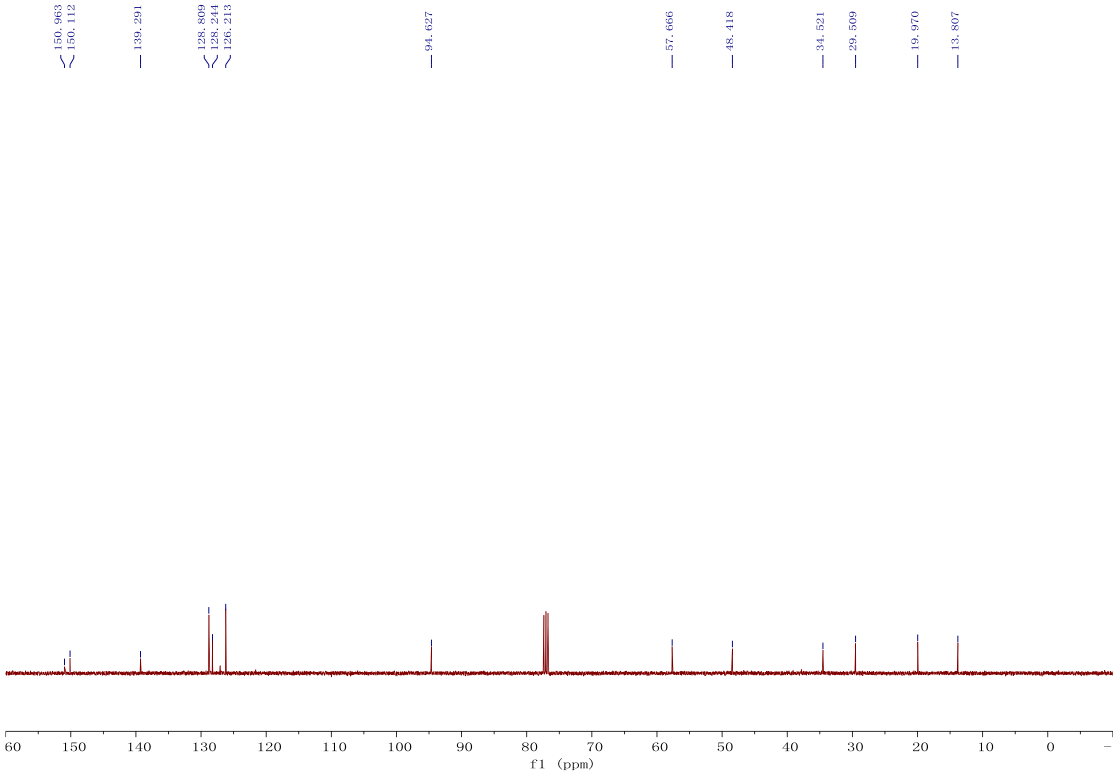
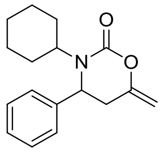
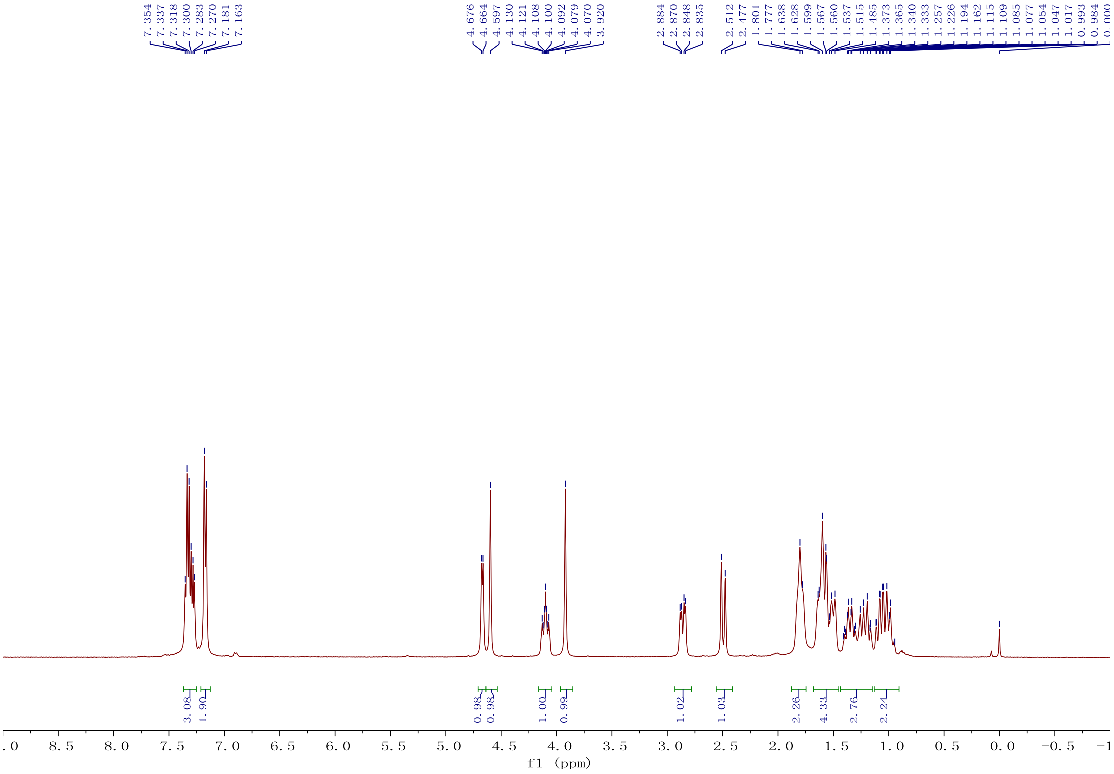
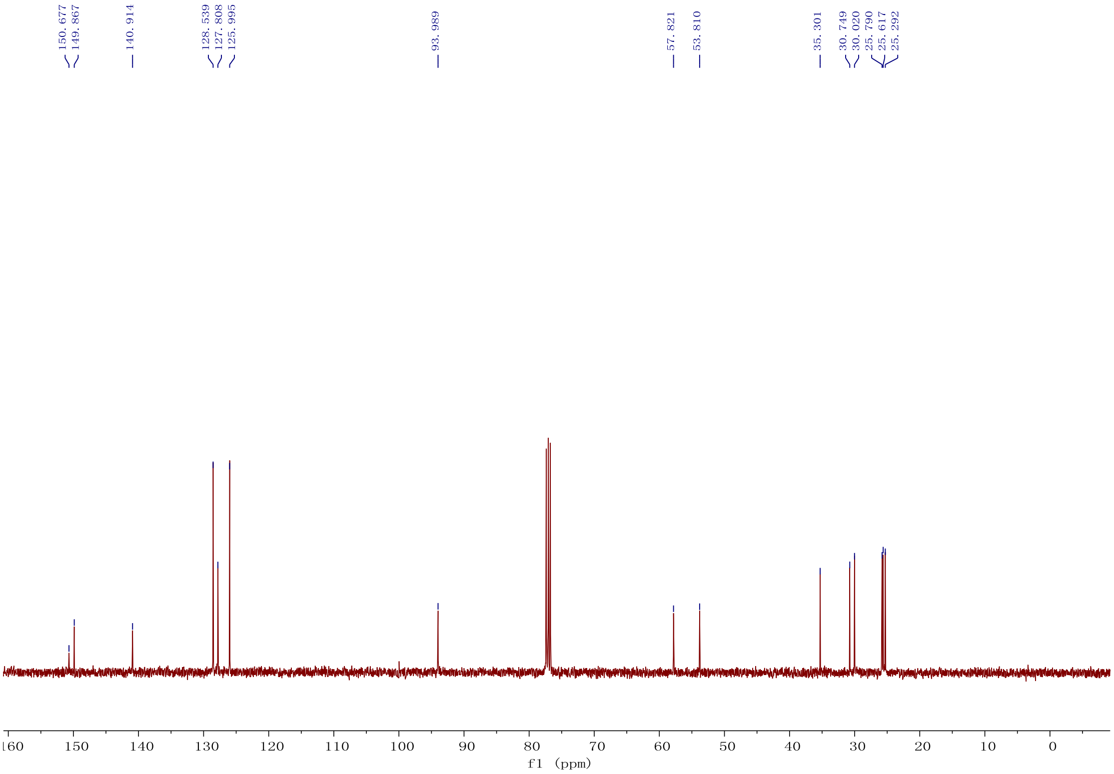
7.379
7.367
7.348
7.334
7.317
7.308
7.301
7.299
7.275
7.188
7.185
7.168
4.655
4.569
4.562
4.553
4.547
4.028
4.025
3.744
3.724
3.709
3.706
3.690
3.670
3.002
2.987
2.966
2.951
2.853
2.835
2.818
2.800
2.781
2.566
2.560
2.531
2.524
1.589
1.571
1.551
1.532
1.513
1.346
1.330
1.325
1.312
1.306
1.294
1.287
1.276
1.268
1.257
1.250
1.237
1.232
1.217
0.901
0.883
0.864
-0.000
3.05
1.97
0.98
1.00
1.00
1.00
1.01
1.04
1.04
2.06
2.26
3.14
.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
-1.0
-1.5
-2
f1 (ppm)


150.963
150.112
139.291
128.809
128.244
126.213
94.627
57.666
48.418
34.521
29.509
19.970
13.807
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


O
N
O

2f


7.354
7.337
7.318
7.300
7.283
7.270
7.181
7.163
4.676
4.664
4.597
4.130
4.121
4.108
4.100
4.092
4.079
4.070
3.920
2.884
2.870
2.848
2.835
2.512
2.477
1.801
1.777
1.638
1.628
1.599
1.567
1.560
1.537
1.515
1.485
1.373
1.365
1.340
1.333
1.257
1.226
1.194
1.162
1.115
1.109
1.085
1.077
1.054
1.047
1.017
0.993
0.984
0.000
3.08
1.90
0.98
0.98
1.00
0.99
1.02
1.03
2.26
4.33
2.76
2.24
.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
−1
f1 (ppm)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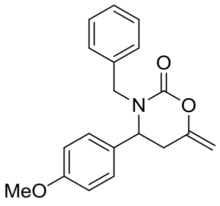
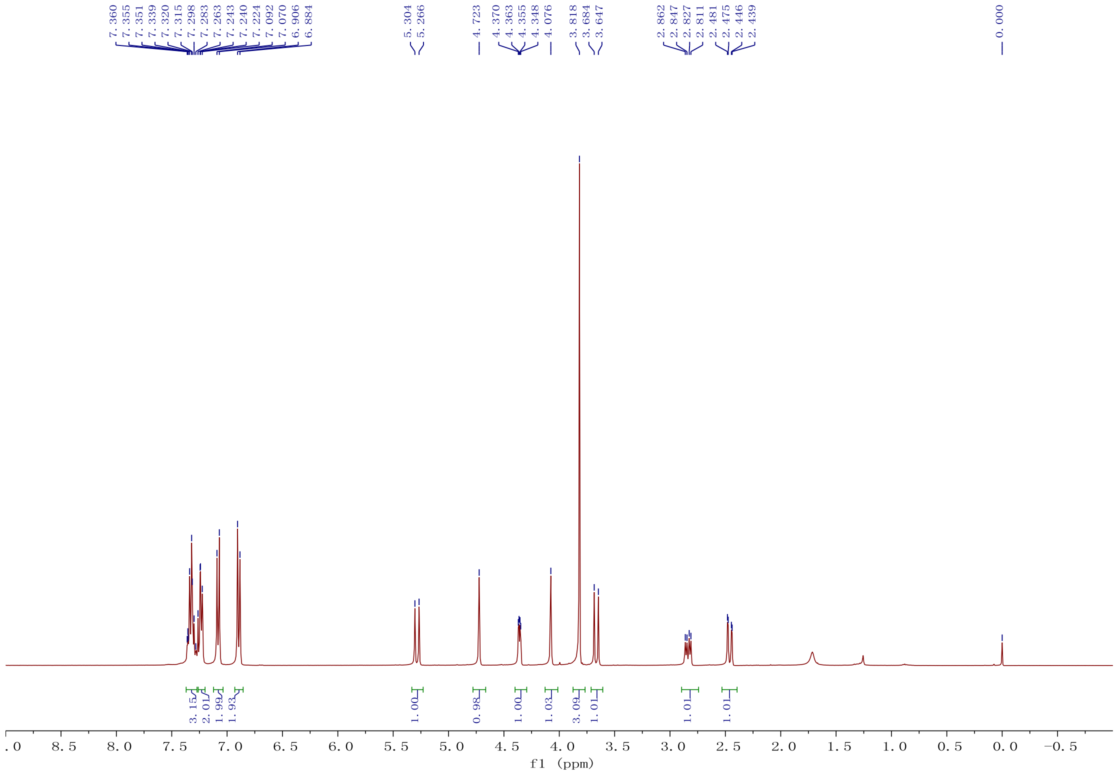
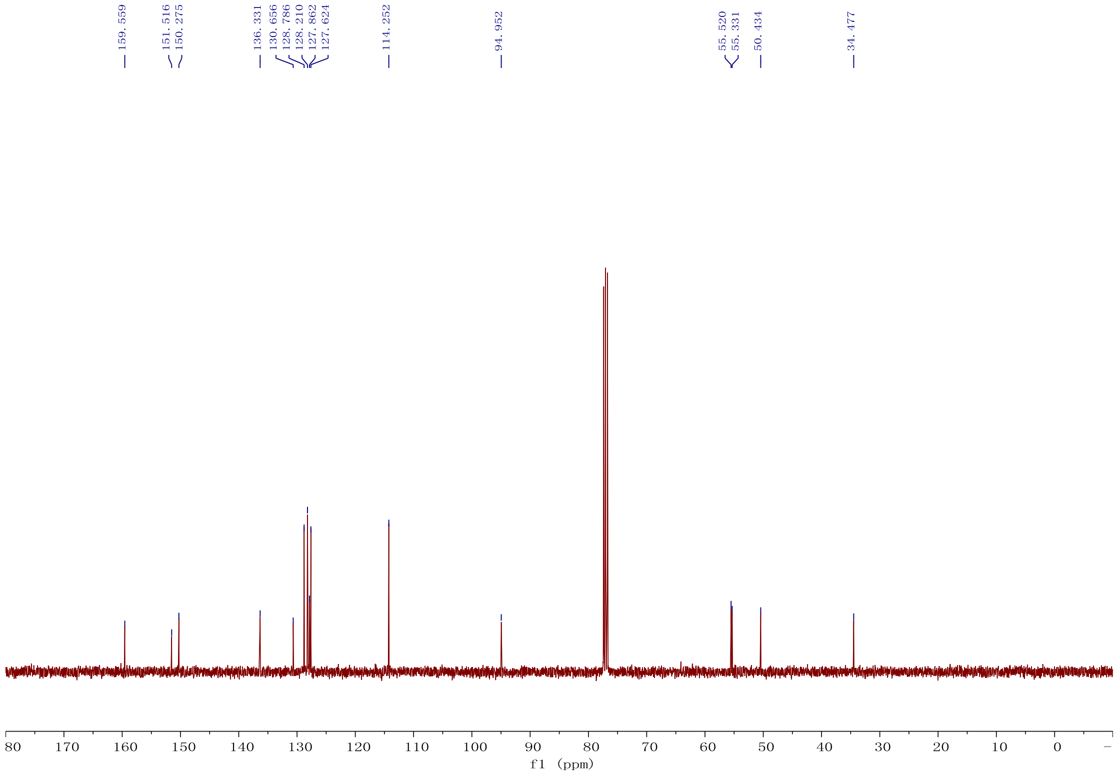
149.867
140.914
128.539
127.808
125.995
93.989
57.821
53.810
35.301
30.749
30.020
25.790
25.617
25.292
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


O
N
O
MeO

2g


7.360
7.355
7.351
7.339
7.320
7.315
7.298
7.283
7.263
7.243
7.240
7.224
7.092
7.070
6.906
6.884
5.304
5.266
4.723
4.370
4.363
4.355
4.348
4.076
3.818
3.684
3.647
2.862
2.847
2.827
2.811
2.481
2.475
2.446
2.439
0.000
3.15
2.01
1.99
1.93
1.00
0.98
1.00
1.03
3.09
1.01
1.01
1.01
.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)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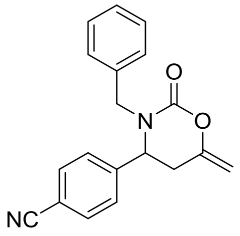
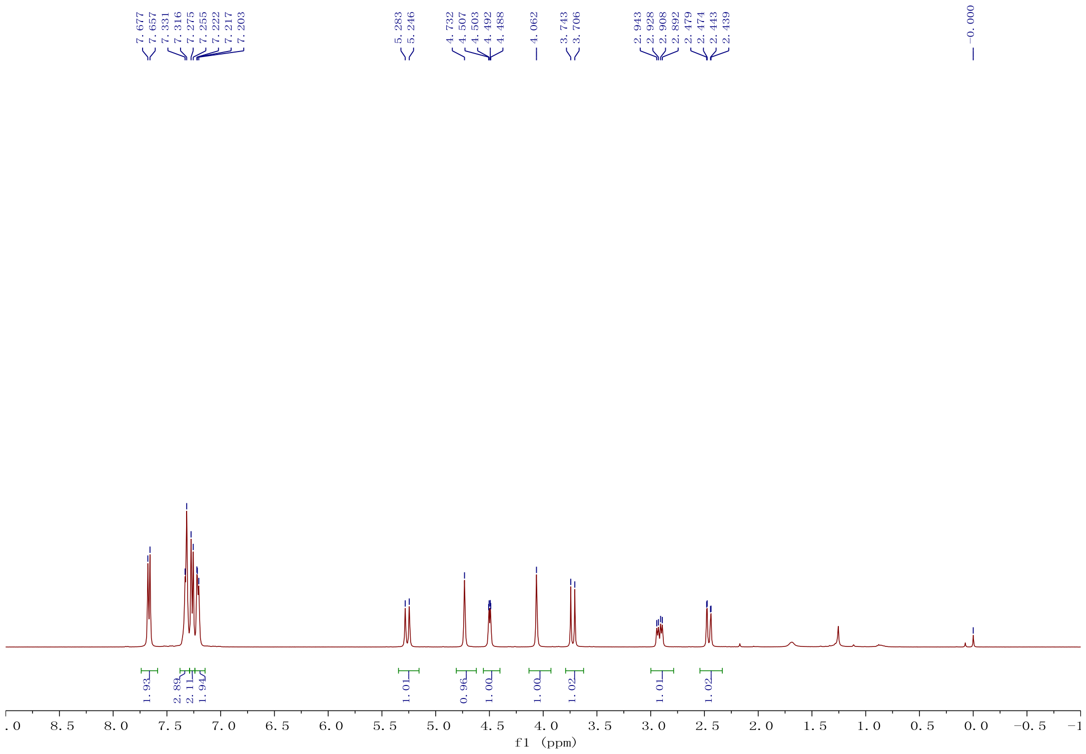
150.275
136.331
130.656
128.786
128.210
127.862
127.624
114.252
94.952
55.520
55.331
50.434
34.477
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
–
f1 (ppm)


O
N
O
NC

2h


7.677
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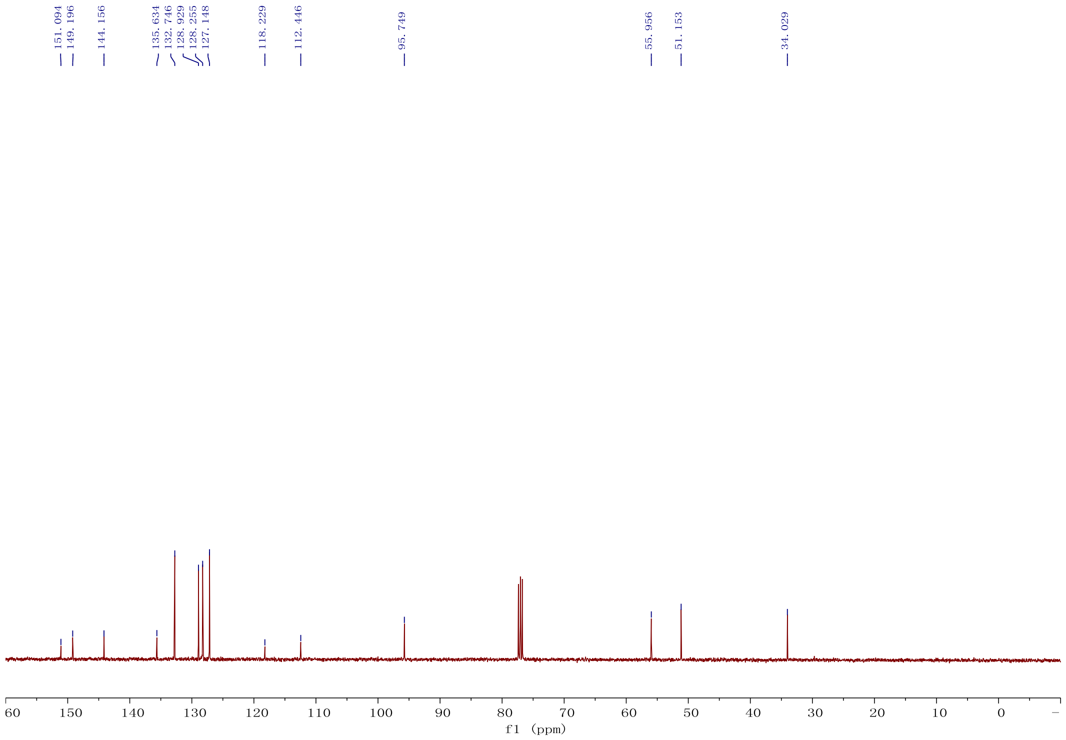
7.316
7.275
7.255
7.222
7.217
7.203
5.283
5.246
4.732
4.507
4.503
4.492
4.488
4.062
3.743
3.706
2.943
2.928
2.908
2.892
2.479
2.474
2.443
2.439
−0.000
1.93
2.89
2.11
1.94
1.01
0.96
1.00
1.00
1.02
1.01
1.02
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1
f1 (ppm)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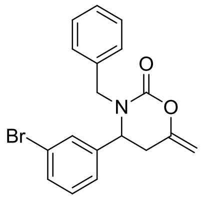
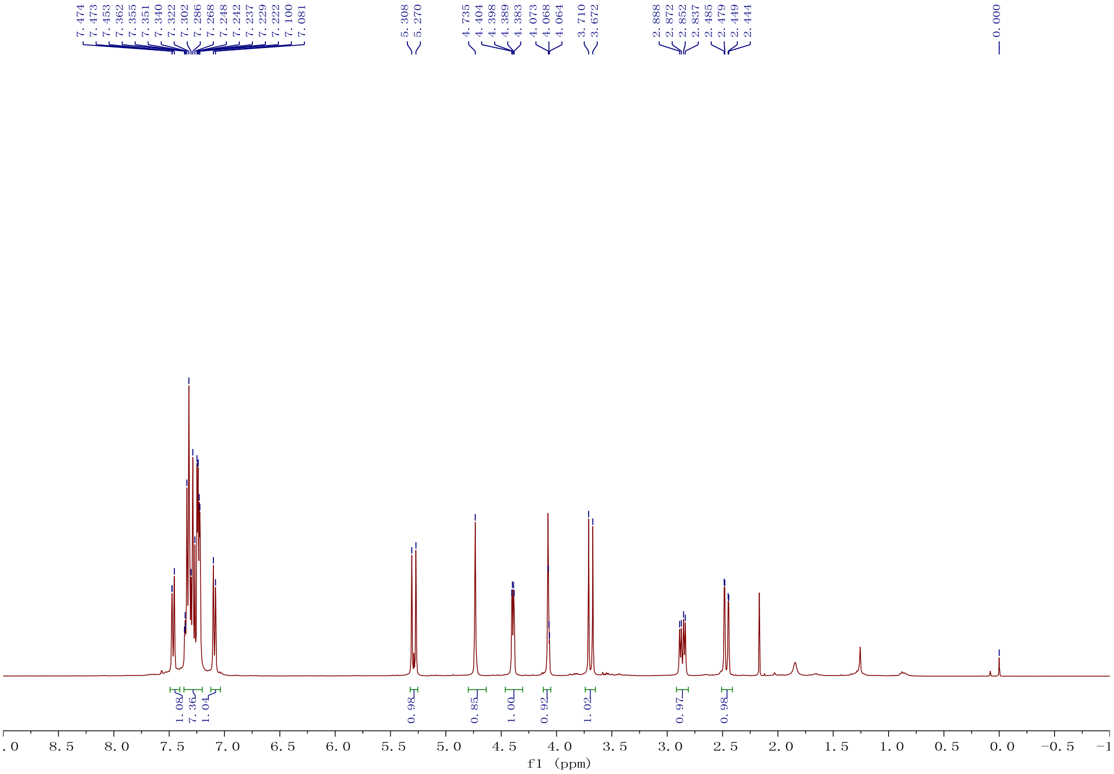
144.156
135.634
132.746
128.929
128.255
127.148
118.229
112.446
95.749
55.956
51.153
34.029
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
–
f1 (ppm)


O
N
O
Br

2i


7.474
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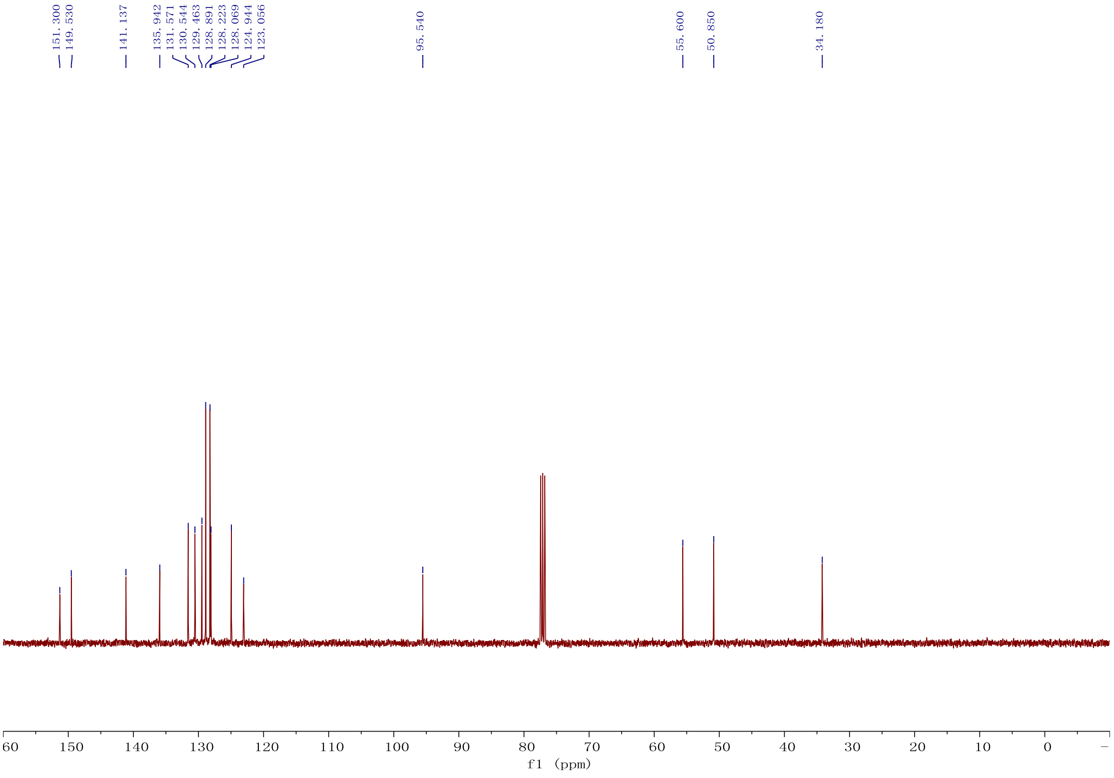
7.340
7.322
7.302
7.286
7.268
7.248
7.242
7.237
7.229
7.222
7.100
7.081
5.308
5.270
4.735
4.404
4.398
4.389
4.383
4.073
4.068
4.064
3.710
3.672
2.888
2.872
2.852
2.837
2.485
2.479
2.449
2.444
0.000
1.08
7.36
1.04
0.98
0.85
1.00
0.92
1.02
0.97
0.98
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1
f1 (ppm)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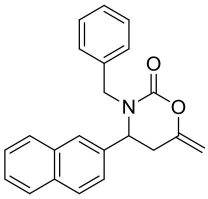
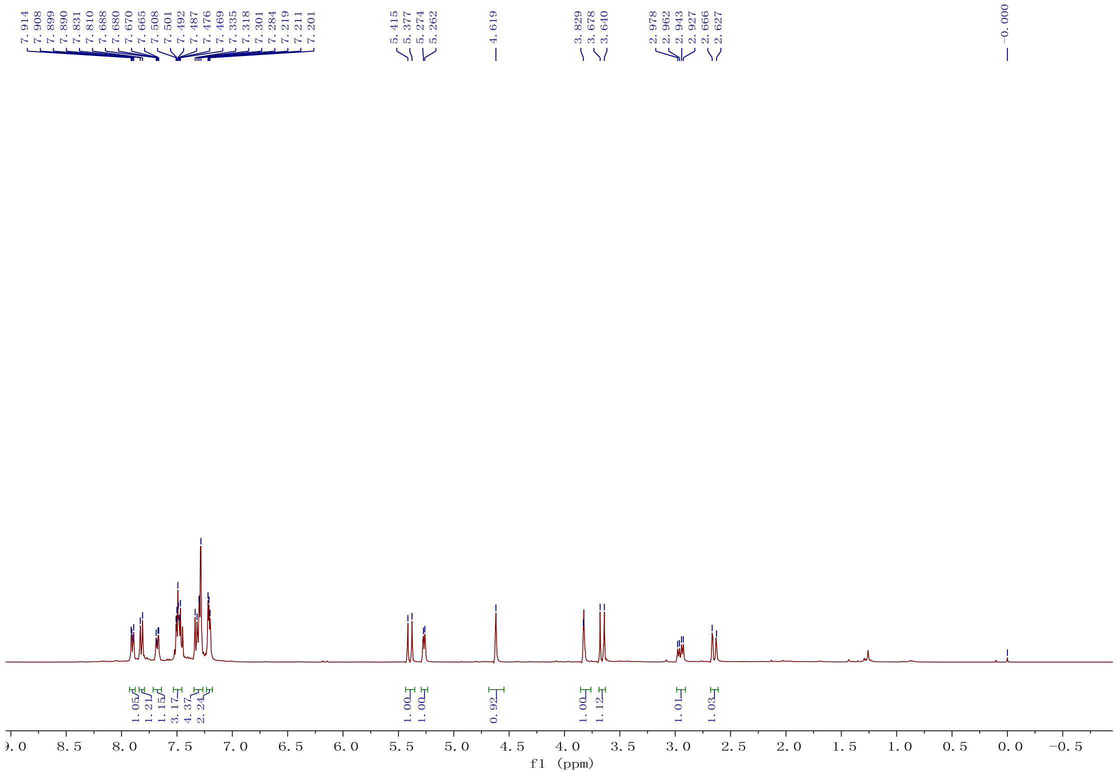
130.544
129.463
128.891
128.223
128.069
124.944
123.056
95.540
55.600
50.850
34.180
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


O
N
O

2j


7.914
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7.831
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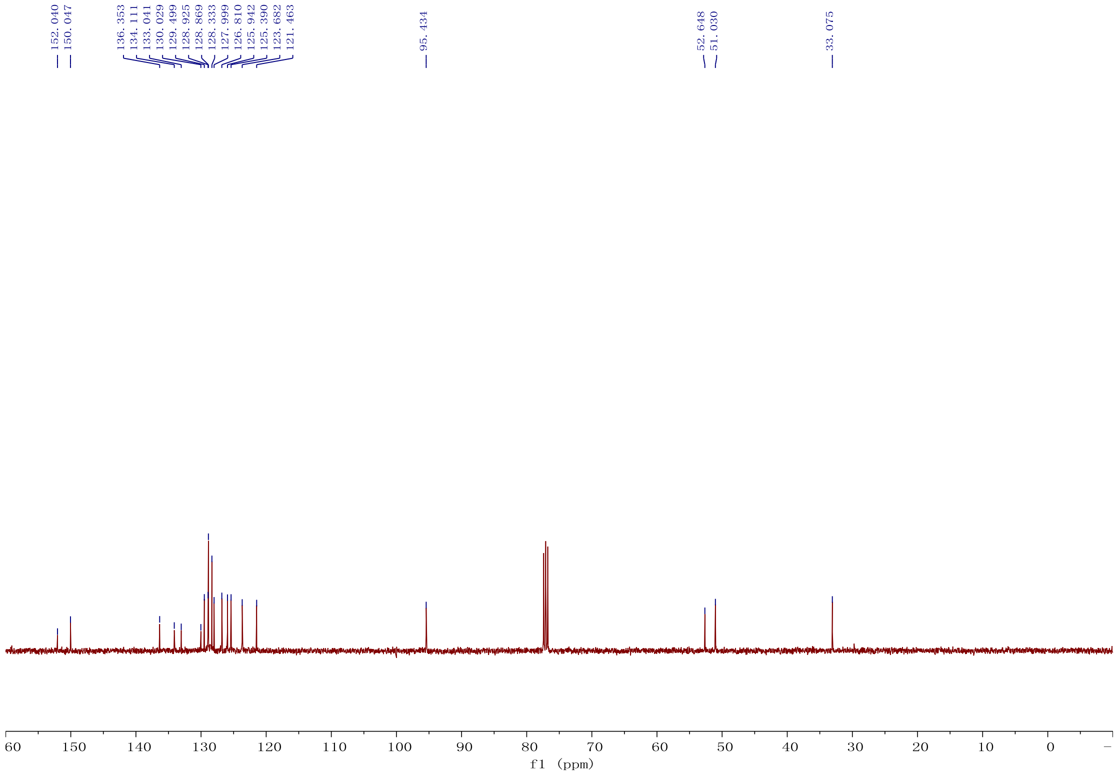
7.688
7.680
7.670
7.665
7.508
7.501
7.492
7.487
7.476
7.469
7.335
7.318
7.301
7.284
7.219
7.211
7.201
5.415
5.377
5.274
5.262
4.619
3.829
3.678
3.640
2.978
2.962
2.943
2.927
2.666
2.627
-0.000
1.05
1.21
1.15
3.17
4.37
2.24
1.00
1.00
0.92
1.00
1.12
1.01
1.03
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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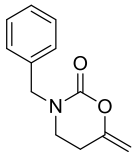
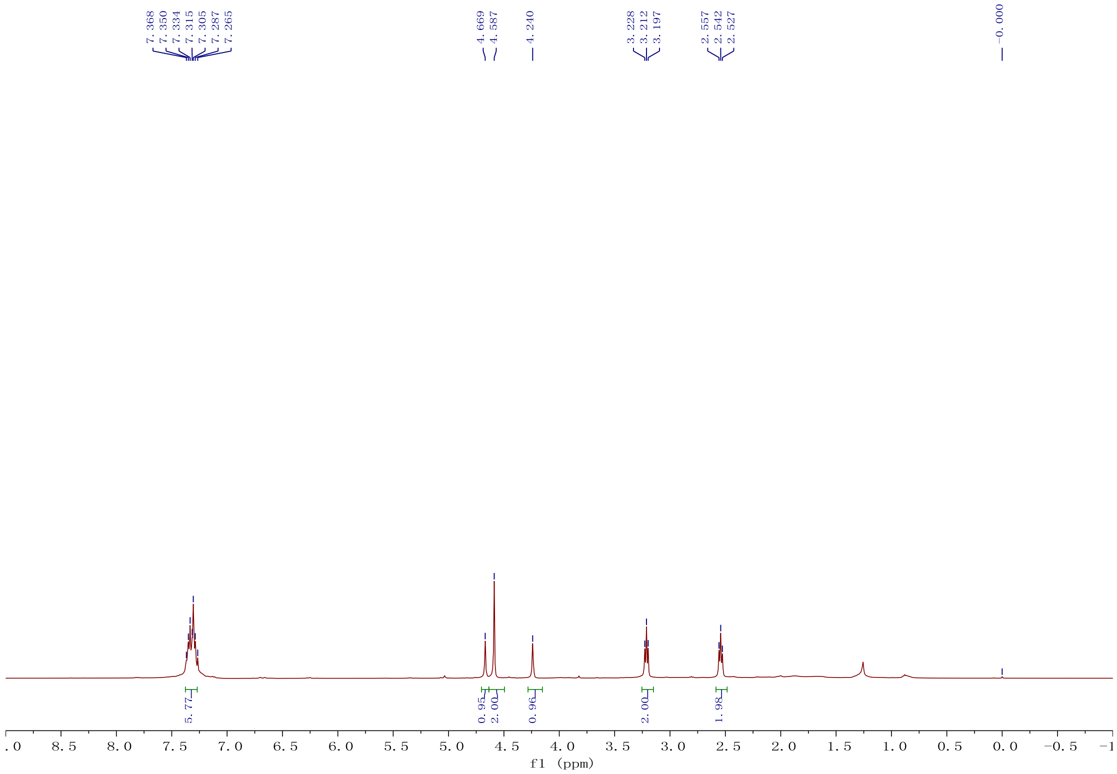
134.111
133.041
130.029
129.499
128.925
128.869
128.333
127.999
126.810
125.942
125.390
123.682
121.463
95.434
52.648
51.030
33.075
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



2k



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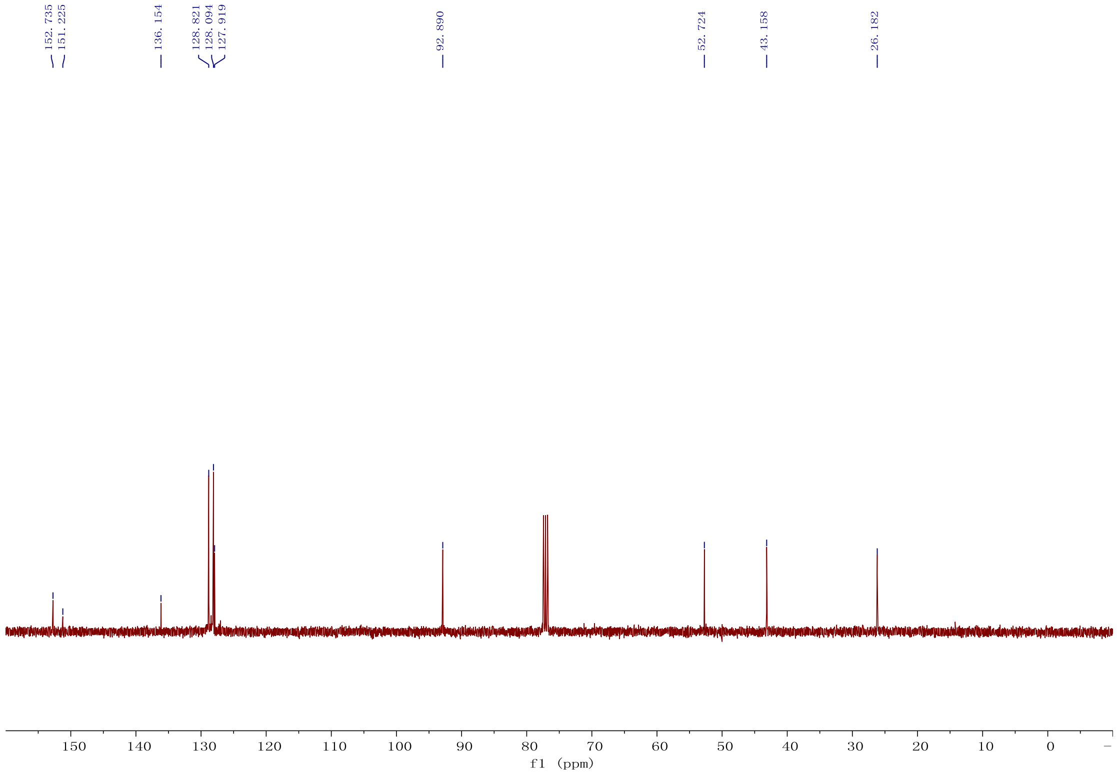
7.334
7.315
7.305
7.287
7.265
4.669
4.587
4.240
3.228
3.212
3.197
2.557
2.542
2.527
−0.000
5.77
0.95
2.00
0.96
2.00
1.98
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1
f1 (ppm)



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136.154
128.821
128.094
127.919
92.890
52.724
43.158
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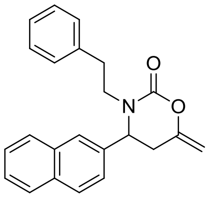
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


O
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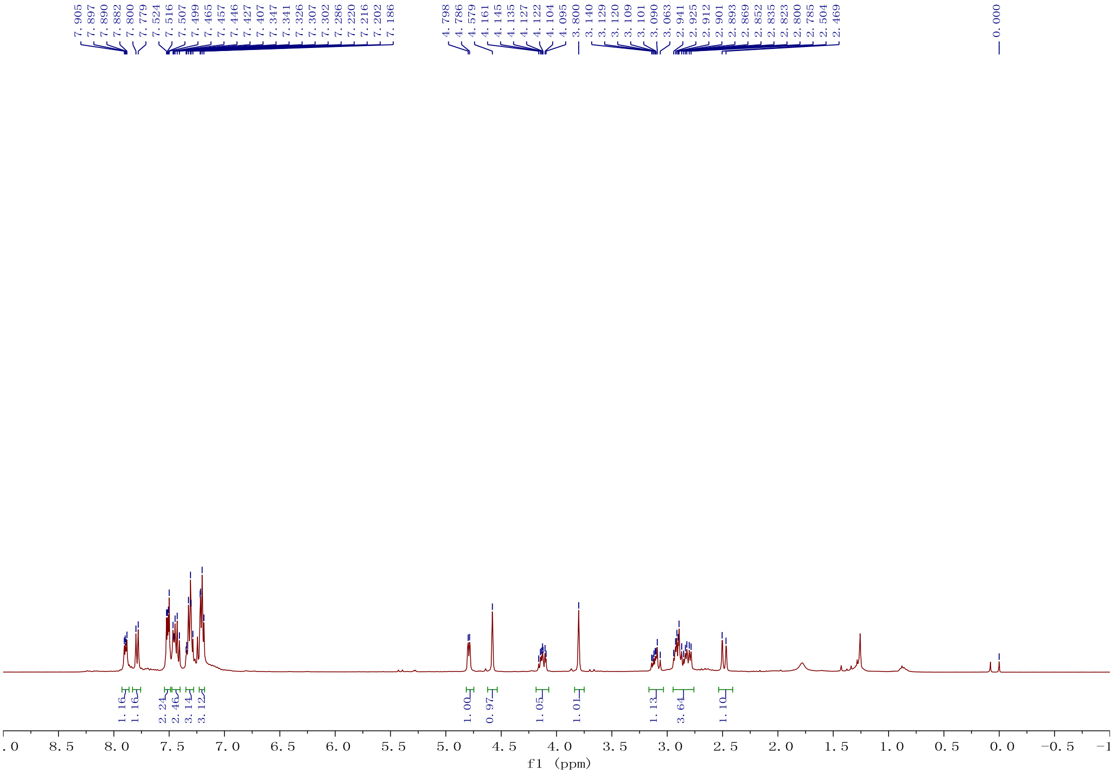
O

2l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7.516
7.507
7.499
7.465
7.457
7.446
7.427
7.407
7.347
7.341
7.326
7.307
7.302
7.286
7.220
7.216
7.202
7.186
4.798
4.786
4.579
4.161
4.145
4.135
4.127
4.122
4.104
4.095
3.800
3.140
3.129
3.120
3.109
3.101
3.090
3.063
2.941
2.925
2.912
2.901
2.893
2.869
2.852
2.835
2.823
2.800
2.785
2.504
2.469
0.000
1.16
1.16
2.21
2.46
3.14
3.12
1.00
0.97
1.05
1.01
1.13
3.64
1.10
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
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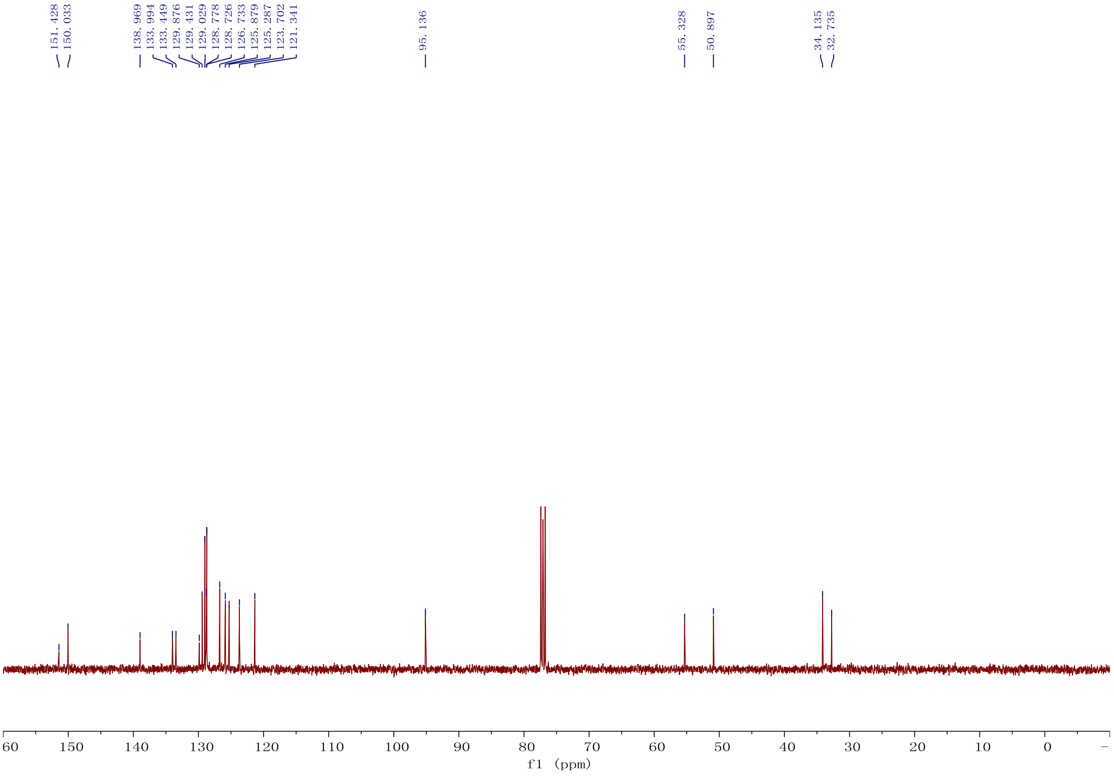
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1
f1 (ppm)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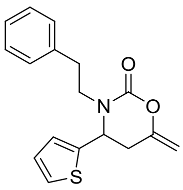
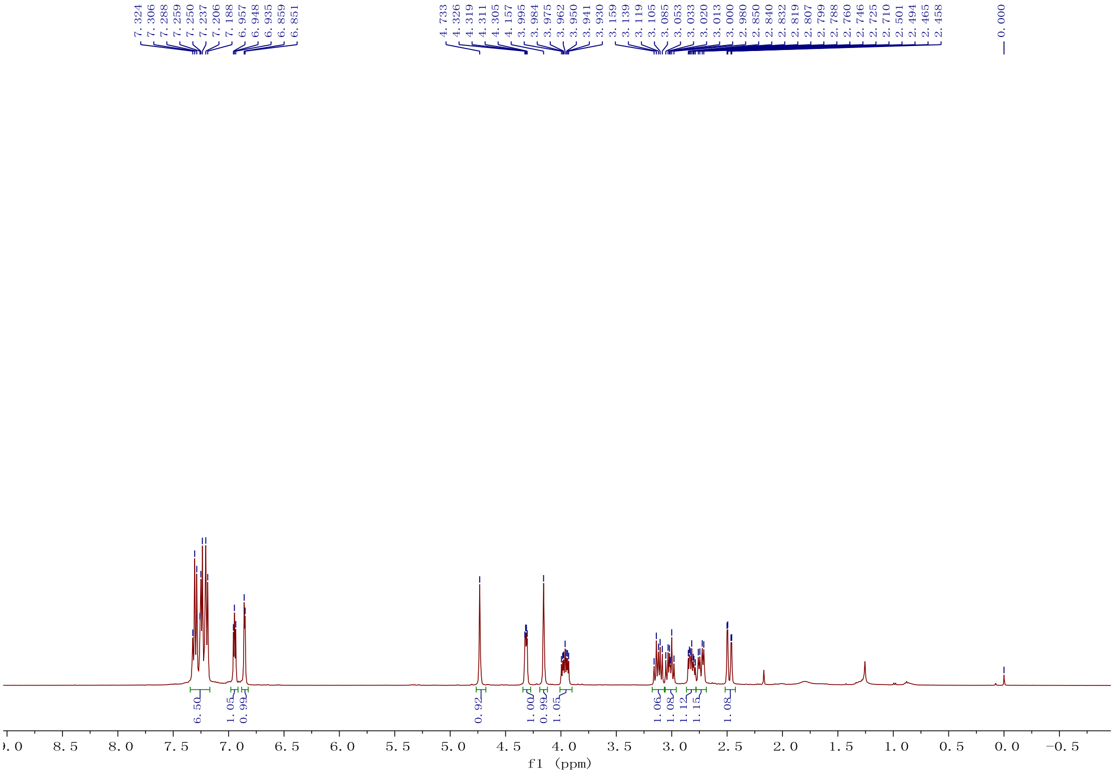
129.029
128.778
128.726
126.733
125.879
125.287
123.702
121.341
95.136
55.328
50.897
34.135
32.735
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
–
f1 (ppm)


O
N
O
S

2m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7.250
7.237
7.206
7.188
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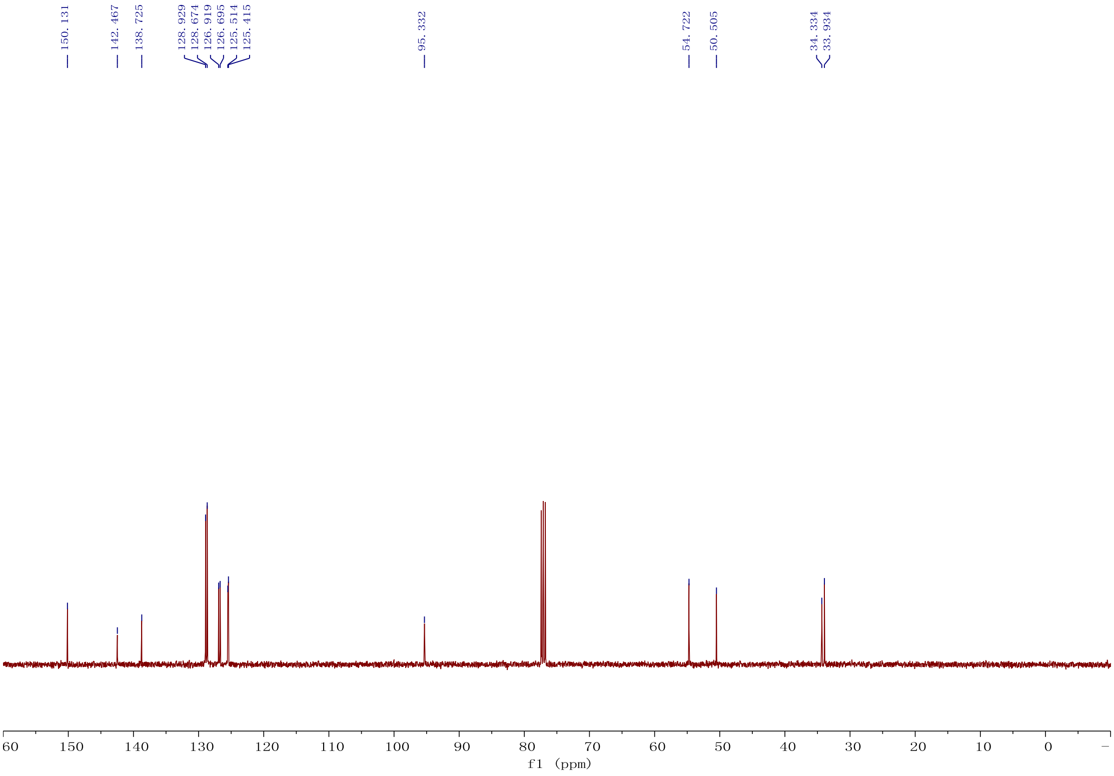
6.935
6.859
6.851
4.733
4.326
4.319
4.311
4.305
4.157
3.995
3.984
3.975
3.962
3.950
3.941
3.930
3.159
3.139
3.119
3.105
3.085
3.053
3.033
3.020
3.013
3.000
2.980
2.850
2.840
2.832
2.819
2.807
2.799
2.788
2.760
2.746
2.725
2.710
2.501
2.494
2.465
2.458
0.000
6.50
1.05
0.99
0.92
1.00
0.99
1.05
1.06
1.08
1.12
1.15
1.08
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)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128.674
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126.695
125.514
125.415
95.332
54.722
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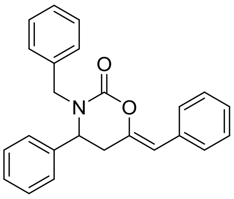
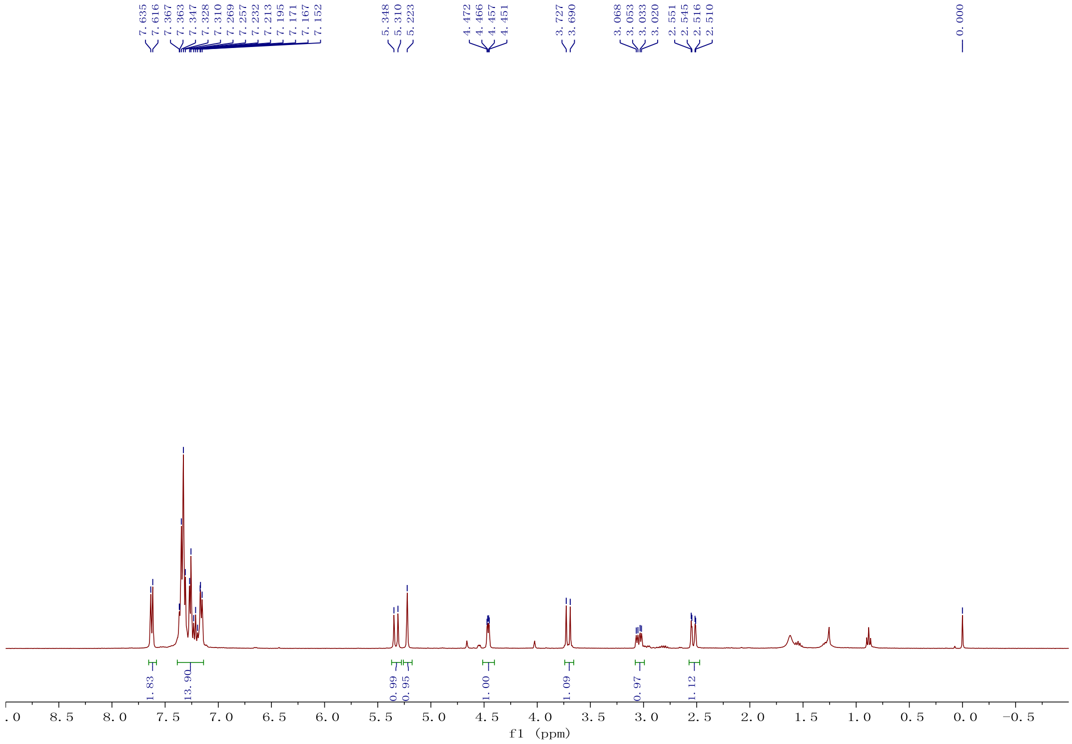
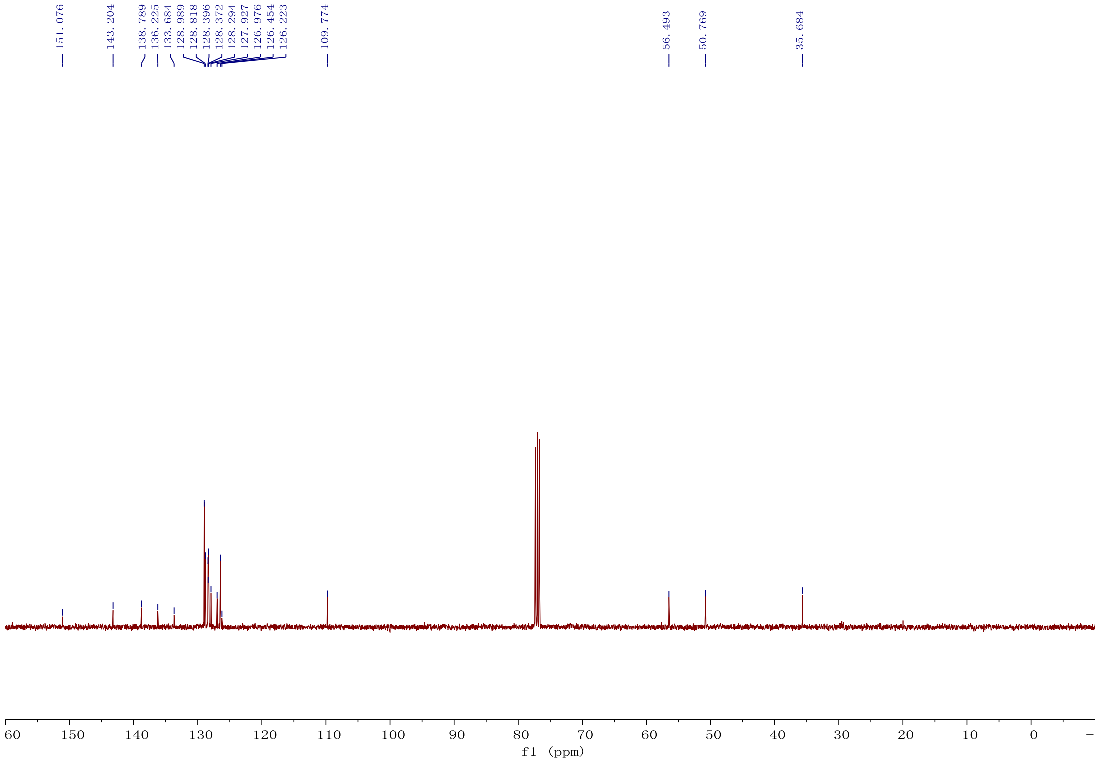
34.334
33.934
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

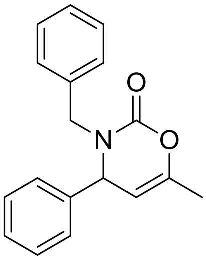


2n

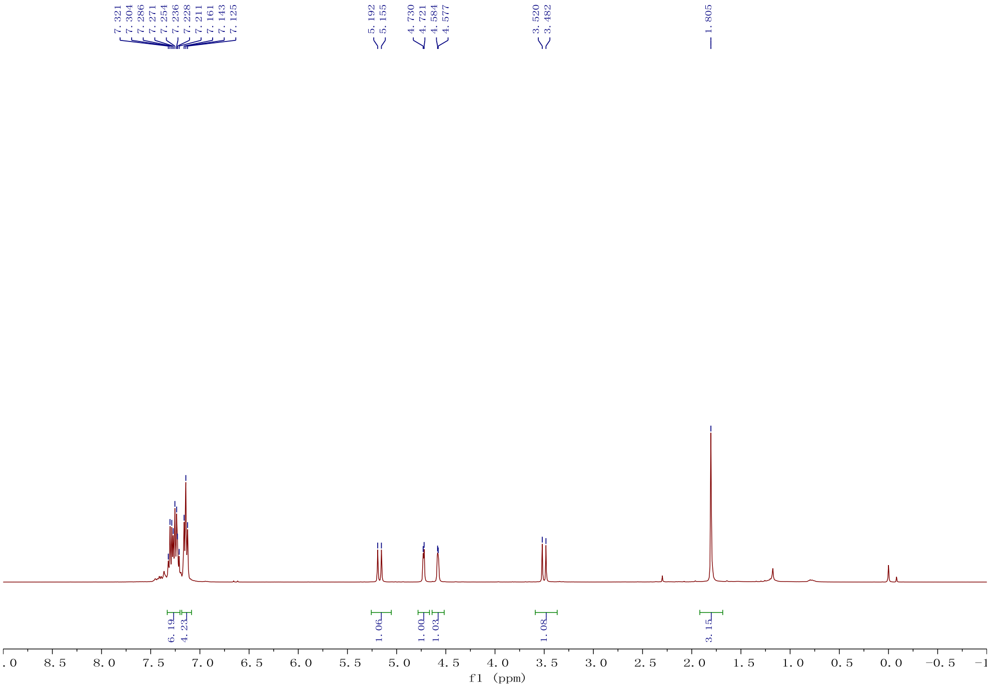

7.635
7.616
7.367
7.363
7.347
7.328
7.310
7.269
7.257
7.232
7.213
7.195
7.171
7.167
7.152
5.348
5.310
5.223
4.472
4.466
4.457
4.451
3.727
3.690
3.068
3.053
3.033
3.020
2.551
2.545
2.516
2.510
0.000
1.83
13.90
0.99
0.95
1.00
1.09
0.97
1.12
. 0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

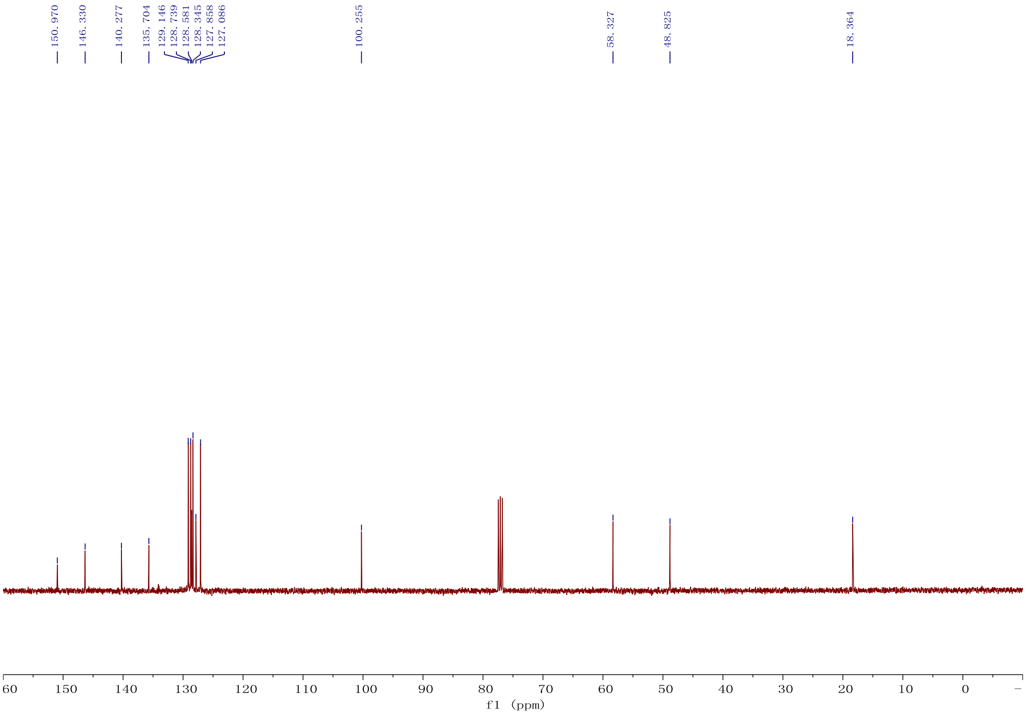

151.076
143.204
138.789
136.225
133.684
128.989
128.818
128.396
128.372
128.294
127.927
126.976
126.454
126.223
109.774
56.493
50.769
35.684
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
–
f1 (ppm)

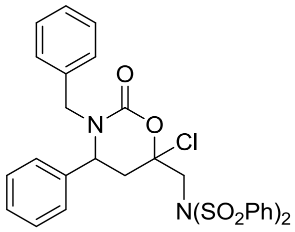
9. The spectra of other compounds 3a, 4a, 5a



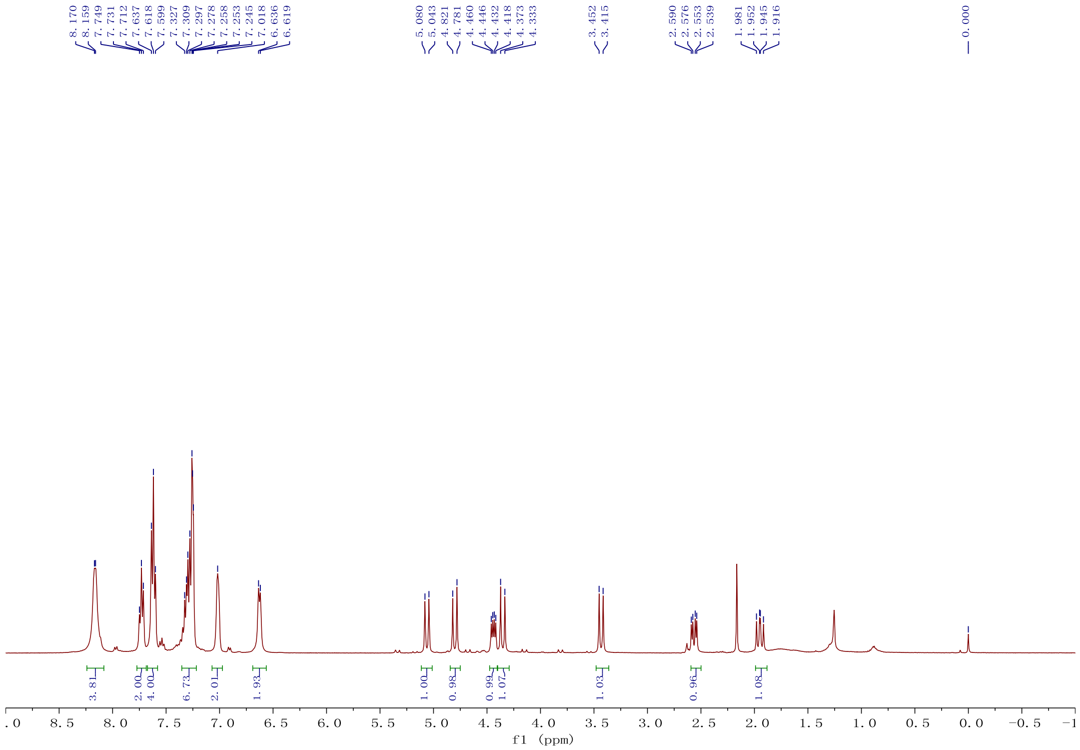
3a

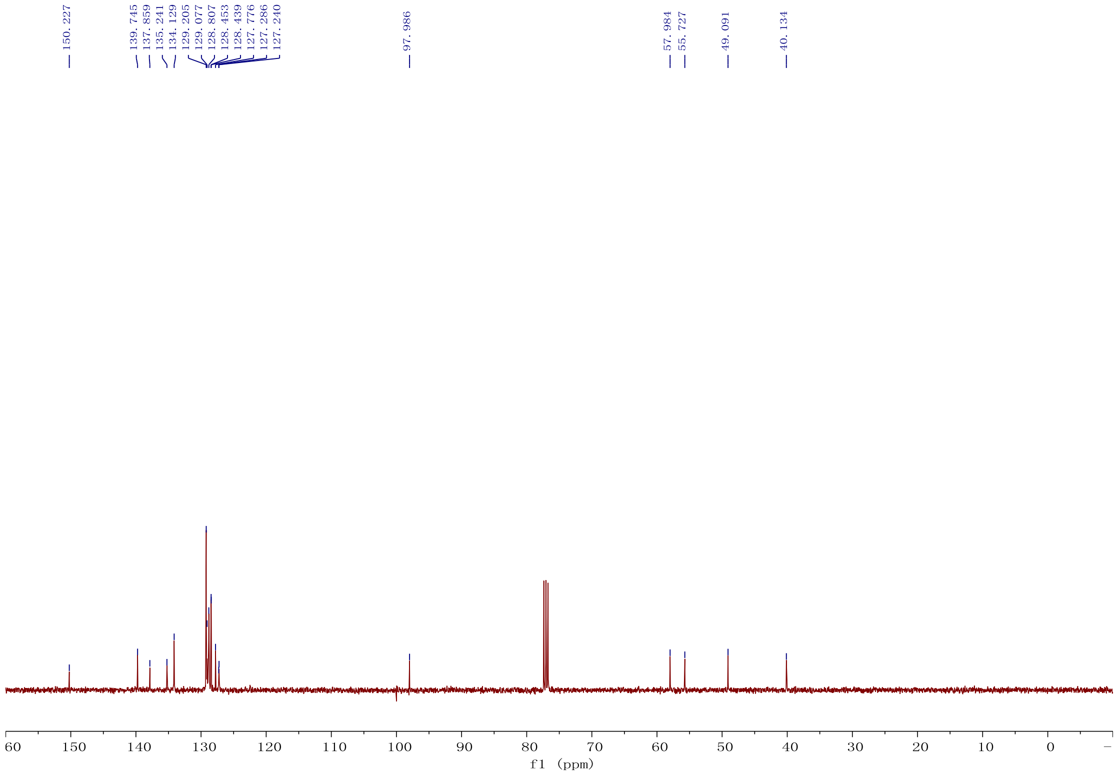


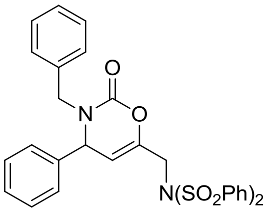



O
N
O
Cl
N(SO$_2$Ph)$_2$

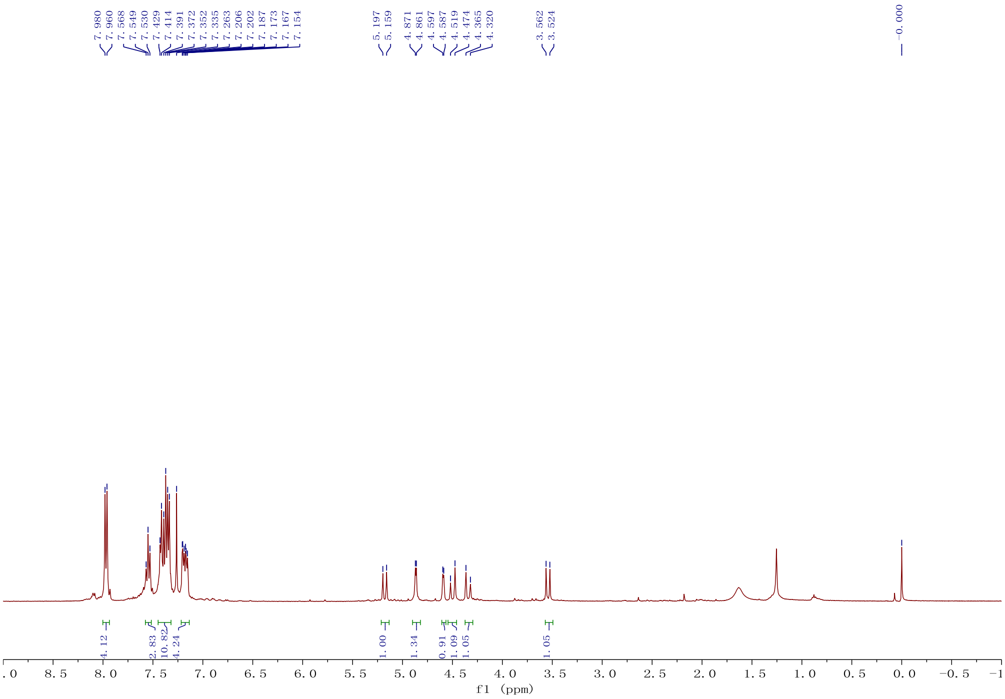
4a

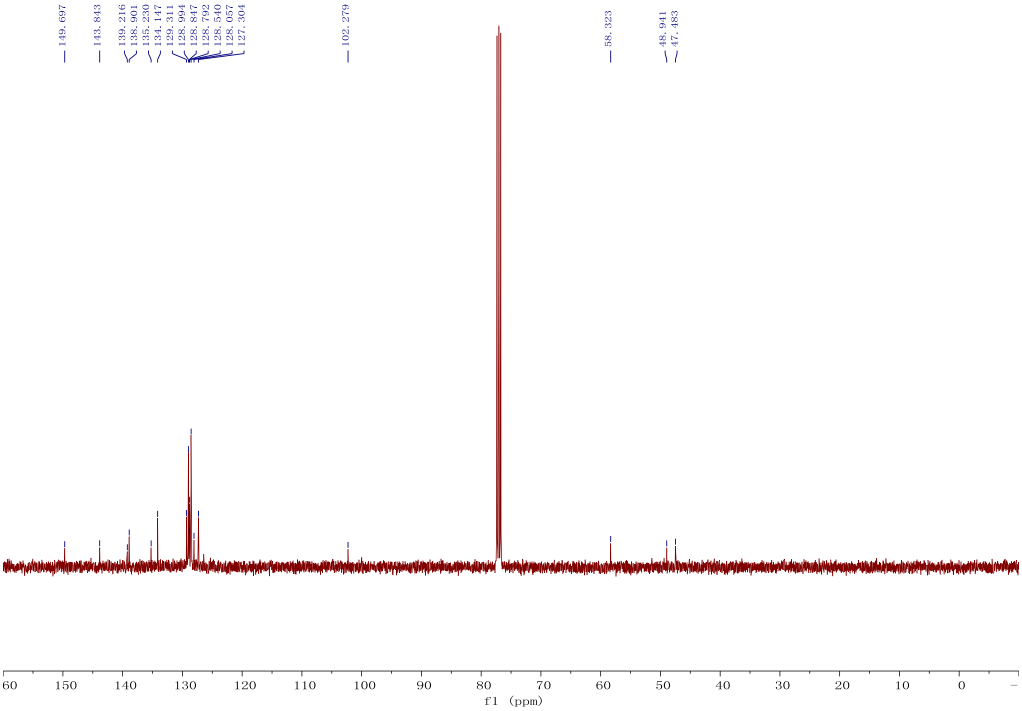

8.170
8.159
7.749
7.731
7.712
7.637
7.618
7.599
7.327
7.309
7.297
7.278
7.258
7.253
7.245
7.018
6.636
6.619
5.080
5.043
4.821
4.781
4.460
4.446
4.432
4.418
4.373
4.333
3.452
3.415
2.590
2.576
2.553
2.539
1.981
1.952
1.945
1.916
0.000
3.81
2.00
4.00
6.73
2.01
1.93
1.00
0.98
0.99
1.07
1.03
0.96
1.08
.0
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
−1
f1 (ppm)


150.227
139.745
137.859
135.241
134.129
129.205
129.077
128.807
128.453
128.439
127.776
127.286
127.240
97.986
57.984
55.727
49.091
40.134
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


O
N
O
N(SO2Ph)2

5a


7.980
7.960
7.568
7.549
7.530
7.429
7.414
7.391
7.372
7.352
7.335
7.263
7.206
7.202
7.187
7.173
7.167
7.154
5.197
5.159
4.871
4.861
4.597
4.587
4.519
4.474
4.365
4.320
3.562
3.524
-0.000
4.12
2.83
10.82
4.24
1.00
1.34
0.91
1.09
1.05
1.05
.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
-1
f1 (ppm)


149.697
143.843
139.216
138.901
135.230
134.147
129.311
128.994
128.847
128.792
128.540
128.057
127.304
102.279
58.323
48.941
47.483
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Reference:

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