

Supporting Information

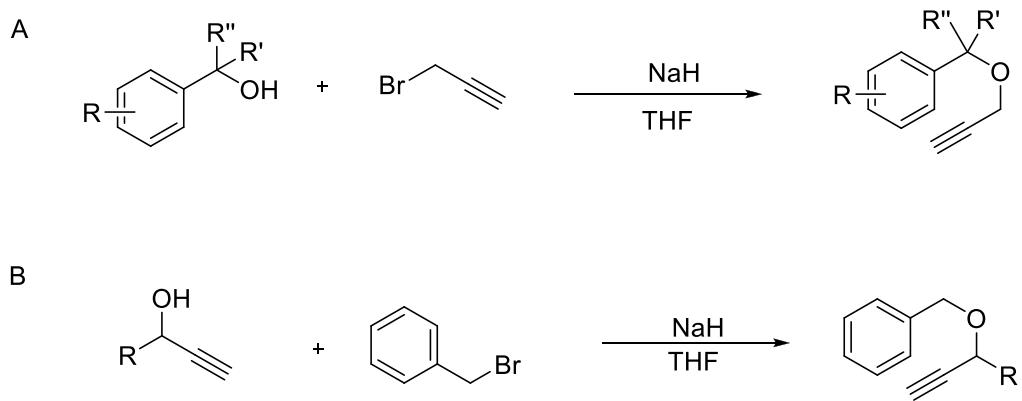
Cyclopropanation of Benzene Rings by Oxidatively Generated α -Oxo Gold Carbene: One-Pot Access to Tetrahydropyranone-Fused Heptatrienes from Propargyl Benzyl Ethers

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General. Ethyl acetate (ACS grade), hexanes (ACS grade), diethyl ether (ACS grade) and anhydrous 1, 2-dichloroethane (anhydride, 99.8%) were purchased from Fisher Scientific and used without further purification. Chlorobenzene (HPLC grade) was purchased from Acros without further purification. Methylene chloride and tetrahydrofuran were purified using MBraun Solvent Purifier. Commercially available reagents were used without further purification. Reactions were monitored by thin layer chromatography (TLC) using Sorbent Technologies' pre-coated silica gel plates. Flash column chromatography was performed over Sorbent Technologies' silica gel (230-400 mesh). ^1H NMR and ^{13}C NMR spectra were recorded on Varian 400 MHz, 500 MHz and 600 MHz spectrometers using residue solvent peaks as internal standards. Infrared spectra were recorded with a Perkin Elmer FT-IR spectrum 2000 spectro-meter and are reported in reciprocal centimeter (cm^{-1}). Mass spectra were recorded with Micromass QTOF₂ Quadrupole/Time-of-Flight Tandem mass spectrometer using electron spray ionization or Waters GCT Premier time-of-flight mass spectrometer with a field ionization (FI) ion source.

General procedure A: Methods for the synthesis ((prop-2-ynyloxy)methyl)benzene derivatives

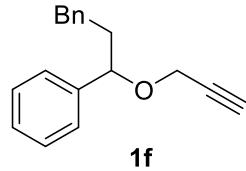


Method A: A solution of benzyl alcohol (5 mmol) was added a solution of NaH (6 mmol) in THF (ca. 20 mL) at 0 °C, after stirring for 30 minutes at room temperature, cool to 0 °C, propargyl bromide (80 % in toluene, 6 mmol) was added dropwise and the resulting slurry was efficiently stirred at room temperature for 6 h (for secondary benzyl alcohol, the reaction was

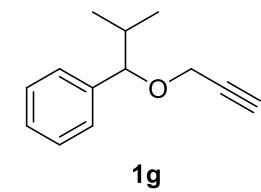
stirred at 50 °C for 6 h). NH₄Cl (10.0 mL), which was extracted with Et₂O. The combined organic phase was washed with water, brine, dried (Na₂SO₄) and concentrated. The mixture was purified by flash chromatography on silica gel (petroleum ether/EtOAc = 10:1) to give pure product as a colorless oil (70% yield).

Method B: To a stirred solution of propargyl alcohol (5 mmol) was added a solution of NaH (6 mmol) in THF (ca. 20 mL). After stirring for 30 minutes, freshly distilled benzyl bromide (6 mmol) was added dropwise and the resulting slurry was efficiently stirred at room temperature for 6 h. the mixture was quenched with aq. NH₄Cl (10.0 mL), which was extracted with Et₂O. The combined organic phase was washed with water, brine, dried (Na₂SO₄) and concentrated. The mixture was purified by flash chromatography on silica gel (petroleum ether/EtOAc = 10:1) to give pure product as a colorless oil (70% yield).

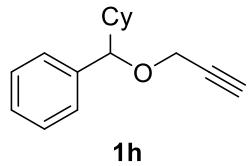
The known compound ((prop-2-ynyoxy)methyl)benzene derivatives **1a**,¹ **1b**,² **1c**,³ **1d**,⁴ **1e**,⁵ **1i**,⁶ **1j**,⁷ **1k**,⁸ **1m**,⁹ **1n**,¹⁰ **1p**,¹¹ was prepared according to the general procedure A and its spectroscopic data were in accordance with the literature data.



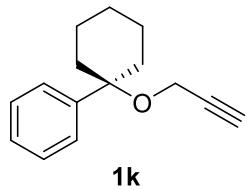
(1-(prop-2-ynyoxy)propane-1,3-diyl)dibenzene 1f: The compound **1f** was prepared in 83% yield through the General Procedure A.¹ ¹H NMR (500 MHz, Chloroform-d) δ 7.39 – 7.34 (m, 2H), 7.33 – 7.26 (m, 5H), 7.22 – 7.16 (m, 3H), 4.47 (dd, *J* = 8.1, 5.3 Hz, 1H), 4.12 (dd, *J* = 15.7, 2.2 Hz, 1H), 3.86 (dd, *J* = 15.6, 2.2 Hz, 1H), 2.78 (ddd, *J* = 14.8, 9.8, 5.5 Hz, 1H), 2.72 – 2.62 (m, 1H), 2.41 (d, *J* = 2.8 Hz, 1H), 2.24 – 2.12 (m, 1H), 2.03 – 1.91 (m, 1H).¹³C NMR (126 MHz, CDCl₃) δ 141.8, 141.1, 128.5, 128.5, 1283, 127.9, 126.9, 125.8, 80.1, 80.0, 74.0, 55.6, 39.4, 32.0. IR (neat, cm⁻¹): 3292, 3028, 2935, 1603, 1495, 1454, 1084, 750. GCMS (EI) calcd for C₁₈H₁₈O: 250.1, found: 250.0.



(2-methyl-1-(prop-2-nyloxy)propyl)benzene 1g: The compound **1g** was prepared in 80% yield through the General Procedure A. ^1H NMR (500 MHz, Chloroform-d) δ 7.34 (t, $J = 7.1$ Hz, 2H), 7.30 – 7.25 (m, 3H), 4.18 – 4.05 (m, 2H), 3.82 (dd, $J = 15.7, 2.3$ Hz, 1H), 2.38 (t, $J = 2.4$ Hz, 1H), 1.96 (dq, $J = 13.8, 6.9$ Hz, 1H), 1.03 (d, $J = 6.6$ Hz, 3H), 0.74 (d, $J = 6.8$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 140.1, 128.1, 127.6, 86.4, 80.2, 73.7, 55.8, 34.5, 19.1, 19.0. IR (neat, cm^{-1}): 3304, 2960, 1453, 1385, 1074, 768. GCMS (EI) calcd for $\text{C}_{13}\text{H}_{16}\text{O}$: 188.1, found: 188.1.

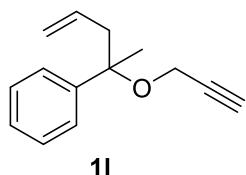


(cyclohexyl(prop-2-nyloxy)methyl)benzene 1h: The compound **1h** was prepared in 80% yield through the General Procedure A. ^1H NMR (600 MHz, Chloroform-d) δ 7.34 (t, $J = 7.3$ Hz, 2H), 7.29 (d, $J = 7.2$ Hz, 1H), 7.26 (d, $J = 7.3$ Hz, 2H), 4.15 (d, $J = 7.7$ Hz, 1H), 4.08 (dd, $J = 15.5, 2.2$ Hz, 1H), 3.80 (dd, $J = 15.7, 1.7$ Hz, 1H), 2.37 (t, $J = 1.5$ Hz, 1H), 2.12 – 2.05 (m, 1H), 1.75 (dd, $J = 14.3, 3.5$ Hz, 1H), 1.64 (ddq, $J = 16.7, 9.0, 4.7, 4.3$ Hz, 3H), 1.29 (d, $J = 13.1$ Hz, 1H), 1.22 (dtd, $J = 12.8, 9.2, 3.3$ Hz, 1H), 1.12 (q, $J = 11.1, 10.6$ Hz, 2H), 1.08 – 1.00 (m, 1H), 0.91 (qd, $J = 12.3, 3.6$ Hz, 1H). ^{13}C NMR (151 MHz, cdcl_3) δ 140.1, 128.1, 127.7, 127.6, 85.7, 80.3, 73.7, 55.7, 44.0, 29.6, 29.3, 26.5, 26.0, 25.9. IR (neat, cm^{-1}): 3307, 2925, 2853, 1451, 1069, 759. GCMS (EI) calcd for $\text{C}_{16}\text{H}_{20}\text{O}$: 228.2, found: 228.2.

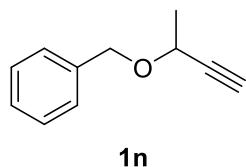


(1-(prop-2-nyloxy)cyclohexyl)benzene 1k: The known compound **1k** was prepared in 45% yield through the General Procedure A and its spectroscopic data were in accordance with the literature data.⁸ ^1H NMR (500 MHz, Chloroform-d) δ 7.44 (d, $J = 7.6$ Hz, 2H), 7.36 (t, $J = 7.6$ Hz, 2H), 7.30 – 7.21 (m, 1H), 3.74 (dd, $J = 2.4, 0.8$ Hz, 2H), 2.36 (td, $J = 2.4, 0.8$ Hz, 1H), 2.04 (dd, $J = 14.1, 3.1$ Hz, 2H), 1.89 – 1.66 (m, 5H), 1.64 – 1.48 (m, 2H), 1.27 (dddd, $J = 16.0, 12.2, 7.7, 3.8$ Hz, 1H). ^{13}C NMR (126 MHz, CDCl_3) δ 145.1, 128.4, 127.2, 126.0, 81.1, 78.8, 73.0,

50.6, 35.7, 25.6, 22.0. IR (neat, cm^{-1}): 3293, 2935, 2859, 1447, 1061, 760. GCMS (EI) calcd for $\text{C}_{15}\text{H}_{18}\text{O}$: 214.1, found: 214.1.

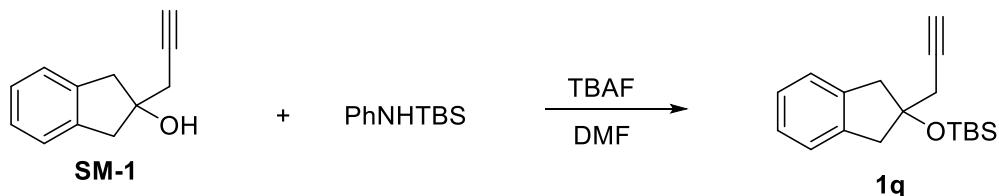


(2-(prop-2-ynyloxy)pent-4-en-2-yl)benzene 1l: The compound **1l** was prepared in 65% yield through the General Procedure A. ^1H NMR (600 MHz, Chloroform-d) δ 7.39 (d, $J = 7.7$ Hz, 2H), 7.36 (t, $J = 7.6$ Hz, 2H), 7.30 – 7.25 (m, 1H), 5.66 (ddt, $J = 17.4, 10.6, 7.1$ Hz, 1H), 5.17 – 4.91 (m, 2H), 3.98 – 3.75 (m, 2H), 2.61 (dd, $J = 14.0, 7.3$ Hz, 1H), 2.54 (dd, $J = 13.9, 7.2$ Hz, 1H), 2.38 (t, $J = 2.5$ Hz, 1H), 1.57 (s, 3H). ^{13}C NMR (151 MHz, CDCl_3) δ 143.9, 133.8, 128.30, 127.3, 126.2, 117.9, 81.1, 80.1, 73.2, 51.3, 47.5, 23.0. IR (neat, cm^{-1}): 3299, 2981, 1447, 1378, 1060, 918, 766. GCMS (EI) calcd for $\text{C}_{14}\text{H}_{16}\text{O}$: 200.12, found: 200.13.

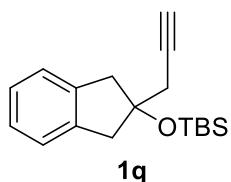


((but-3-yn-2-yloxy)methyl)benzene 1n: The known compound **1n** was prepared in 90% yield through the General Procedure A, method B and its spectroscopic data were in accordance with the literature data.¹⁰ ^1H NMR (500 MHz, Chloroform-d) δ 7.40 – 7.33 (m, 4H), 7.32 – 7.26 (m, 1H), 4.80 (d, $J = 11.6$ Hz, 1H), 4.52 (d, $J = 11.6$ Hz, 1H), 4.22 (qd, $J = 6.5, 2.0$ Hz, 1H), 2.47 (d, $J = 2.4$ Hz, 1H), 1.49 (d, $J = 6.6$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 137.8, 128.4, 128.0, 127.7, 83.7, 73.1, 70.5, 64.2, 22.0. IR (neat, cm^{-1}): 3295, 2989, 1455, 1328, 1065, 1099, 738. GCMS (EI) calcd for $\text{C}_{11}\text{H}_{12}\text{O}$: 160.1, found: 160.0.

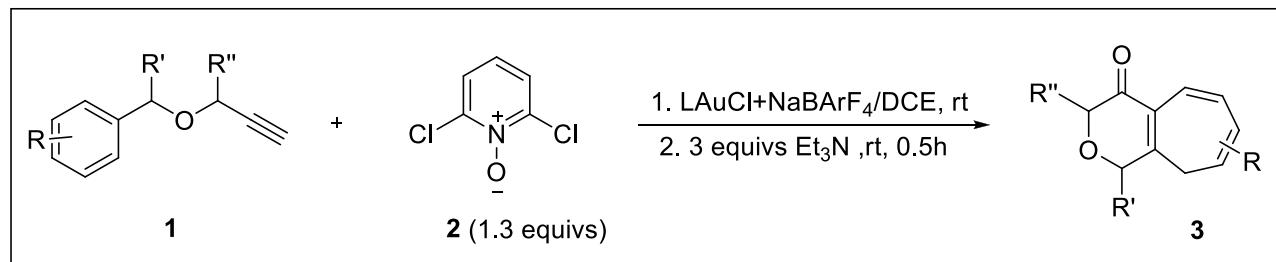
General procedure B: for the preparation of tert-butyldimethyl(2-(prop-2-ynyl)-2,3-dihydro-1H-inden-2-yloxy)silane 1q:



TBAF (1 M THF solution; 0.2 mL, 0.2 mmol) was added to a stirred solution of 2-(prop-2-ynyl)-2,3-dihydro-1H-inden-2-ol (2.0 mmol) and PhNHTBS (3.0 mmol) in DMF (4.0 mL) at 20–25 °C under an Ar atmosphere. After stirring at the same temperature for 4 hours, the mixture was quenched with water (10.0 mL), which was extracted with Et₂O. The combined organic phase was washed with water, brine, dried (Na₂SO₄) and concentrated. The obtained crude product was purified by SiO₂ column chromatography (hexane) to tert-butyldimethyl(2-(prop-2-ynyl)-2,3-dihydro-1H-inden-2-yloxy)silane **1q** (75%); colorless oil.

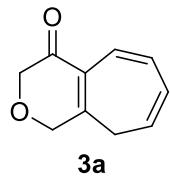


tert-butyldimethyl(2-(prop-2-ynyl)-2,3-dihydro-1H-inden-2-yloxy)silane 1q: ¹H NMR (600 MHz, Chloroform-d) δ 7.16 (q, *J* = 5.0 Hz, 4H), 3.22 (d, *J* = 16.0 Hz, 2H), 3.02 (d, *J* = 16.0 Hz, 2H), 2.56 (d, *J* = 2.7 Hz, 2H), 2.01 (d, *J* = 2.7 Hz, 1H), 0.83 (s, 9H), -0.03 (s, 6H). ¹³C NMR (151 MHz, cdcl₃) δ 141.3, 126.5, 124.7, 83.6, 81.9, 70.6, 46.1, 31.6, 25.7, 18.1, -2.8. IR (neat, cm⁻¹): 3312, 2955, 2929, 1462, 1254, 1120, 1085, 774. GCMS (EI) calcd for C₁₈H₂₆OSi: 286.18, found: 286.20.

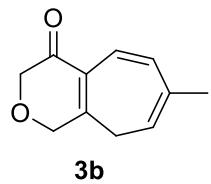


General procedure C for gold-catalyzed oxidative cyclopropanation and ring expansion: 2,6-dichloropyridine N-oxide **2c** (42.4 mg, 0.26 mmol), and Me₄^tBuXPhosAuCl (7.1 mg, 0.010 mmol, 5 mol %) and NaBArF₄ (13 mg, 0.015 mmol, 7.5 mol %) were added sequentially to a solution of the propargyl benzyl ethers **1** (0.20 mmol) in DCE (4 mL, 0.05M) at room temperature. The resulting reaction mixture was stirred at RT, and the progress of the reaction was monitored by TLC. The reaction typically took 1–3 h. Upon completion, the reaction mixture was added 3 equiv. Et₃N and stirred for 0.5 h at room temperature. The reaction mixture was concentrated under vacuum. The residue was purified by chromatography on silica gel

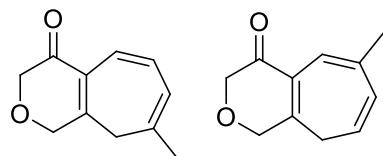
(eluent: hexanes/ethyl acetate) to afford the desired product **3**.



3,9-dihydrocyclohepta[c]pyran-4(1H)-one 3a: The compound **3a** was prepared in 69% yield according to the general procedure C (eluents: ethyl acetate: hexanes = 1:10). ¹H NMR (500 MHz, Chloroform-d) δ 7.23 (d, *J* = 11.4 Hz, 1H), 6.70 (dd, *J* = 11.4, 5.6 Hz, 1H), 6.30 (dd, *J* = 9.3, 5.5 Hz, 1H), 5.47 (dt, *J* = 9.3, 6.7 Hz, 1H), 4.56 (s, 2H), 4.17 (s, 2H), 2.42 (d, *J* = 6.7 Hz, 2H). ¹³C NMR (126 MHz, CDCl₃) δ 193.3, 144.9, 131.2, 129.3, 128.8, 124.9, 119.9, 71.7, 69.0, 29.5. IR (neat, cm⁻¹): 3028, 1683, 1435, 1314, 1121, 722. MS (ESI/[M+Na]⁺) calcd for C₁₀H₁₀NaO₂⁺: 185.06, found: 185.06.



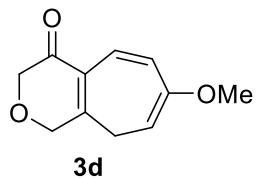
7-methyl-3,9-dihydrocyclohepta[c]pyran-4(1H)-one 3b: The compound **3b** was prepared in 65% yield according to the general procedure C (eluents: ethyl acetate: hexanes = 1:10). ¹H NMR (600 MHz, Chloroform-d) δ 7.10 (d, *J* = 11.5 Hz, 1H), 6.58 (d, *J* = 11.5 Hz, 1H), 5.21 (t, *J* = 6.8 Hz, 1H), 4.54 (s, 1H), 4.14 (s, 1H), 2.34 (d, *J* = 6.8 Hz, 2H), 1.89 (s, 2H). ¹³C NMR (151 MHz, cdcl₃) δ 193.1, 147.0, 136.9, 134.4, 128.8, 123.9, 116.4, 71.6, 68.7, 29.2, 21.4. IR (neat, cm⁻¹): 2939, 1681, 1440, 1301, 1172, 958, 735. GCMS (EI) calcd for C₁₁H₁₂O₂: 176.08, found: 176.09.



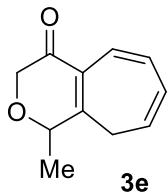
3c:3c'=1.7:1

8-methyl-3,9-dihydrocyclohepta[c]pyran-4(1H)-one 3c and 6-methyl-3,9-dihydrocyclohepta[c]pyran-4(1H)-one 3c': The compound **3c** and **3c'** was prepared in 39% yield according to the general procedure C (eluents: ethyl acetate: hexanes = 1:10). **3c (major)**

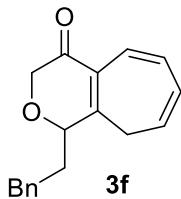
¹H NMR (500 MHz, Chloroform-d) δ 7.12 (d, *J* = 11.3 Hz, 1H), 6.62 (dd, *J* = 11.4, 5.8 Hz, 1H), 6.11 (t, *J* = 8.1 Hz, 1H), 4.49 (s, 2H), 4.16 (s, 2H), 2.33 (s, 2H), 2.02 (s, 3H). **3c'** (minor) ¹H NMR (500 MHz, Chloroform-d) δ 7.01 (s, 1H), 6.11 (t, *J* = 8.1 Hz, 1H), 5.44 (dt, *J* = 9.5, 6.8 Hz, 1H), 4.54 (s, 2H), 4.15 (s, 2H), 2.39 (d, *J* = 6.7 Hz, 2H), 2.11 (s, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 193.6, 193.4, 143.6, 142.8, 140.6, 131.9, 131.2, 130.7, 129.2, 128.9, 124.0, 122.8, 122.5, 121.7, 119.1, 71.7, 71.5, 69.2, 68.9, 35.3, 29.4, 24.7, 24.4. IR (neat, cm⁻¹): 2966, 1683, 1437, 1346, 1120, 958, 767. MS (ESI/[M+Na]⁺) calcd for C₁₁H₁₂NaO₂⁺: 199.07, found: 199.07.



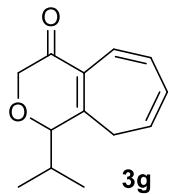
7-methoxy-3,9-dihydrocyclohepta[c]pyran-4(1H)-one 3d: The compound **3d** was prepared in 50 % yield according to the general procedure **C** (eluents: ethyl acetate: hexanes = 1:10). ¹H NMR (600 MHz, Chloroform-d) δ 6.43 (d, *J* = 7.0 Hz, 1H), 6.35 (t, *J* = 7.7 Hz, 1H), 5.47 (d, *J* = 6.9 Hz, 1H), 4.58 (s, 2H), 4.18 (s, 2H), 3.61 (s, 3H), 2.62 (d, *J* = 7.8 Hz, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 197.1, 149.5, 134.1, 129.9, 125.5, 123.3, 98.0, 74.1, 70.9, 56.5, 32.8. IR (neat, cm⁻¹): 2964, 2837, 1701, 1601, 1507, 1292, 1164, 1098, 1036, 765. MS (ESI/[M+Na]⁺) calcd for C₁₁H₁₂NaO₃⁺: 215.07, found: 215.08.



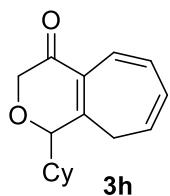
1-methyl-3,9-dihydrocyclohepta[c]pyran-4(1H)-one 3e: The compound **3e** was prepared in 83% yield according to the general procedure **C** (eluents: ethyl acetate: hexanes = 1:10). ¹H NMR (500 MHz, CDCl₃) δ 7.27 (d, *J* = 11.3 Hz, 1H), 6.74 (dd, *J* = 11.3, 5.5 Hz, 1H), 6.32 (dd, *J* = 9.1, 5.5 Hz, 1H), 5.47 (dd, *J* = 16.0, 6.9 Hz, 1H), 4.65 (q, *J* = 6.6 Hz, 1H), 4.30 – 4.22 (m, 1H), 4.12 (ddd, *J* = 13.0, 12.5, 8.6 Hz, 1H), 2.78 (dd, *J* = 12.1, 7.5 Hz, 1H), 1.93 – 1.82 (m, 1H), 1.49 (d, *J* = 6.7 Hz, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 193.5, 148.4, 131.3, 129.0, 128.4, 124.8, 119.4, 73.5, 70.1, 29.9, 21.0. IR (neat, cm⁻¹): 2984, 1683, 1437, 1311, 1296, 1120, 743. MS (ESI/[M+Na]⁺) calcd for C₁₁H₁₂NaO₂⁺: 199.07, found: 199.07.



1-phenethyl-3,9-dihydrocyclohepta[c]pyran-4(1H)-one 3f: The compound **3f** was prepared in 82% yield according to the general procedure **C** (eluents: ethyl acetate: hexanes = 1:10). ¹H NMR (500 MHz, Chloroform-d) δ 7.36 – 7.32 (m, 2H), 7.29 (d, *J* = 11.4 Hz, 1H), 7.26 – 7.20 (m, 3H), 6.75 (dd, *J* = 11.3, 5.5 Hz, 1H), 6.33 (dd, *J* = 9.2, 5.5 Hz, 1H), 5.46 (dt, *J* = 9.1, 6.8 Hz, 1H), 4.49 (dd, *J* = 9.7, 2.7 Hz, 1H), 4.33 (d, *J* = 16.2 Hz, 1H), 4.14 (d, *J* = 16.3 Hz, 1H), 2.92 (ddd, *J* = 14.0, 9.6, 4.5 Hz, 1H), 2.78 (dt, *J* = 13.8, 8.3 Hz, 1H), 2.72 (dd, *J* = 12.2, 7.4 Hz, 1H), 2.27 – 2.13 (m, 1H), 2.05 – 1.87 (m, 2H). ¹³C NMR (126 MHz, CDCl₃) δ 193.4, 147.2, 141.2, 131.3, 129.5, 128.5, 128.5, 128.4, 126.1, 125.1, 119.7, 76.1, 69.5, 36.0, 31.7, 29.8. IR (neat, cm⁻¹): 3028, 2930, 1686, 1496, 1454, 1310, 1113, 750. MS (ESI/[M+Na]⁺) calcd for C₁₈H₁₈NaO₂⁺: 289.12, found: 289.12.



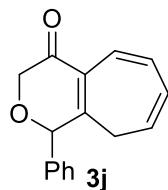
1-isopropyl-3,9-dihydrocyclohepta[c]pyran-4(1H)-one 3g: The compound **3g** was prepared in 77% yield according to the general procedure **C** (eluents: ethyl acetate: hexanes = 1:10). ¹H NMR (500 MHz, Chloroform-d) δ 7.26 (d, *J* = 11.3 Hz, 1H), 6.72 (dd, *J* = 11.4, 5.5 Hz, 1H), 6.41 – 6.25 (m, 1H), 5.44 (td, *J* = 8.6, 6.1 Hz, 1H), 4.40 (s, 1H), 4.26 (d, *J* = 16.0 Hz, 1H), 4.06 (dd, *J* = 16.0, 1.8 Hz, 1H), 2.91 (dd, *J* = 12.2, 7.7 Hz, 1H), 2.19 (pd, *J* = 6.8, 2.6 Hz, 1H), 1.94 – 1.84 (m, 1H), 1.15 (d, *J* = 6.9 Hz, 3H), 0.77 (d, *J* = 6.8 Hz, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 193.6, 146.8, 131.2, 130.6, 128.3, 125.2, 120.7, 82.0, 70.4, 31.8, 29.7, 20.4, 15.7. IR (neat, cm⁻¹): 2971, 1685, 1437, 1313, 1109, 953, 722. MS (ESI/[M+Na]⁺) calcd for C₁₃H₁₆NaO₂⁺: 227.10, found: 227.10.



1-cyclohexyl-3,9-dihydrocyclohepta[c]pyran-4(1H)-one 3h: The compound **3h** was prepared in 78% yield according to the general procedure **C** (eluents: ethyl acetate: hexanes = 1:10). ¹H NMR (500 MHz, Chloroform-d) δ 7.26 (d, *J* = 11.4 Hz, 1H), 6.72 (dd, *J* = 11.4, 5.5 Hz, 1H), 6.33 (dd, *J* = 9.3, 5.4 Hz, 1H), 5.42 (td, *J* = 8.6, 6.3 Hz, 1H), 4.38 (s, 1H), 4.25 (d, *J* = 16.1 Hz, 1H), 4.10 – 4.00 (m, 1H), 2.90 (dd, *J* = 12.2, 7.7 Hz, 1H), 1.89 (dd, *J* = 12.3, 6.1 Hz, 1H), 1.85 – 1.74 (m, 2H), 1.71 – 1.64 (m, 3H), 1.59 – 1.44 (m, 2H), 1.32 (tdd, *J* = 12.9, 9.1, 3.7 Hz, 1H), 1.19 – 1.02 (m, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 193.6, 146.7, 131.2, 130.5, 128.4, 125.4, 120.5, 82.1, 70.3, 42.1, 30.8, 29.9, 26.8, 26.3, 26.2, 26.1. IR (neat, cm⁻¹): 2932, 2853, 1686, 1438, 1311, 1140, 716. MS (ESI/[M+Na]⁺) calcd for C₁₆H₂₀NaO₂⁺: 267.14, found: 267.14.

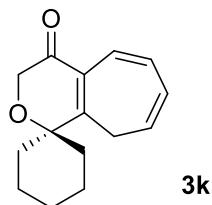


1-allyl-3,9-dihydrocyclohepta[c]pyran-4(1H)-one 3i: The compound **3i** was prepared in 71% yield according to the general procedure **C** (eluents: ethyl acetate: hexanes = 1:10). ¹H NMR (600 MHz, Chloroform-d) δ 7.26 (d, *J* = 11.3 Hz, 1H), 6.74 (dd, *J* = 11.4, 5.5 Hz, 1H), 6.32 (dd, *J* = 9.3, 5.5 Hz, 1H), 5.89 (ddt, *J* = 17.0, 10.2, 6.8 Hz, 1H), 5.47 (dt, *J* = 9.1, 6.9 Hz, 1H), 5.23 – 5.09 (m, 2H), 4.59 (dd, *J* = 8.8, 3.6 Hz, 1H), 4.29 (d, *J* = 16.4 Hz, 1H), 4.11 (d, *J* = 16.4 Hz, 1H), 2.75 (dd, *J* = 12.3, 7.3 Hz, 1H), 2.70 – 2.62 (m, 1H), 2.47 (dt, *J* = 15.1, 7.7 Hz, 1H), 2.00 (dd, *J* = 12.3, 6.3 Hz, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 193.3, 146.6, 133.7, 131.5, 129.6, 128.4, 125.0, 119.8, 117.8, 76.8, 69.6, 38.6, 29.9. IR (neat, cm⁻¹): 2977, 1684, 1436, 1310, 1119, 995, 919, 754. MS (ESI/[M+Na]⁺) calcd for C₁₃H₁₄NaO₂⁺: 225.09, found: 225.09.

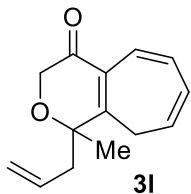


1-phenyl-3,9-dihydrocyclohepta[c]pyran-4(1H)-one 3j: The compound **3j** was prepared in 84% yield according to the general procedure **C** (eluents: ethyl acetate: hexanes = 1:10). ¹H

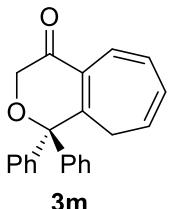
¹H NMR (600 MHz, Chloroform-d) δ 7.42 – 7.35 (m, 5H), 7.30 (d, *J* = 11.5 Hz, 1H), 6.74 (dd, *J* = 11.4, 5.5 Hz, 1H), 6.24 (dd, *J* = 9.3, 5.5 Hz, 1H), 5.52 (s, 1H), 4.97 (dt, *J* = 9.3, 6.8 Hz, 1H), 4.25 (d, *J* = 16.4 Hz, 1H), 4.18 (d, *J* = 16.5 Hz, 1H), 2.49 (dd, *J* = 12.2, 7.2 Hz, 1H), 2.09 (dd, *J* = 12.2, 6.3 Hz, 1H). ¹³C NMR (151 MHz, cdcl₃) δ 193.4, 147.1, 138.5, 131.6, 130.1, 129.1, 128.9, 128.6, 128.1, 124.4, 121.8, 80.7, 69.6, 30.4. IR (neat, cm⁻¹): 3029, 1686, 1439, 1340, 1111, 995, 748, 720. MS (ESI/[M+Na]⁺) calcd for C₁₆H₁₄NaO₂⁺: 261.09, found: 261.09.



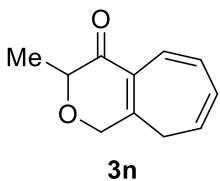
3H-spiro[cyclohepta[c]pyran-1,1'-cyclohexan]-4(9H)-one 3k: The compound **3k** was prepared in 80% yield according to the general procedure **C** (eluents: ethyl acetate: hexanes = 1:10). ¹H NMR (500 MHz, Chloroform-d) δ 7.29 (d, *J* = 11.4 Hz, 1H), 6.72 (dd, *J* = 11.3, 5.4 Hz, 1H), 6.30 (dd, *J* = 9.1, 5.4 Hz, 1H), 5.49 – 5.30 (m, 1H), 4.20 (s, 2H), 2.31 (d, *J* = 6.9 Hz, 2H), 1.89 (d, *J* = 11.5 Hz, 2H), 1.79 – 1.60 (m, 7H), 1.35 – 1.21 (m, 1H). ¹³C NMR (126 MHz, CDCl₃) δ 194.3, 152.1, 131.0, 128.3, 128.1, 125.2, 119.8, 76.3, 65.6, 32.5, 30.1, 25.0, 21.1. IR (neat, cm⁻¹): 2933, 1682, 1439, 1310, 1108, 937, 753. MS (ESI/[M+Na]⁺) calcd for C₁₅H₁₈NaO₂⁺: 253.12, found: 253.13.



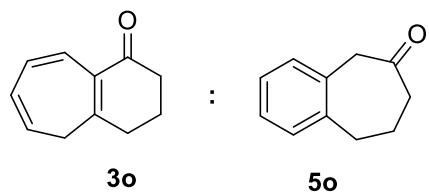
1-allyl-1-methyl-3,9-dihydrocyclohepta[c]pyran-4(1H)-one 3l: The compound **3l** was prepared in 65% yield according to the general procedure **C** (eluents: ethyl acetate: hexanes = 1:10). ¹H NMR (500 MHz, Chloroform-d) δ 7.27 (d, *J* = 11.4 Hz, 1H), 6.72 (dd, *J* = 11.4, 5.4 Hz, 1H), 6.30 (dd, *J* = 9.2, 5.4 Hz, 1H), 5.91 – 5.77 (m, 1H), 5.46 (dt, *J* = 9.1, 6.9 Hz, 1H), 5.22 – 5.14 (m, 1H), 5.14 (s, 1H), 4.36 – 4.13 (m, 2H), 2.70 (dd, *J* = 14.7, 6.2 Hz, 1H), 2.51 (dd, *J* = 14.6, 7.9 Hz, 1H), 2.43 (dd, *J* = 12.2, 7.0 Hz, 1H), 2.30 (dd, *J* = 12.3, 6.9 Hz, 1H), 1.48 (s, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 193.7, 152.0, 132.6, 131.3, 128.6, 128.2, 125.2, 120.7, 118.6, 77.3, 66.4, 42.2, 30.4, 23.7. IR (neat, cm⁻¹): 2980, 1686, 1437, 1310, 1109, 920, 756. MS (ESI/[M+Na]⁺) calcd for C₁₄H₁₆NaO₂⁺: 239.10, found: 239.11.



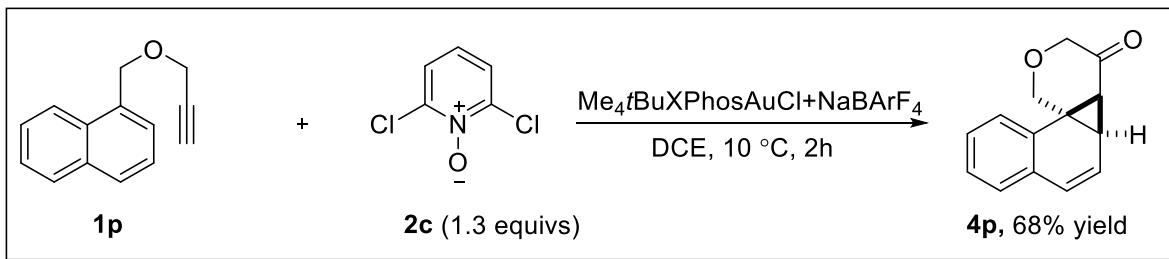
1,1-diphenyl-3,9-dihydrocyclohepta[c]pyran-4(1H)-one 3m: The compound **3m** was prepared in 70% yield according to the general procedure **C** (eluents: ethyl acetate: hexanes = 1:10). The polar of the compound **3n** and 2,6-dichloropyridine is the same, and can't be separated. For detail, see the HNMR. ^1H NMR (500 MHz, Chloroform-d) δ 7.34 (ddd, J = 16.6, 7.1, 3.5 Hz, 1H), 6.72 (dd, J = 11.4, 5.4 Hz, 1H), 6.08 (dd, J = 9.2, 5.4 Hz, 1H), 4.30 (dt, J = 9.2, 6.9 Hz, 1H), 4.02 (s, 2H), 2.46 (d, J = 6.8 Hz, 2H). ^{13}C NMR (126 MHz, CDCl_3) δ 193.9, 151.2, 150.6, 140.7, 131.6, 130.0, 129.2, 128.5, 128.1, 127.9, 127.3, 124.2, 122.8, 122.8, 85.9, 67.0, 32.8. IR (neat, cm^{-1}): 3045, 1687, 1565, 1438, 1339, 1162, 989, 760. MS (ESI/[M+Na] $^+$) calcd for $\text{C}_{22}\text{H}_{18}\text{NaO}_2^+$: 337.12, found: 337.13.



3-methyl-3,9-dihydrocyclohepta[c]pyran-4(1H)-one 3n: The compound **3n** was prepared in 40% yield according to the general procedure **C** (eluents: ethyl acetate: hexanes = 1:10). ^1H NMR (600 MHz, Chloroform-d) δ 7.22 (d, J = 11.4 Hz, 1H), 6.68 (dd, J = 11.4, 5.5 Hz, 1H), 6.28 (dd, J = 9.3, 5.5 Hz, 1H), 5.46 (dt, J = 8.8, 6.5 Hz, 1H), 4.65 (d, J = 18.7 Hz, 1H), 4.48 (d, J = 18.7 Hz, 1H), 4.09 (q, J = 6.7 Hz, 1H), 2.71 (dd, J = 12.4, 7.5 Hz, 1H), 2.11 (dd, J = 12.5, 5.9 Hz, 1H), 1.41 (d, J = 6.7 Hz, 3H). ^{13}C NMR (151 MHz, cdcl_3) δ 195.3, 144.7, 131.0, 128.6, 128.6, 125.5, 119.9, 76.5, 67.9, 29.4, 15.6. IR (neat, cm^{-1}): 3030, 2939, 1682, 1436, 1371, 1265, 1130, 1116, 1036, 734. MS (ESI/[M+Na] $^+$) calcd for $\text{C}_{11}\text{H}_{12}\text{NaO}_2^+$: 199.07, found: 199.08.

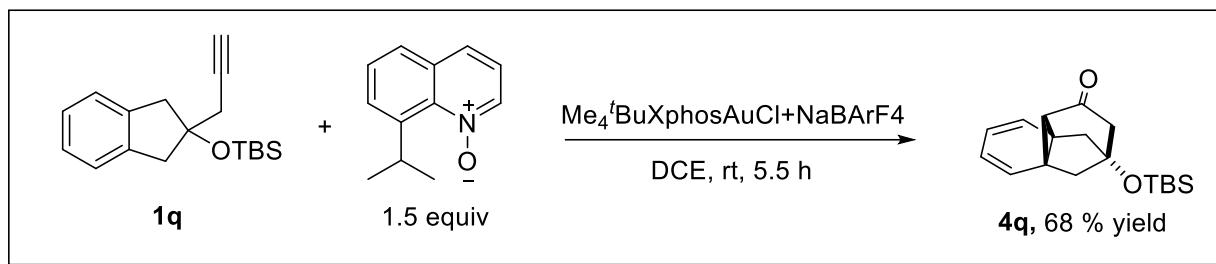


2,3,4,5-tetrahydro-1*H*-benzo[7]annulen-1-one **3o and 8,9-dihydro-5*H*-benzo[7]annulen-6(*7H*)-one **5o****. The ratio of **3o** to **5o** is 3.3:1 from the crude NMR. The compound **3o** and **5o** was prepared in 59% yield according to the general procedure C at 60°C for 4h, without adding 3 equivs Et₃N (eluent: ethyl acetate: hexanes = 1:10). **3o (major)**: ¹H NMR (400 MHz, Chloroform-d) δ 7.24 (d, *J* = 11.5 Hz, 1H), 6.61 (dd, *J* = 11.5, 5.3 Hz, 1H), 6.21 (dd, *J* = 9.2, 5.3 Hz, 1H), 5.49 (dt, *J* = 9.3, 6.8 Hz, 1H), 2.65 (t, *J* = 6.0 Hz, 2H), 2.45 (dd, *J* = 14.8, 7.0 Hz, 4H), 1.96 (dt, *J* = 12.7, 6.3 Hz, 2H). ¹³C NMR (101 MHz, Chloroform-d) δ 198.0, 149.4, 131.5, 130.0, 128.0, 127.4, 120.6, 37.7, 34.9, 32.6, 22.2. **5o(minor)**: ¹H NMR (400 MHz, Chloroform-d) δ 7.17 (dtd, *J* = 13.3, 6.3, 2.6 Hz, 4H), 3.73 (s, 2H), 3.05 – 2.88 (m, 2H), 2.57 (t, *J* = 6.9 Hz, 2H), 2.03 – 1.97 (m, 2H). ¹³C NMR (101 MHz, Chloroform-d) δ 208.8, 140.4, 133.5, 129.5, 129.2, 127.5, 127.1, 126.7, 50.1, 43.7, 33.0, 26.2. IR (neat, cm⁻¹): 2951, 1708, 1671, 1434, 1345, 1324, 1277, 1126, 754. GCMS (EI) calcd for C₁₁H₁₂O: 160.1, found: 160.0.

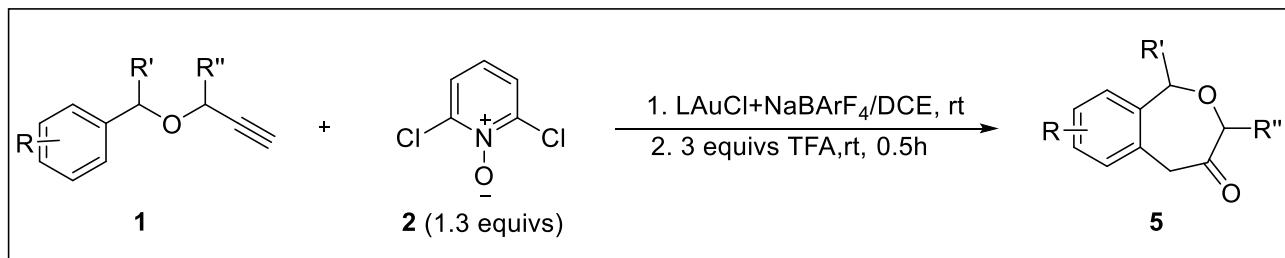


General procedure D for gold-catalyzed oxidative cyclopropanation of **1p:** To a 3 dram vial containing 6 mL of DCE were added sequentially a 1-((prop-2-ynyl)oxy)methyl)naphthalene **1q** (0.2 mmol), 2,6-dichloropyridine N-oxide (42.4 mg, 0.26 mmol), Me₄tBuXPhosAuCl (7.1 mg, 0.010 mmol) and NaBArF₄ (13.0 mg, 0.015 mmol). The resulting mixture was stirred 10 °C and the reaction was monitored by TLC. Upon completion (2h), the reaction mixture was concentrated under vacuum. The residue was purified by chromatography on silica gel (eluent: hexanes/ethyl acetate) to afford the desired product **4p** in 68% isolated yield. ¹H NMR (500 MHz, Chloroform-d) δ 7.48 – 7.37 (m, 1H), 7.33 – 7.24 (m, 2H), 7.24 – 7.18 (m, 1H), 6.47 (d, *J* = 9.5 Hz, 1H), 6.34 (dd, *J* = 9.5, 5.2 Hz, 1H), 4.49 (d, *J* = 11.3 Hz, 1H), 4.28 (d, *J* = 18.4 Hz, 1H), 4.24 (d, *J* = 11.3 Hz, 1H), 3.96 (d, *J* = 18.3 Hz, 1H), 3.49 – 3.36 (m, 1H), 1.27 (d, *J* = 3.8 Hz, 1H). ¹³C NMR (126 MHz, CDCl₃) δ 205.6, 131.6, 131.0, 128.7, 128.0, 127.3, 126.9, 125.6,

124.53, 72.8, 64.6, 35.6, 33.9, 28.6. IR (neat, cm^{-1}): 2861, 1688, 1287, 1256, 1111, 913, 758. MS (ESI/[M+Na] $^{+}$) calcd for $\text{C}_{14}\text{H}_{12}\text{NaO}_2^{+}$: 235.07, found: 235.08.

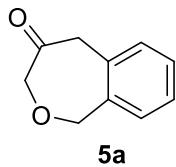


General procedure E for gold-catalyzed oxidative cyclopropanation of 1q: To a 3 dram vial containing 4 mL of DCE were added sequentially a tert-butyldimethyl(2-(prop-2-ynyl)-2,3-dihydro-1H-inden-2-yloxy)silane **1q** (0.2 mmol), 8-isopropylquinoline N-oxide (56.1 mg, 0.3 mmol), $\text{Me}_4^t\text{BuXPhosAuCl}$ (7.1 mg, 0.010 mmol) and NaBArF_4 (13.0 mg, 0.015 mmol). The resulting mixture was stirred at room temperature and the reaction was monitored by TLC. Upon completion, the reaction mixture was concentrated under vacuum. The residue was purified by chromatography on silica gel (eluent: hexanes/ethyl acetate) to afford the desired product **4q**. ^1H NMR (500 MHz, Chloroform-d) δ 6.16 (dd, $J = 7.2, 2.8 \text{ Hz}$, 2H), 6.04 – 5.94 (m, 2H), 2.38 (s, 2H), 2.12 (s, 4H), 0.89 (s, 1H), 0.84 (d, $J = 2.7 \text{ Hz}$, 9H), 0.08 (s, 6H). ^{13}C NMR (126 MHz, CDCl_3) δ 210.9, 126.8, 122.9, 72.2, 52.2, 43.1, 41.2, 38.1, 25.6, 17.8, -2.4. IR (neat, cm^{-1}): 2954, 2931, 2858, 1693, 1468, 1315, 1258, 1188, 1123, 983, 918, 838, 773. MS (ESI/[M+Na] $^{+}$) calcd for $\text{C}_{18}\text{H}_{26}\text{NaO}_2\text{Si}^{+}$: 325.16, found: 325.16.

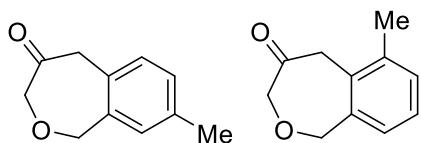


General procedure F for gold-catalyzed oxidative cyclopropanation and ring expansion: To a 3 dram vial containing 6 mL of DCE were added sequentially a ((prop-2-ynyoxy)methyl) benzene derivatives **1** (0.2 mmol), 2,6-dichloropyridine N-oxide (42.4 mg, 0.26 mmol), $\text{Me}_4^t\text{BuXPhosAuCl}$ (7.1 mg, 0.010 mmol) and NaBArF_4 (13.0 mg, 0.015 mmol). The resulting

mixture was stirred at room temperature and the reaction was monitored by TLC. Upon completion, the reaction mixture was added 3 equivs TFA and stirred for 0.5 h at room temperature. The reaction mixture was concentrated under vacuum. The residue was purified by chromatography on silica gel (eluent: hexanes/ethyl acetate) to afford the desired product **5a**.



3,5-dihydrobenzo[c]oxepin-4(1H)-one 5a: The compound **5a** was prepared in 65% yield according to the general procedure F (eluents: ethyl acetate: hexanes = 1:10). ^1H NMR (500 MHz, Chloroform-d) δ 7.26 – 7.18 (m, 2H), 7.13 – 7.09 (m, 1H), 7.03 (d, J = 7.2 Hz, 1H), 5.11 (s, 2H), 4.19 (s, 2H), 4.08 (s, 2H). ^{13}C NMR (126 MHz, CDCl₃) δ 209.1, 135.7, 130.9, 129.2, 127.7, 127.4, 125.9, 76.1, 74.9, 48.5. IR (neat, cm⁻¹): 2893, 1725, 1475, 1263, 1116, 955, 752. MS (ESI/[M+Na]⁺) calcd for C₁₀H₁₀NaO₂⁺: 185.06, found: 185.05.



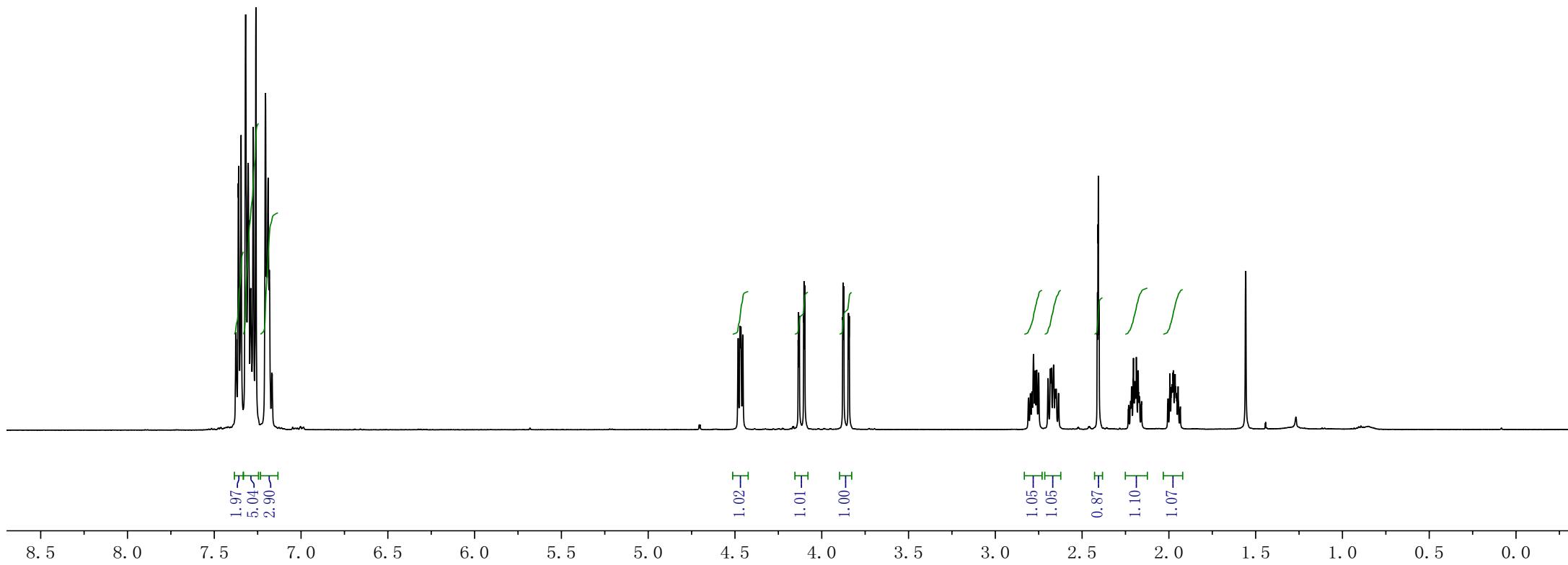
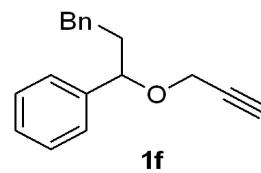
5c:5c'=3.8:1

The compound **5c** and **5c'** was prepared in 73% yield according to the general procedure F (eluents: ethyl acetate: hexanes = 1:10). **5c (major)** ^1H NMR (500 MHz, Chloroform-d) δ 7.04 – 6.97 (m, 2H), 6.84 (s, 1H), 5.07 (s, 2H), 4.17 (s, 2H), 4.03 (s, 2H), 2.30 (s, 3H). **5c' (minor)** ^1H NMR (500 MHz, Chloroform-d) δ 7.11 (d, J = 5.0 Hz, 2H), 6.89 (t, J = 4.6 Hz, 1H), 5.10 (s, 2H), 4.17 (s, 2H), 4.12 (s, 2H), 2.38 (s, 3H). ^{13}C NMR (126 MHz, CDCl₃) δ 209.2, 137.1, 135.5, 130.8, 129.7, 128.4, 126.9, 126.4, 126.2, 124.3, 76.0, 75.5, 74.8, 74.8, 48.0, 42.5, 20.9, 20.8. IR (neat, cm⁻¹): 2923, 1726, 1614, 1504, 1417, 1263, 1121, 819. MS (ESI/[M+Na]⁺) calcd for C₁₁H₁₂KO₂⁺: 215.05, found: 215.06.

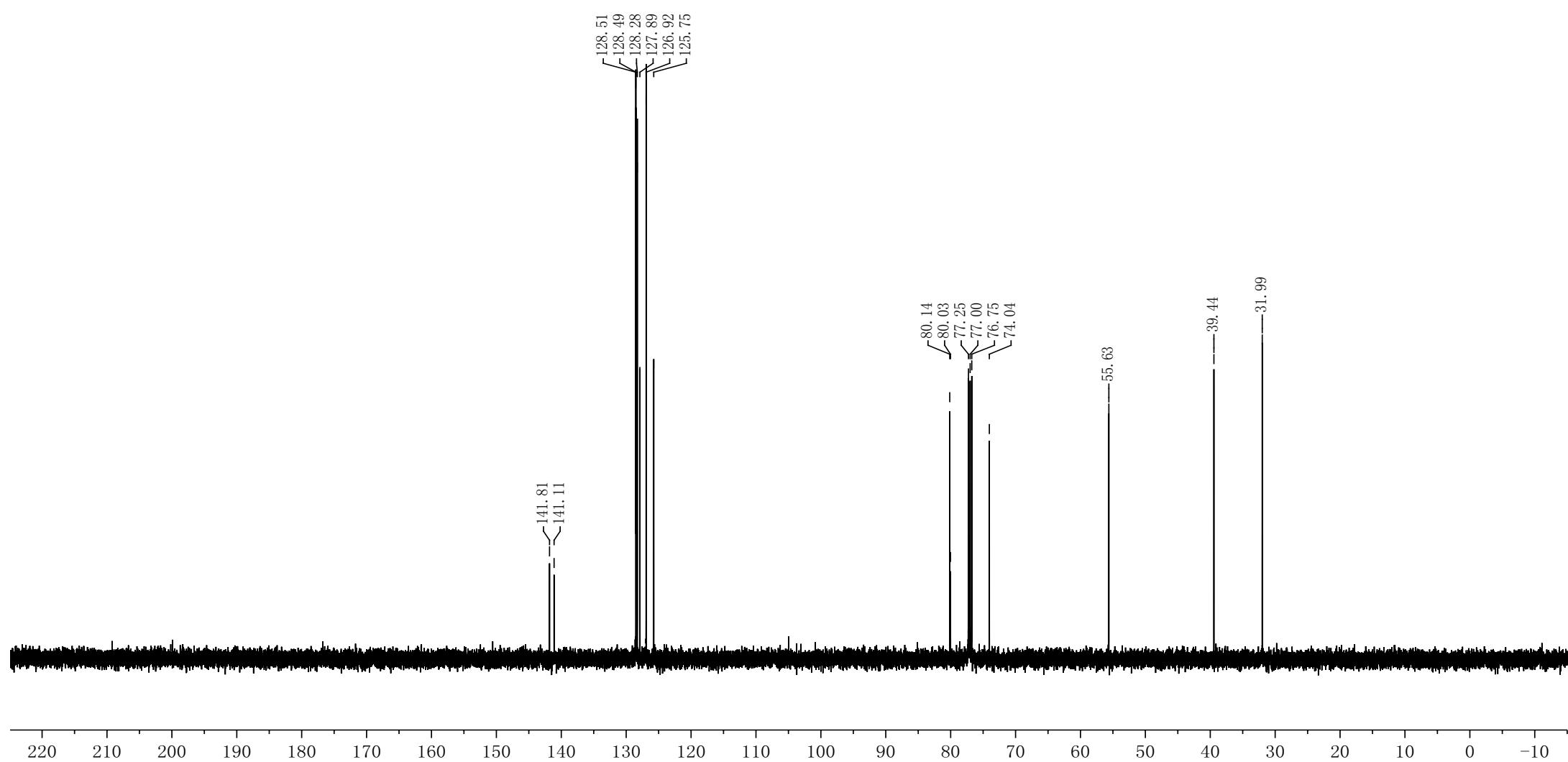
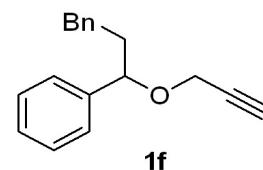
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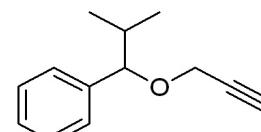
Parameter	Value
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Solvent	CDCl ₃
Spectrometer Frequency	499.86
Nucleus	¹ H



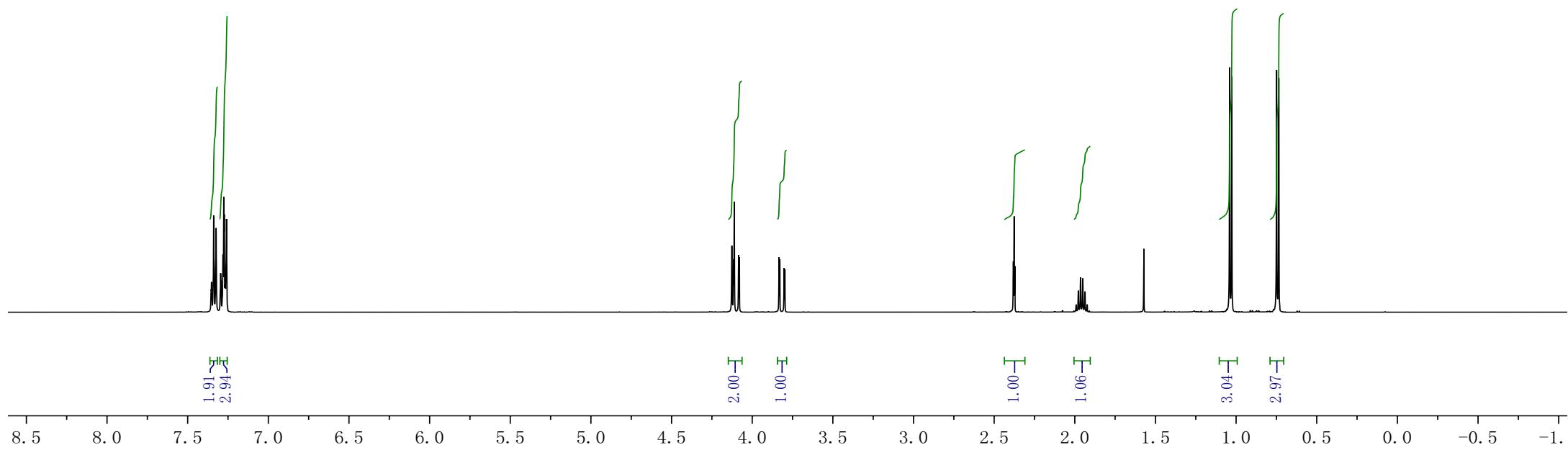
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Solvent	CDCl ₃
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Nucleus	¹³ C



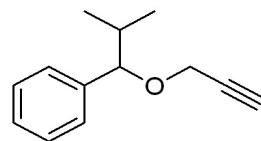
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Solvent	CDCl ₃
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Nucleus	¹ H



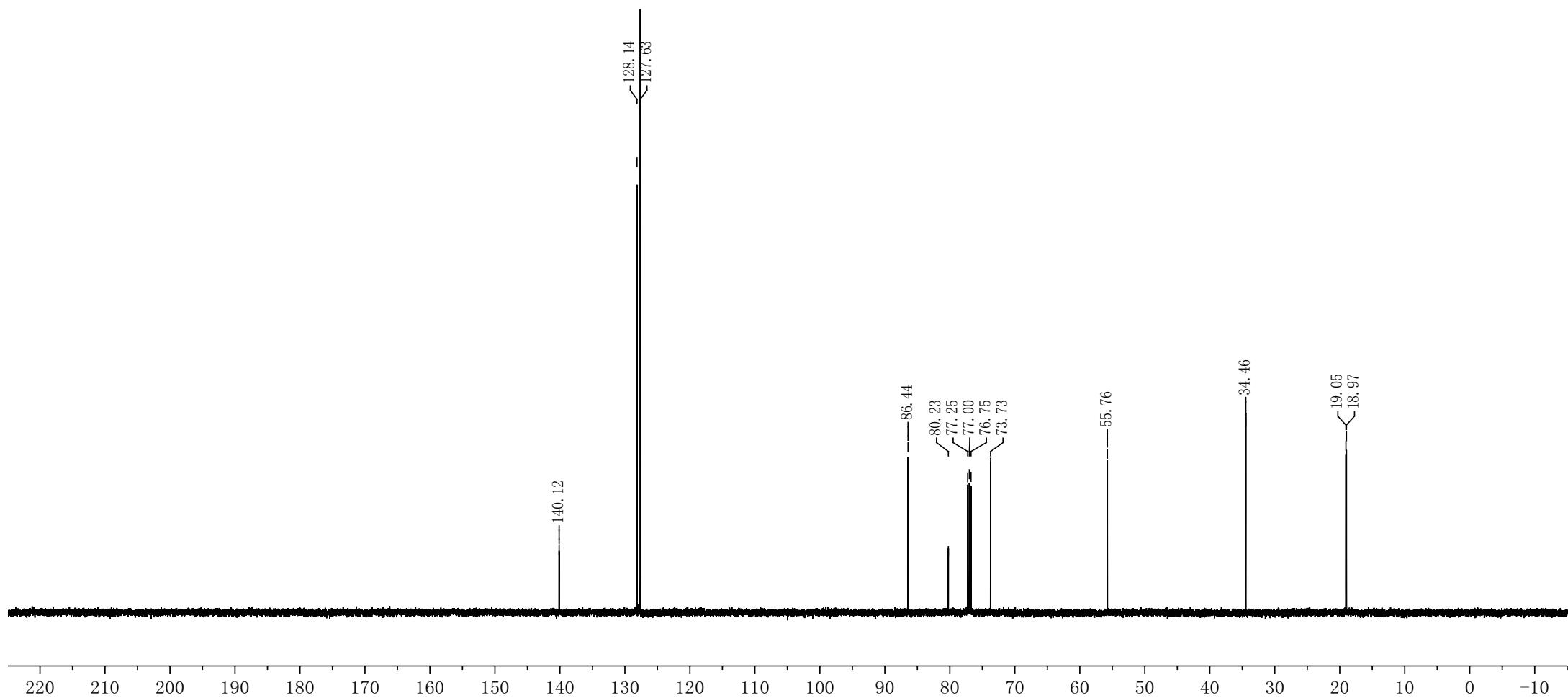
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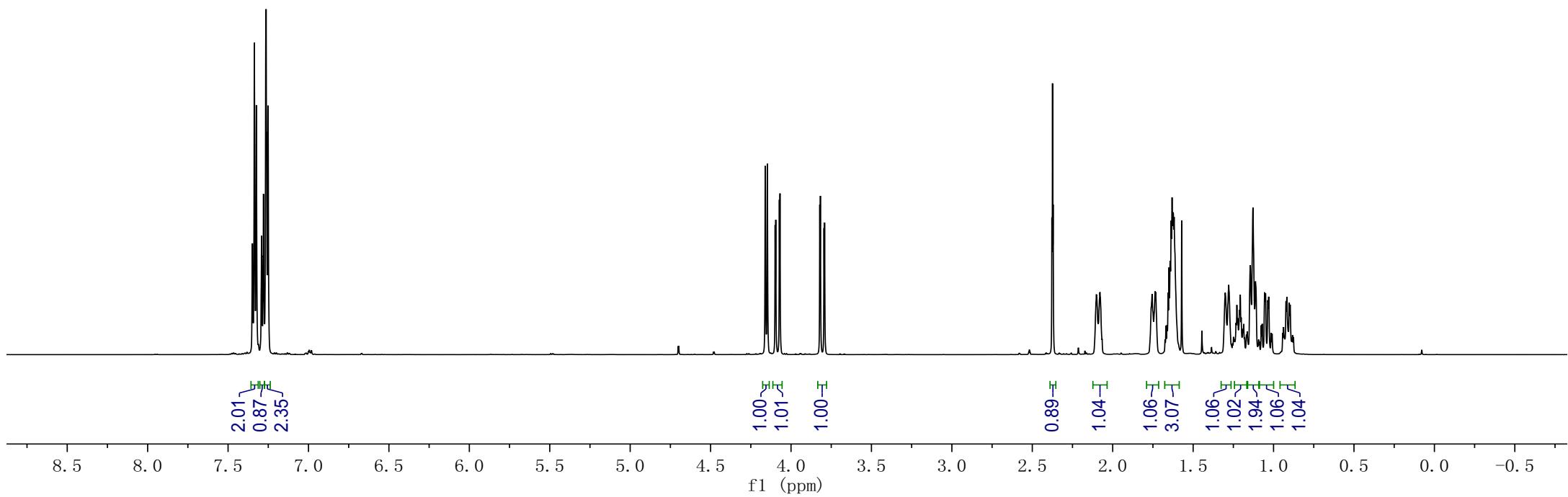
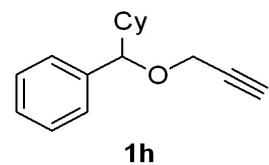
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Solvent	CDCl ₃
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Nucleus	¹³ C



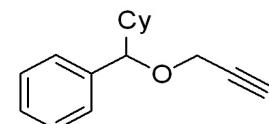
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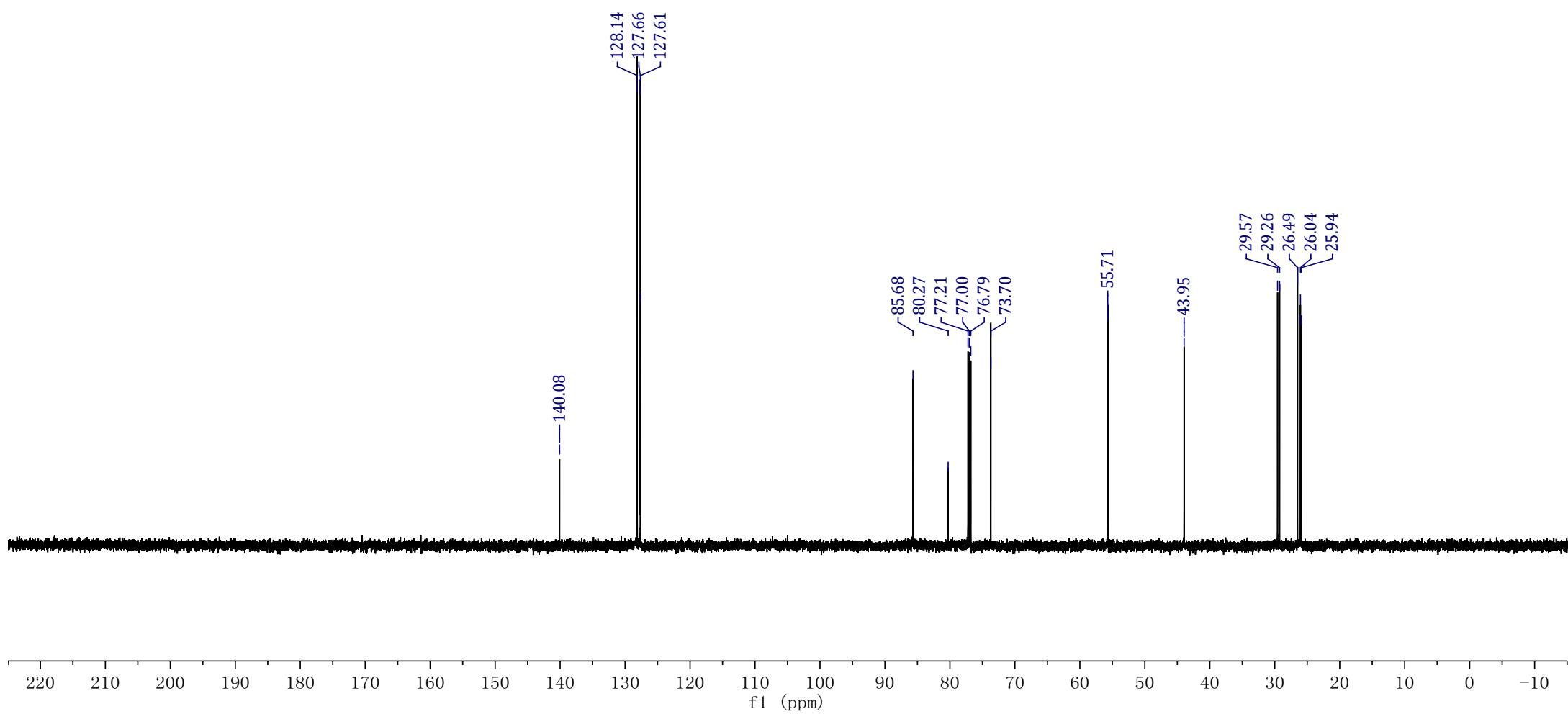
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4 Relaxation Delay	10.0000
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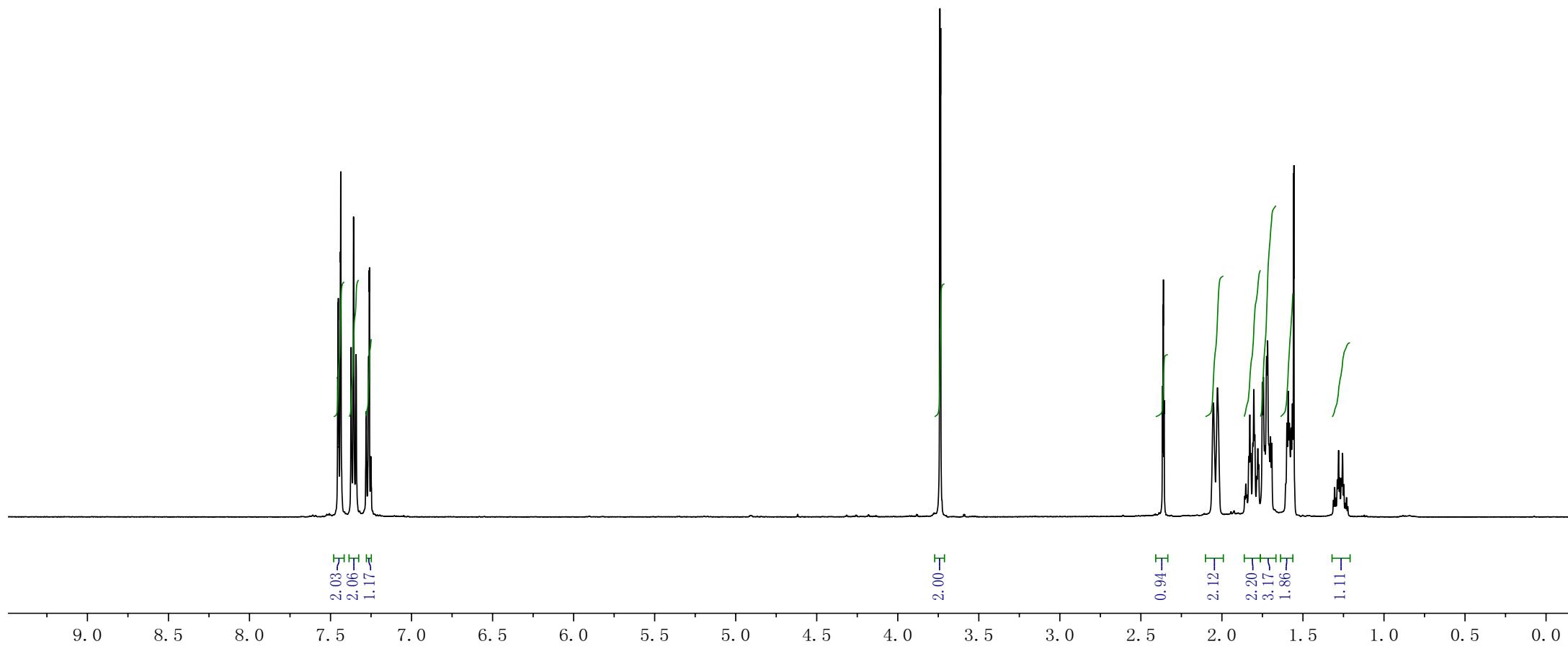
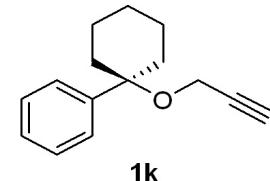
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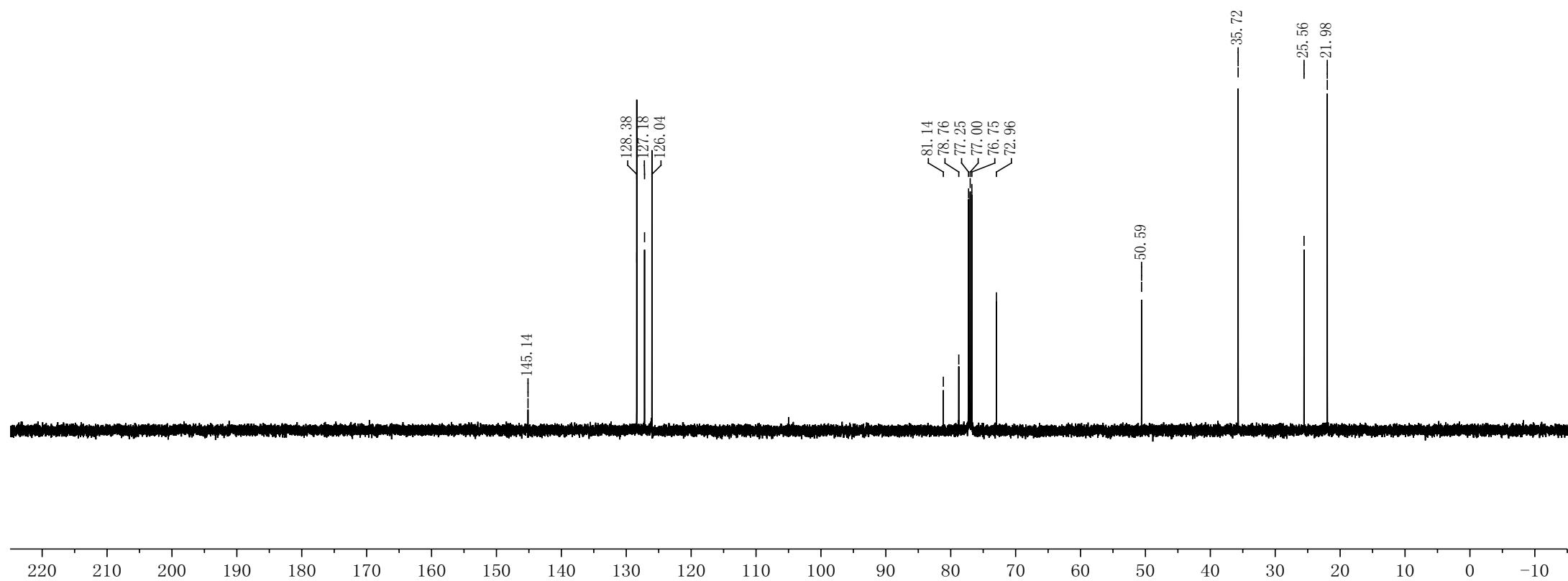
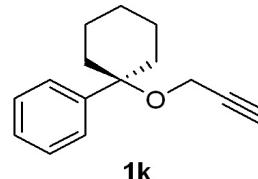
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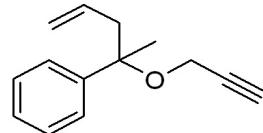
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Spectrometer Frequency	499.86
Nucleus	¹ H



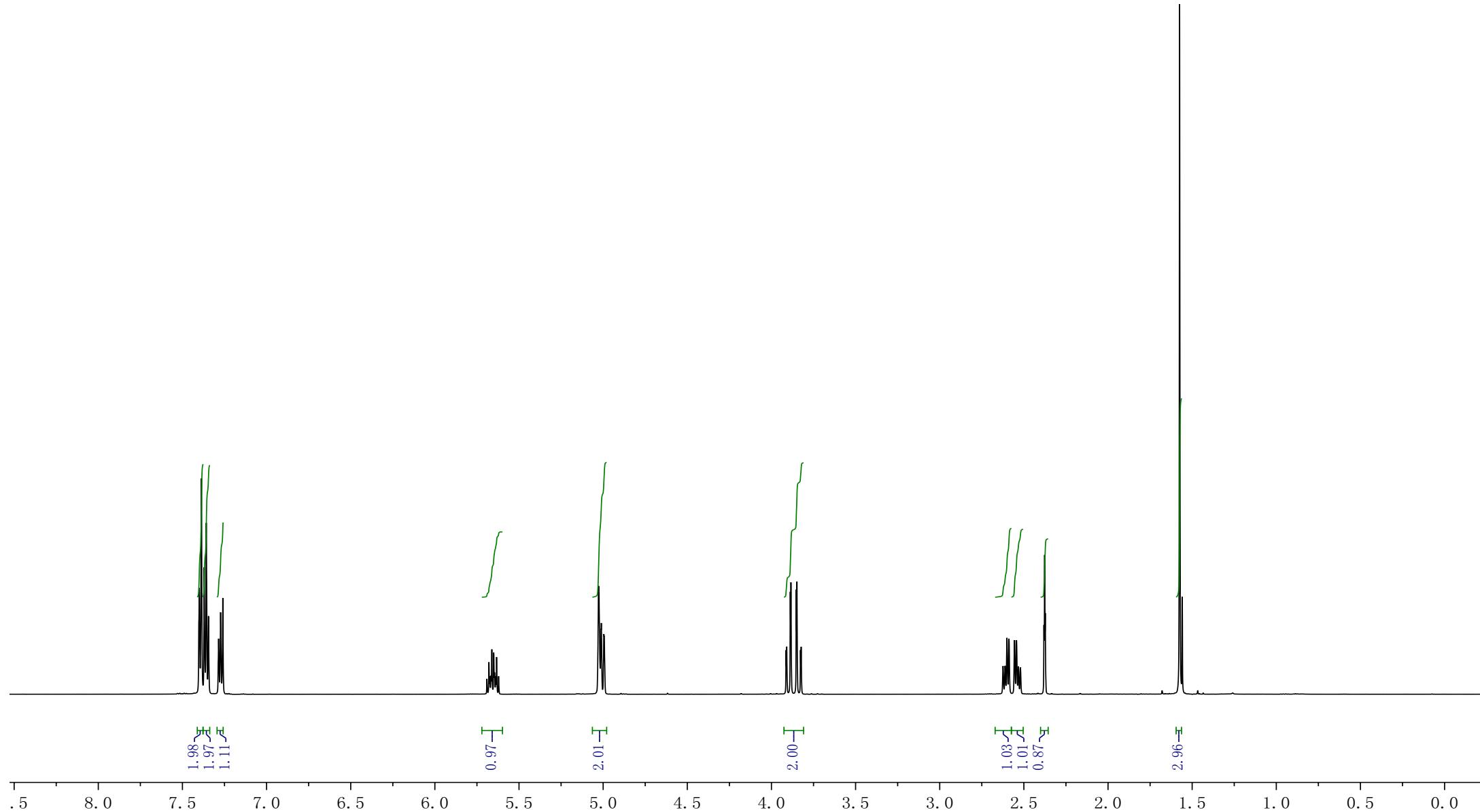
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Solvent	CDCl ₃
Spectrometer Frequency	125.70
Nucleus	¹³ C



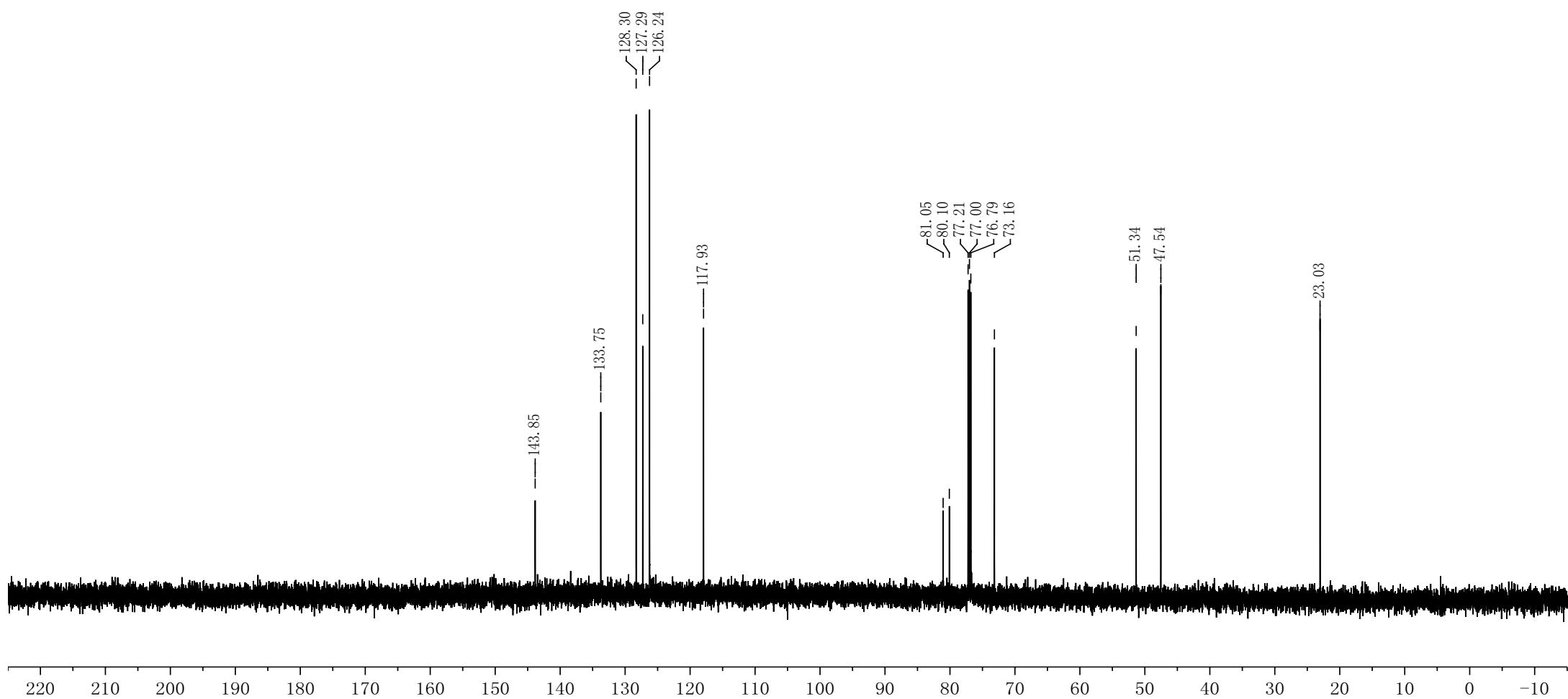
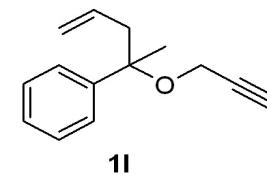
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Solvent	cdcl3
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Nucleus	1H



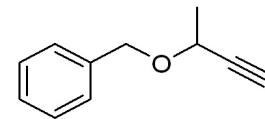
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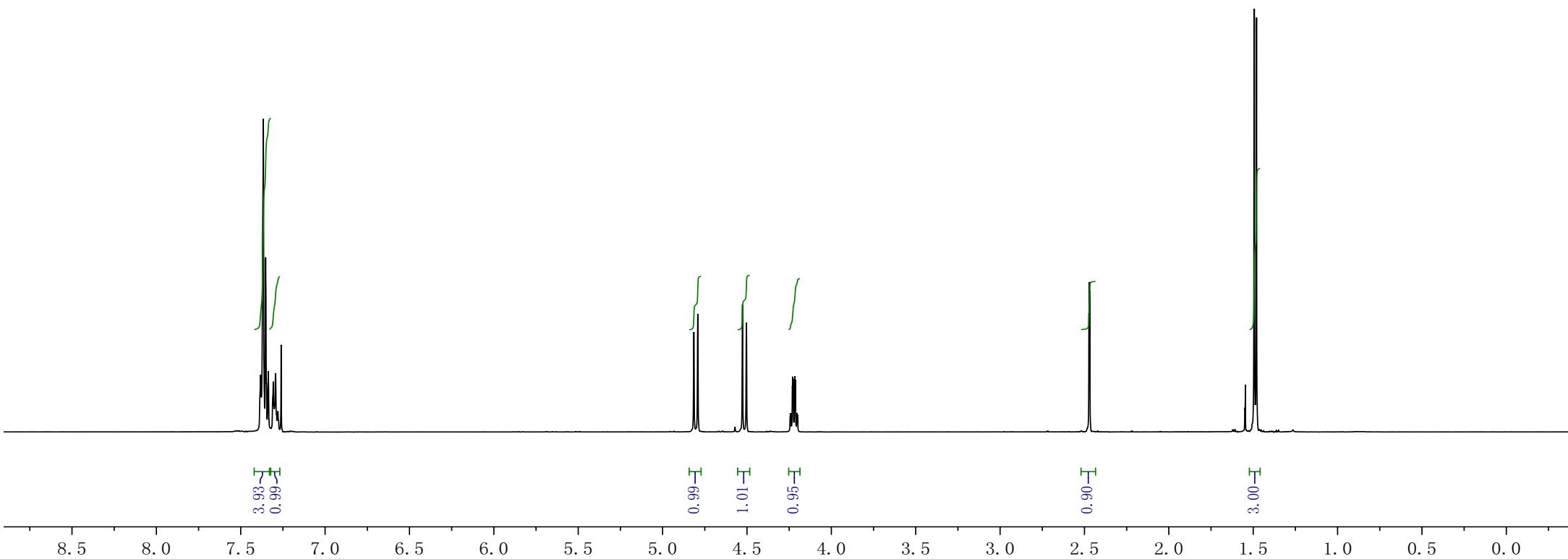
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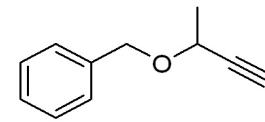
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Solvent	CDCl ₃
Spectrometer Frequency	499.86
Nucleus	¹ H



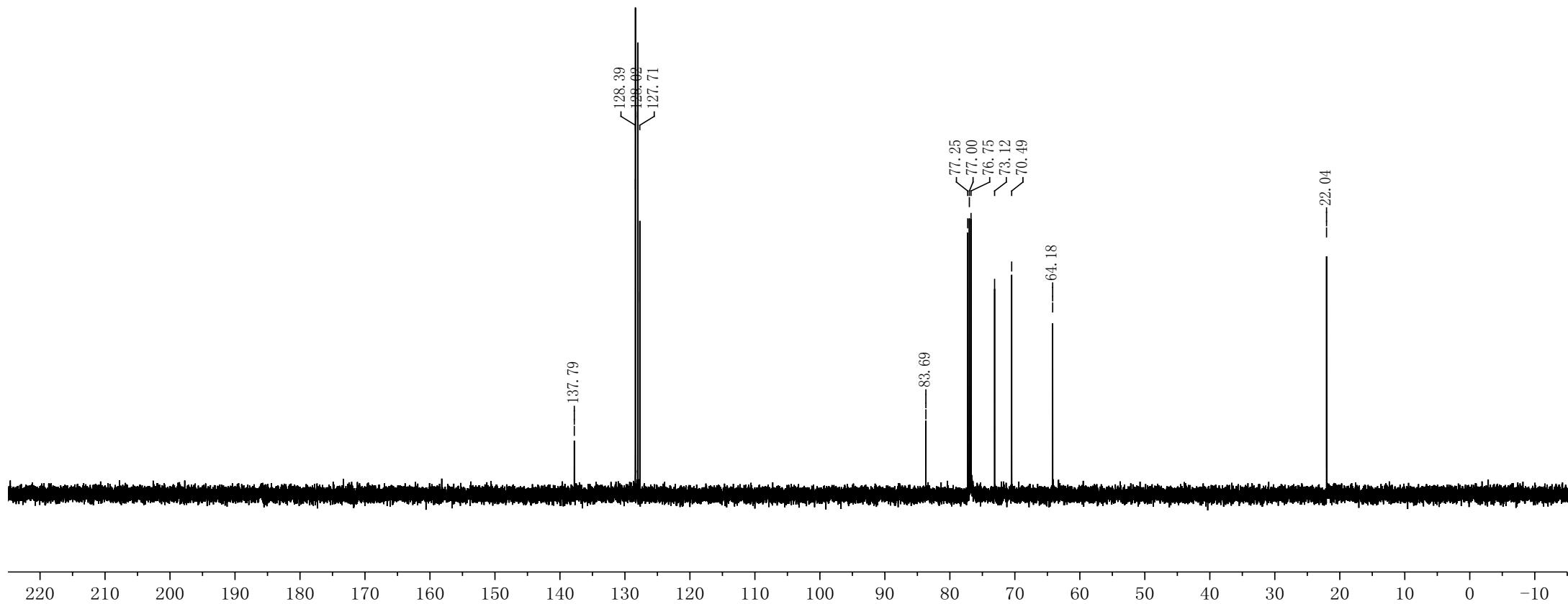
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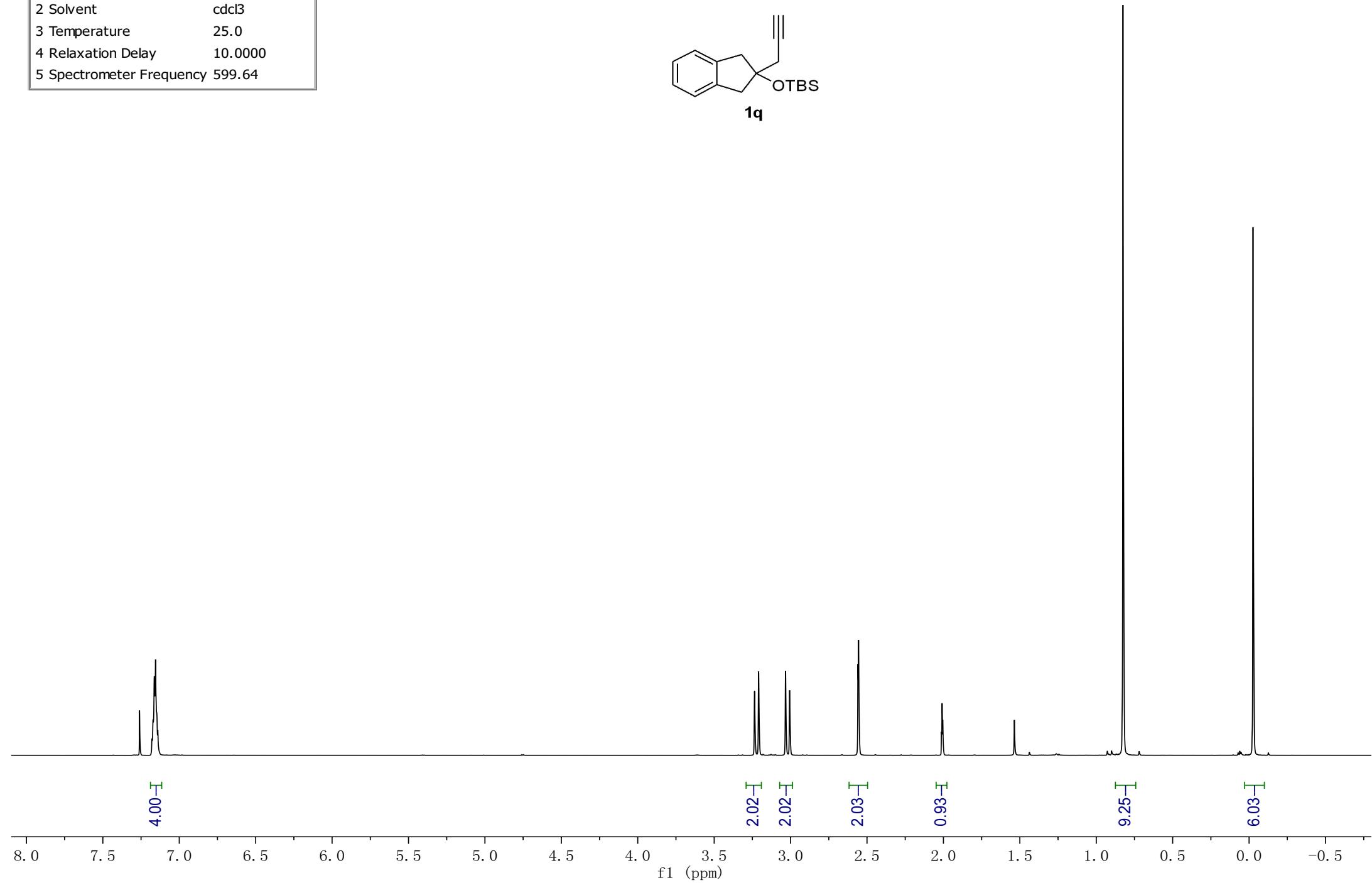
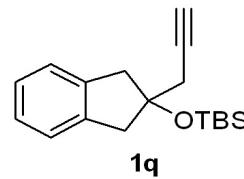
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Title	jkg-V-151-1-C
Solvent	CDCl ₃
Spectrometer Frequency	125.70
Nucleus	¹³ C



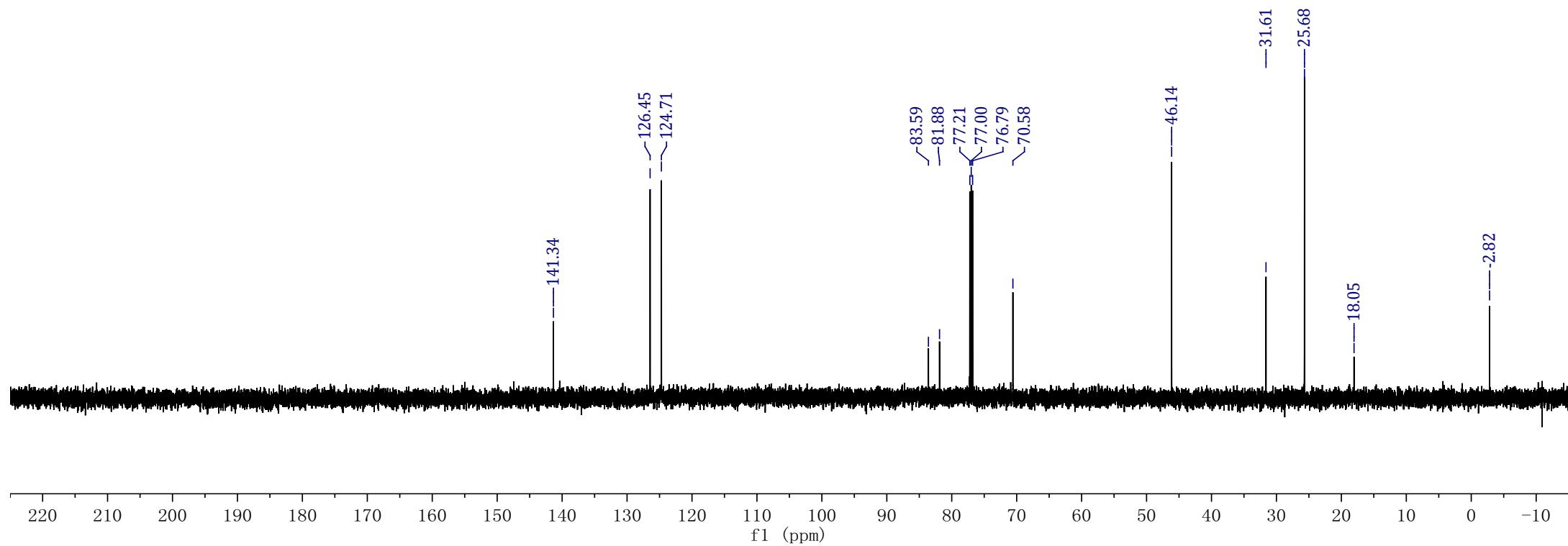
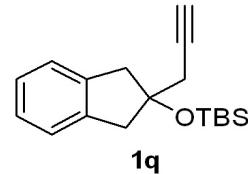
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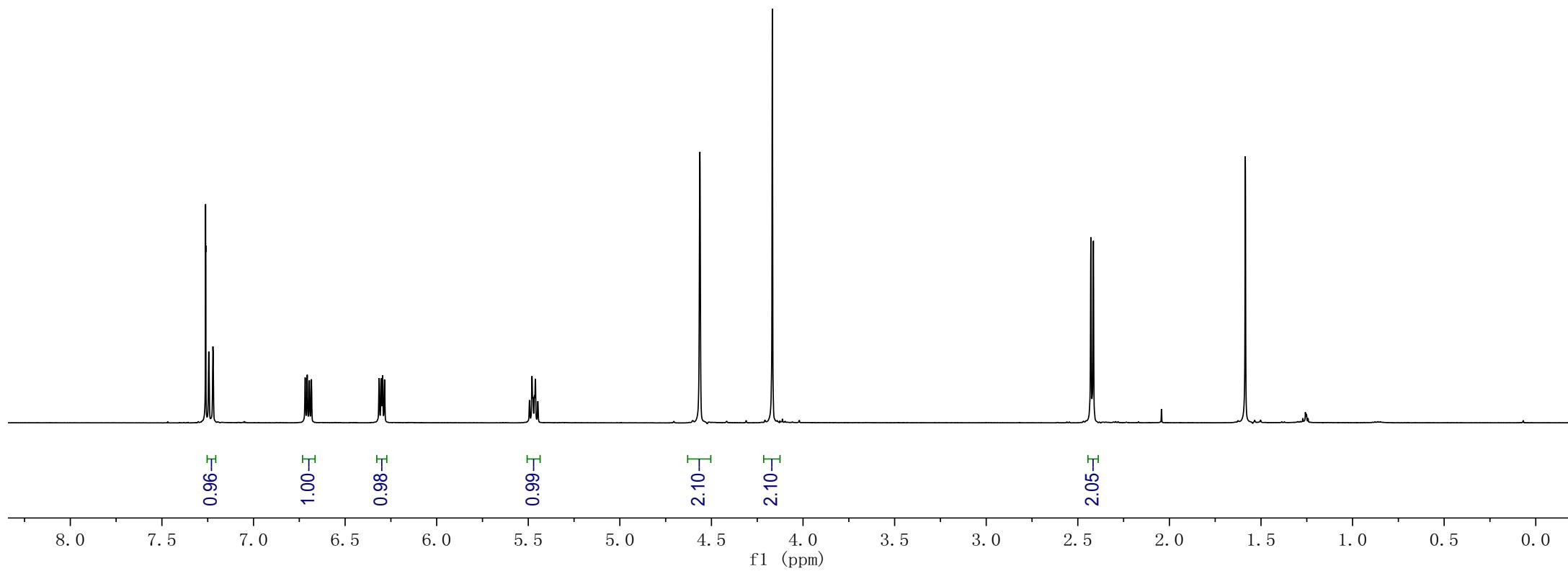
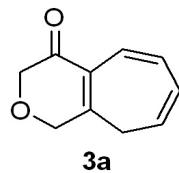
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2 Solvent	cdcl3
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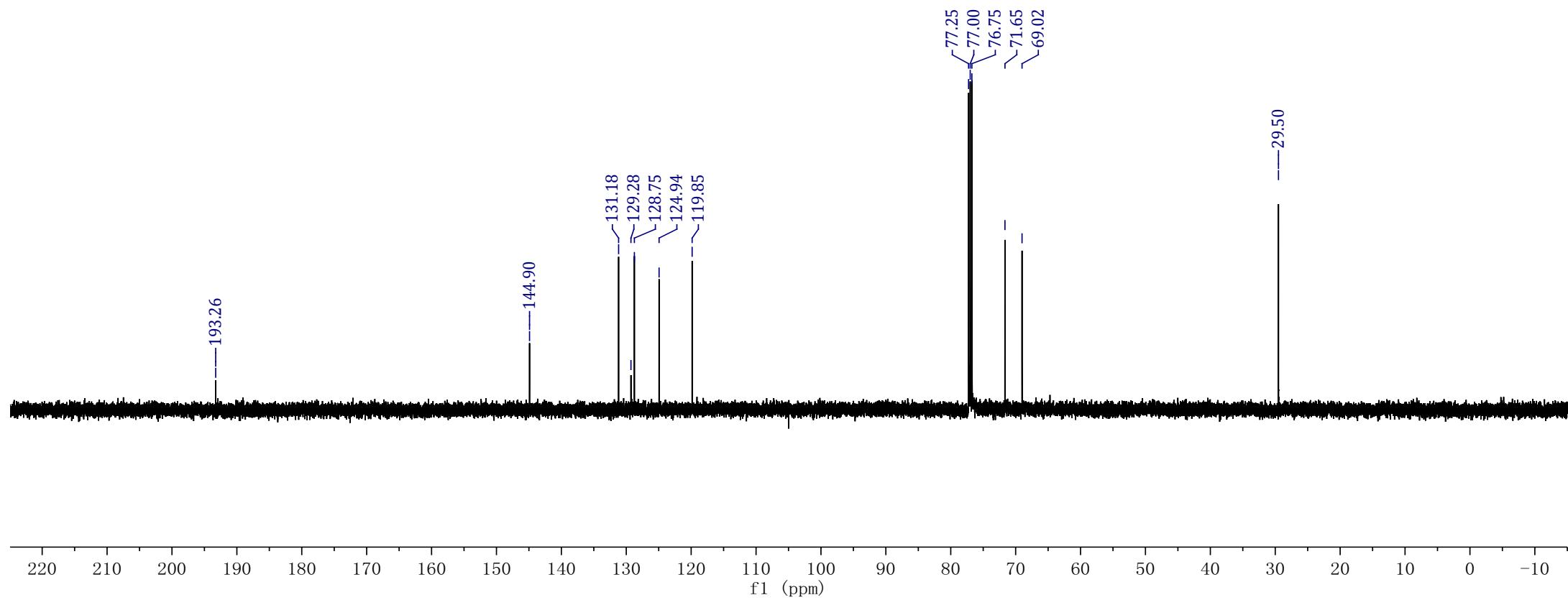
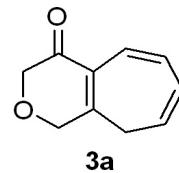
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2 Solvent	cdcl3
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5 Spectrometer Frequency	150.79

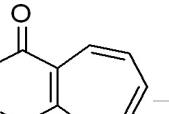
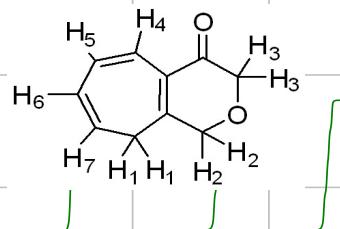


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5 Spectrometer Frequency	499.86



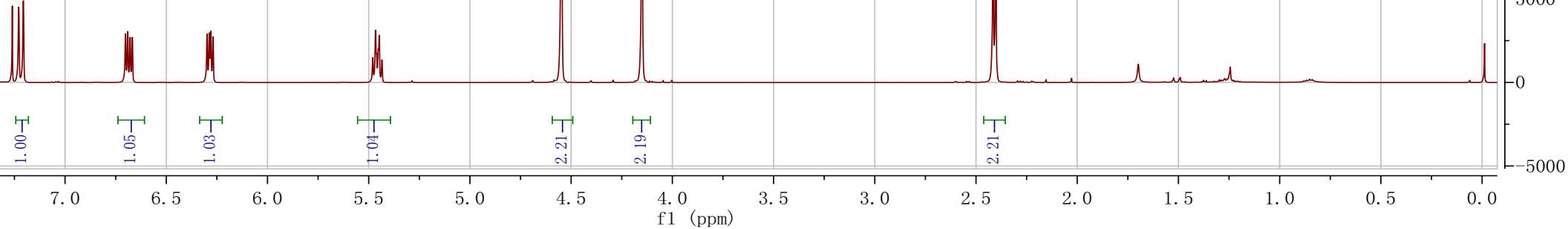
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5 Spectrometer Frequency	125.70

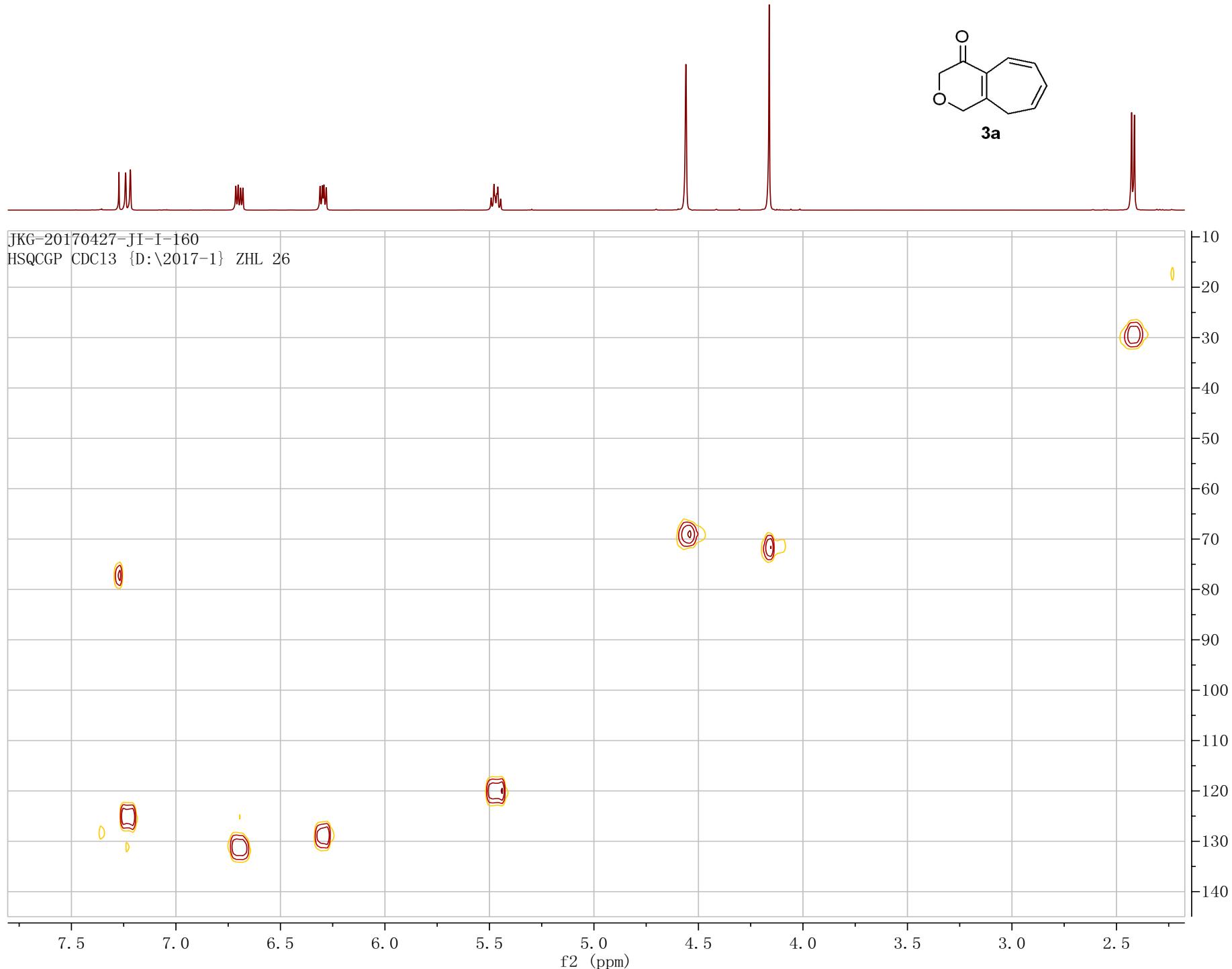
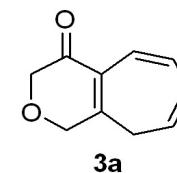
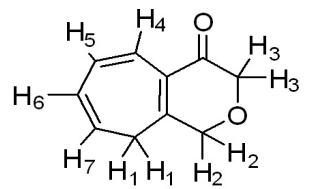


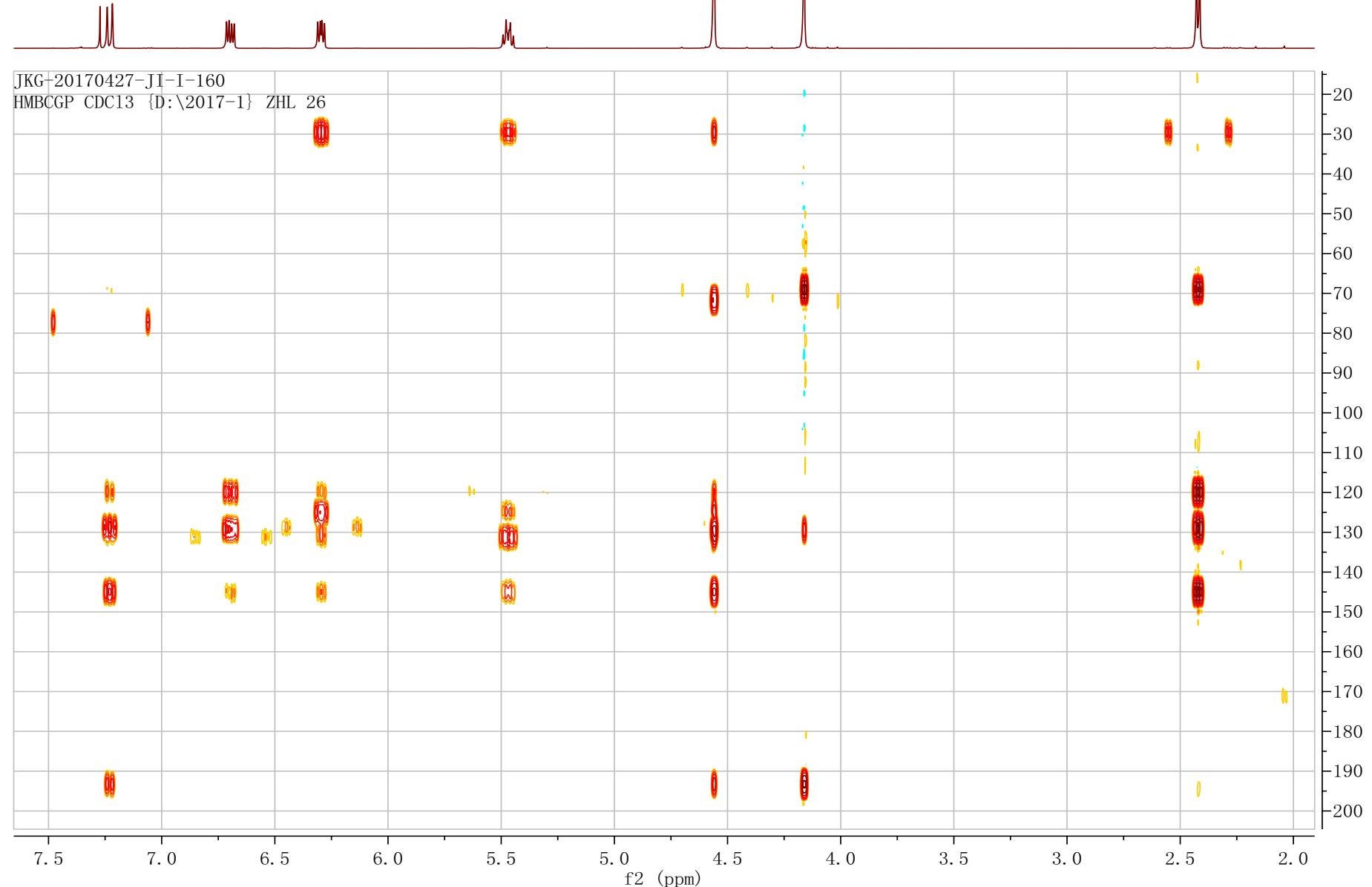
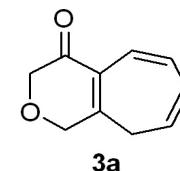
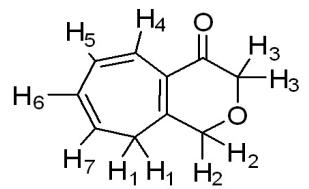


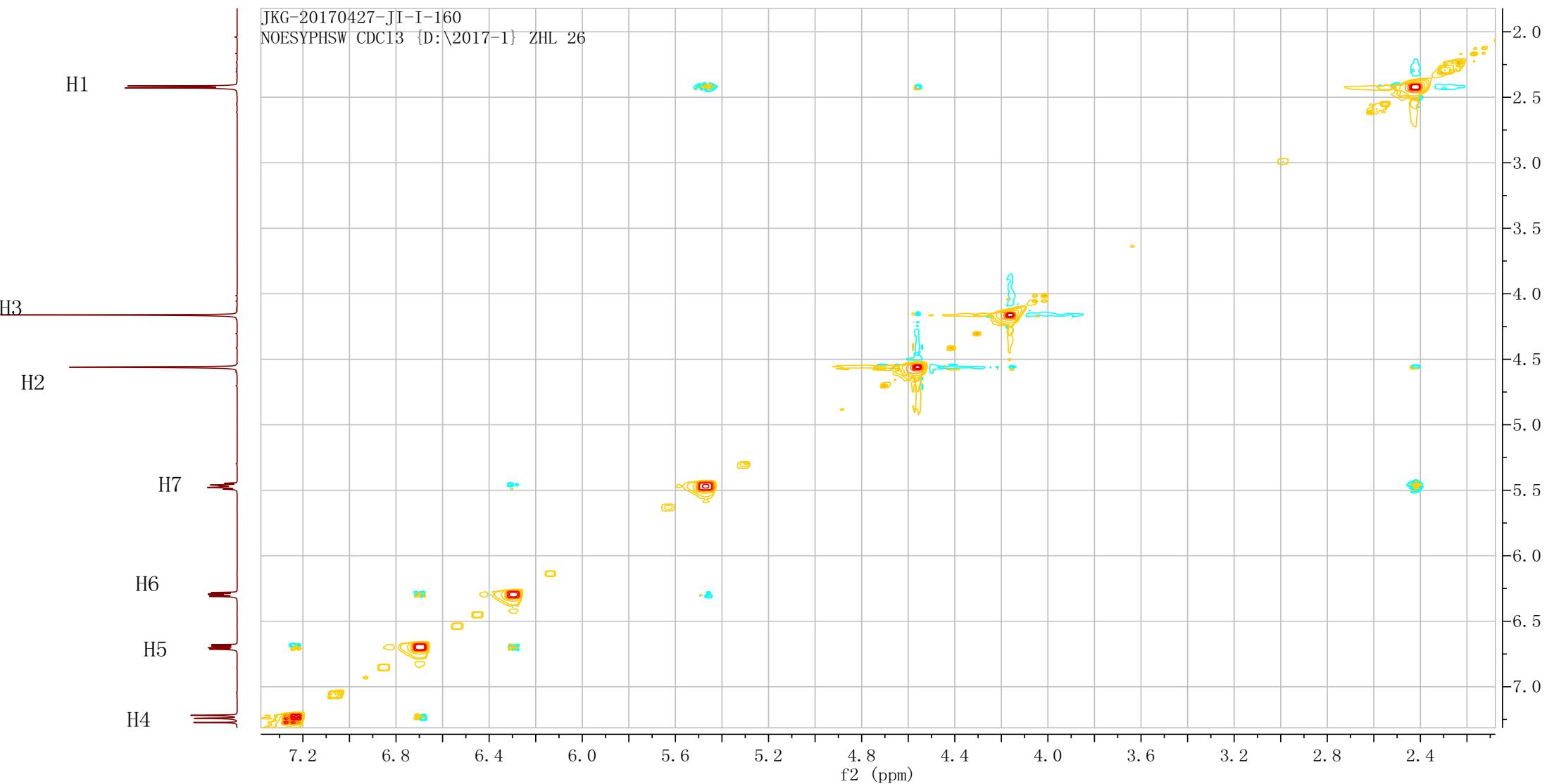
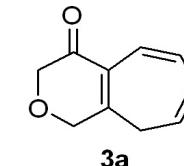
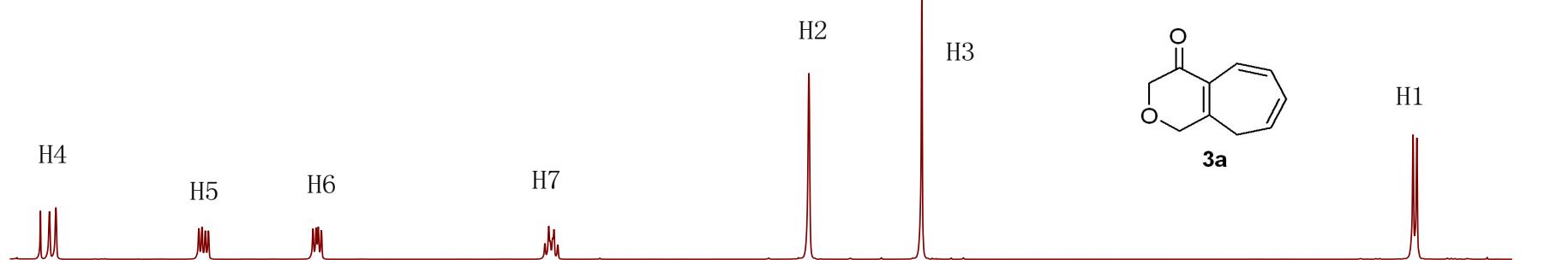
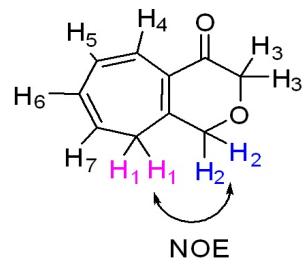
3a

A (d) 7.22	B (dd) 6.68	C (dd) 6.28	D (dt) 5.46	E (s) 4.55	F (s) 4.15	G (d) 2.41
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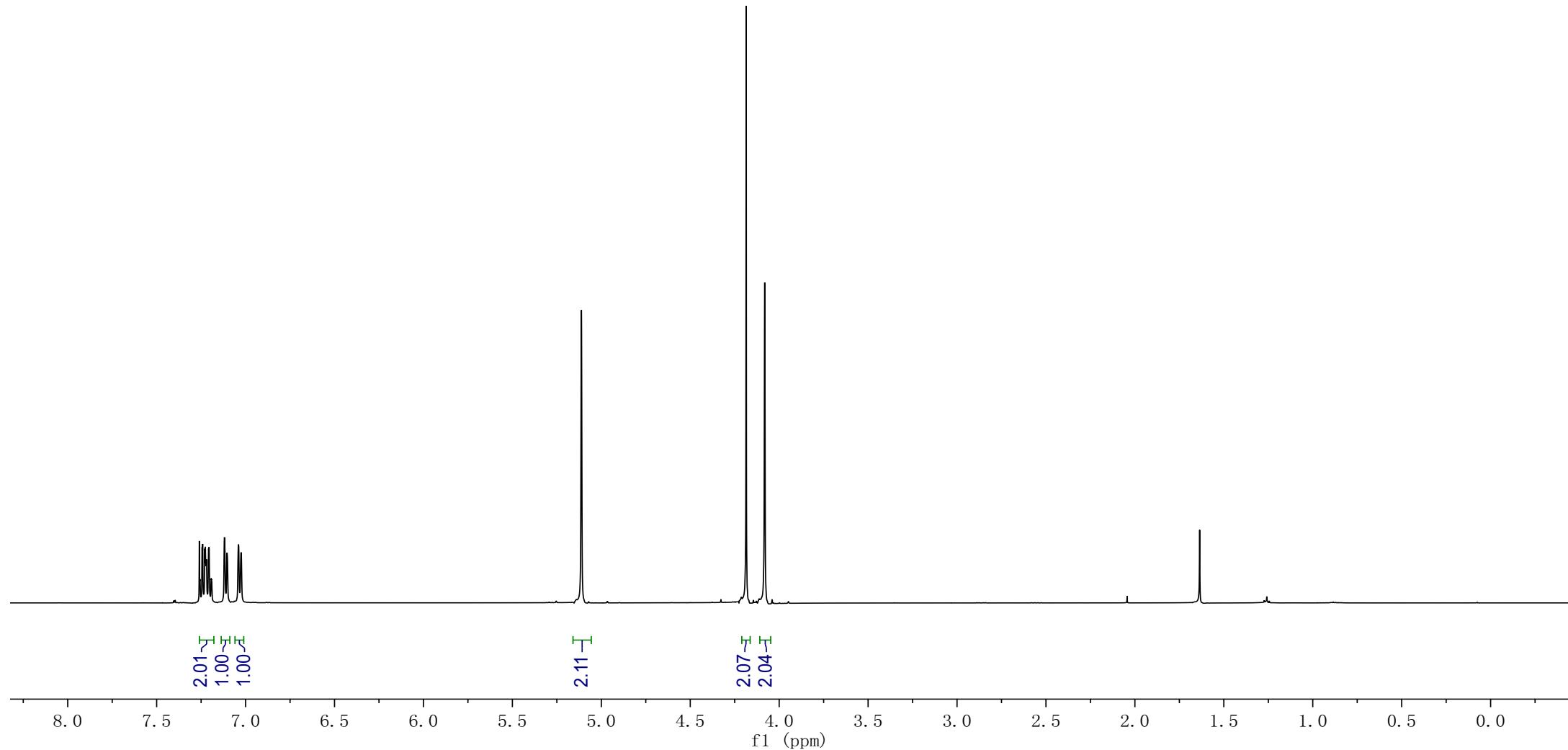
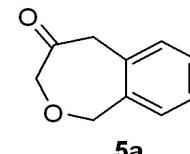




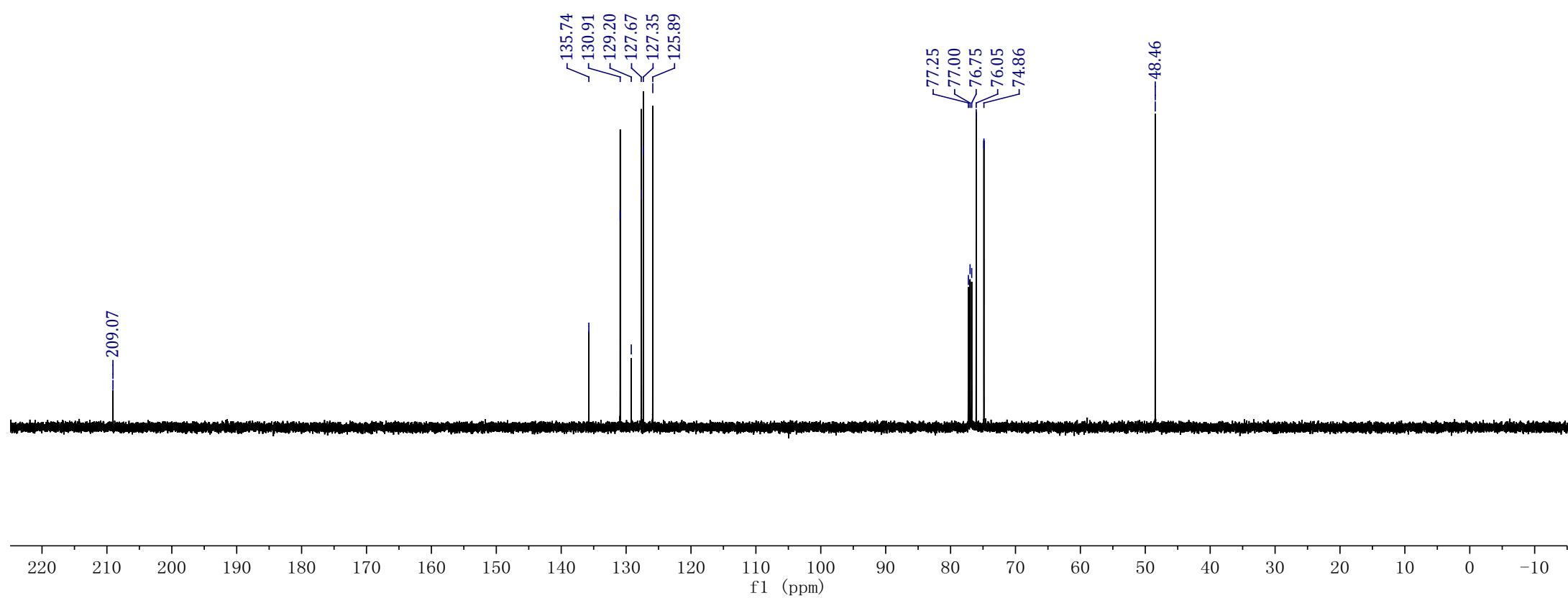
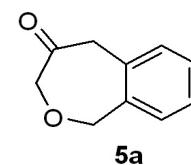




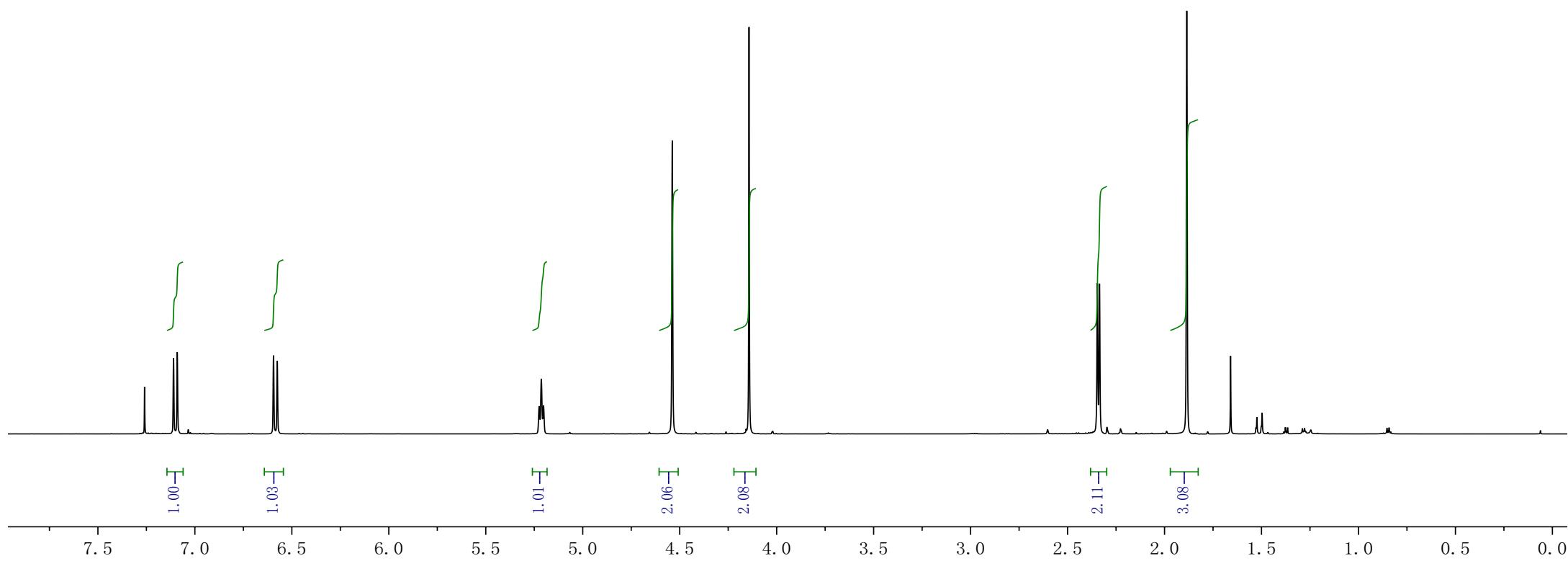
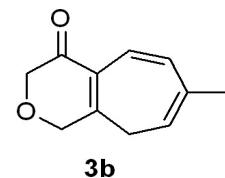
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2 Solvent	CDCl ₃
3 Temperature	80.0
4 Relaxation Delay	10.0000
5 Spectrometer Frequency	499.86



Parameter	Value
1 Title	jkg-VI-5a-C
2 Solvent	CDCl ₃
3 Temperature	80.0
4 Relaxation Delay	1.0000
5 Spectrometer Frequency	125.70



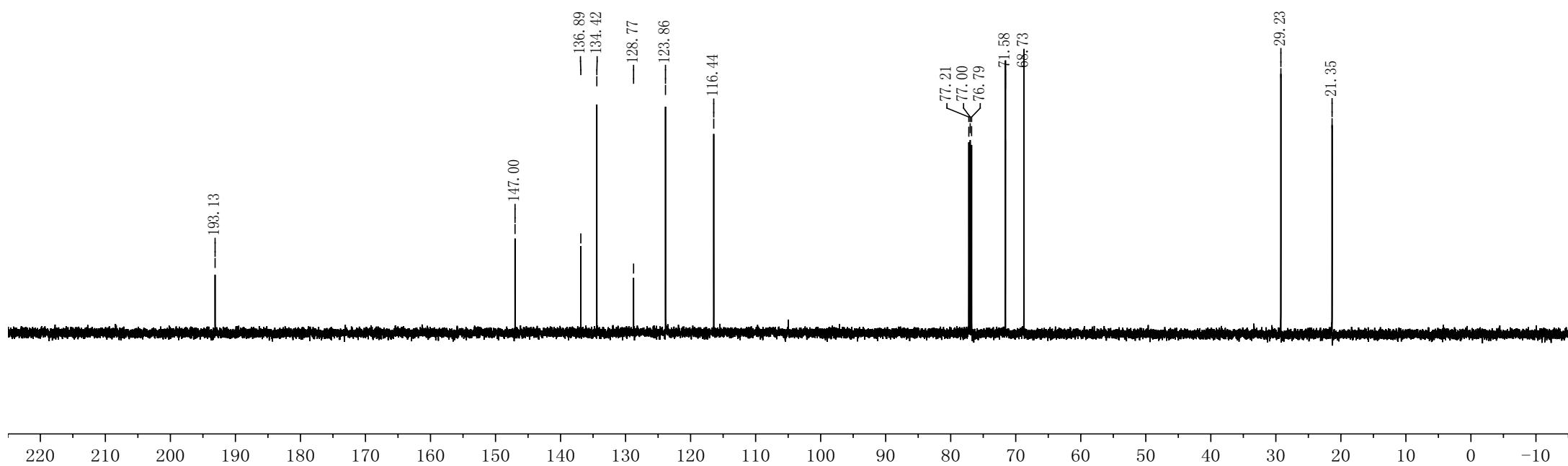
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Title	jkg-VI-6A-H
Solvent	cdcl3
Spectrometer Frequency	599.64
Nucleus	1H



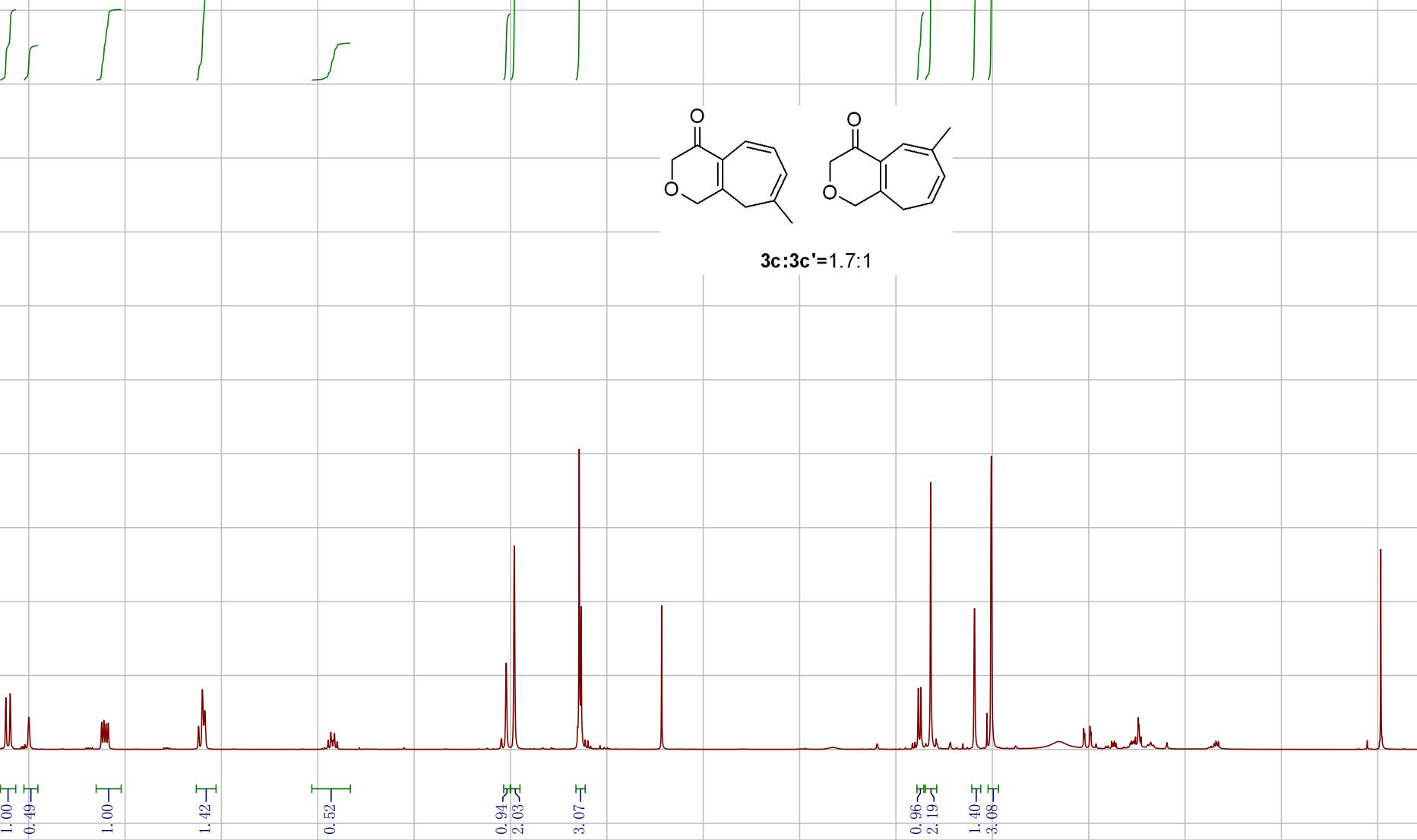
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Solvent	cdcl3
Spectrometer Frequency	150.79
Nucleus	13C



3b



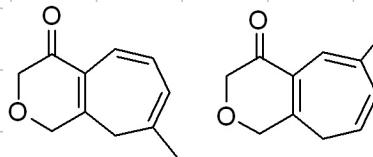
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20000
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16000
14000
12000
10000
8000
6000
4000
2000
0
-2000



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

f1 (ppm)

JKG-20170504-JI¹³C 164
C13CPD CDC13 {D:\2017-1} ZHL 5



3c:3c'=1.7:1

193.58
193.40
164.00
143.62
142.77
140.56
131.87
131.17
130.73
129.17
128.95
123.97
122.84
121.71
119.06

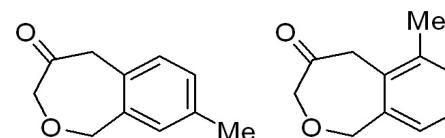
71.68
71.48
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68.91
35.28
29.42
24.69
24.33

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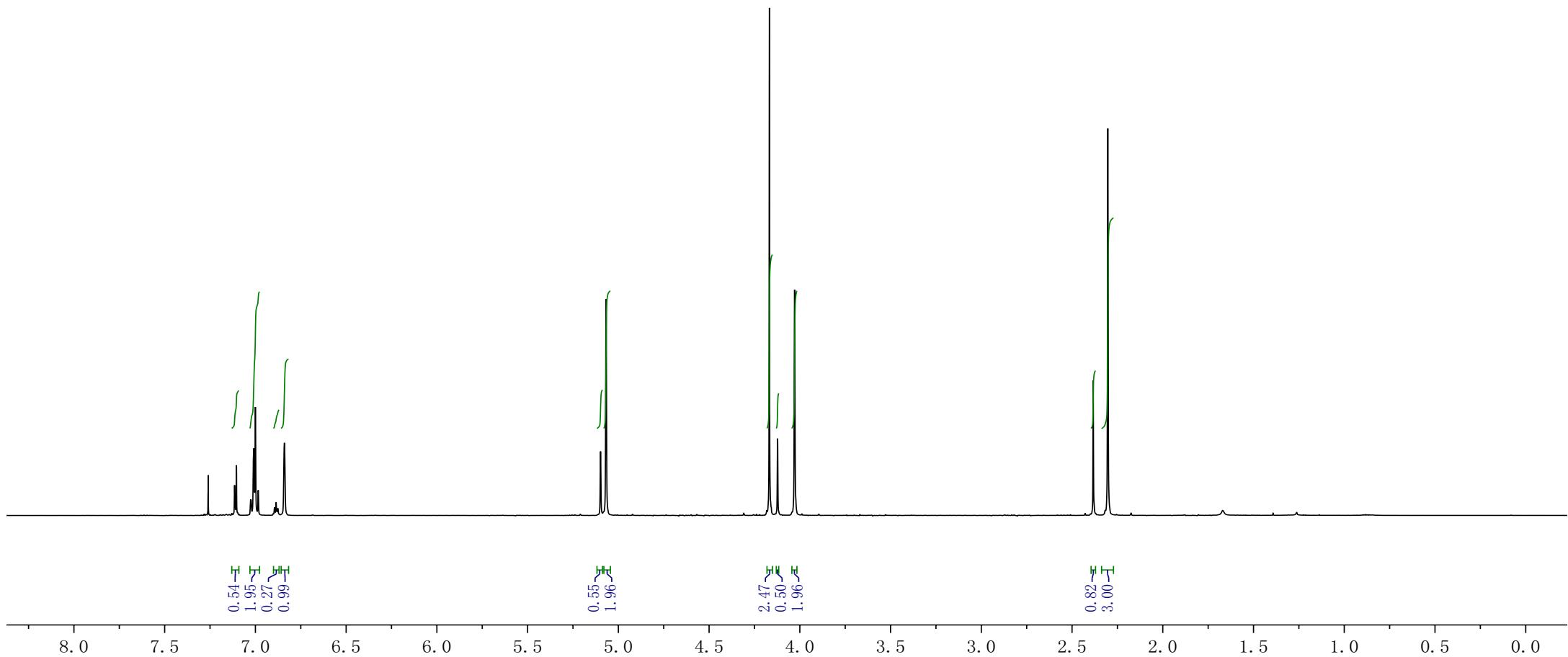
f1 (ppm)

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-100
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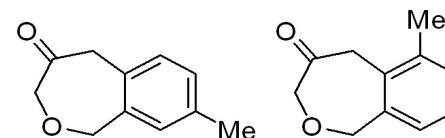
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Solvent	CDCl ₃
Spectrometer Frequency	499.86
Nucleus	¹ H



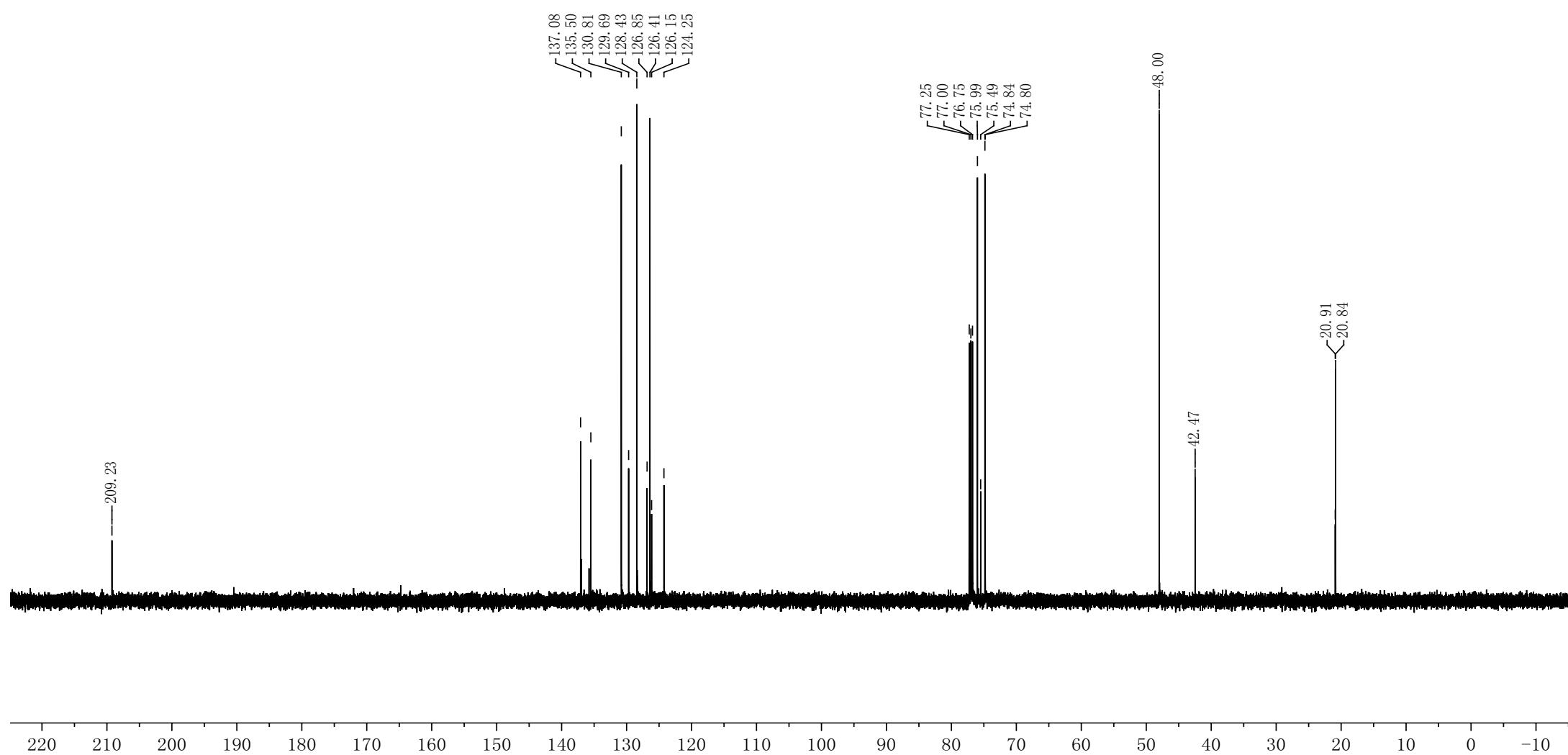
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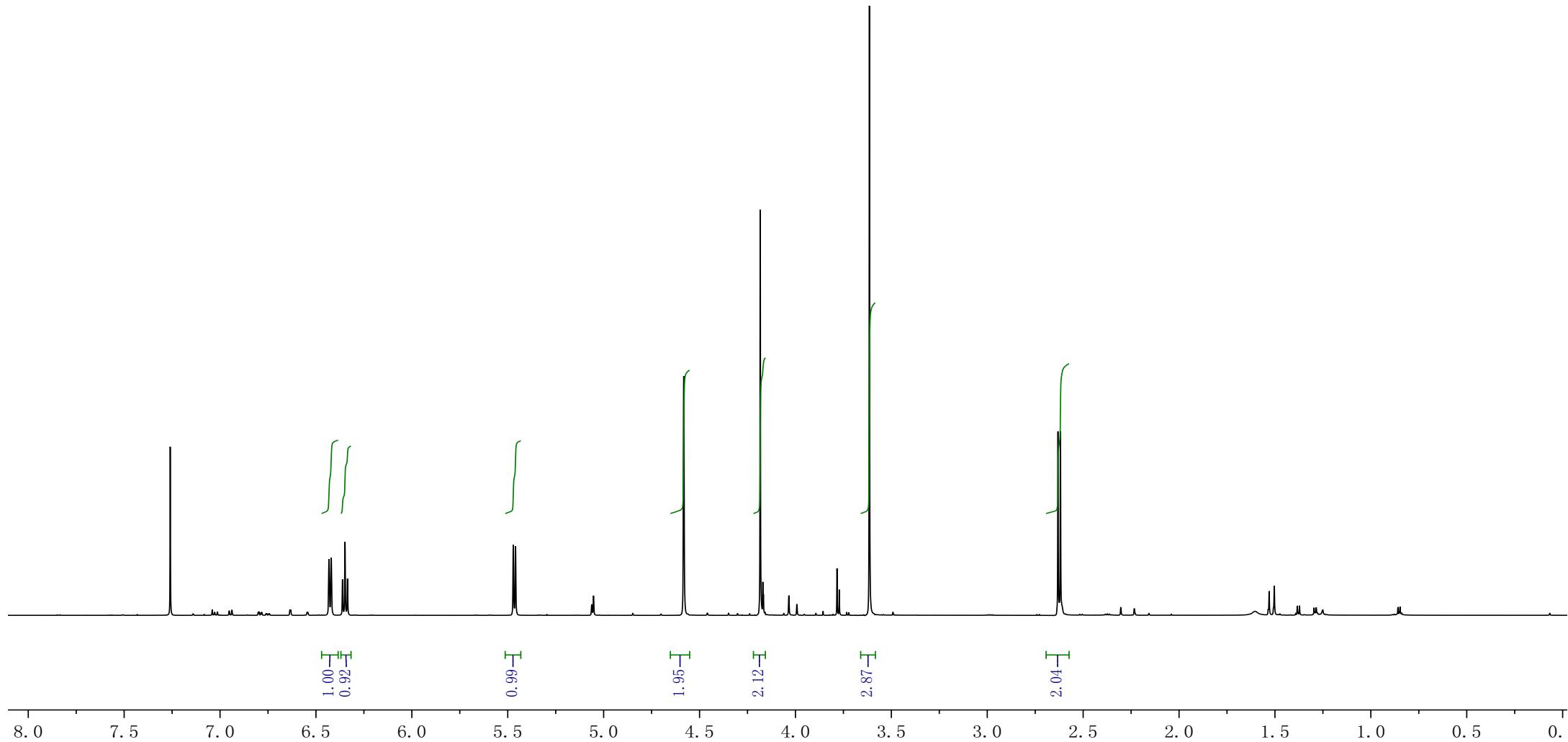
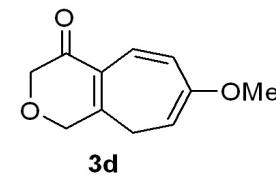
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Solvent	CDCl ₃
Spectrometer Frequency	125.70
Nucleus	¹³ C



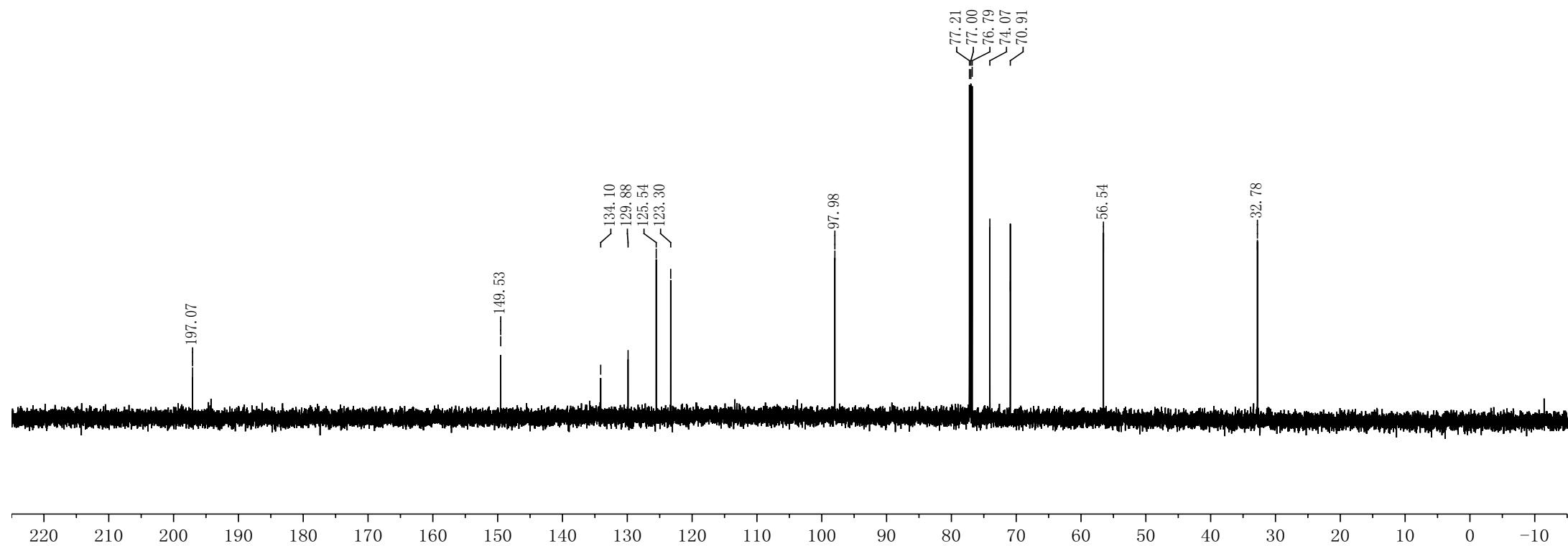
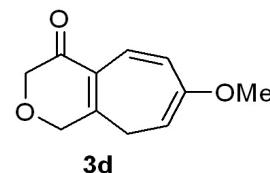
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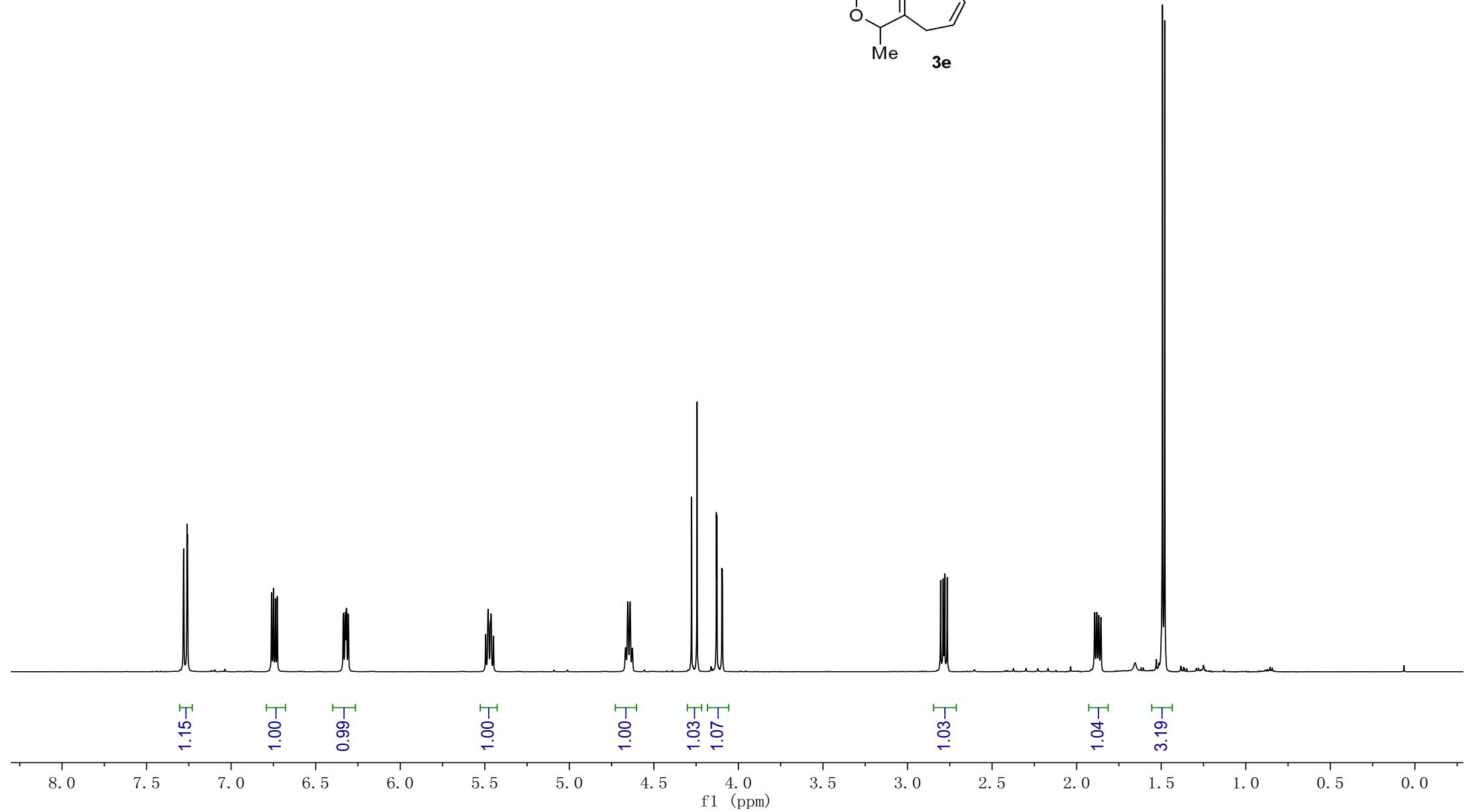
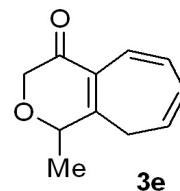
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Title	jkg-VI-8B-H
Solvent	cdcl3
Spectrometer Frequency	599.64
Nucleus	1H



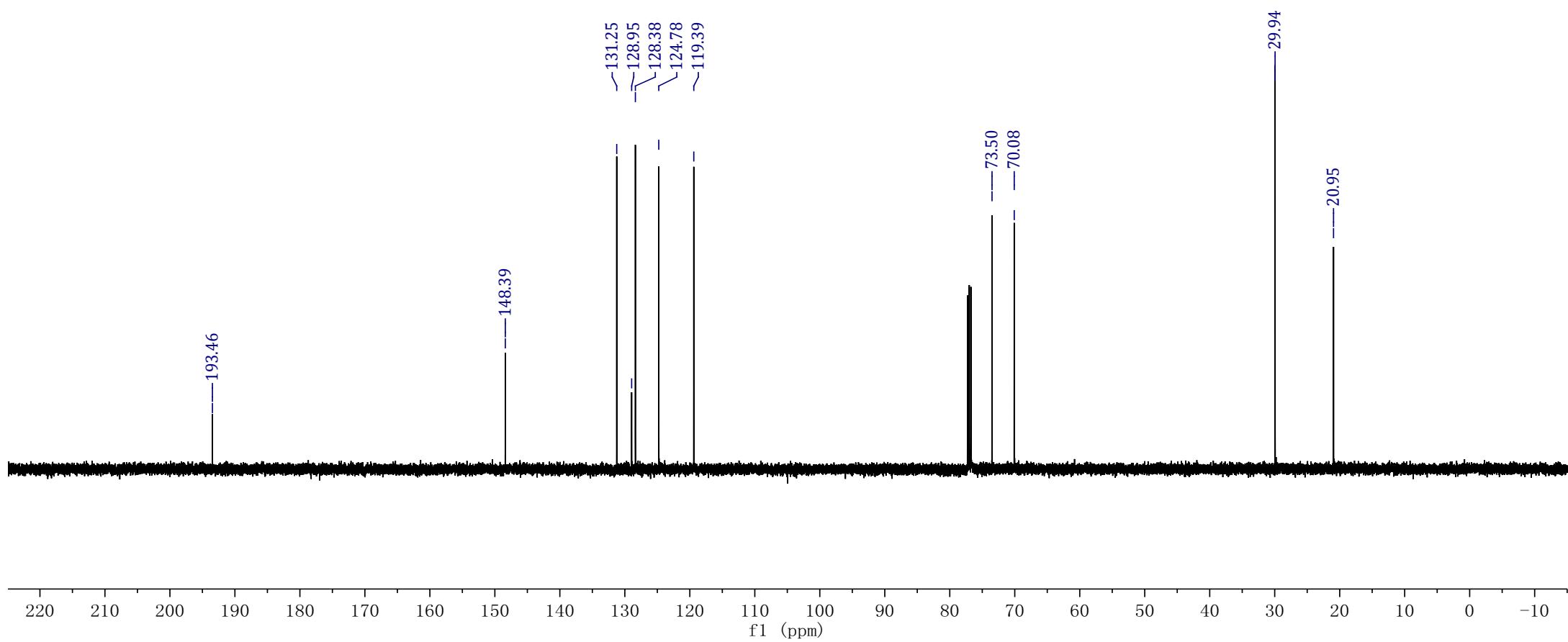
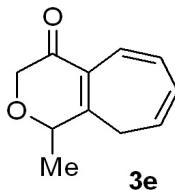
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Title	jkg-VI-8B-C
Solvent	cdcl3
Spectrometer Frequency	150.79
Nucleus	13C



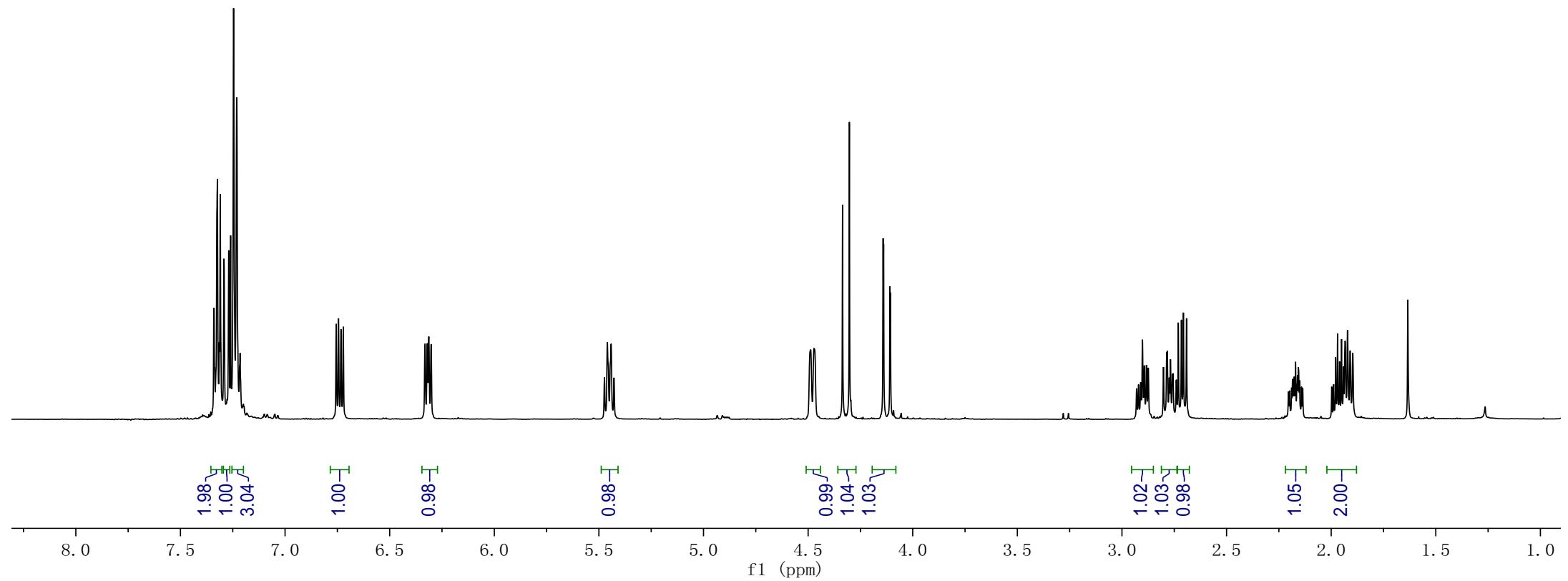
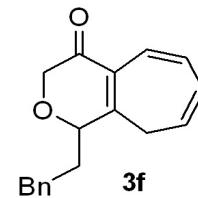
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2 Solvent	CDCl ₃
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4 Relaxation Delay	10.0000
5 Spectrometer Frequency	499.86



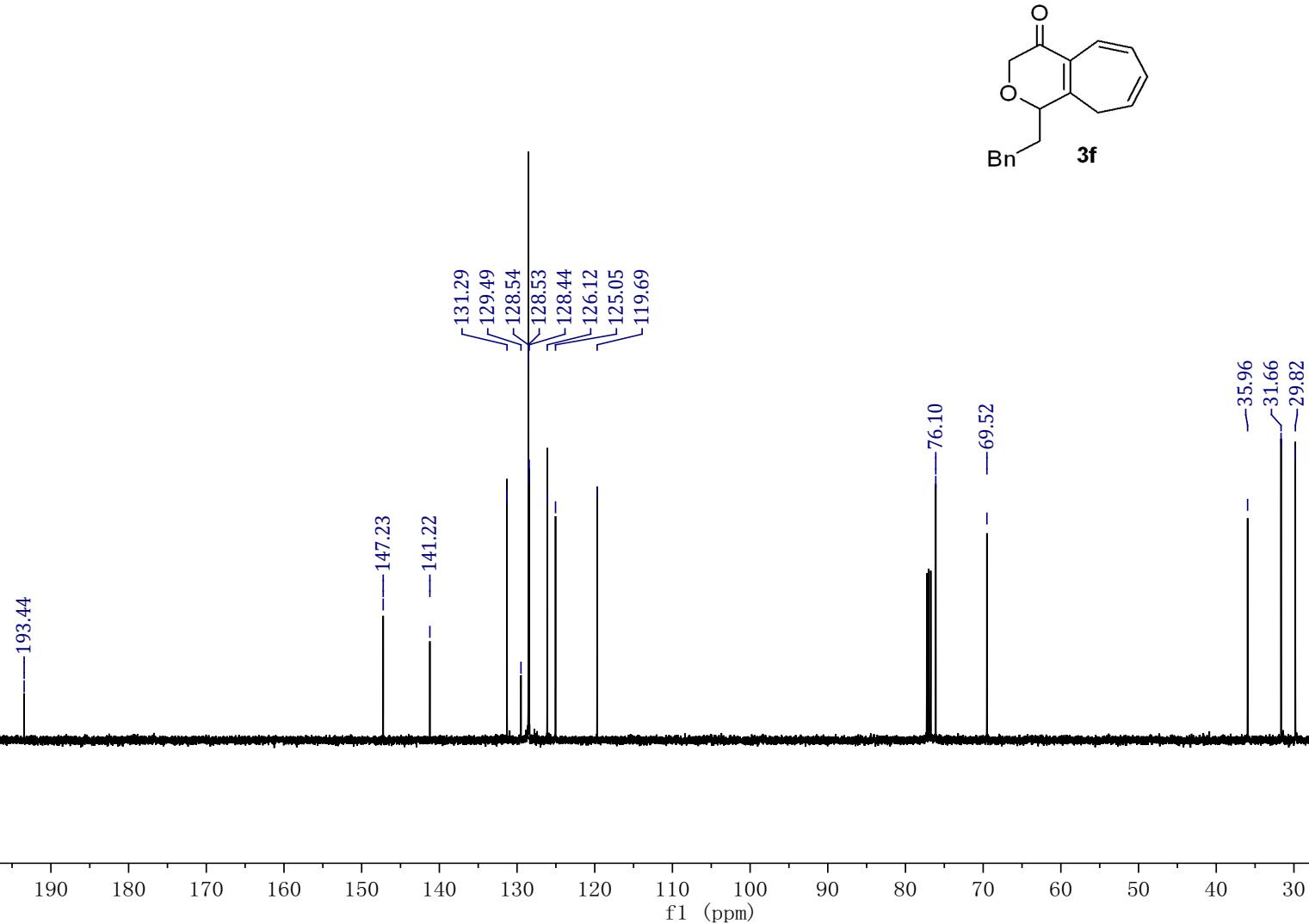
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2 Solvent	CDCl ₃
3 Temperature	25.0
4 Relaxation Delay	1.0000
5 Spectrometer Frequency	125.70



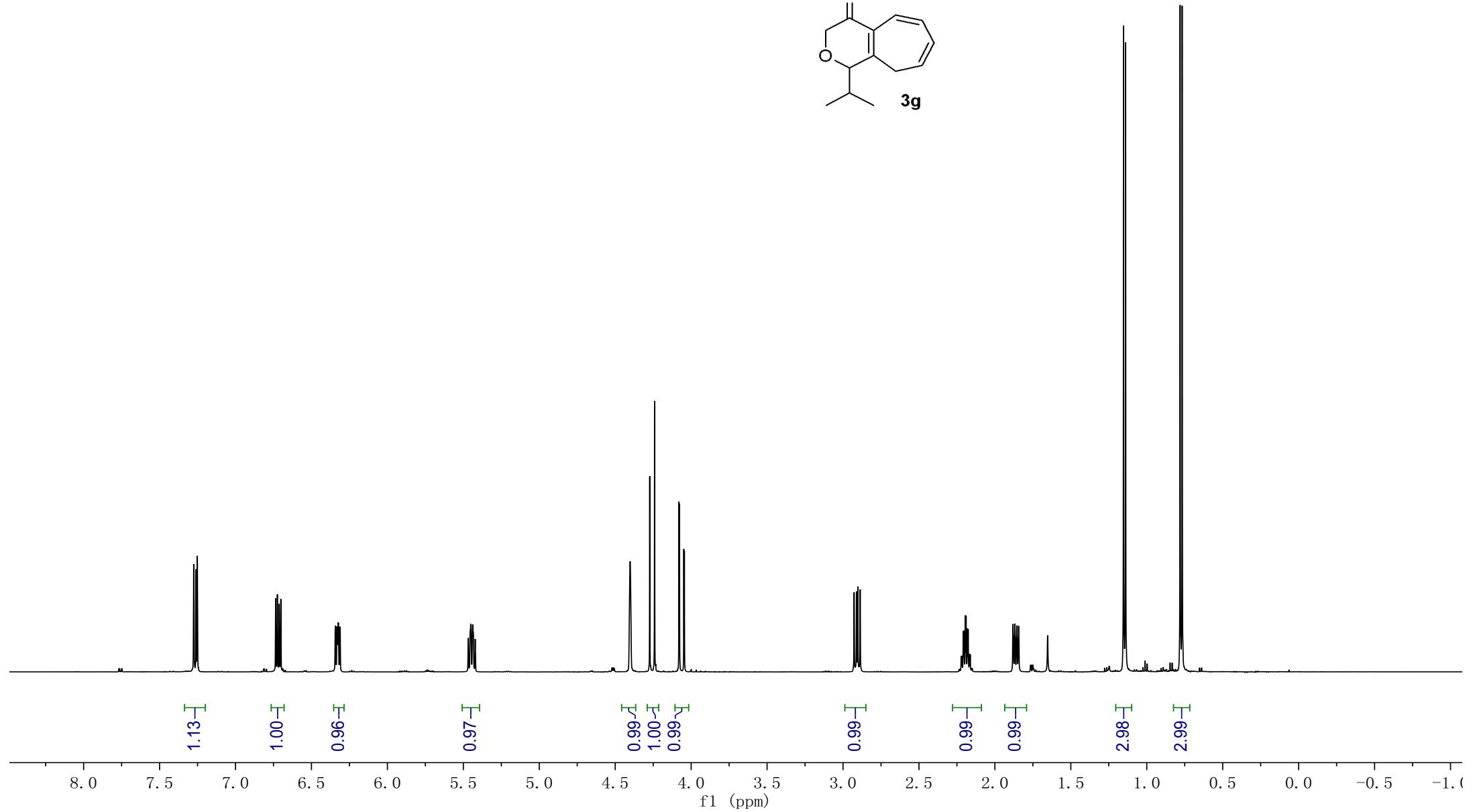
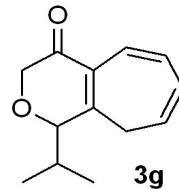
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2 Solvent	CDCl ₃
3 Temperature	25.0
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5 Spectrometer Frequency	499.86



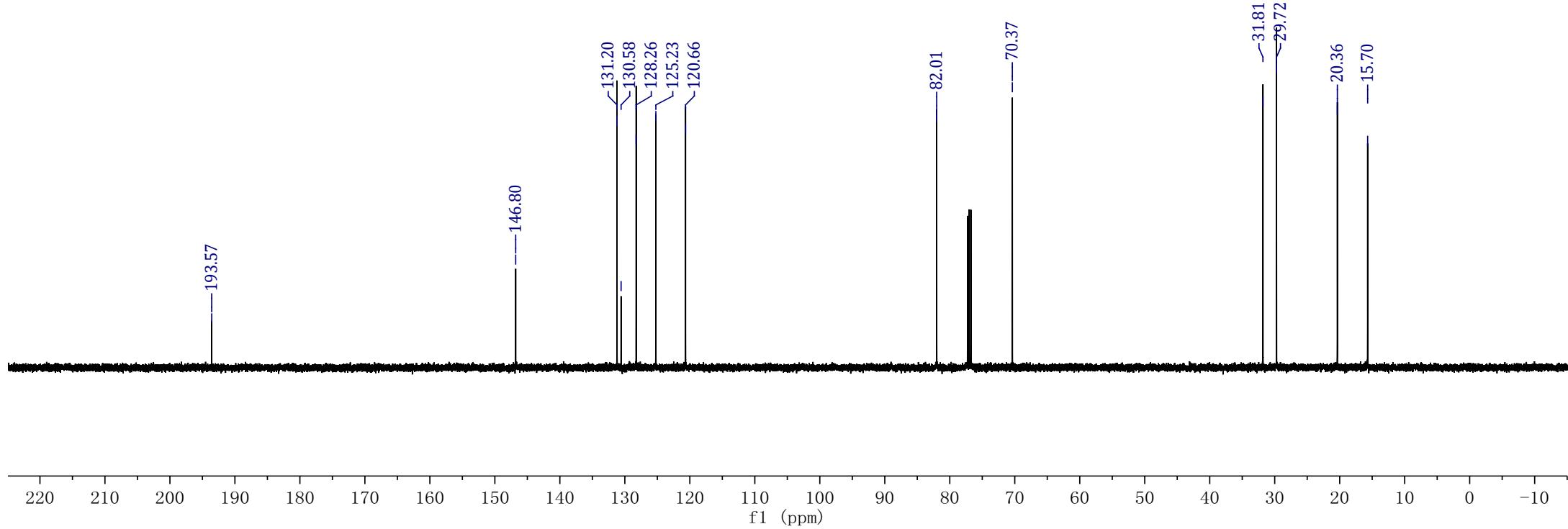
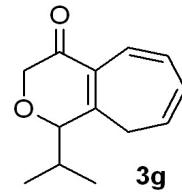
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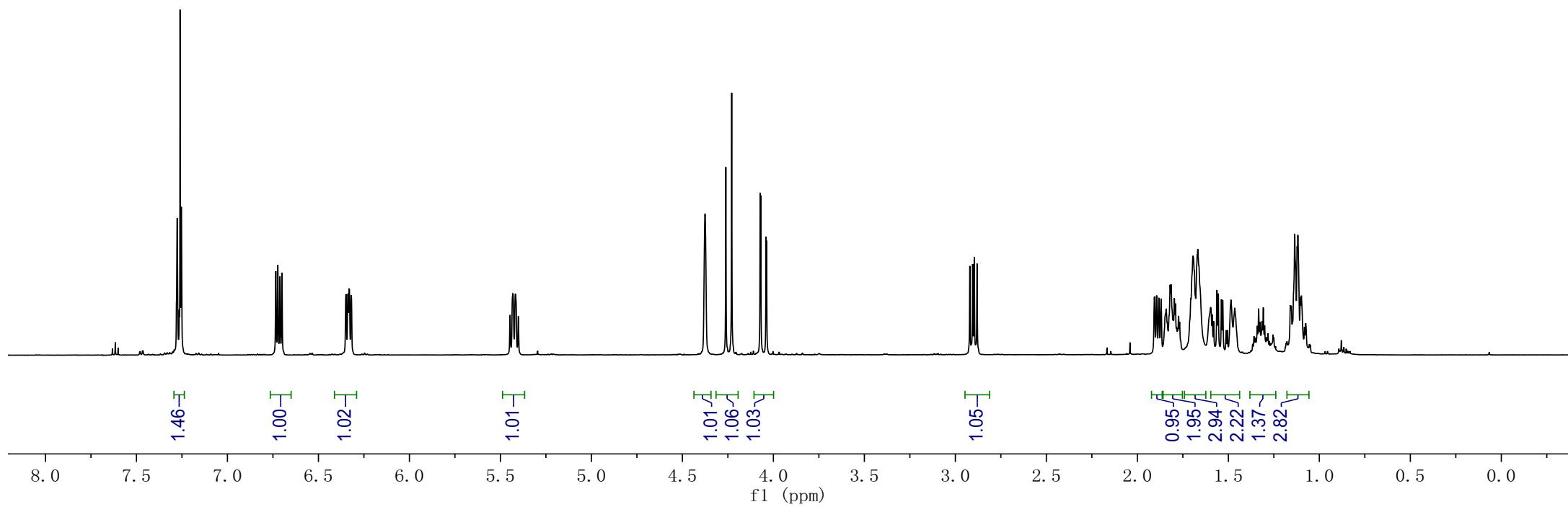
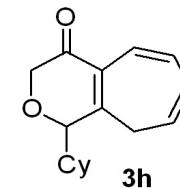
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5 Spectrometer Frequency	499.86



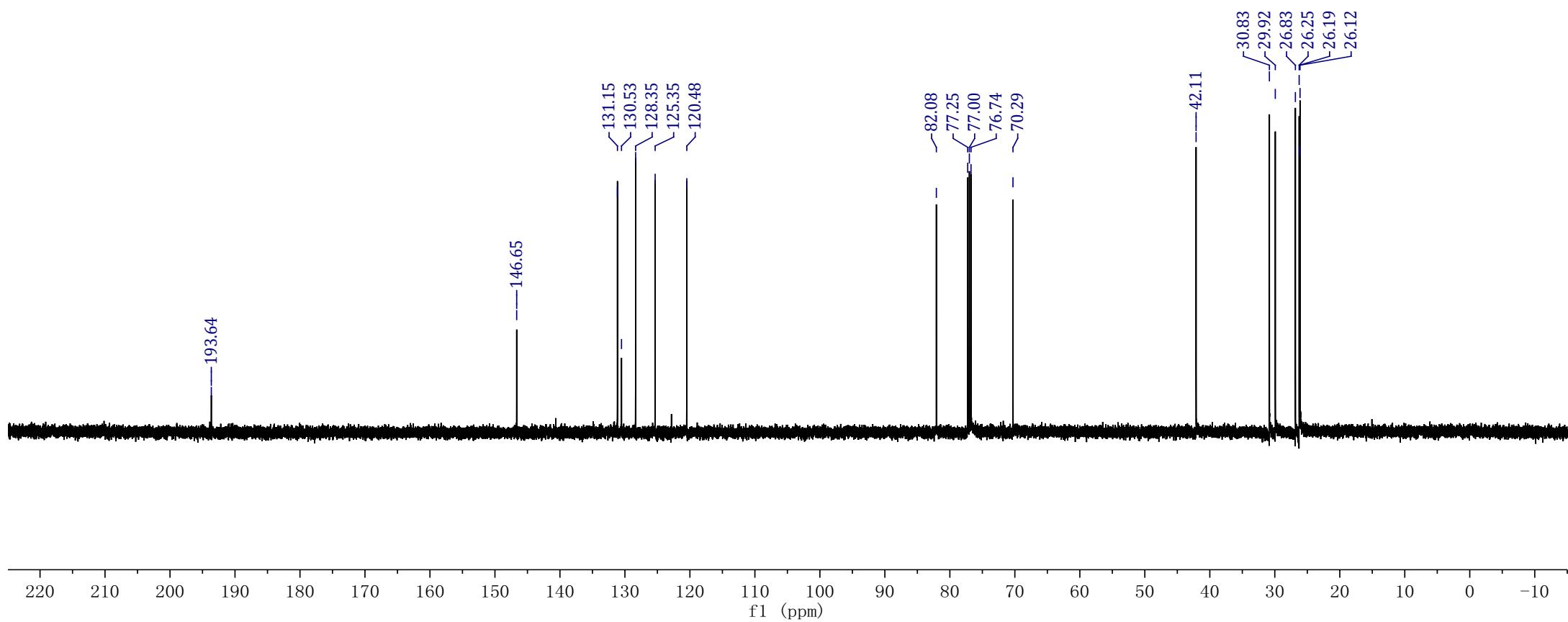
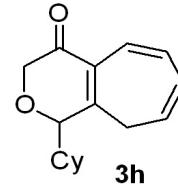
Parameter	Value
1 Title	jkg-VI-14A-C
2 Solvent	CDCl ₃
3 Temperature	25.0
4 Relaxation Delay	1.0000
5 Spectrometer Frequency	125.70



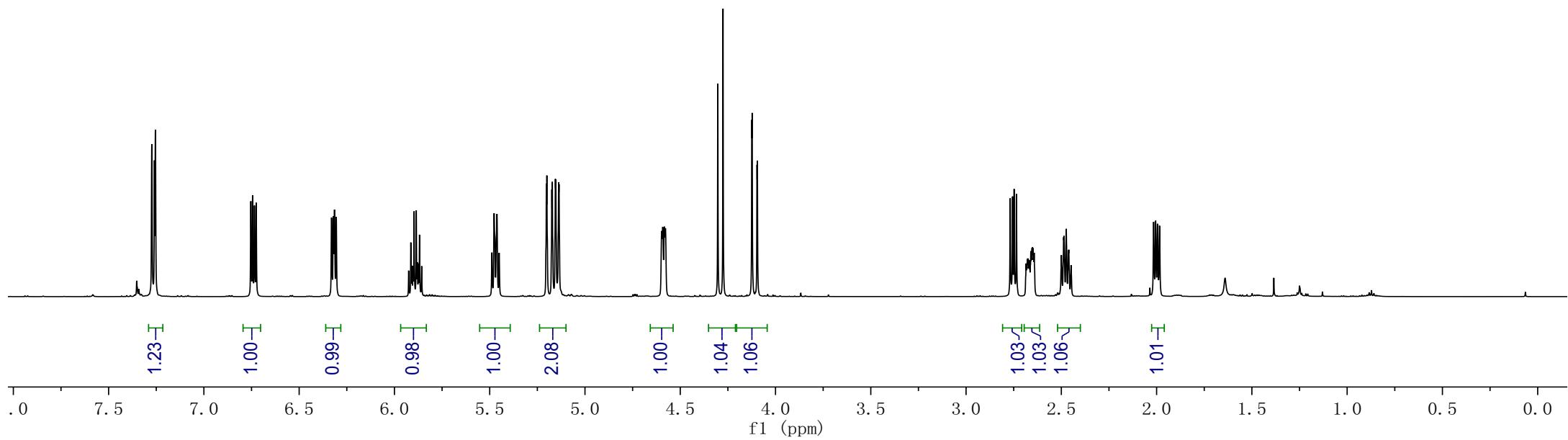
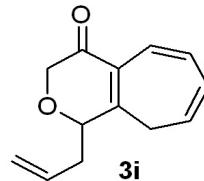
Parameter	Value
1 Title	jkg-VI-23C-H
2 Solvent	CDCl ₃
3 Temperature	25.0
4 Relaxation Delay	10.0000
5 Spectrometer Frequency	499.86



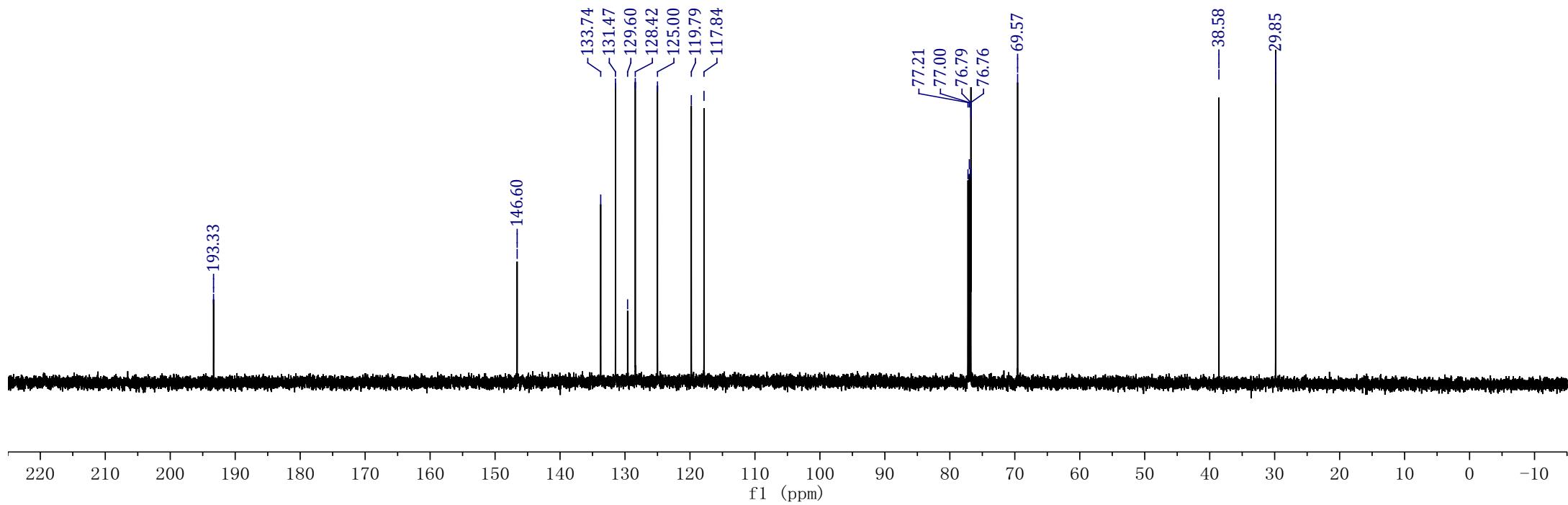
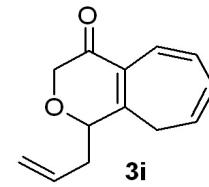
Parameter	Value
1 Title	jkg-VI-23C-C
2 Solvent	CDCl ₃
3 Temperature	25.0
4 Relaxation Delay	1.0000
5 Spectrometer Frequency	125.70



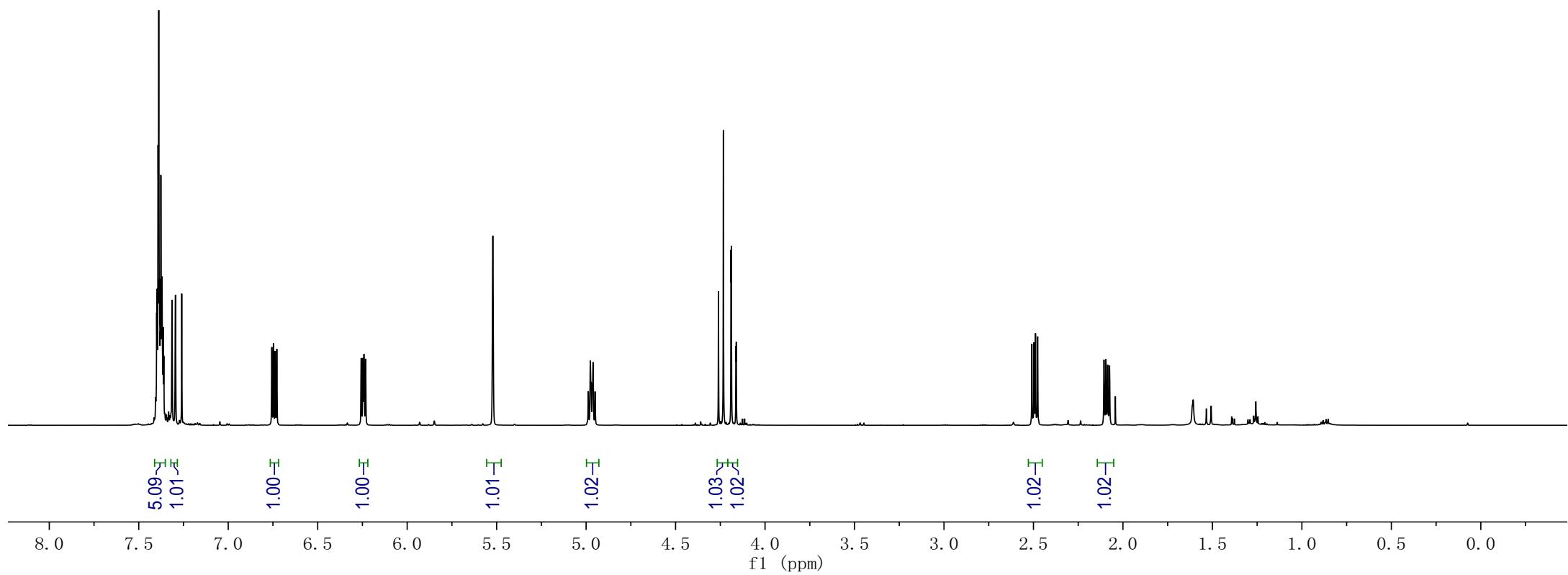
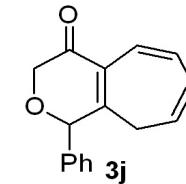
Parameter	Value
1 Title	jkg-VI-15B-H
2 Solvent	cdcl3
3 Temperature	25.0
4 Relaxation Delay	10.0000
5 Spectrometer Frequency	599.64



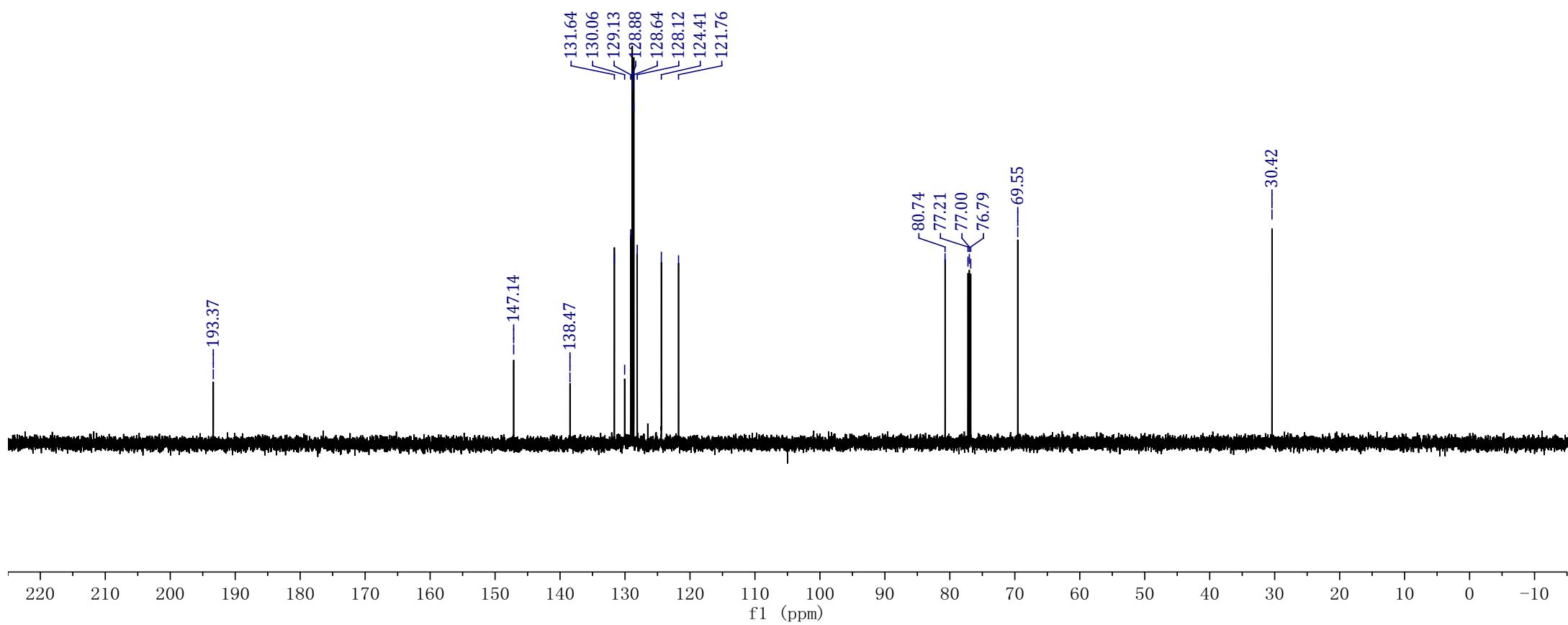
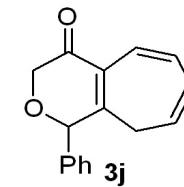
Parameter	Value
1 Title	jkg-VI-15B-C
2 Solvent	cdcl3
3 Temperature	25.0
4 Relaxation Delay	1.0000
5 Spectrometer Frequency	150.79



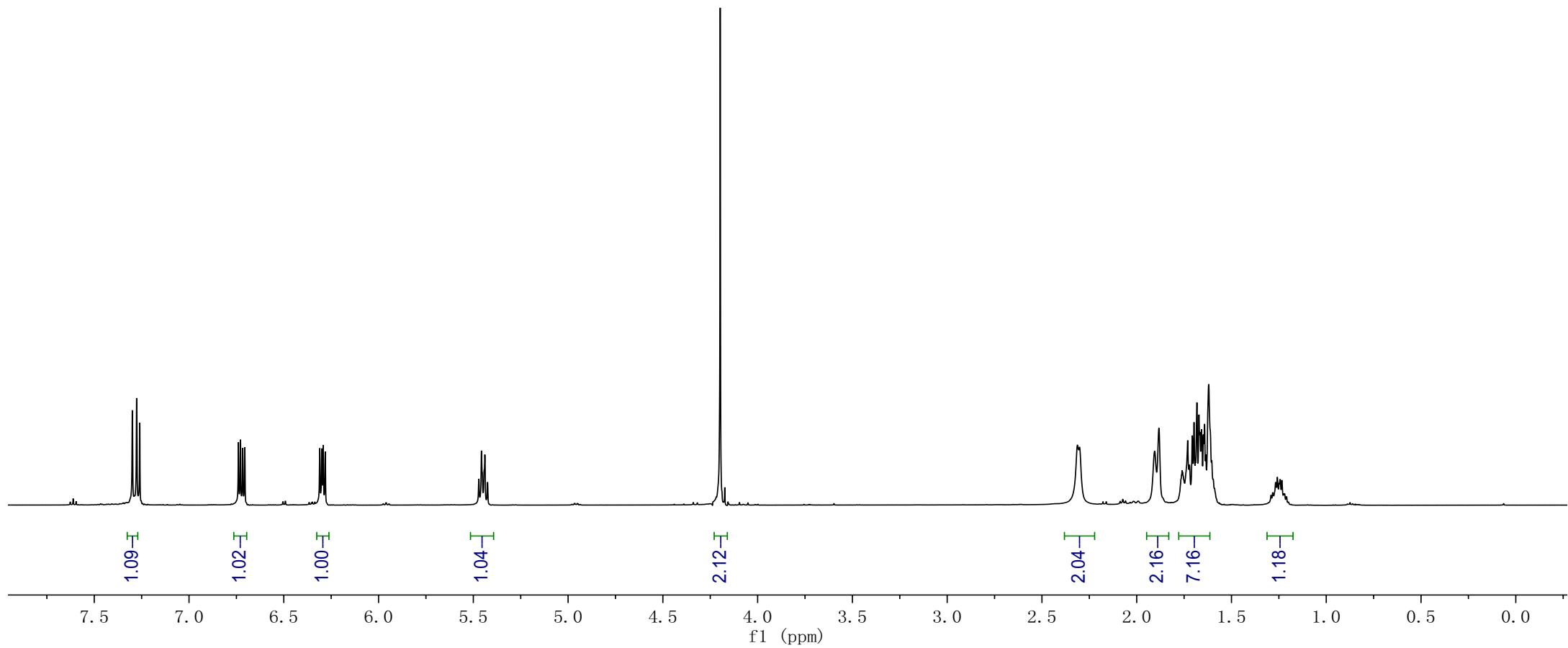
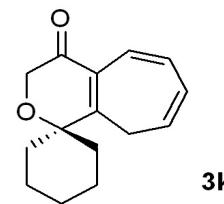
Parameter	Value
1 Title	jkg-VI-14B-H
2 Solvent	cdcl3
3 Temperature	25.0
4 Relaxation Delay	10.0000
5 Spectrometer Frequency	599.64



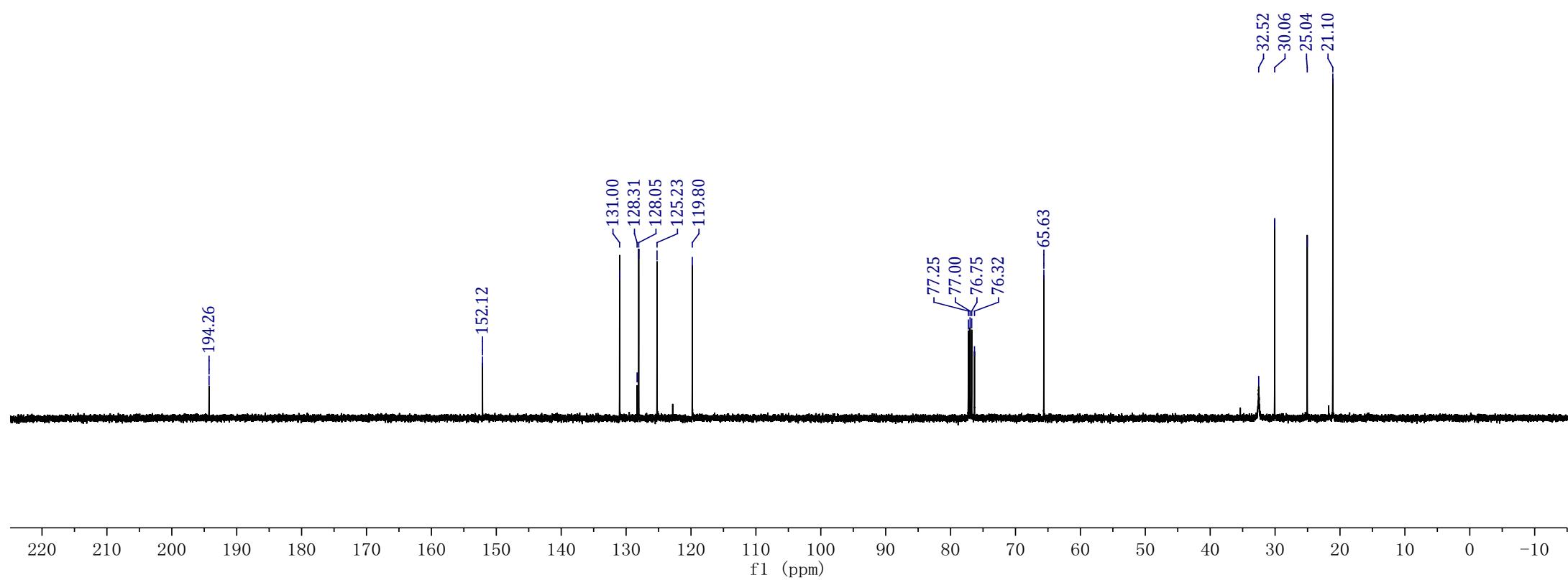
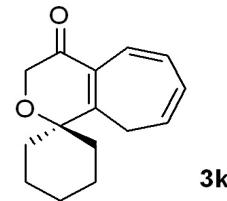
Parameter	Value
1 Title	jkg-VI-14B-C
2 Solvent	cdcl3
3 Temperature	25.0
4 Relaxation Delay	1.0000
5 Spectrometer Frequency	150.79



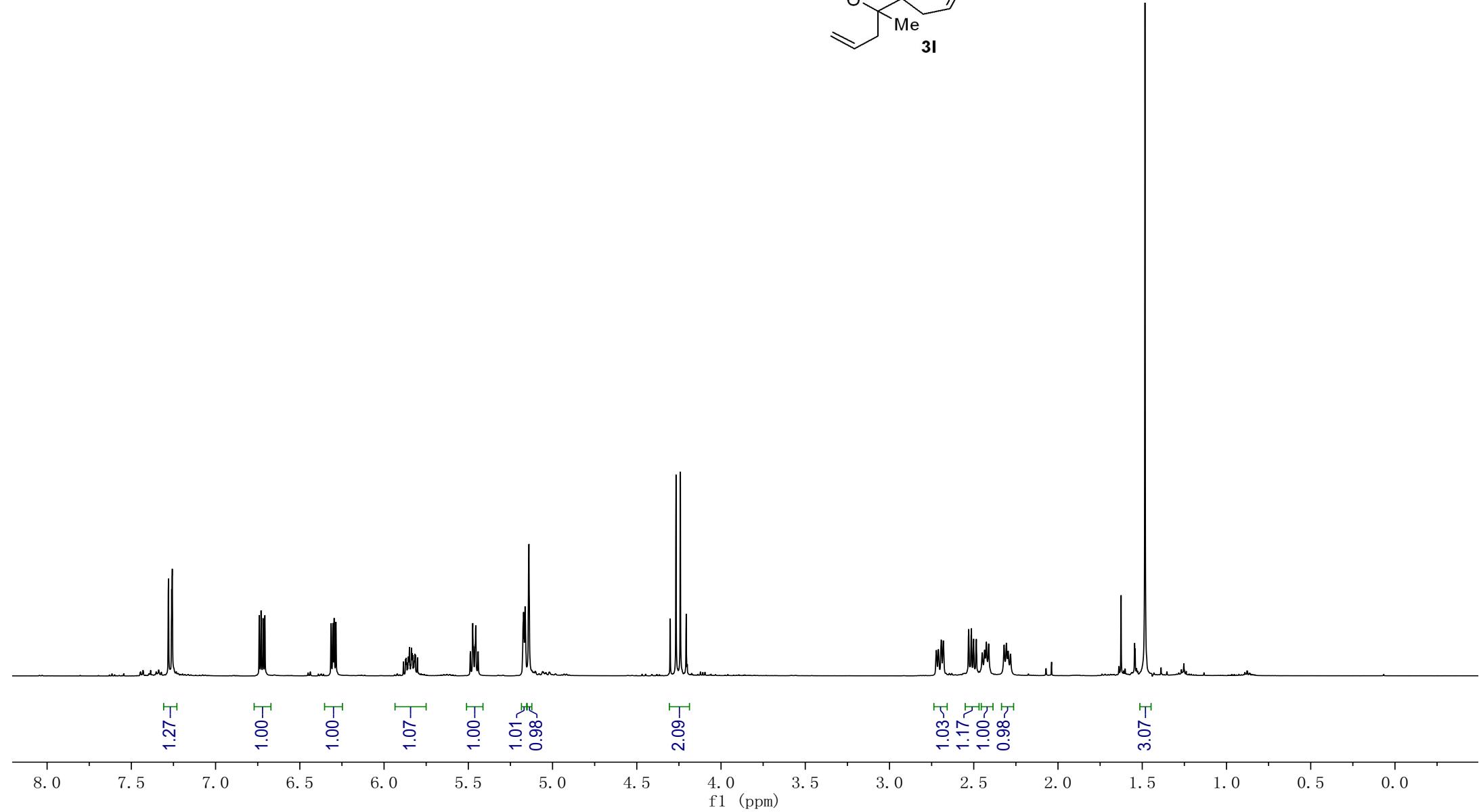
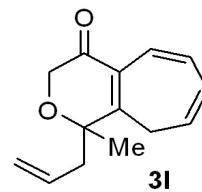
Parameter	Value
1 Title	jkg-VI-22B-H1
2 Solvent	CDCl ₃
3 Temperature	25.0
4 Relaxation Delay	10.0000
5 Spectrometer Frequency	499.86



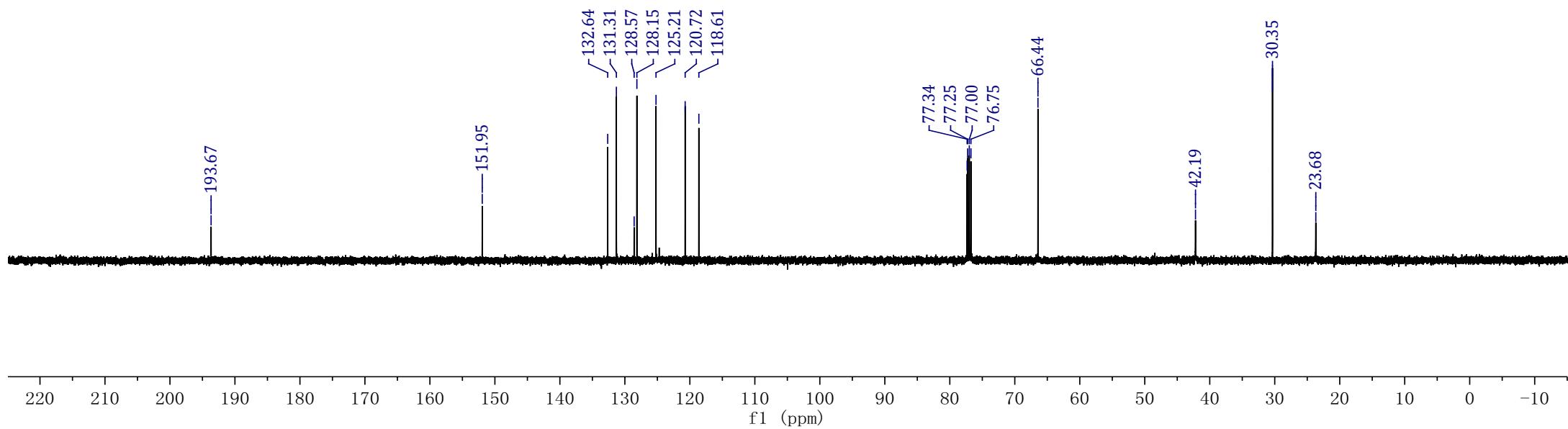
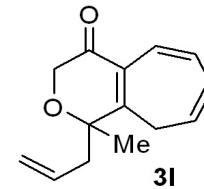
Parameter	Value
1 Title	jkg-VI-22B-C
2 Solvent	CDCl ₃
3 Temperature	25.0
4 Relaxation Delay	1.0000
5 Spectrometer Frequency	125.70



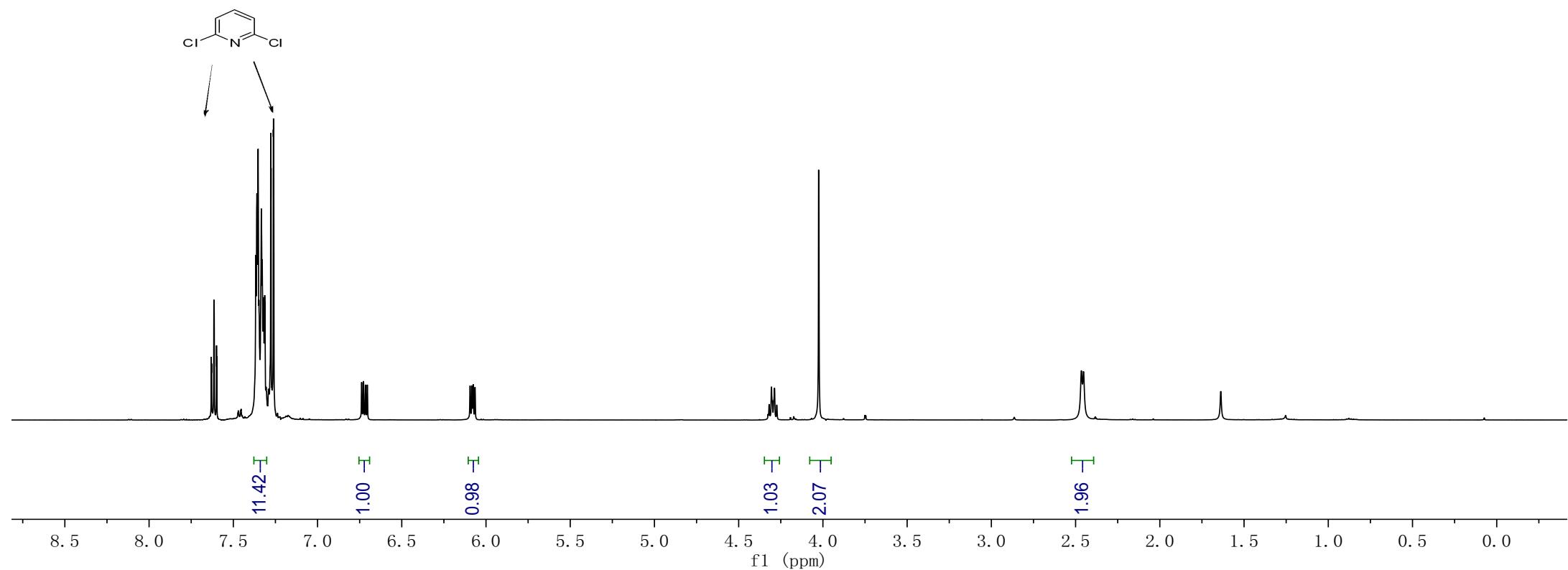
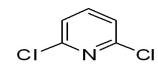
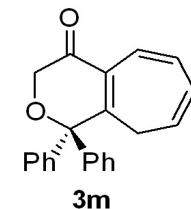
Parameter	Value
1 Title	jkg-VI-17B-H
2 Solvent	CDCl ₃
3 Temperature	20.0
4 Relaxation Delay	10.0000
5 Spectrometer Frequency	499.86



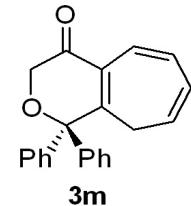
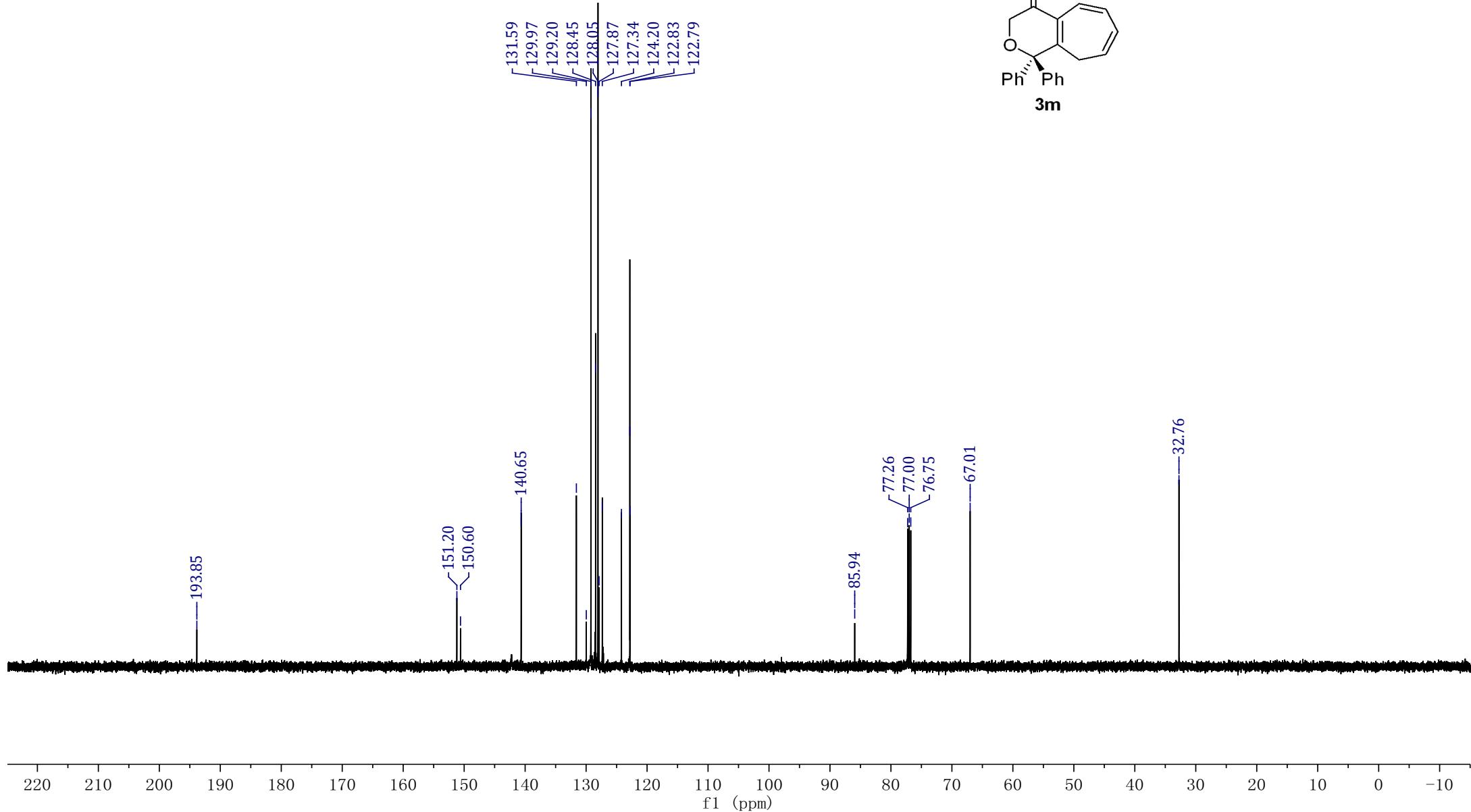
Parameter	Value
1 Title	jkg-VI-17B-C
2 Solvent	CDCl ₃
3 Temperature	20.0
4 Relaxation Delay	1.0000
5 Spectrometer Frequency	125.70



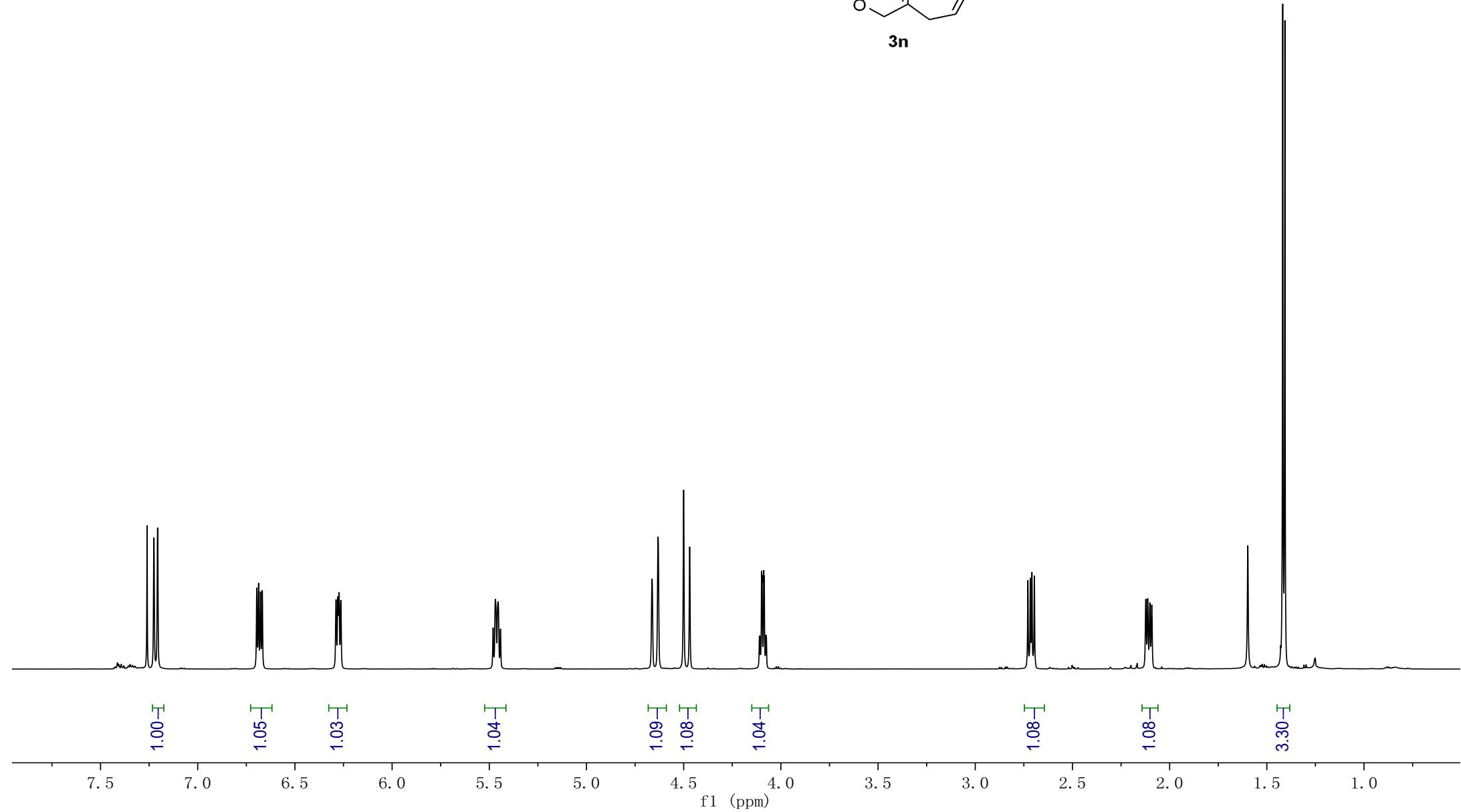
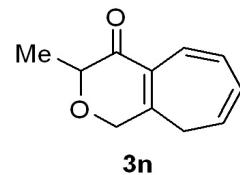
Parameter	Value
1 Title	jkg-Vi-18B-H
2 Solvent	CDCl ₃
3 Temperature	20.0
4 Relaxation Delay	10.0000
5 Spectrometer Frequency	499.86



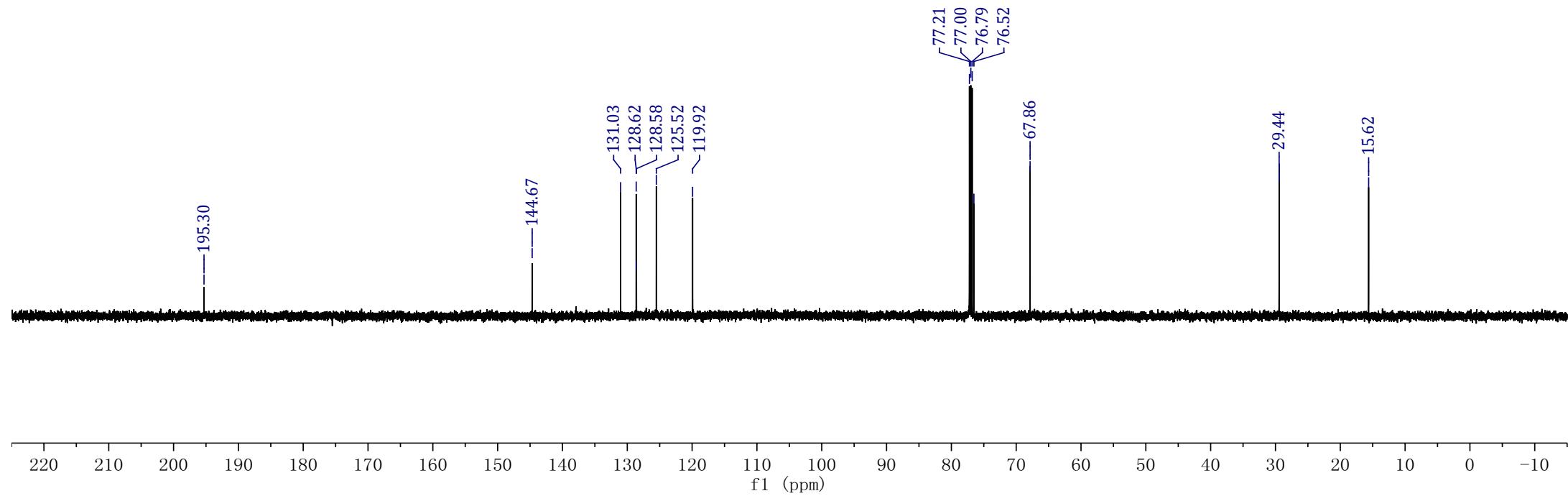
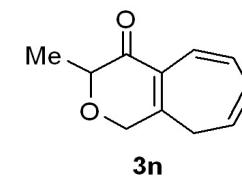
Parameter	Value
1 Title	jkg-Vi-18B-C
2 Solvent	CDCl ₃
3 Temperature	20.0
4 Relaxation Delay	1.0000
5 Spectrometer Frequency	125.70



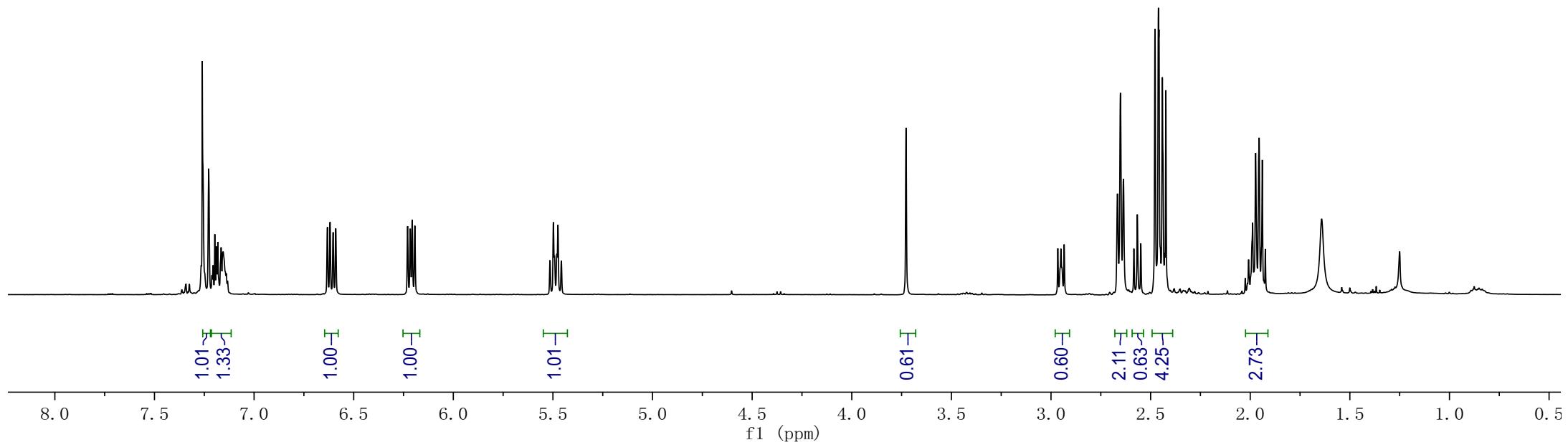
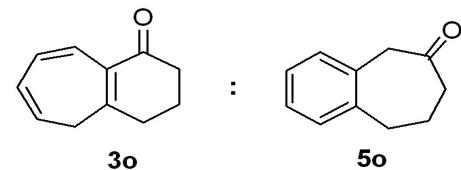
Parameter	Value
1 Title	jkg-VI-20A-H
2 Solvent	cdcl3
3 Temperature	25.0
4 Relaxation Delay	10.0000
5 Spectrometer Frequency	599.64



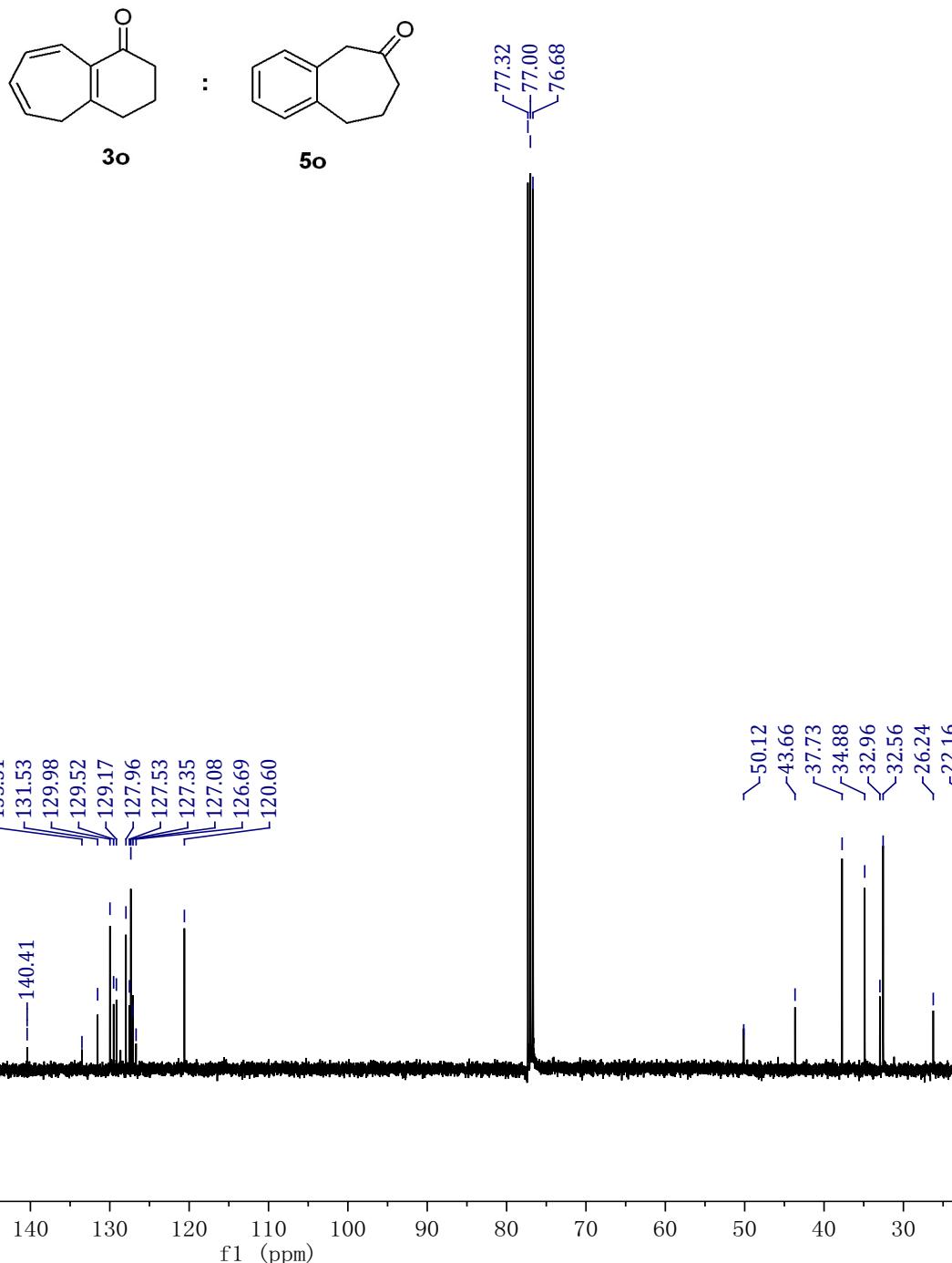
Parameter	Value
1 Title	jkg-VI-20A-C
2 Solvent	cdcl3
3 Temperature	25.0
4 Relaxation Delay	1.0000
5 Spectrometer Frequency	150.79



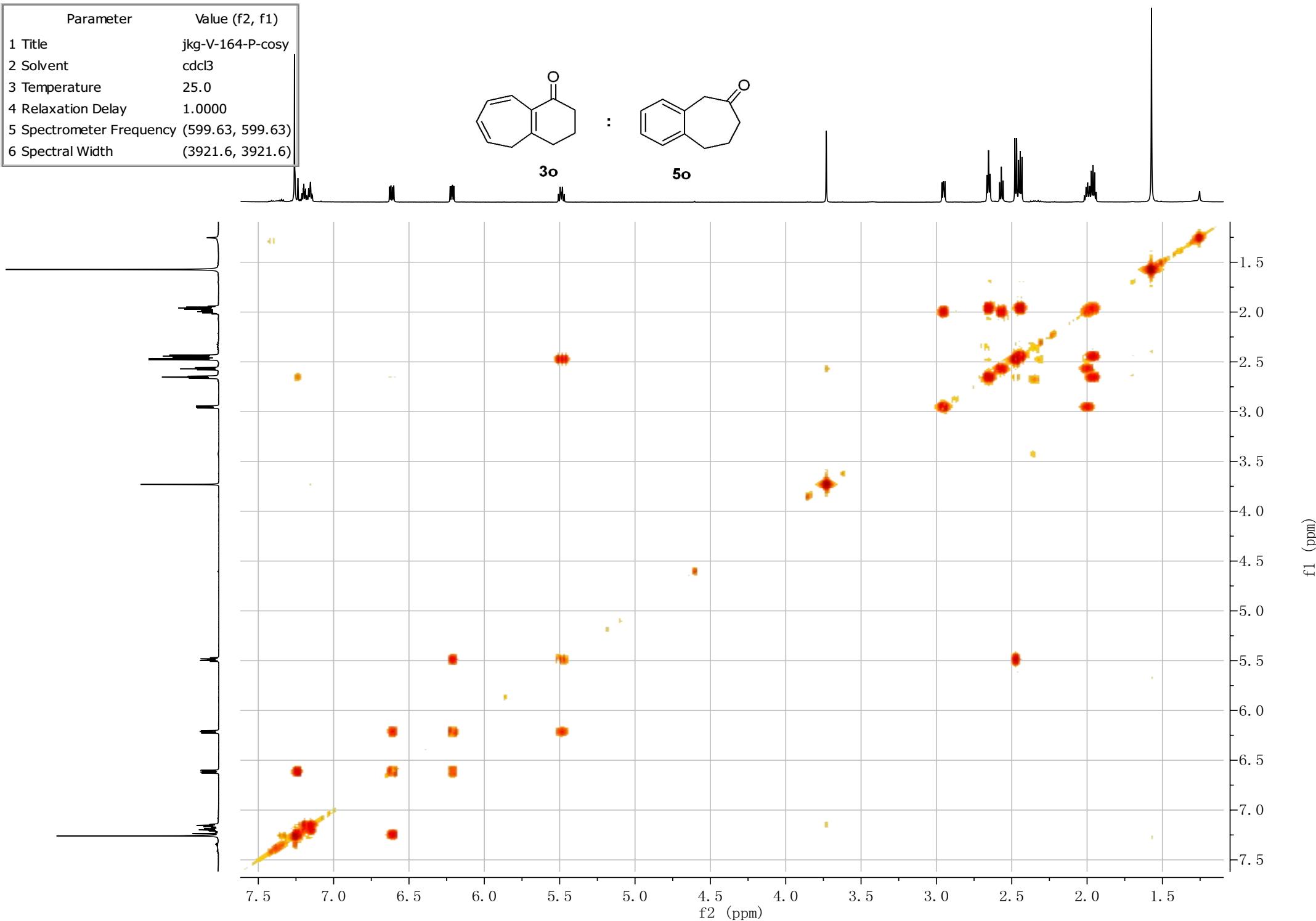
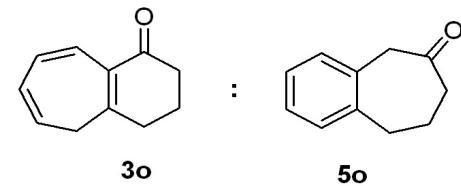
Parameter	Value
1 Title	jkg-VII-227D-H
2 Solvent	cdcl3
3 Temperature	26.0
4 Relaxation Delay	10.0000
5 Spectrometer Frequency	399.78



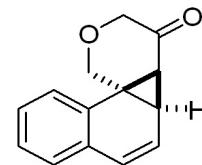
Parameter	Value
1 Title	jkg-VII-227D-C13
2 Solvent	cdcl3
3 Temperature	26.0
4 Relaxation Delay	1.0000
5 Spectrometer Frequency	100.53



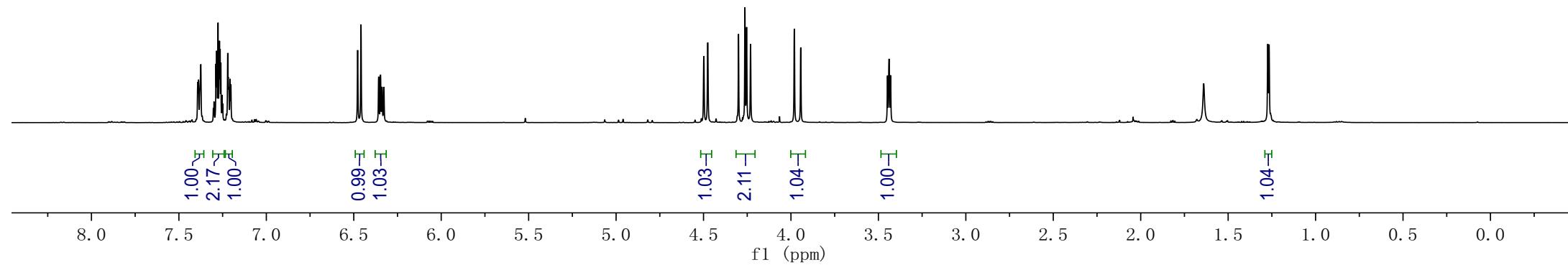
Parameter	Value (f2, f1)
1 Title	jkg-V-164-P-cosy
2 Solvent	cdcl3
3 Temperature	25.0
4 Relaxation Delay	1.0000
5 Spectrometer Frequency (599.63, 599.63)	
6 Spectral Width	(3921.6, 3921.6)



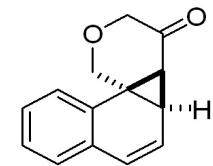
Parameter	Value
1 Title	jkg-VII-227C-H
2 Solvent	CDCl ₃
3 Temperature	80.0
4 Relaxation Delay	10.0000
5 Spectrometer Frequency	499.86



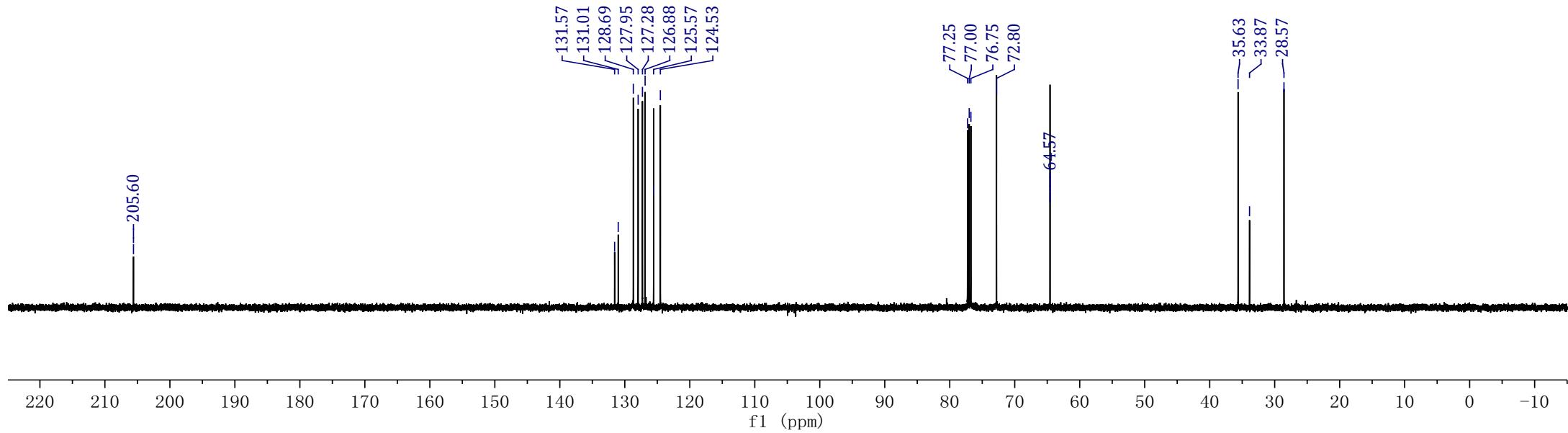
4p



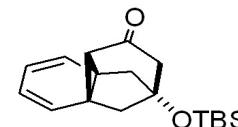
Parameter	Value
1 Title	jkg-VII-227C-C13
2 Solvent	CDCl ₃
3 Temperature	80.0
4 Relaxation Delay	1.0000
5 Spectrometer Frequency	125.70



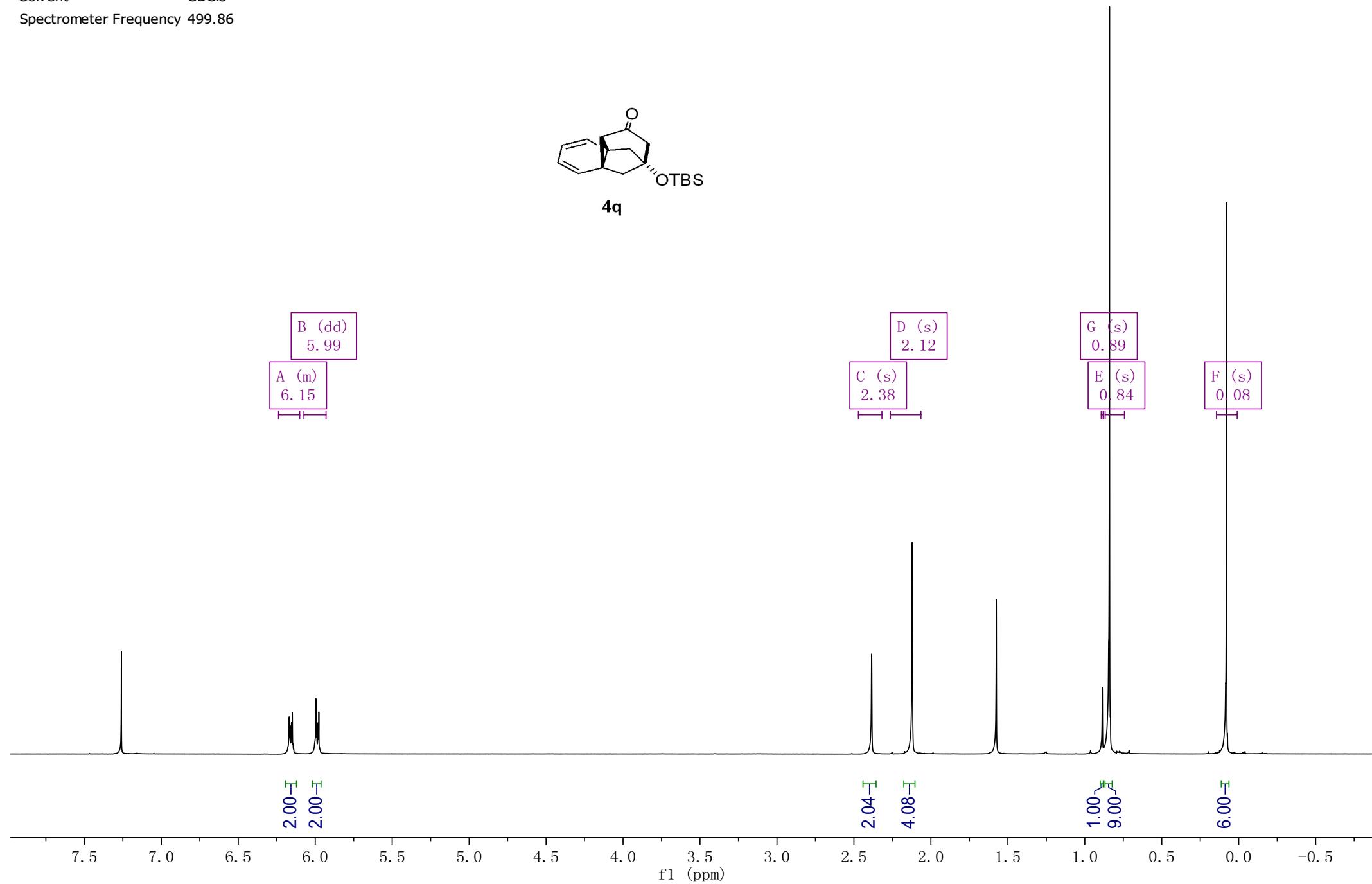
4p



Parameter	Value
Title	jkg-VI-73-H
Solvent	CDCl ₃
Spectrometer Frequency	499.86



4q



Parameter	Value
Title	jkg-VI-73-C
Solvent	CDCl ₃
Spectrometer Frequency	125.70

