

Supporting Information

Gold-catalyzed selective oxidation of 4-Oxahepta-1,6-diynes to 2*H*-pyran-3(6*H*)-ones and chromen-3(4*H*)-ones via the β -gold vinyl cation intermediates

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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. 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 ¹³C NMR spectra were recorded on Bruker 500 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.

¹³C NMR spectra were recorded on a Bruker AV-500 spectrometer and a Bruker AV-500 spectrometer in chloroform-d₃. Chemical shifts are reported in ppm with the internal chloroform signal at 7.26 and 77.0 ppm as a standard.

Table 1 Screening conditions

Reaction scheme: **1a** $\xrightarrow[\text{N-Oxide, DCE, rt, 10h}]{[\text{Au}]/\text{additive}}$ **3a**

2a

2b

2c

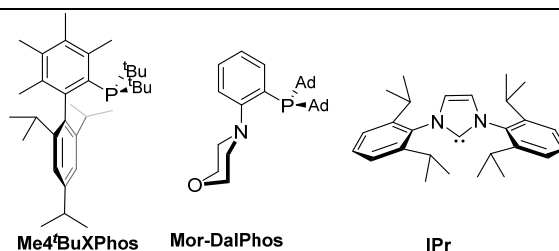
2d

2e

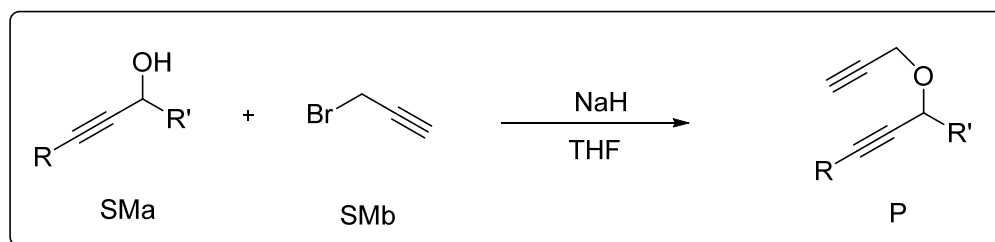
Entry	N-Oxide (equiv)	Catalyst (mol %)	Additive (mol%)	Yield ^b
1	2a (2.5)	Me ₄ ^t BuXPhosAuCl(5)	NaBARF ₄ (10)	82% ^c
2	2b (2.5)	Me ₄ ^t BuXPhosAuCl(5)	NaBARF ₄ (10)	58%
3	2c (2.5)	Me ₄ ^t BuXPhosAuCl(5)	NaBARF ₄ (10)	55%
4	2d (2.5)	Me ₄ ^t BuXPhosAuCl(5)	NaBARF ₄ (10)	57%
5	2e (2.5)	Me ₄ ^t BuXPhosAuCl(5)	NaBARF ₄ (10)	73%
6	2a (1.5)	Me ₄ ^t BuXPhosAuCl(5)	NaBARF ₄ (10)	60%
7	2a (2.0)	Me ₄ ^t BuXPhosAuCl(5)	NaBARF ₄ (10)	78%

8	2a (3.0)	Me ₄ ^t BuXPhosAuCl(5)	NaBARF ₄ (10)	79%
9	2a (2.5)	Me₄^tBuXPhosAuCl(2)	NaBARF₄ (4)	82%
10	2a (2.5)	Ph ₃ PAuCl(2)	NaBARF ₄ (4)	< 3%
11	2a (2.5)	IPrAuCl(2)	NaBARF ₄ (4)	< 5%
12	2a (2.5)	Mor-DalPhosAuNTf ₂ (2)	-	72%
13	2a (2.5)	Me ₄ ^t BuXPhosAuCl(2)	NaBARF ₄ (4)	< 3% ^d
14	2a (2.5)	Me ₄ ^t BuXPhosAuCl(2)	NaBARF ₄ (4)	45% ^e
15	2a (2.5)	Me ₄ ^t BuXPhosAuCl(2)	NaBARF ₄ (4)	< 3% ^f

^a The reaction was run with everything in a vial capped with a septum, Initially, [1a]=0.1M. ^b Isolated yield. ^c Reaction time 5h. ^d Acetonitrile as the solvent. ^e Toluene as the solvent. ^f Acetone as the solvent.



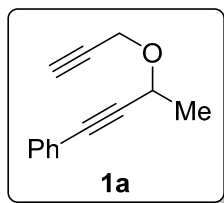
General procedure A: Methods for the synthesis 4-Oxahepta-1,6-diyne derivatives



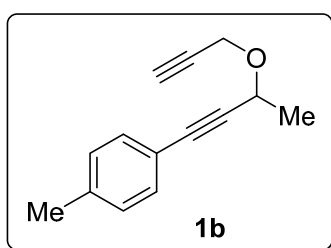
A solution of propargyl alcohol **SMa** (5 mmol) was added a solution of NaH (6 mmol) in THF (ca. 20 mL) at 0 °C, after stirring for 30 minutes at room temperature, cool to 0 °C, propargyl bromide **SMb** (80 % in toluene, 6 mmol) was added dropwise and the resulting slurry was efficiently stirred at room temperature 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 4-oxahepta-1,6-diynes as a colorless oil (70% yield).

SM NMR data

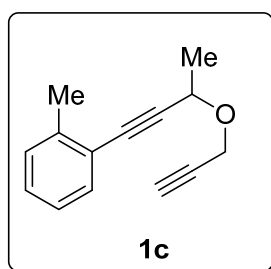
The known compound 4-oxahepta-1,6-diynes **1a**,¹ was prepared according to the general procedure **A** and its spectroscopic data were in accordance with the literature data.



(3-(prop-2-yn-1-yloxy)but-1-yn-1-yl)benzene **1a**¹ is known compound. ¹H NMR (500 MHz, CDCl₃) δ 7.48 – 7.41 (m, 2H), 7.35 – 7.29 (m, 3H), 4.64 (q, *J* = 6.6 Hz, 1H), 4.43 – 4.29 (m, 2H), 2.51 – 2.41 (m, 1H), 1.56 (d, *J* = 6.6 Hz, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 131.71, 128.41, 128.23, 122.44, 87.89, 85.61, 79.55, 74.40, 64.59, 55.72, 21.98.



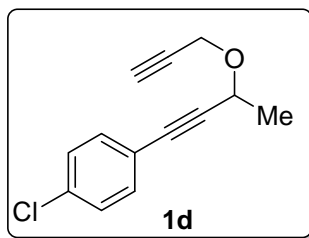
1-methyl-4-(3-(prop-2-yn-1-yloxy)but-1-yn-1-yl)benzene 1b: The compound **1b** was prepared in 78% yield through the General Procedure A. ¹H NMR (500 MHz, CDCl₃) δ 7.33 (d, *J* = 8.1 Hz, 2H), 7.11 (d, *J* = 7.9 Hz, 2H), 4.68 – 4.56 (m, 1H), 4.49 – 4.25 (m, 2H), 2.51 – 2.40 (m, 1H), 2.34 (s, 3H), 1.54 (t, *J* = 7.1 Hz, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 138.55, 131.65, 131.62, 129.00, 119.38, 87.17, 85.76, 79.64, 74.34, 64.67, 55.69, 22.04, 21.42. IR (neat, cm⁻¹): 3295, 2987, 2928, 1615, 1509, 1369, 1095, 756. GCMS (*m/z*): 198.10



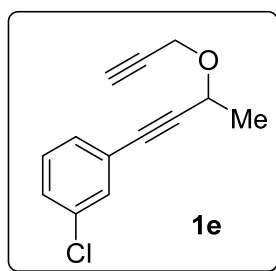
1-methyl-2-(3-(prop-2-yn-1-yloxy)but-1-yn-1-yl)benzene 1c : The compound **1c** was prepared in 75% yield through the General Procedure A. ¹H NMR (500 MHz, CDCl₃) δ 7.41 (d, *J* = 7.5 Hz, 1H), 7.26 – 7.18 (m, 2H), 7.17 – 7.11 (m, 1H), 4.75 – 4.64 (m, 1H), 4.44 – 4.31 (m, 2H), 2.45 (q, *J* = 2.7 Hz, 1H), 2.43 (s, 3H), 1.58 (d, *J* = 6.6 Hz, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 140.23, 132.03, 129.41, 128.46, 125.51, 122.24, 91.84, 84.54, 74.41, 64.71,

55.72, 22.18, 20.68. IR (neat, cm^{-1}): 3295, 2988, 2927, 1617, 1509, 1368, 1224, 1095, 756.

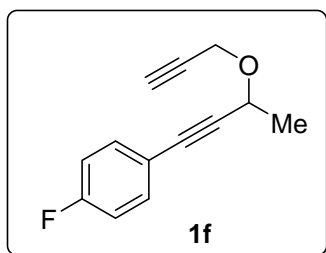
GCMS (m/z): 198.10



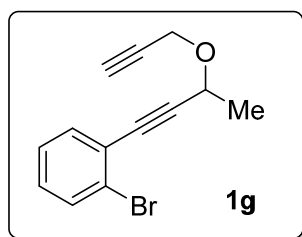
1-chloro-4-(3-(prop-2-yn-1-yloxy)but-1-yn-1-yl)benzene **1d**: The compound **1d** was prepared in 70% yield through the General Procedure A. ^1H NMR (500 MHz, CDCl_3) δ 7.35 (t, $J = 9.2$ Hz, 2H), 7.28 (dd, $J = 8.4, 1.8$ Hz, 2H), 4.74 – 4.54 (m, 1H), 4.44 – 4.26 (m, 2H), 2.46 (t, $J = 2.4$ Hz, 1H), 1.54 (t, $J = 7.1$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 134.50, 132.98, 132.95, 128.60, 128.58, 120.94, 88.94, 84.49, 79.45, 74.52, 64.54, 55.80. IR (neat, cm^{-1}): 3298, 2930, 2224, 1620, 1519, 1368, 1224, 1095, 760. GCMS (m/z): 218.05



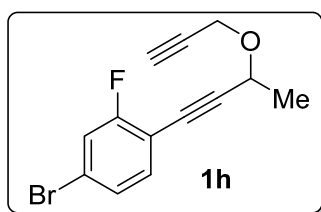
1-chloro-3-(3-(prop-2-yn-1-yloxy)but-1-yn-1-yl)benzene **1e**: The compound **1e** was prepared in 70% yield through the General Procedure A. ^1H NMR (500 MHz, CDCl_3) δ 7.44 (t, $J = 1.6$ Hz, 1H), 7.34 – 7.28 (m, 2H), 7.25 (dd, $J = 14.0, 6.2$ Hz, 1H), 4.63 (q, $J = 6.6$ Hz, 1H), 4.35 (ddd, $J = 36.8, 15.7, 2.4$ Hz, 2H), 2.47 (t, $J = 2.4$ Hz, 1H), 1.55 (d, $J = 6.6$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 134.10, 131.61, 129.83, 129.49, 128.73, 124.16, 89.21, 84.20, 79.40, 74.56, 64.47, 55.83, 21.87. IR (neat, cm^{-1}): 3297, 2928, 2224, 1620, 1519, 1368, 1224, 1093, 758. GCMS (m/z): 218.05



1-fluoro-4-(3-(prop-2-yn-1-yloxy)but-1-yn-1-yl)benzene **1f**: The compound **1f** was prepared in 68 % yield through the General Procedure A. ^1H NMR (500 MHz, CDCl_3) δ 7.46 – 7.36 (m, 2H), 7.00 (t, $J = 8.7$ Hz, 2H), 4.62 (q, $J = 6.6$ Hz, 1H), 4.35 (ddd, $J = 36.0, 15.7, 2.4$ Hz, 2H), 2.45 (t, $J = 2.3$ Hz, 1H), 1.58 – 1.49 (m, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 162.58 (d, $J_{\text{C-F}} = 249.7$ Hz), 133.66 (d, $J_{\text{C-F}} = 8.4$ Hz), 118.55 (d, $J_{\text{C-F}} = 3.6$ Hz), 115.55 (d, $J_{\text{C-F}} = 22.1$ Hz), 87.64, 84.56, 79.51, 74.46, 64.57, 55.78, 21.97. IR (neat, cm^{-1}): 3436, 3290, 2222, 1616, 1518, 1368, 1224, 758. GCMS (m/z): 202.08



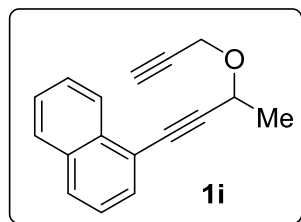
1-bromo-2-(3-(prop-2-yn-1-yloxy)but-1-yn-1-yl)benzene 1g: The compound **1g** was prepared in 50 % yield through the General Procedure A. ^1H NMR (500 MHz, CDCl_3) δ 7.59 (dd, $J = 8.0, 0.9$ Hz, 1H), 7.46 (dt, $J = 10.2, 5.1$ Hz, 1H), 7.32 – 7.23 (m, 1H), 7.18 (td, $J = 7.8, 1.7$ Hz, 1H), 4.80 – 4.64 (m, 1H), 4.49 – 4.35 (m, 2H), 2.47 (t, $J = 2.4$ Hz, 1H), 1.58 (t, $J = 7.1$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 133.38, 132.36, 129.60, 126.95, 125.59, 124.60, 92.64, 84.16, 79.50, 74.51, 64.56, 55.88, 21.81. IR (neat, cm^{-1}): 3299, 2932, 2228, 1627, 1524, 1368, 1224, 1095, 763. GCMS (m/z): 262.00



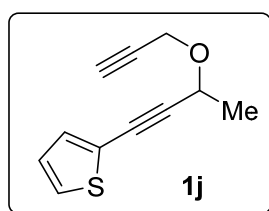
4-bromo-2-fluoro-1-(3-(prop-2-yn-1-yloxy)but-1-yn-1-yl)benzene **1h**: The compound **1h** was prepared in 53 % yield through the General Procedure A. ^1H NMR (500 MHz, CDCl_3) δ 7.33 – 7.20 (m, 3H), 4.65 (q, $J = 6.6$ Hz, 1H), 4.35 (ddd, $J = 36.4, 15.7, 2.4$ Hz, 2H), 2.46 (t, $J = 2.4$ Hz, 1H), 1.56 (d, $J = 6.6$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 162.48 (d, $J_{\text{C-F}} = 256.4$ Hz), 134.23 (d, $J_{\text{C-F}} = 1.7$ Hz), 127.38 (d, $J_{\text{C-F}} = 3.8$ Hz), 122.82 (d, $J_{\text{C-F}} = 9.0$ Hz), 119.29 (d, $J_{\text{C-F}} = 24.1$ Hz), 110.30 (d, $J_{\text{C-F}} = 15.9$ Hz), 94.43 (d, $J_{\text{C-F}} = 3.4$ Hz), 79.36, 78.09, 74.59,

64.56, 55.86, 21.75. IR (neat, cm^{-1}): 3230, 2933, 2226, 1627, 1527, 1365, 1224, 1095, 760.

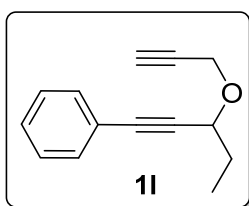
GCMS (m/z): 280.00



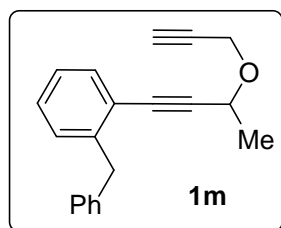
1-(3-(prop-2-yn-1-yloxy)but-1-yn-1-yl)naphthalene **1i**: The compound **1i** was prepared in 68 % yield through the General Procedure A. ^1H NMR (500 MHz, CDCl_3) δ 8.31 (d, $J = 8.3$ Hz, 1H), 7.85 (t, $J = 8.1$ Hz, 2H), 7.69 (d, $J = 7.1$ Hz, 1H), 7.58 (t, $J = 7.5$ Hz, 1H), 7.55 – 7.50 (m, 1H), 7.43 (dd, $J = 8.1, 7.3$ Hz, 1H), 4.81 (q, $J = 6.6$ Hz, 1H), 4.55 – 4.40 (m, 2H), 2.49 (t, $J = 1.9$ Hz, 1H), 1.67 (d, $J = 6.6$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 133.29, 133.13, 130.69, 128.96, 128.29, 126.84, 126.41, 125.99, 125.13, 120.11, 92.90, 83.75, 79.61, 74.53, 64.87, 55.91, 22.23. IR (neat, cm^{-1}): 3292, 3056, 2855, 1714, 1585, 1500, 1076, 801, 745. GCMS (m/z): 234.10.



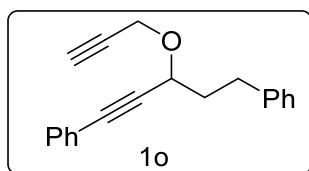
2-(3-(prop-2-yn-1-yloxy)but-1-yn-1-yl)thiophene **1j**: The compound **1j** was prepared in 80 % yield through the General Procedure A. ^1H NMR (500 MHz, CDCl_3) δ 7.28 – 7.22 (m, 1H), 6.97 (dd, $J = 5.1, 3.7$ Hz, 1H), 4.64 (q, $J = 6.6$ Hz, 1H), 4.33 (ddd, $J = 38.2, 15.7, 2.4$ Hz, 2H), 2.45 (t, $J = 2.4$ Hz, 1H), 1.55 (t, $J = 7.3$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 132.36, 127.30, 126.91, 122.36, 91.82, 79.48, 78.89, 74.51, 64.72, 55.84, 21.85. IR (neat, cm^{-1}): 3290, 3045, 2856, 1718, 1585, 1512, 1096, 745. HRMS (ESI $\text{M}+\text{Na}^+$) calcd for $\text{C}_{11}\text{H}_{11}\text{NaOS}^+$: 213.0345, found: 213.0349.



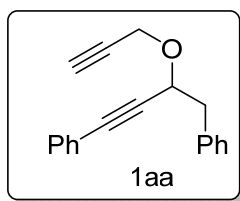
(3-(prop-2-yn-1-yloxy)pent-1-yn-1-yl)benzene **1l**: The compound **1l** was prepared in 70 % yield through the General Procedure A. ^1H NMR (500 MHz, CDCl_3) δ 7.40 – 7.30 (m, 2H), 7.28 – 7.18 (m, 3H), 4.36 (dd, $J = 16.2, 9.8$ Hz, 1H), 4.27 (qd, $J = 15.7, 2.3$ Hz, 2H), 2.35 (t, $J = 2.3$ Hz, 1H), 1.83 – 1.68 (m, 2H), 0.99 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 131.77, 128.40, 128.26, 122.59, 87.06, 86.37, 79.69, 74.33, 70.14, 55.83, 28.80, 9.67. IR (neat, cm^{-1}): 3294, 2989, 2929, 1613, 1500, 1367, 1095, 755. GCMS (m/z): 198.10.



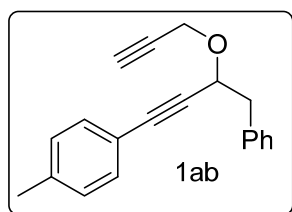
1-benzyl-2-(3-(prop-2-yn-1-yloxy)but-1-yn-1-yl)benzene 1m: The compound **1m** was prepared in 70 % yield through the General Procedure A. ^1H NMR (500 MHz, CDCl_3) δ 7.45 (d, $J = 7.6$ Hz, 1H), 7.25 (q, $J = 7.4$ Hz, 3H), 7.22 – 7.12 (m, 5H), 4.63 (q, $J = 6.6$ Hz, 1H), 4.23 (ddt, $J = 18.7, 13.1, 6.6$ Hz, 2H), 4.15 (s, 2H), 2.42 (t, $J = 2.4$ Hz, 1H), 1.52 (d, $J = 6.6$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 143.01, 140.37, 132.57, 129.49, 128.85, 128.73, 128.38, 126.13, 126.06, 122.23, 91.99, 84.52, 79.58, 74.41, 64.66, 55.71, 40.23, 22.04. IR (neat, cm^{-1}): 3293, 3060, 1492, 1446, 1076, 818, 693. GCMS (m/z): 274.14.



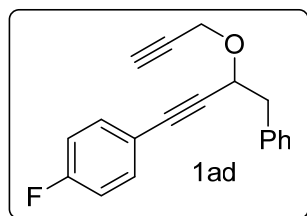
(3-(prop-2-yn-1-yloxy)pent-1-yne-1,5-diyl)dibenzene 1o: The compound **1o** was prepared in 78 % yield through the General Procedure A. ^1H NMR (500 MHz, CDCl_3) δ 7.51 – 7.40 (m, 2H), 7.37 – 7.14 (m, 8H), 4.52 (t, $J = 6.4$ Hz, 1H), 4.39 (ddd, $J = 45.3, 15.7, 2.1$ Hz, 2H), 3.02 – 2.80 (m, 2H), 2.45 (d, $J = 2.2$ Hz, 1H), 2.27 – 2.08 (m, 2H). ^{13}C NMR (126 MHz, CDCl_3) δ 141.33, 131.78, 128.57, 128.49, 128.38, 128.29, 125.94, 122.47, 86.93, 86.68, 79.60, 74.49, 68.11, 55.89, 37.21, 31.43. IR (neat, cm^{-1}): 3292, 3061, 1493, 1448, 1077, 817, 693. GCMS (m/z): 274.14.



(3-(prop-2-yn-1-yloxy)but-1-yne-1,4-diyl)dibenzene 1aa: The compound **1aa** was prepared in 72 % yield through the General Procedure **A**. ^1H NMR (500 MHz, CDCl_3) δ 7.40 – 7.21 (m, 10H), 4.72 (t, $J = 6.7$ Hz, 1H), 4.36 (tt, $J = 15.8, 7.8$ Hz, 2H), 3.22 – 3.07 (m, 2H), 2.42 (t, $J = 2.3$ Hz, 1H). ^{13}C NMR (126 MHz, CDCl_3) δ 136.86, 131.68, 129.74, 128.46, 128.24, 128.15, 126.66, 122.43, 87.33, 86.64, 79.42, 74.57, 69.75, 55.92, 42.02. IR (neat, cm^{-1}): 3293, 3060, 1492, 1446, 1077, 816, 693. GCMS (m/z): 260.11.

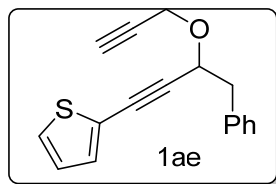


1-methyl-4-(4-phenyl-3-(prop-2-yn-1-yloxy)but-1-yn-1-yl)benzene **1ab**: The compound **1ab** was prepared in 72 % yield through the General Procedure **A**. ^1H NMR (500 MHz, CDCl_3) δ 7.48 – 7.31 (m, 8H), 7.19 (d, $J = 7.9$ Hz, 2H), 4.83 (t, $J = 6.7$ Hz, 1H), 4.46 (qd, $J = 15.8, 2.4$ Hz, 2H), 3.32 – 3.18 (m, 2H), 2.50 (dt, $J = 8.1, 2.4$ Hz, 1H), 2.42 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 138.45, 136.81, 131.47, 129.65, 128.90, 128.02, 126.52, 119.24, 87.37, 85.87, 79.38, 74.53, 69.64, 55.73, 41.94, 21.32. IR (neat, cm^{-1}): 3448, 32943, 3060, 2927, 1492, 1446, 1337, 1077, 917, 816. GCMS (m/z): 274.13.

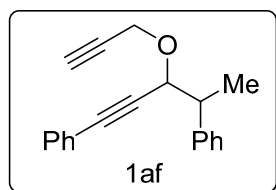


1-fluoro-4-(4-phenyl-3-(prop-2-yn-1-yloxy)but-1-yn-1-yl)benzene **1ad**: The compound **1ad** was prepared in 72 % yield through the General Procedure **A**. ^1H NMR (500 MHz, CDCl_3) δ 7.41 – 7.26 (m, 7H), 7.02 (t, $J = 8.7$ Hz, 2H), 4.76 (t, $J = 6.6$ Hz, 1H), 4.40 (qd, $J = 15.7, 1.1$ Hz, 2H), 3.26 – 3.09 (m, 2H), 2.51 – 2.39 (m, 1H). ^{13}C NMR (126 MHz, CDCl_3) δ 163.52,

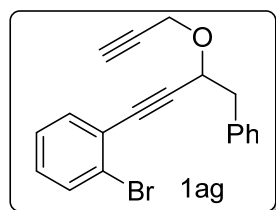
161.54, 136.76, 133.60, 133.53, 129.70, 128.13, 126.66, 118.45, 118.42, 115.60, 115.42. IR (neat, cm^{-1}): 3290, 3056, 1490, 1446, 1338, 1076, 816, 693, 637. GCMS (m/z): 278.10.



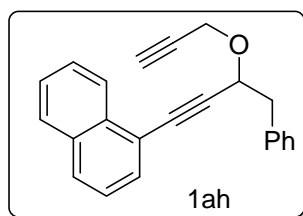
2-(4-phenyl-3-(prop-2-yn-1-yloxy)but-1-yn-1-yl)thiophene **1ae**: The compound **1ae** was prepared in 70 % yield through the General Procedure A. ^1H NMR (500 MHz, CDCl_3) δ 7.35 – 7.28 (m, 4H), 7.26 – 7.22 (m, 2H), 7.17 (dd, $J = 3.6, 1.0$ Hz, 1H), 6.95 (dd, $J = 5.1, 3.7$ Hz, 1H), 4.72 (t, $J = 6.6$ Hz, 1H), 4.47 – 4.21 (m, 2H), 3.13 (qd, $J = 13.6, 6.7$ Hz, 2H), 2.42 (t, $J = 2.4$ Hz, 1H). ^{13}C NMR (126 MHz, CDCl_3) δ 136.68, 132.34, 129.72, 128.19, 127.36, 126.90, 126.69, 122.27, 90.60, 80.59, 79.30, 74.69, 69.81, 56.01, 41.86. IR (neat, cm^{-1}): 3448, 3063, 1492, 1446, 1075, 816, 712. HRMS (ESI $\text{M}+\text{Na}^+$) calcd for $\text{C}_{17}\text{H}_{14}\text{NaOS}^+$: 289.0658, found: 289.0662.



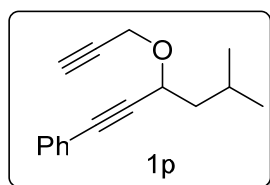
(3-(prop-2-yn-1-yloxy)pent-1-yn-1,4-diyl)dibenzene **1af**: The compound **1af** was prepared in 76 % yield through the General Procedure A. ^1H NMR (500 MHz, CDCl_3) δ 7.43 – 7.24 (m, 10H), 4.66 (ddd, $J = 6.2, 5.5, 3.3$ Hz, 1H), 4.43 – 4.31 (m, 2H), 3.30 – 3.12 (m, 1H), 2.50 – 2.39 (m, 1H), 1.50 (dt, $J = 7.1, 3.7$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 142.64, 131.71, 131.64, 128.38, 128.34, 128.26, 128.19, 128.15, 128.11, 128.00, 126.70, 122.53, 87.50, 86.25, 79.57, 74.47, 73.60, 56.05, 44.74, 17.22. IR (neat, cm^{-1}): 3448, 3292, 3060, 1492, 1446, 1076, 816, 695. GCMS (m/z): 274.13.



(3-(prop-2-yn-1-yloxy)pent-1-yne-1,4-diyl)dibenzene **1ag**: The compound **1ag** was prepared in 66% yield through the General Procedure A. ^1H NMR (500 MHz, CDCl_3) δ 7.59 (dd, $J = 8.0, 1.0$ Hz, 1H), 7.44 – 7.38 (m, 3H), 7.35 (dd, $J = 10.2, 4.7$ Hz, 2H), 7.30 – 7.24 (m, 2H), 7.18 (td, $J = 7.8, 1.7$ Hz, 1H), 4.85 (dt, $J = 13.5, 6.8$ Hz, 1H), 4.55 – 4.40 (m, 2H), 3.21 (ddd, $J = 20.8, 13.6, 6.8$ Hz, 2H), 2.47 (t, $J = 2.4$ Hz, 1H). ^{13}C NMR (126 MHz, CDCl_3) δ 136.63, 133.41, 132.30, 129.74, 129.60, 128.16, 126.89, 126.66, 125.42, 124.54, 91.29, 85.76, 79.32, 74.69, 69.63, 55.96, 41.73. IR (neat, cm^{-1}): 3295, 3060, 1492, 1446, 1075, 817, 700. HRMS (ESI $\text{M}+\text{Na}^+$) calcd for $\text{C}_{19}\text{H}_{15}\text{BrNaO}^+$: 361.0198, found: 361.0199.



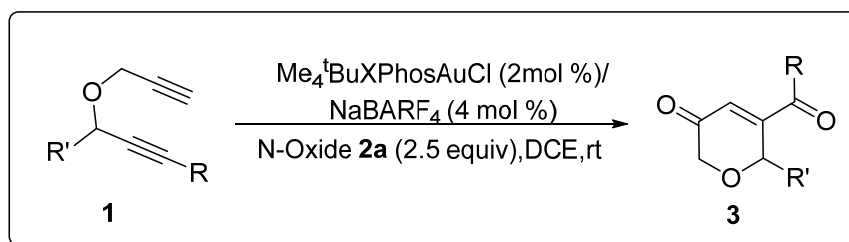
(3-(prop-2-yn-1-yloxy)pent-1-yne-1,4-diyl)dibenzene **1ah**: The compound **1ah** was prepared in 66% yield through the General Procedure A. ^1H NMR (500 MHz, CDCl_3) δ 8.16 – 8.05 (m, 1H), 7.89 – 7.81 (m, 2H), 7.67 (dd, $J = 7.1, 0.9$ Hz, 1H), 7.57 – 7.51 (m, 2H), 7.48 – 7.31 (m, 6H), 5.03 – 4.92 (m, 1H), 4.58 – 4.47 (m, 2H), 3.30 (ddd, $J = 20.9, 13.6, 6.7$ Hz, 2H), 2.52 (t, $J = 2.4$ Hz, 1H). ^{13}C NMR (126 MHz, CDCl_3) δ 136.85, 133.18, 133.01, 130.57, 129.82, 128.91, 128.26, 128.16, 126.73, 126.70, 126.35, 126.08, 125.06, 120.01, 91.41, 85.52, 79.41, 74.74, 69.98, 56.02, 42.05. IR (neat, cm^{-1}): 3292, 3057, 1715, 1077, 801, 699. HRMS (ESI $\text{M}+\text{Na}^+$) calcd for $\text{C}_{23}\text{H}_{18}\text{NaO}^+$: 333.1250, found: 333.1258.



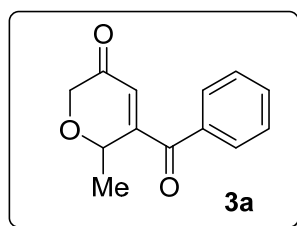
(5-methyl-3-(prop-2-yn-1-yloxy)hex-1-yn-1-yl)benzene **1p**: The compound **1p** was prepared in 77 % yield through the General Procedure A. ^1H NMR (500 MHz, CDCl_3) δ 7.44 (dd, $J = 6.6, 3.1$ Hz, 2H), 7.39 – 7.29 (m, 3H), 4.57 (t, $J = 7.1$ Hz, 1H), 4.37 (qd, $J = 15.7, 2.3$ Hz, 2H), 2.45 (t, $J = 2.3$ Hz, 1H), 1.94 (tt, $J = 13.4, 6.8$ Hz, 1H), 1.80 (dt, $J = 14.2, 7.2$ Hz, 1H), 1.67

(dt, $J = 13.7, 6.9$ Hz, 1H), 0.98 (t, $J = 6.3$ Hz, 6H). ^{13}C NMR (126 MHz, CDCl_3) δ 131.74, 128.38, 128.26, 122.61, 87.51, 86.13, 79.70, 74.32, 67.36, 55.72, 44.55, 24.70, 22.69, 22.33. IR (neat, cm^{-1}): 3060, 2970, 1732, 1358, 808, 725. GCMS (m/z): 226.12.

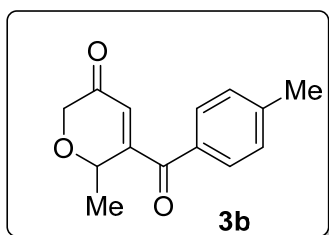
General procedure B: gold catalyzed selective oxidation of 4-Oxahepta-1,6-diyne derivatives to 2H-pyran-3(6H)-ones 3



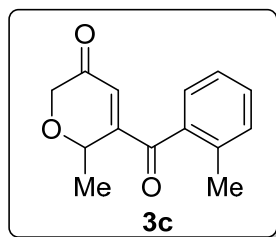
To a 3 dram vial containing 2 mL of DCE were added sequentially the 4-Oxahepta-1,6-diyne 1 (0.2 mmol), 2,6-dichloropyridine *N*-oxide 2a (82 mg, 0.5 mmol), $\text{Me}_4\text{tBuXphosAuCl}$ (4.0 mg, 0.004 mmol) and NaBARF_4 (7.0 mg, 0.008 mmol). The resulting mixture was stirred at 25 °C or the indicated temperature, and the progress of 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 2H-pyran-3(6H)-ones 3.



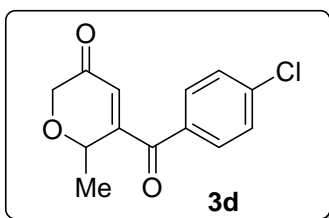
5-benzoyl-6-methyl-2H-pyran-3(6H)-one 3a was prepared in 82% yield according to the general procedure B. ^1H NMR (500 MHz, CDCl_3) δ 7.87 (dd, $J = 8.3, 1.1$ Hz, 2H), 7.70 – 7.61 (m, 1H), 7.52 (t, $J = 7.8$ Hz, 2H), 6.23 (d, $J = 1.9$ Hz, 1H), 4.95 (dtd, $J = 6.8, 5.2, 1.6$ Hz, 1H), 4.37 (d, $J = 16.6$ Hz, 1H), 4.18 (dd, $J = 16.6, 1.4$ Hz, 1H), 1.45 (d, $J = 6.8$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 194.96, 194.77, 158.85, 135.16, 134.25, 129.71, 128.92, 127.40, 70.65, 70.17, 18.14. IR (neat, cm^{-1}): 3061, 1698, 1659, 1249, 1134, 722. HRMS ($\text{M}+\text{H}^+$) calcd for $\text{C}_{14}\text{H}_{15}\text{O}_3^+$: 217.0859, found: 217.0862.



6-methyl-5-(4-methylbenzoyl)-2H-pyran-3(6H)-one **3b** was prepared in 72% yield according to the general procedure B. ^1H NMR (500 MHz, CDCl_3) δ 7.83 (d, $J = 7.3$ Hz, 2H), 7.36 (d, $J = 7.8$ Hz, 2H), 6.26 (s, 1H), 4.99 (dd, $J = 12.9, 6.1$ Hz, 1H), 4.41 (d, $J = 16.6$ Hz, 1H), 4.22 (d, $J = 16.6$ Hz, 1H), 2.49 (s, 3H), 1.50 – 1.45 (m, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 194.87, 194.54, 159.28, 145.64, 132.58, 129.95, 129.68, 126.90, 70.79, 70.34, 21.85, 18.19. IR (neat, cm^{-1}): 3035, 1698, 1656, 1254, 1133, 752. HRMS ($\text{M}+\text{H}^+$) calcd for $\text{C}_{14}\text{H}_{15}\text{O}_3^+$: 231.1016, found: 231.1018.

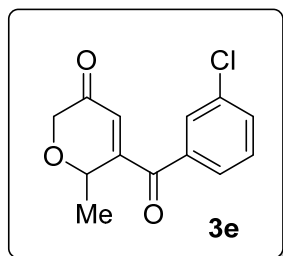


6-methyl-5-(2-methylbenzoyl)-2H-pyran-3(6H)-one **3c** was prepared in 70% yield according to the general procedure B. ^1H NMR (500 MHz, CDCl_3) δ 7.47 (dd, $J = 19.9, 7.3$ Hz, 2H), 7.39 – 7.27 (m, 2H), 6.20 (s, 1H), 5.02 (d, $J = 6.2$ Hz, 1H), 4.40 (d, $J = 16.9$ Hz, 1H), 4.20 (d, $J = 16.8$ Hz, 1H), 2.48 (s, 3H), 1.58 (d, $J = 6.2$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 197.91, 195.71, 158.93, 138.39, 135.58, 132.00, 131.79, 129.71, 129.35, 125.58, 69.85, 69.21, 20.41, 17.95. IR (neat, cm^{-1}): 3035, 1698, 1657, 1254, 1133, 745. HRMS ($\text{M}+\text{H}^+$) calcd for $\text{C}_{14}\text{H}_{15}\text{O}_3^+$: 231.1016, found: 231.1018.

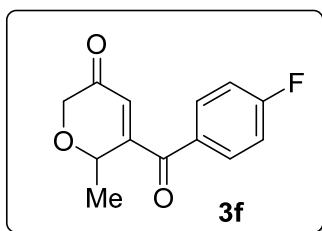


5-(4-chlorobenzoyl)-6-methyl-2H-pyran-3(6H)-one **3d** was prepared in 65% yield according to the general procedure B. ^1H NMR (500 MHz, CDCl_3) δ 7.92 – 7.82 (m, 2H), 7.62 – 7.51 (m, 2H), 6.26 (d, $J = 1.9$ Hz, 1H), 5.06 – 4.93 (m, 1H), 5.05 – 4.92 (m, 1H), 4.42 (d, $J = 16.7$ Hz, 1H), 4.22 (dd, $J = 16.7, 1.3$ Hz, 1H), 1.48 (d, $J = 6.8$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ

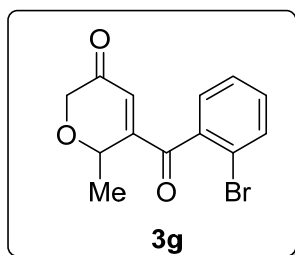
194.58, 193.70, 158.36, 141.03, 133.37, 131.03, 129.33, 127.43, 70.58, 70.17, 18.13. IR (neat, cm^{-1}): 3060, 1705, 1671, 1370, 1230, 751. HRMS ($\text{M}+\text{H}^+$) calcd for $\text{C}_{13}\text{H}_{12}\text{ClO}_3^+$: 251.0469, found: 251.0472.



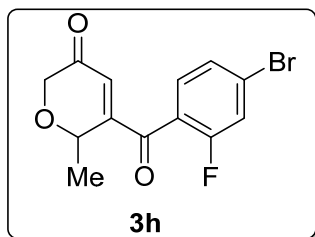
5-(3-chlorobenzoyl)-6-methyl-2H-pyran-3(6H)-one **3e** was prepared in 62% yield according to the general procedure B. ^1H NMR (500 MHz, CDCl_3) δ 7.83 (t, $J = 1.7$ Hz, 1H), 7.74 – 7.69 (m, 1H), 7.62 (ddd, $J = 8.0, 2.0, 0.9$ Hz, 1H), 7.47 (t, $J = 7.9$ Hz, 1H), 6.24 (d, $J = 1.8$ Hz, 1H), 4.98 – 4.88 (m, 1H), 4.36 (t, $J = 16.1$ Hz, 1H), 4.18 (dt, $J = 16.7, 3.8$ Hz, 1H), 1.45 (d, $J = 6.8$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 194.62, 193.69, 158.01, 136.66, 135.36, 134.16, 130.22, 129.43, 127.86, 127.80, 70.49, 70.09, 18.12. IR (neat, cm^{-1}): 2978, 1703, 1671, 1370, 1229, 751. HRMS ($\text{M}+\text{H}^+$) calcd for $\text{C}_{13}\text{H}_{12}\text{ClO}_3^+$: 251.0469, found: 251.0471.



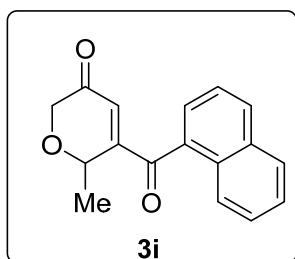
5-(4-fluorobenzoyl)-6-methyl-2H-pyran-3(6H)-one **3f** was prepared in 77% yield according to the general procedure B. ^1H NMR (500 MHz, CDCl_3) δ 7.91 (ddd, $J = 8.0, 5.0, 2.3$ Hz, 2H), 7.19 (dd, $J = 14.1, 5.6$ Hz, 2H), 6.21 (d, $J = 1.8$ Hz, 1H), 4.93 (q, $J = 6.8$ Hz, 1H), 4.37 (d, $J = 16.6$ Hz, 1H), 4.27 – 4.11 (m, 1H), 1.41 (dd, $J = 16.4, 4.5$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 193.94 (d, $J = 162.5$ Hz), 166.43 (d, $J = 257.6$ Hz), 158.62, 132.46 (d, $J = 9.6$ Hz), 131.45 (d, $J = 2.9$ Hz), 127.19 (s), 116.25 (d, $J = 22.1$ Hz), 70.63, 70.22, 18.12. IR (neat, cm^{-1}): 3060, 1708, 1672, 1368, 1230, 751. HRMS ($\text{M}+\text{H}^+$) calcd for $\text{C}_{13}\text{H}_{12}\text{FO}_3^+$: 236.0765, found: 236.0768.



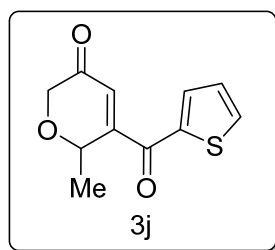
5-(2-bromobenzoyl)-6-methyl-2H-pyran-3(6H)-one **3g** was prepared in 50% yield according to the general procedure B. ^1H NMR (500 MHz, CDCl_3) δ 7.62 (dt, $J = 15.1, 7.4$ Hz, 1H), 7.47 – 7.36 (m, 2H), 7.33 (dd, $J = 7.4, 1.8$ Hz, 1H), 6.15 (d, $J = 1.5$ Hz, 1H), 5.07 – 4.96 (m, 1H), 4.37 (d, $J = 17.0$ Hz, 1H), 4.15 (d, $J = 16.8$ Hz, 1H), 1.62 (d, $J = 6.8$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 196.36, 196.06, 156.49, 138.35, 133.51, 132.35, 130.94, 129.44, 127.55, 119.61, 69.24, 68.34, 17.73. IR (neat, cm^{-1}): 3059, 1703, 1670, 1368, 1228, 751. HRMS ($\text{M}+\text{H}^+$) calcd for $\text{C}_{13}\text{H}_{12}\text{BrO}_3^+$: 294.9964, found: 294.9968.



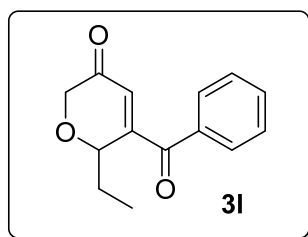
5-(4-bromo-2-fluorobenzoyl)-6-methyl-2H-pyran-3(6H)-one **3h** was prepared in 66% yield according to the general procedure B. ^1H NMR (500 MHz, CDCl_3) δ 7.51 – 7.47 (m, 1H), 7.44 (dd, $J = 8.3, 1.6$ Hz, 1H), 7.41 – 7.34 (m, 1H), 6.20 (s, 1H), 4.94 (q, $J = 6.7$ Hz, 1H), 4.34 (dd, $J = 16.7, 9.1$ Hz, 1H), 4.13 (dt, $J = 14.1, 4.9$ Hz, 1H), 1.50 (d, $J = 6.8$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 195.26, 191.92, 160.36 (d, $J = 259.6$ Hz), 158.43, 131.76 (d, $J = 2.4$ Hz), 128.62 (d, $J = 9.5$ Hz), 128.40 (d, $J = 3.6$ Hz), 128.20 (d, $J = 3.3$ Hz), 123.75 (d, $J = 12.7$ Hz), 120.43 (d, $J = 24.8$ Hz), 69.78, 69.33, 17.98. IR (neat, cm^{-1}): 3060, 1709, 1672, 1370, 1233, 755. HRMS ($\text{M}+\text{H}^+$) calcd for $\text{C}_{13}\text{H}_{11}\text{BrFO}_3^+$: 312.9870, found: 312.9873.



5-(1-naphthoyl)-6-methyl-2*H*-pyran-3(6*H*)-one **3i** was prepared in 66% yield according to the general procedure B. ¹H NMR (500 MHz, CDCl₃) δ 8.44 (t, *J* = 15.4 Hz, 1H), 8.08 (t, *J* = 8.6 Hz, 1H), 7.96 – 7.88 (m, 1H), 7.72 (dt, *J* = 7.8, 3.9 Hz, 1H), 7.67 – 7.56 (m, 2H), 7.57 – 7.48 (m, 1H), 6.22 (d, *J* = 1.7 Hz, 1H), 5.08 (q, *J* = 6.7 Hz, 1H), 5.08 (q, *J* = 6.7 Hz, 1H), 4.39 (d, *J* = 16.8 Hz, 1H), 4.26 – 4.14 (m, 1H), 1.60 (d, *J* = 6.8 Hz, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 197.20, 195.54, 159.71, 133.90, 133.75, 132.98, 130.70, 130.27, 129.32, 128.67, 128.40, 126.96, 125.13, 124.13, 70.16, 69.45, 18.08. IR (neat, cm⁻¹): 3054, 1698, 1656, 1234, 1140, 782. HRMS (M+H⁺) calcd for C₁₇H₁₅O₃⁺: 267.1016, found: 267.1019.

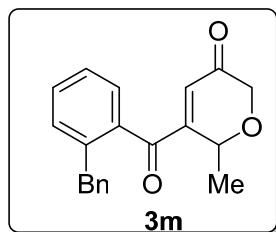


6-methyl-5-(thiophene-2-carbonyl)-2*H*-pyran-3(6*H*)-one **3j** was prepared in 70% yield according to the general procedure B. ¹H NMR (500 MHz, CDCl₃) δ 7.93 – 7.77 (m, 1H), 7.71 (dd, *J* = 3.8, 0.9 Hz, 1H), 7.24 – 7.16 (m, 1H), 6.40 (d, *J* = 1.8 Hz, 1H), 4.92 (q, *J* = 6.9 Hz, 1H), 4.36 (d, *J* = 16.6 Hz, 1H), 4.17 (dd, *J* = 16.6, 1.2 Hz, 1H), 1.44 (d, *J* = 6.8 Hz, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 194.72, 186.28, 158.88, 142.06, 136.60, 135.32, 128.61, 126.48, 70.59, 70.16, 18.16. IR (neat, cm⁻¹): 3055, 1698, 1659, 1508, 1230, 1140, 897, 780. HRMS (M+H⁺) calcd for C₁₁H₁₁O₃⁺: 223.0423, found: 223.0425.

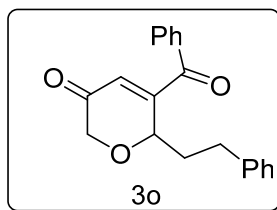


5-benzoyl-6-ethyl-2*H*-pyran-3(6*H*)-one **3i** was prepared in 76% yield according to the general procedure B. ¹H NMR (500 MHz, CDCl₃) δ 7.97 – 7.88 (m, 2H), 7.70 (t, *J* = 7.4 Hz, 1H), 7.56 (t, *J* = 7.8 Hz, 2H), 6.30 (d, *J* = 1.8 Hz, 1H), 4.93 – 4.77 (m, 1H), 4.42 (dd, *J* = 16.8, 6.7 Hz, 1H), 4.22 (dt, *J* = 7.3, 3.3 Hz, 1H), 1.95 – 1.80 (m, 2H), 1.07 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 195.08, 194.92, 158.27, 134.98, 134.19, 129.74, 128.88, 128.13, 75.28,

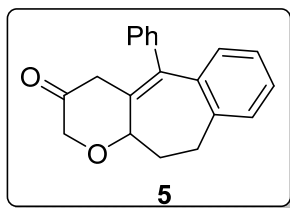
69.82, 25.04, 9.99. IR (neat, cm^{-1}): 3058, 1698, 1658, 1249, 1134, 725. HRMS ($\text{M}+\text{H}^+$) calcd for $\text{C}_{14}\text{H}_{15}\text{O}_3^+$: 231.1016, found: 231.1018.



5-(2-benzylbenzoyl)-6-methyl-2H-pyran-3(6H)-one **3m** was prepared in 55% yield according to the general procedure B. ^1H NMR (500 MHz, CDCl_3) δ 7.49 – 7.43 (m, 1H), 7.34 – 7.28 (m, 3H), 7.21 (t, $J = 7.5$ Hz, 2H), 7.13 (t, $J = 7.4$ Hz, 1H), 7.05 (t, $J = 6.9$ Hz, 2H), 5.91 (d, $J = 1.6$ Hz, 1H), 4.85 (q, $J = 6.6$ Hz, 1H), 4.23 (dd, $J = 25.9, 16.1$ Hz, 2H), 4.15 – 4.01 (m, 2H), 1.44 (d, $J = 6.8$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 198.14, 195.76, 157.95, 141.21, 140.05, 136.29, 131.70, 131.67, 130.10, 129.26, 128.40, 126.24, 126.01, 69.41, 68.63, 38.95, 17.87. IR (neat, cm^{-1}): 2977, 1698, 1658, 1230, 1079, 780. HRMS ($\text{M}+\text{H}^+$) calcd for $\text{C}_{20}\text{H}_{19}\text{O}_3^+$: 307.1329, found: 307.1332.

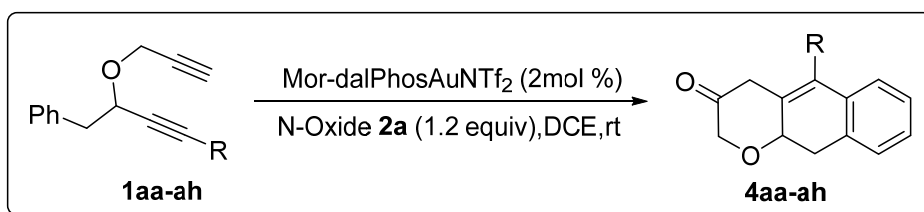


5-benzoyl-6-phenethyl-2H-pyran-3(6H)-one **3o** was prepared in 30% yield according to the general procedure B with Mor-DalPhosAuNTf₂ as the catalyst. ^1H NMR (500 MHz, CDCl_3) δ 7.89 – 7.81 (m, 2H), 7.68 – 7.60 (m, 1H), 7.50 (dd, $J = 10.7, 4.9$ Hz, 2H), 7.26 (dd, $J = 10.2, 4.7$ Hz, 2H), 7.20 – 7.17 (m, 1H), 7.15 (dd, $J = 6.1, 4.9$ Hz, 2H), 6.27 (d, $J = 1.9$ Hz, 1H), 4.83 (ddd, $J = 19.0, 9.2, 7.2$ Hz, 1H), 4.41 (d, $J = 16.7$ Hz, 1H), 4.27 – 4.12 (m, 1H), 2.94 – 2.70 (m, 2H), 2.14 – 1.98 (m, 2H). ^{13}C NMR (126 MHz, CDCl_3) δ 194.87, 194.82, 158.04, 140.75, 134.97, 134.26, 129.72, 128.91, 128.47, 128.44, 128.11, 126.14, 73.49, 69.83, 33.44, 31.70. IR (neat, cm^{-1}): 2934, 1698, 1659, 1232, 1135, 781. HRMS ($\text{M}+\text{H}^+$) calcd for $\text{C}_{20}\text{H}_{19}\text{O}_3^+$: 307.1329, found: 307.1332.

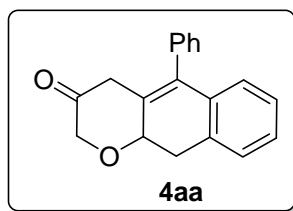


5-phenyl-4,10,11,11a-tetrahydrobenzo[4,5]cyclohepta[1,2-b]pyran-3(2H)-one **5** was prepared in 30% yield according to the general procedure **B** with Mor-DalPhosAuNTf₂ as the catalyst. ¹H NMR (500 MHz, CDCl₃) δ 7.36 (t, *J* = 7.3 Hz, 2H), 7.32 – 7.30 (m, 1H), 7.28 (d, *J* = 8.3 Hz, 1H), 7.18 (td, *J* = 7.4, 1.2 Hz, 1H), 7.13 – 7.06 (m, 3H), 6.74 (dd, *J* = 7.7, 0.9 Hz, 1H), 4.19 (d, *J* = 17.9 Hz, 1H), 4.16 – 4.07 (m, 1H), 3.81 (d, *J* = 17.9 Hz, 1H), 3.57 (dd, *J* = 14.7, 1.1 Hz, 1H), 3.46 (d, *J* = 14.7 Hz, 1H), 3.07 – 2.93 (m, 1H), 2.81 – 2.62 (m, 2H), 2.41 (tt, *J* = 16.5, 8.4 Hz, 1H). ¹³C NMR (126 MHz, CDCl₃) δ 209.77, 140.46, 140.43, 139.85, 137.91, 129.98, 129.66, 129.46, 128.40, 128.36, 127.45, 127.33, 126.28, 77.00, 72.55, 41.83, 40.38, 30.19. IR (neat, cm⁻¹): 2948, 1729, 1222, 1109, 732. HRMS (M+H⁺) calcd for C₂₀H₁₉O₂⁺: 291.1380, found: 291.1383.

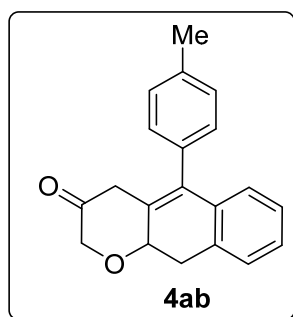
General procedure C: gold catalyzed selective oxidation of 4-Oxahepta-1,6-diyne derivatives 1a-1ah to chromen-3(4H)-ones 4



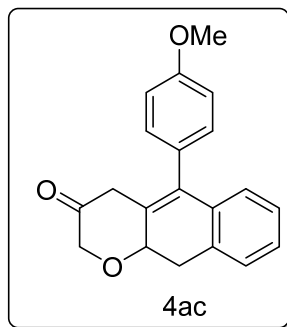
To a 3 dram vial containing 2 mL of DCE were added sequentially the 4-Oxahepta-1,6-diyne **1aa-ah** (0.1 mmol), 2,6-dichloropyridine *N*-oxide **2a** (20 mg, 0.24 mmol), Mor-DalPhosAuNTf₂ (1.8 mg, 0.002 mmol). The resulting mixture was stirred at 25 °C or the indicated temperature, and the progress of 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 chromen-3(4H)-ones **4aa-ah**.



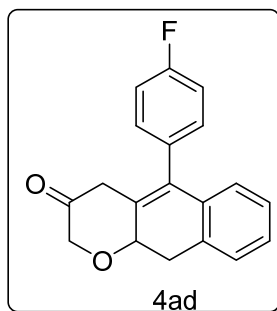
5-phenyl-10,10a-dihydro-2H-benzo[g]chromen-3(4H)-one **4aa** was prepared in 63% yield according to the general procedure C. ^1H NMR (500 MHz, CDCl_3) δ 7.48 (t, $J = 7.5$ Hz, 2H), 7.43 – 7.41 (m, 1H), 7.29 (d, $J = 7.4$ Hz, 1H), 7.19 (td, $J = 7.4, 1.1$ Hz, 3H), 7.12 (dd, $J = 13.3, 5.8$ Hz, 1H), 6.72 (d, $J = 7.6$ Hz, 1H), 4.80 – 4.71 (m, 1H), 4.48 – 4.37 (m, 1H), 4.07 (d, $J = 18.0$ Hz, 1H), 3.42 – 3.28 (m, 3H), 3.10 (dd, $J = 16.5, 10.0$ Hz, 1H). ^{13}C NMR (126 MHz, CDCl_3) δ 208.27, 137.10, 135.62, 135.47, 132.87, 129.72, 129.49, 128.81, 128.10, 127.56, 127.20, 127.03, 126.06, 75.28, 72.48, 41.36, 33.68. IR (neat, cm^{-1}): 2948, 1728, 1220, 1108, 717. HRMS ($\text{M}+\text{H}^+$) calcd for $\text{C}_{19}\text{H}_{17}\text{O}_2^+$: 277.1223, found: 277.1228.



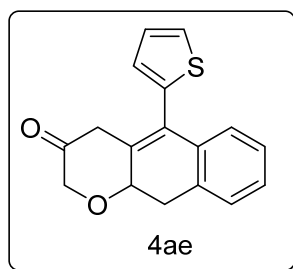
5-(p-tolyl)-10,10a-dihydro-2H-benzo[g]chromen-3(4H)-one **4ab** was prepared in 58% yield according to the general procedure C. ^1H NMR (500 MHz, CDCl_3) δ 7.26 (dd, $J = 15.6, 7.6$ Hz, 3H), 7.18 (td, $J = 7.4, 1.0$ Hz, 1H), 7.12 (t, $J = 7.5$ Hz, 1H), 7.07 (d, $J = 6.4$ Hz, 2H), 6.75 (d, $J = 7.5$ Hz, 1H), 4.74 (td, $J = 14.7, 4.6$ Hz, 1H), 4.42 (d, $J = 17.9$ Hz, 1H), 4.08 (dd, $J = 21.3, 13.2$ Hz, 1H), 3.40 – 3.35 (m, 2H), 3.32 (dd, $J = 16.8, 12.5$ Hz, 1H), 3.17 – 3.03 (m, 1H), 2.45 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 208.37, 137.20, 135.62, 135.57, 134.02, 132.88, 129.57, 129.47, 129.36, 128.05, 127.12, 126.98, 126.07, 75.29, 72.41, 41.37, 33.65, 21.21. IR (neat, cm^{-1}): 2949, 1729, 1220, 1109, 732. HRMS ($\text{M}+\text{H}^+$) calcd for $\text{C}_{20}\text{H}_{19}\text{O}_2^+$: 291.1380, found: 291.1383.



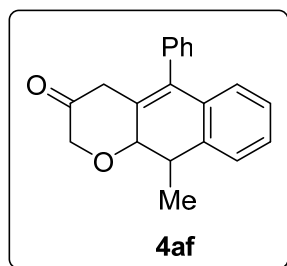
5-(4-methoxyphenyl)-10,10a-dihydro-2H-benzo[g]chromen-3(4H)-one **4ac** was prepared in 56% yield according to the general procedure C. ¹H NMR (500 MHz, CDCl₃) δ 7.28 – 7.23 (m, 1H), 7.18 (t, *J* = 7.1 Hz, 1H), 7.14 – 7.05 (m, 3H), 7.05 – 6.98 (m, 2H), 6.74 (dd, *J* = 15.2, 4.7 Hz, 1H), 4.75 (dt, *J* = 17.7, 8.9 Hz, 1H), 4.40 (dd, *J* = 16.8, 12.5 Hz, 1H), 4.06 (d, *J* = 17.9 Hz, 1H), 3.90 (s, 3H), 3.41 – 3.35 (m, 2H), 3.34 – 3.25 (m, 1H), 3.08 (dt, *J* = 20.2, 10.1 Hz, 1H). ¹³C NMR (126 MHz, CDCl₃) δ 208.43, 158.94, 135.74, 135.26, 132.90, 130.66, 129.73, 129.19, 128.07, 127.13, 127.00, 126.06, 114.22, 75.29, 72.35, 55.28, 41.41, 33.61. IR (neat, cm⁻¹): 3024, 1731, 1220, 1109, 732. HRMS (M+H⁺) calcd for C₂₀H₁₉O₃⁺: 307.1329, found: 307.1332.



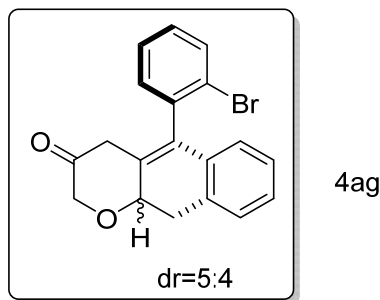
5-(4-fluorophenyl)-10,10a-dihydro-2H-benzo[g]chromen-3(4H)-one **4ad** was prepared in 55% yield according to the general procedure C. ¹H NMR (500 MHz, CDCl₃) δ 7.29 (d, *J* = 7.4 Hz, 1H), 7.24 – 7.11 (m, 6H), 6.69 (d, *J* = 7.6 Hz, 1H), 4.75 (dd, *J* = 14.7, 6.4 Hz, 1H), 4.48 – 4.37 (m, 1H), 4.07 (d, *J* = 18.0 Hz, 1H), 3.42 – 3.26 (m, 3H), 3.17 – 3.06 (m, 1H). ¹³C NMR (126 MHz, CDCl₃) δ 208.02, 162.20 (d, *J* = 246.8 Hz), 135.33, 134.64, 132.91 (d, *J* = 3.7 Hz), 132.87, 131.22 (d, *J* = 8.0 Hz), 130.34, 128.19, 127.36, 127.08, 125.89, 75.23, 72.46, 41.38, 33.59. IR (neat, cm⁻¹): 2970, 1733, 1229, 1200, 702. HRMS (M+H⁺) calcd for C₁₉H₁₆FO₂⁺: 295.1129, found: 295.1132.



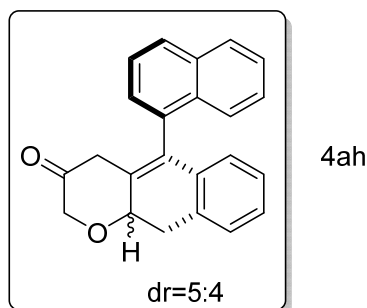
5-(thiophen-2-yl)-10,10a-dihydro-2H-benzo[g]chromen-3(4H)-one **4ae** was prepared in 76% yield according to the general procedure C. ^1H NMR (500 MHz, CDCl_3) δ 7.44 (t, $J = 8.0$ Hz, 1H), 7.26 (t, $J = 8.4$ Hz, 1H), 7.18 (ddd, $J = 10.1, 8.5, 5.5$ Hz, 3H), 6.94 (t, $J = 4.8$ Hz, 2H), 4.73 (dd, $J = 14.8, 6.5$ Hz, 1H), 4.42 (d, $J = 18.0$ Hz, 1H), 4.06 (d, $J = 18.0$ Hz, 1H), 3.56 – 3.45 (m, 2H), 3.38 – 3.25 (m, 1H), 3.17 – 3.02 (m, 1H). ^{13}C NMR (126 MHz, CDCl_3) δ 207.73, 137.14, 135.33, 133.86, 132.46, 128.42, 128.03, 127.77, 127.48, 127.28, 127.19, 126.21, 125.83, 75.34, 72.54, 41.60, 33.42. IR (neat, cm^{-1}): 2949, 1730, 1360, 1227, 1110, 701. HRMS ($\text{M}+\text{H}^+$) calcd for $\text{C}_{17}\text{H}_{15}\text{O}_2\text{S}^+$: 238.0787, found: 238.0791.



10-methyl-5-phenyl-10,10a-dihydro-2H-benzo[g]chromen-3(4H)-one **4af** was prepared in 75% yield according to the general procedure C. ^1H NMR (500 MHz, CDCl_3) δ 7.44 (ddd, $J = 18.3, 14.9, 7.4$ Hz, 4H), 7.27 (t, $J = 7.1$ Hz, 1H), 7.16 (qt, $J = 10.4, 5.0$ Hz, 3H), 6.75 (dd, $J = 17.7, 9.4$ Hz, 1H), 4.44 (dd, $J = 18.0, 14.2$ Hz, 1H), 4.30 (dd, $J = 16.6, 8.8$ Hz, 1H), 4.05 (d, $J = 18.0$ Hz, 1H), 3.44 – 3.31 (m, 3H), 1.59 (t, $J = 11.6$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 208.70, 137.40, 137.24, 135.54, 135.32, 129.68, 129.60, 128.77, 127.53, 127.45, 126.67, 126.06, 124.97, 122.85, 80.03, 72.05, 41.55, 36.04, 14.06. IR (neat, cm^{-1}): 2949, 1728, 1218, 1109, 733. HRMS ($\text{M}+\text{H}^+$) calcd for $\text{C}_{20}\text{H}_{19}\text{O}_2^+$: 291.1380, found: 291.1383.

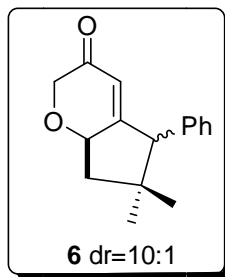


5-(2-bromophenyl)-10,10a-dihydro-2H-benzo[g]chromen-3(4H)-one **4ag** was prepared in 45% yield with dr=5:4 according to the general procedure C. ^1H NMR (500 MHz, CDCl_3) δ 7.71 (ddd, $J = 24.8, 12.4, 4.6$ Hz, 1H), 7.50 – 7.36 (m, 1H), 7.30 – 7.08 (m, 5H), 6.58 (dt, $J = 37.8, 19.0$ Hz, 1H), 4.88 – 4.68 (m, 1H), 4.53 – 4.36 (m, 1H), 4.08 (dd, $J = 17.9, 14.6$ Hz, 1H), 3.48 – 3.09 (m, 4H). ^{13}C NMR (126 MHz, CDCl_3) δ 207.89, 207.43, 137.93, 137.49, 134.59, 134.35, 134.04, 133.32, 133.01, 132.87, 132.66, 131.38, 131.15, 131.07, 130.76, 129.45, 129.42, 128.21, 128.18, 128.05, 127.75, 127.37, 127.35, 127.20, 127.13, 125.57, 124.82, 124.21, 124.01, 75.13, 75.10, 72.78, 72.72, 41.38, 41.06, 33.71, 33.59. IR (neat, cm^{-1}): 2857, 1733, 1732, 1227, 1198, 764. HRMS ($\text{M}+\text{H}^+$) calcd for $\text{C}_{19}\text{H}_{16}\text{BrO}_2^+$: 355.0328, found: 355.0331.



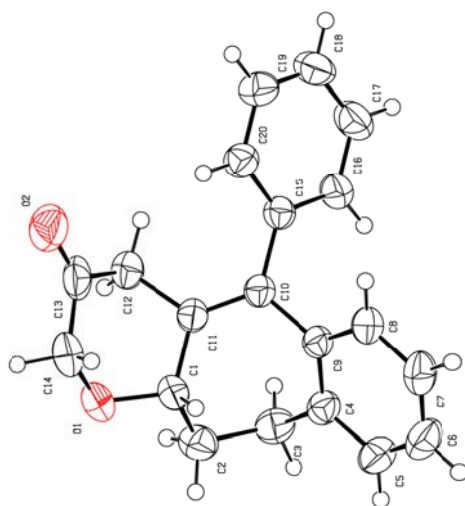
5-(naphthalen-1-yl)-10,10a-dihydro-2H-benzo[g]chromen-3(4H)-one **4ah** was prepared in 81% yield with dr=5:4 according to the general procedure C. ^1H NMR (500 MHz, CDCl_3) δ 8.01 – 7.91 (m, 2H), 7.73 – 7.54 (m, 3H), 7.53 – 7.44 (m, 1H), 7.41 – 7.29 (m, 2H), 7.25 – 7.13 (m, 1H), 7.09 – 6.96 (m, 1H), 6.54 (dd, $J = 57.0, 7.7$ Hz, 1H), 5.00 – 4.77 (m, 1H), 4.50 – 4.40 (m, 1H), 4.10 (dd, $J = 17.9, 4.6$ Hz, 1H), 3.56 – 3.36 (m, 1H), 3.33 – 3.17 (m, 2H), 3.09 – 2.87 (m, 1H). ^{13}C NMR (126 MHz, CDCl_3) δ 208.01, 207.83, 135.52, 135.16, 134.81, 134.14, 134.01, 133.72, 133.65, 133.56, 132.63, 132.42, 131.78, 131.63, 131.48, 131.42, 128.58, 128.48, 128.21, 128.16, 128.09, 128.03, 127.28, 127.21, 127.16, 127.04, 126.73, 126.37, 126.18, 126.06, 125.87, 125.62, 125.57, 125.14, 124.88, 75.53, 75.22, 73.13, 72.77, 41.39, 41.12,

34.21, 33.90. IR (neat, cm^{-1}): 3028, 1729, 1728, 1234, 1100, 702. HRMS ($\text{M}+\text{H}^+$) calcd for $\text{C}_{23}\text{H}_{19}\text{O}_2^+$: 327.1380, found: 327.1382.



6,6-dimethyl-5-phenyl-5,6,7,7a-tetrahydrocyclopenta[b]pyran-3(2H)-one **6** was prepared in 80% yield according to the general procedure C. ^1H NMR (500 MHz, CDCl_3) δ 7.52 – 7.26 (m, 3H), 7.16 (dd, $J = 20.0, 6.3$ Hz, 2H), 6.12 (d, $J = 177.8$ Hz, 1H), 4.82 (d, $J = 31.9$ Hz, 1H), 4.37 (d, $J = 16.7$ Hz, 1H), 4.26 – 4.09 (m, 1H), 3.99 – 3.53 (m, 1H), 2.21 (dd, $J = 21.0, 12.7$ Hz, 1H), 1.91 – 1.75 (m, 1H), 1.28 (d, $J = 19.7$ Hz, 3H), 0.75-0.72 (m, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 195.07, 174.17, 137.67, 129.13, 128.34, 127.12, 122.30, 77.98, 77.25, 77.00, 76.75, 72.87, 60.08, 44.73, 41.30, 28.62, 24.42. IR (neat, cm^{-1}): 2970, 1700, 1591, 1248, 722. HRMS ($\text{M}+\text{H}^+$) calcd for $\text{C}_{16}\text{H}_{19}\text{O}_2^+$: 243.1380, found: 243.1382.

X-ray structure of **5**



Bond precision:	C-C = 0.0030 Å	Wavelength=0.71073
Cell:	a=15.2594(7)	b=10.4298(5)
	alpha=90	beta=90
		gamma=90
Temperature:	294 K	
	Calculated	Reported

Volume	3093.2(3)	3093.2(3)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C20 H18 O2	C20 H18 O2
Sum formula	C20 H18 O2	C20 H18 O2
Mr	290.34	290.34
Dx,g cm-3	1.247	1.247
Z	8	8
Mu (mm-1)	0.079	0.079
F000	1232.0	1232.0
F000'	1232.55	
h,k,lmax	18,12,23	18,12,23
Nref	3039	3032
Tmin,Tmax	0.973,0.976	0.686,1.000
Tmin'	0.973	

Correction method= # Reported T Limits: Tmin=0.686 Tmax=1.000 AbsCorr =
MULTI-SCAN

Data completeness= 0.998

Theta(max)= 26.020

R(reflections)= 0.0536(2077)

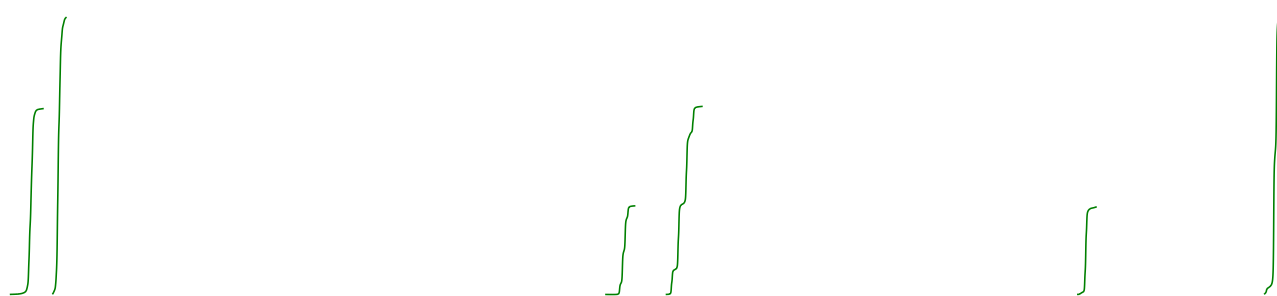
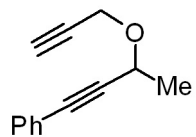
wR2(reflections)= 0.1393(3032)

S = 1.069

Npar= 199

Reference:

1. T. C. Johnson , G. J. Clarkson , and M. Wills *Organometallics*, **2011**, 30 ,1859–1868

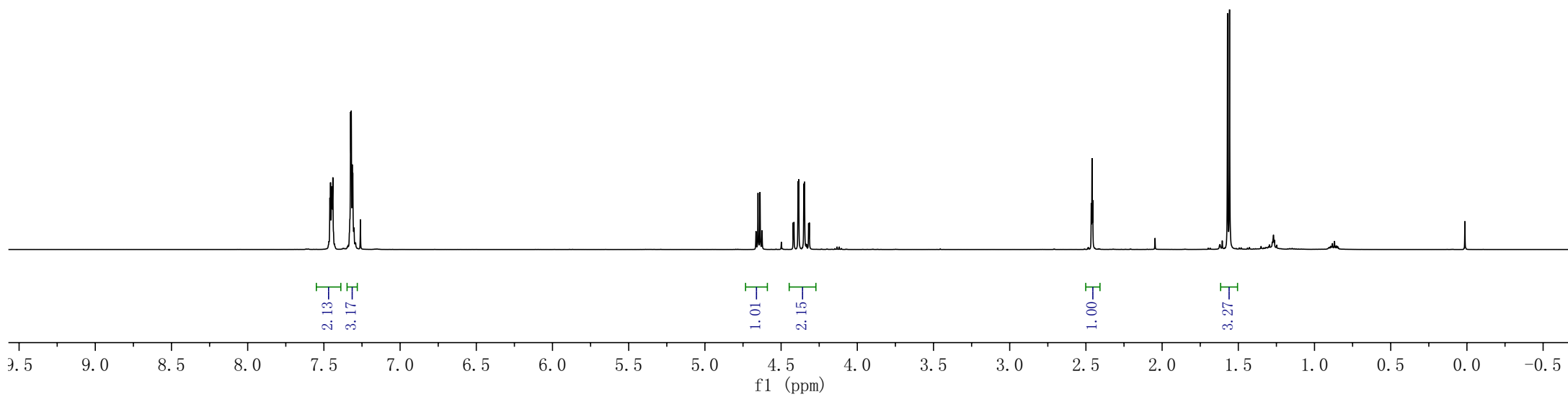


D (m)
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C (m)
7.45
HH

B (m)
4.36
A (q)
4.64
HH

E (m)
2.47
H

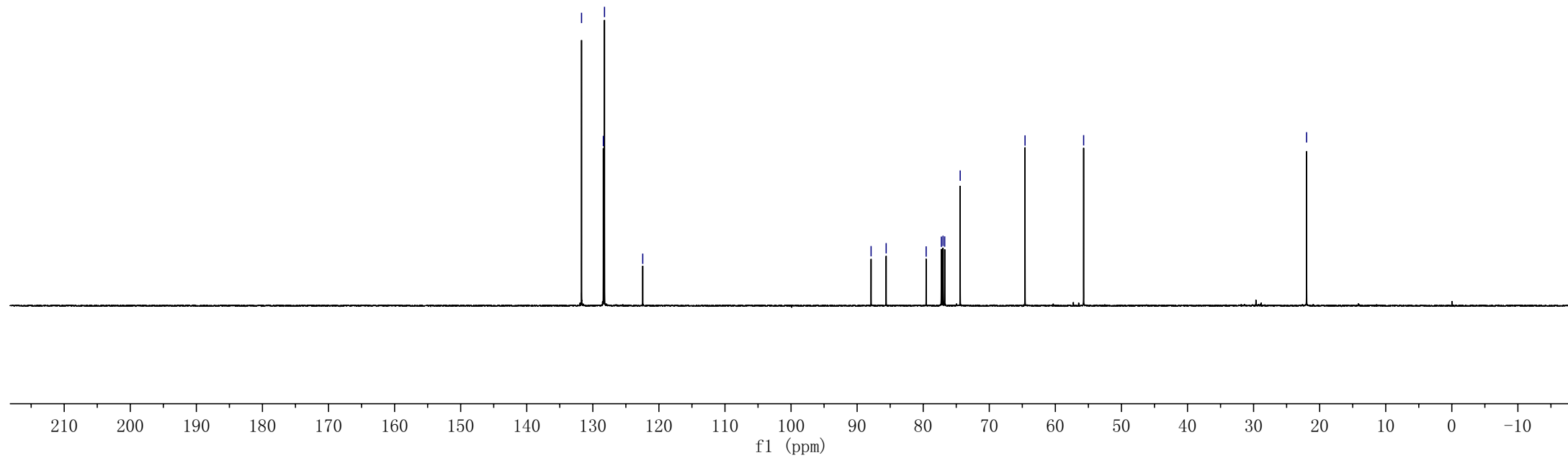
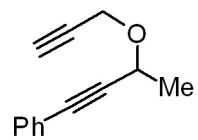
F (d)
1.56
H

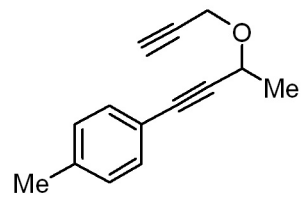


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128.23
122.44

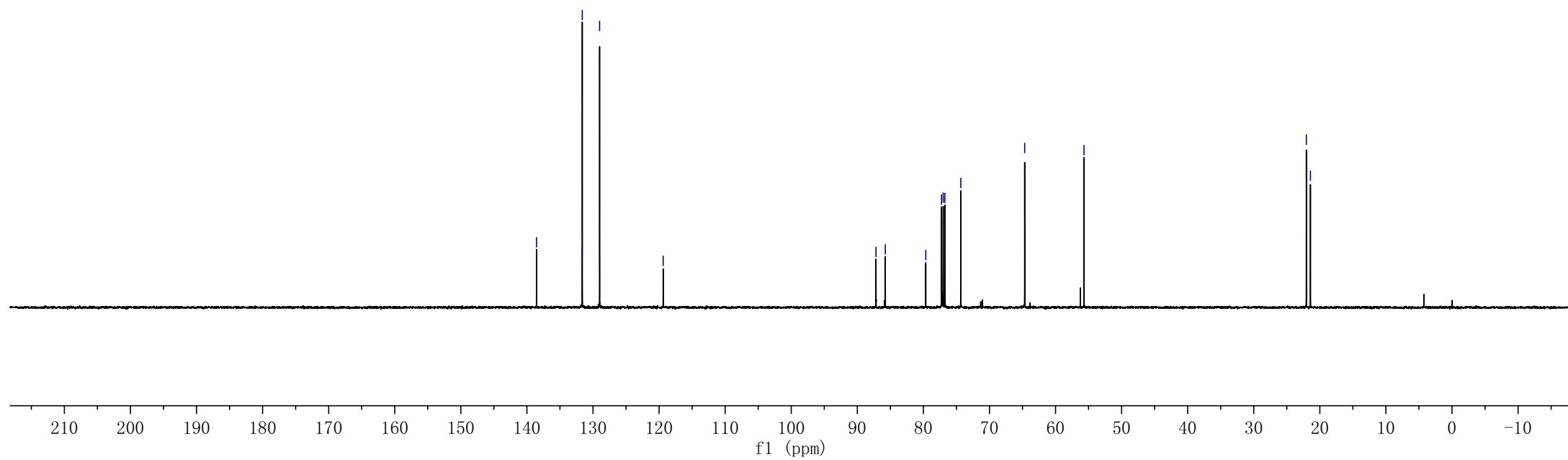
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77.25
77.00
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55.72

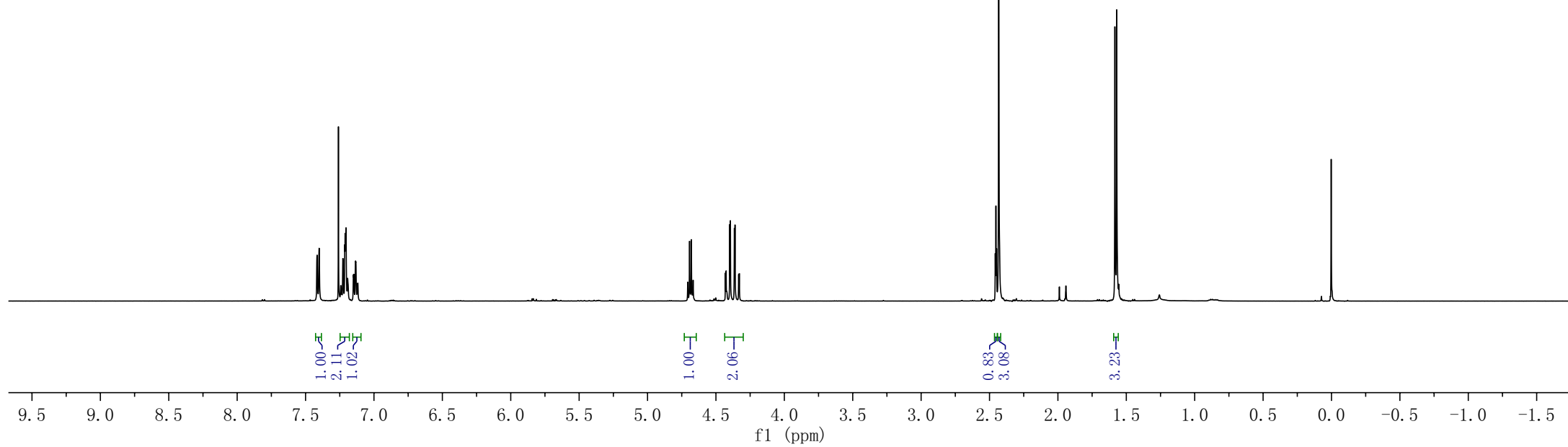
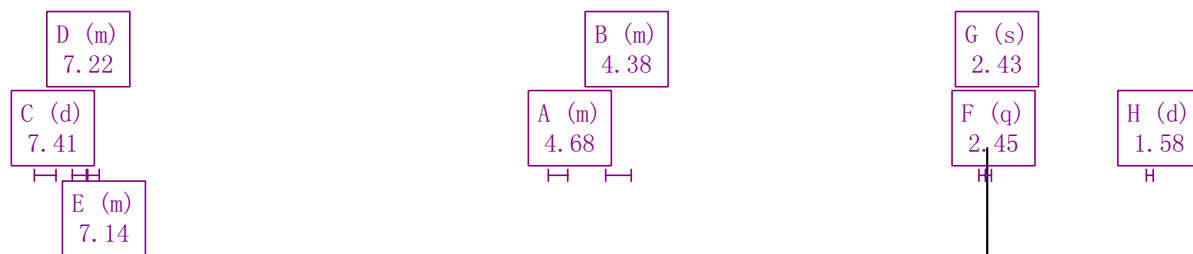
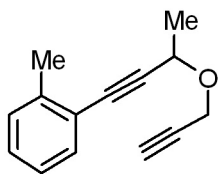
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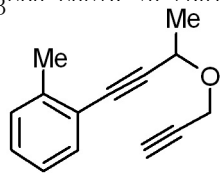


138.55
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74.34
64.67
55.69
22.04
21.42





JKG-20150311-I-52B
C13 NMR (CDCl₃, 125 MHz, 25 °C) { 2015-1 } ZHL 18



140.23

132.03

129.41

128.46

125.51

122.24

91.84

84.54

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77.00

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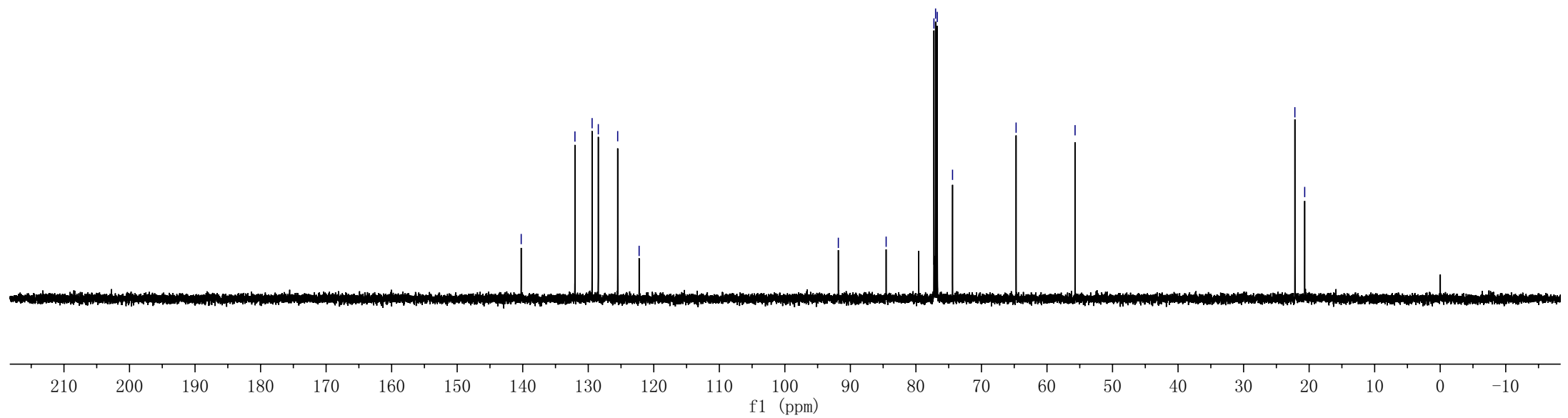
74.41

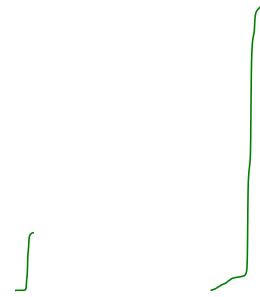
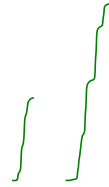
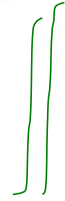
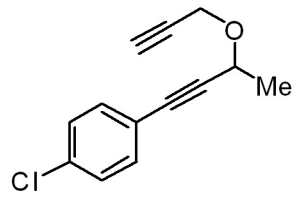
64.71

55.72

22.18

20.68



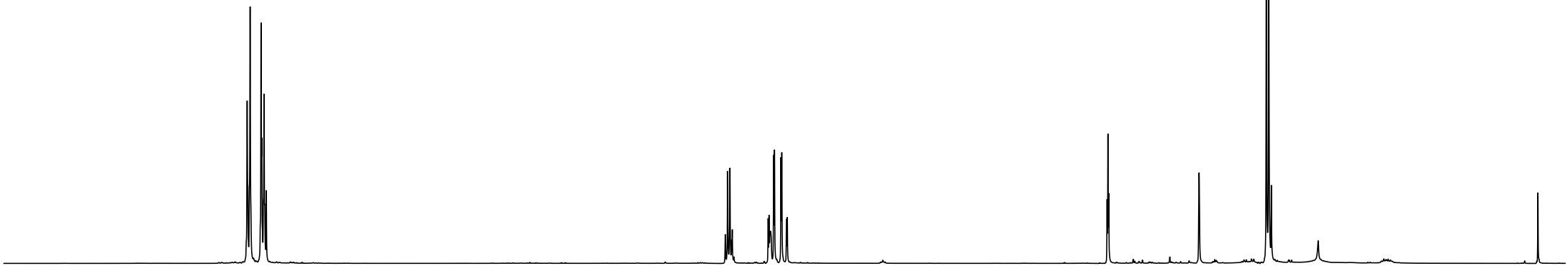


F (dd)
7.28
E (t)
7.35

B (m)
4.35
A (m)
4.61

C (t)
2.46

D (t)
1.54



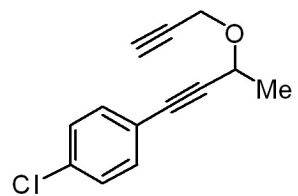
2.14
2.32

1.00
2.14

0.70

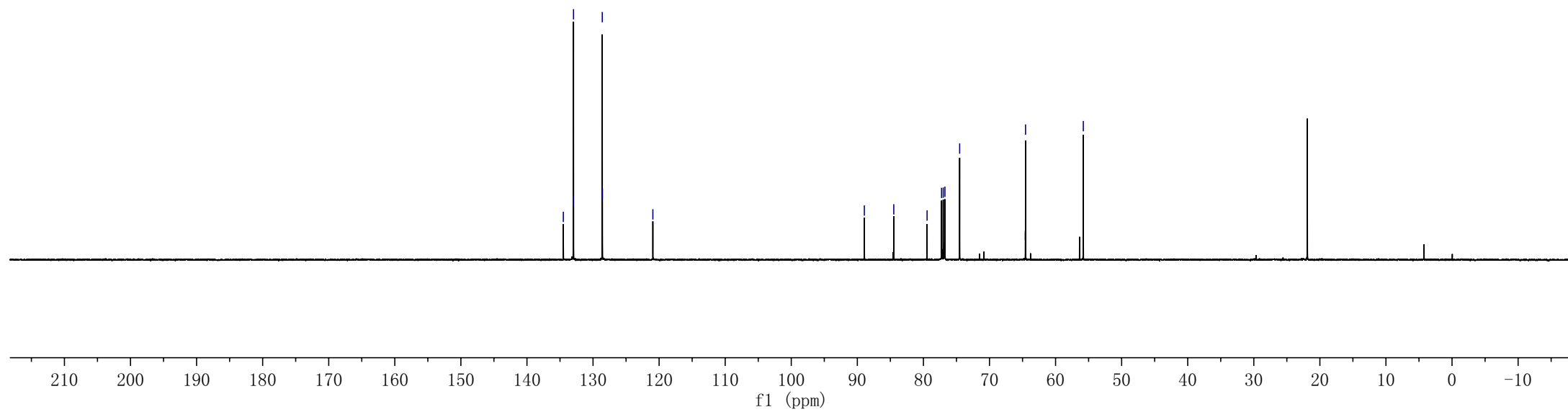
3.46

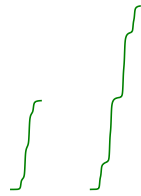
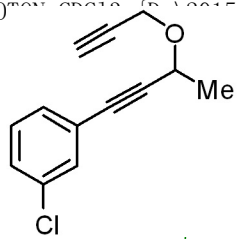
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)



134.50
132.98
132.95
128.60
128.58
120.94

88.94
84.49
79.45
77.25
77.00
76.75
74.52
64.54
55.80





F (m)
7.31

E (t)
7.44

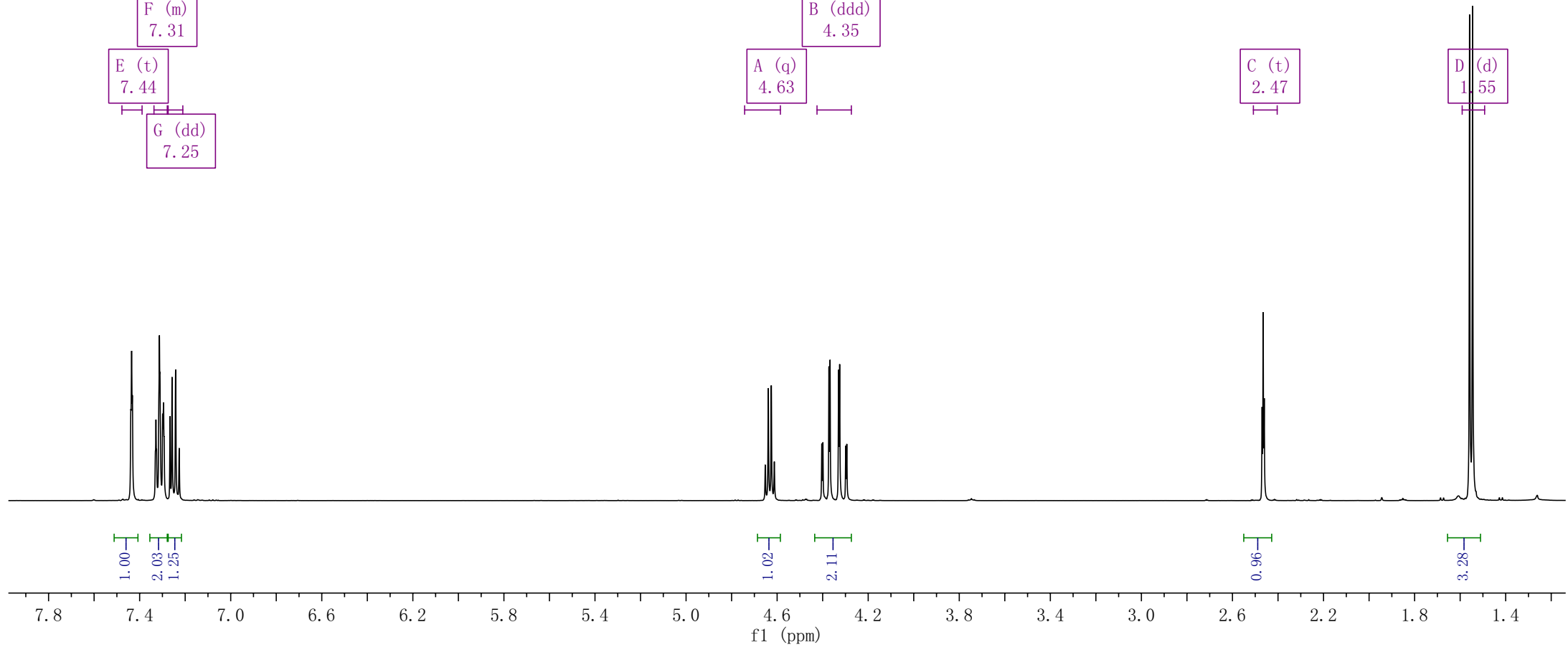
G (dd)
7.25

A (q)
4.63

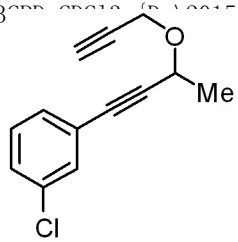
B (ddd)
4.35

C (t)
2.47

D (d)
1.55



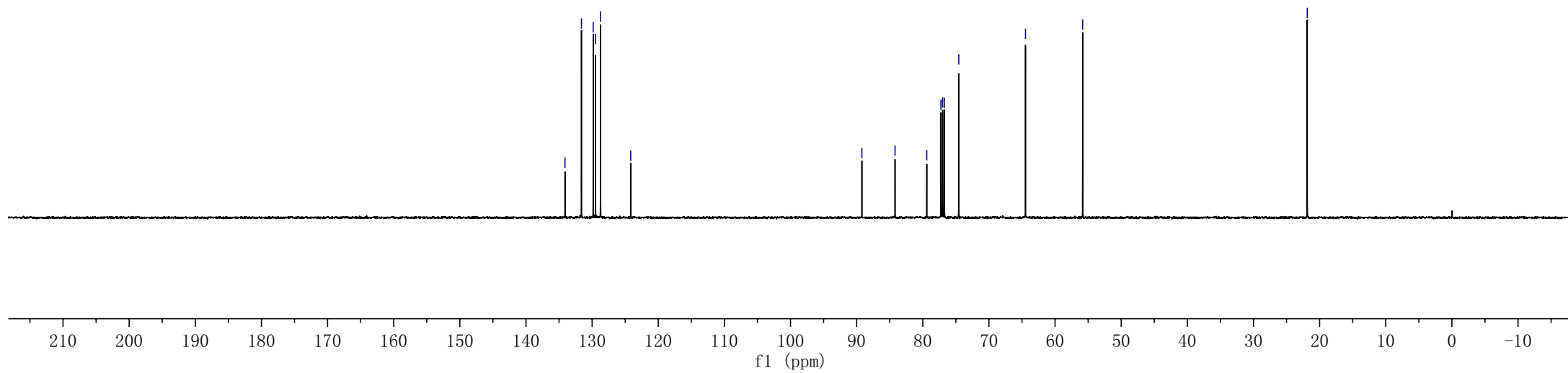
JKG-20150316-2B
C13 NMR (CDCl3) {S: 2015-1} ZHL 39

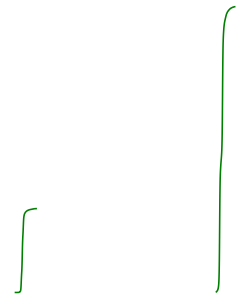
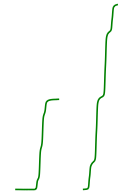
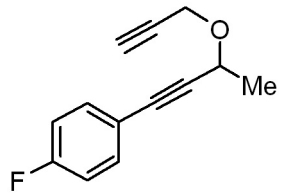


134.10
131.61
129.83
129.49
128.73
124.16

89.21
84.20
79.40
77.25
77.00
76.75
74.56
64.47
55.83

21.87





C (m)
7.42

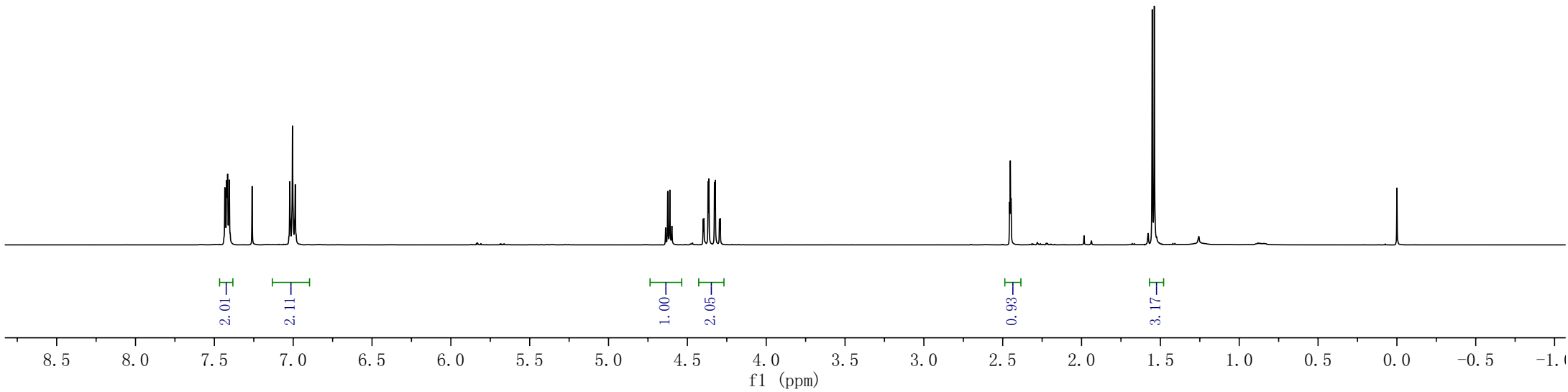
D (t)
7.00

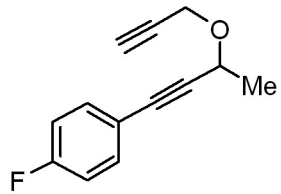
A (q)
4.62

B (ddd)
4.35

E (t)
2.45

F (m)
1.55





163.57
161.58

133.69
133.63

118.56
118.54
115.64
115.47

87.64
84.56
79.51
77.25
77.00
76.75
74.46

64.57

55.78

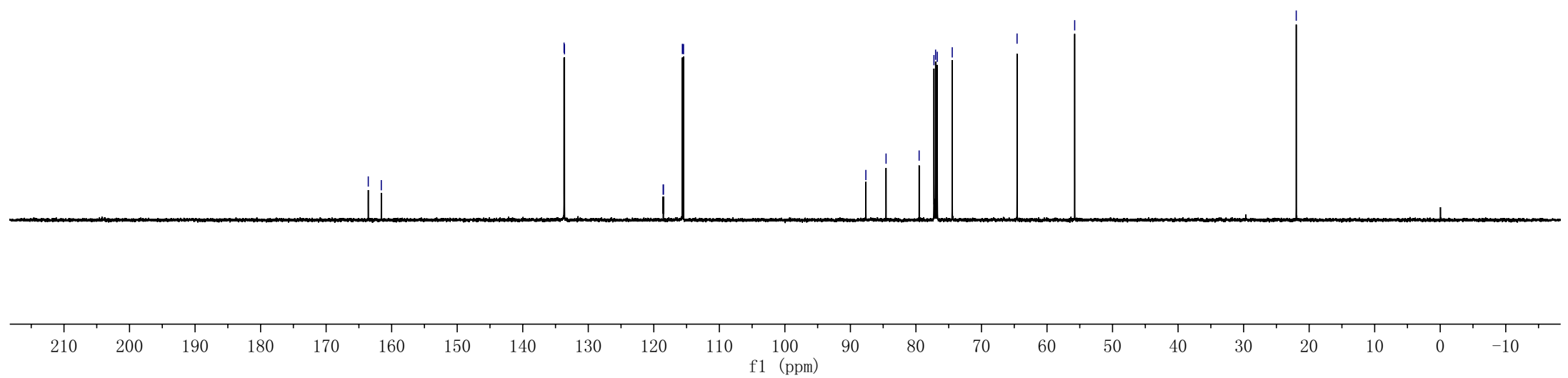
21.97

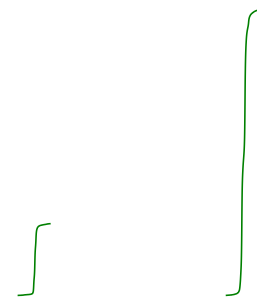
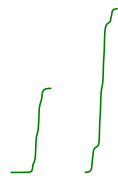
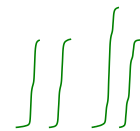
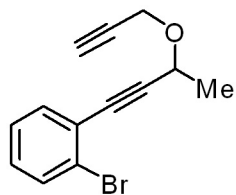
A (d)
162.58

B (d)
133.66

C (d)
118.55

D (d)
115.55





D (dt)
7.46
C (dd)
7.59
F (td)
7.18
E (m)
7.26

B (m)
4.43
A (m)
4.69

G (t)
2.47

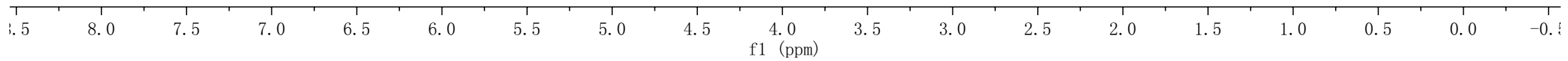
H (t)
1.58

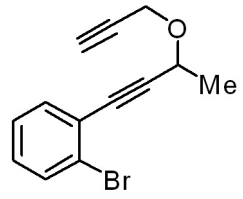
1.04
1.05
1.43
1.04

1.00
1.95

0.85

3.40





133.38
132.36
129.60
126.95
125.59
124.60

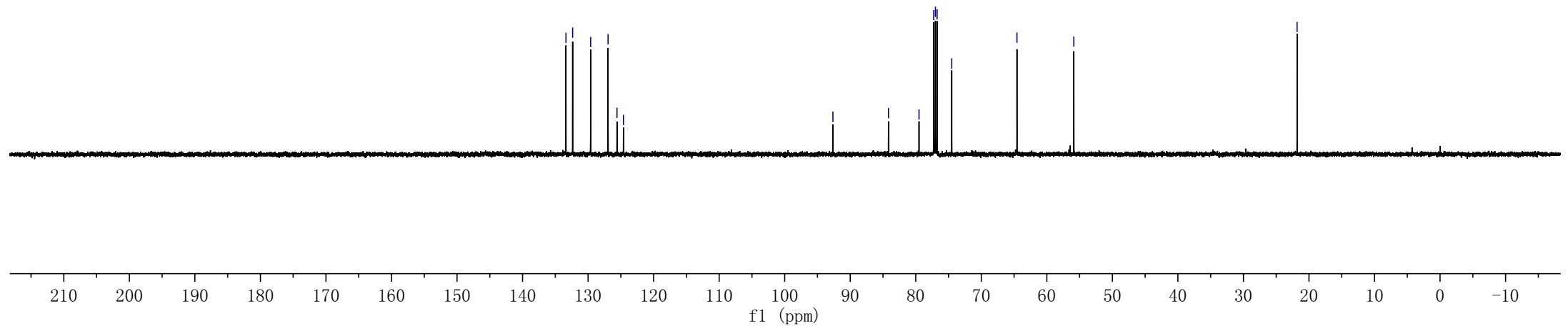
92.64

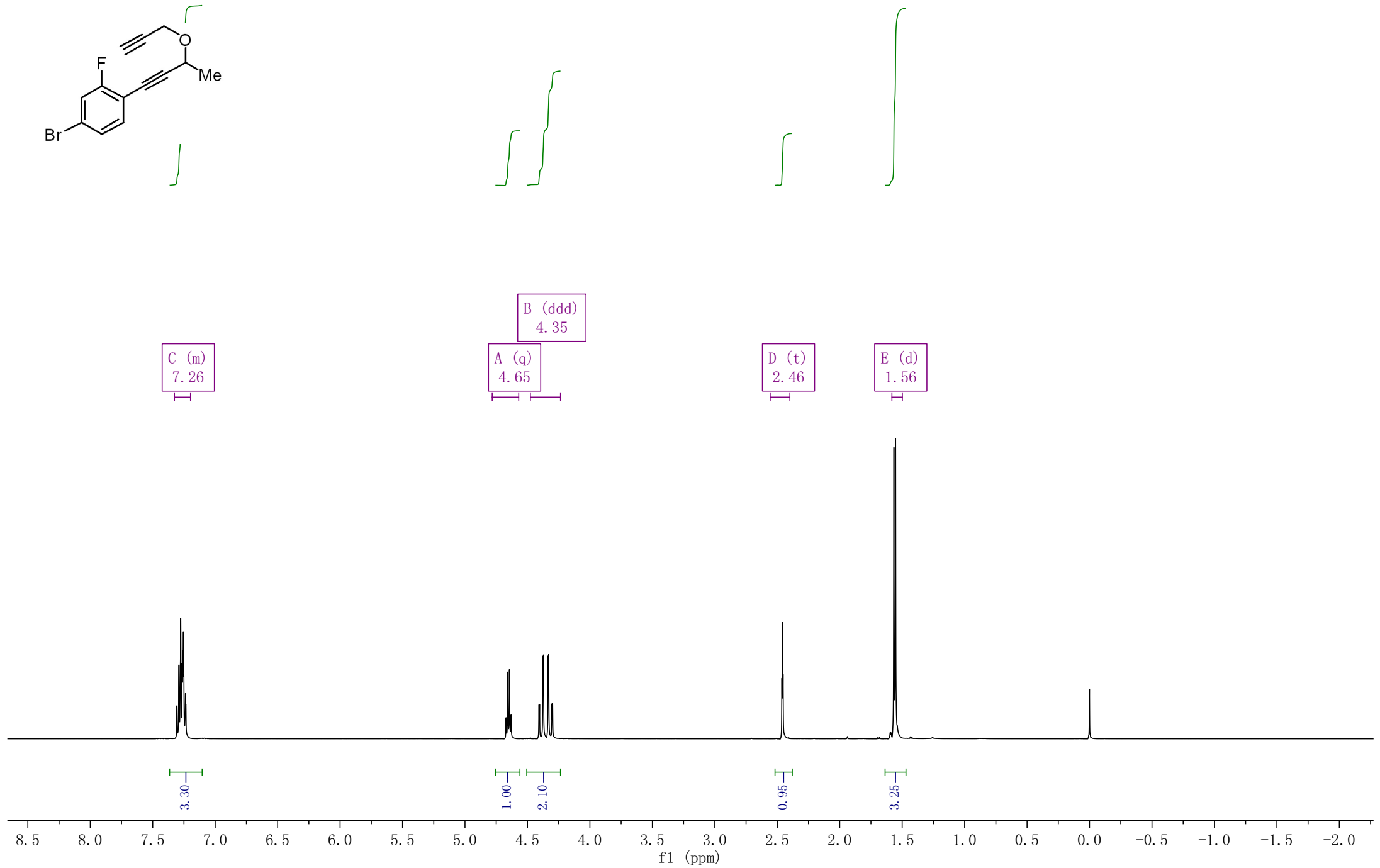
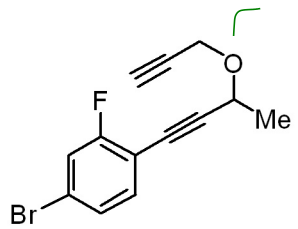
84.16
79.50
77.25
77.00
76.75
74.51

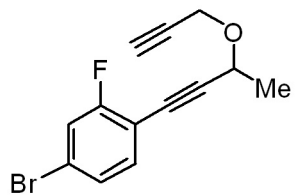
64.56

55.88

21.81







163.50
161.46

134.24
134.22
127.39
127.36
122.85
122.78
119.39
119.20

110.36
110.24

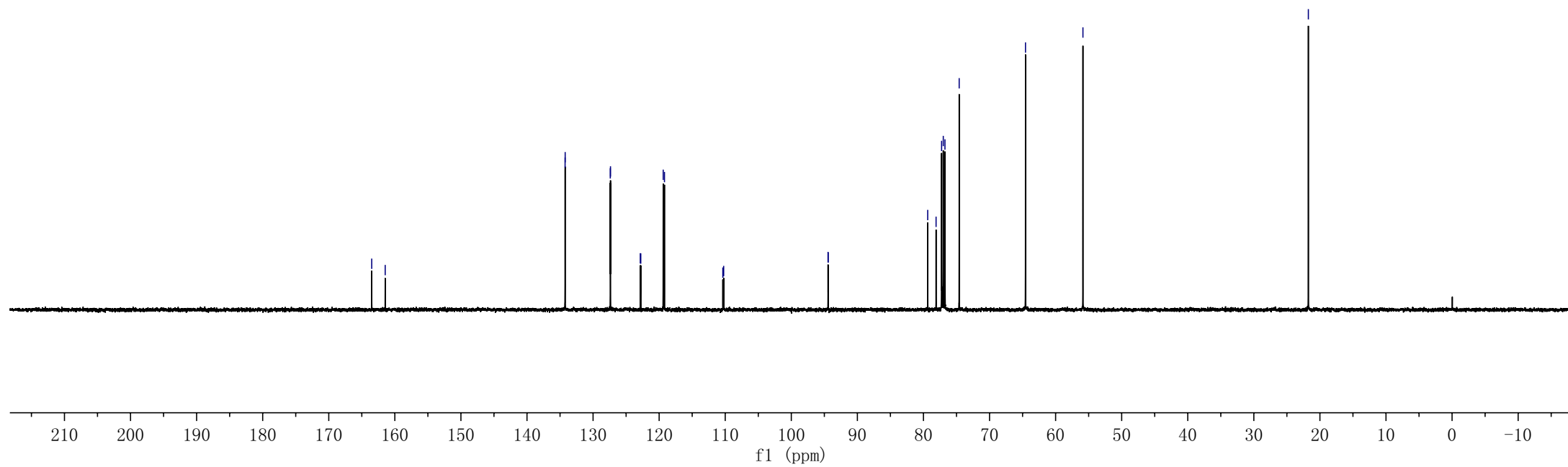
94.44
94.41

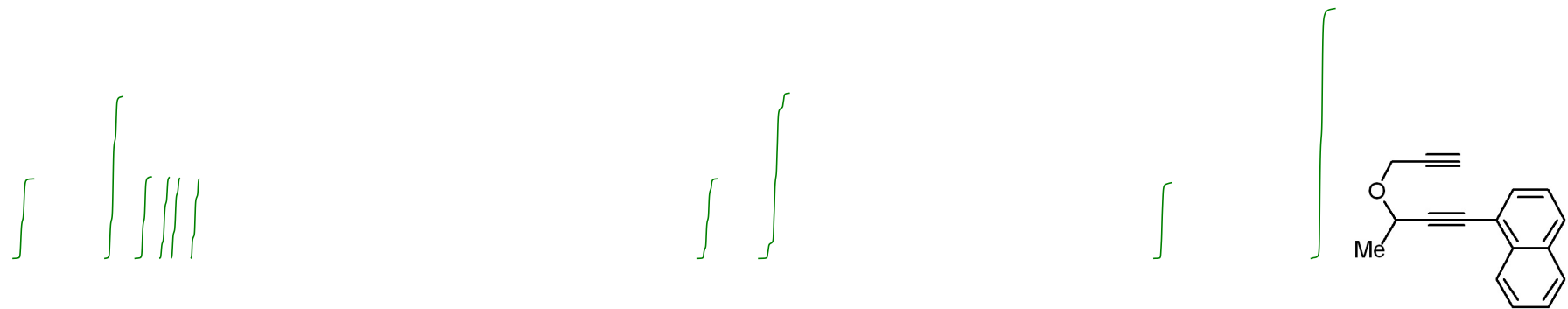
79.36
78.09
77.25
77.00
76.75
74.59

64.56

55.86

21.75





A (d)
8.31

B (t)
7.85

C (d)
7.69

D (t)
7.58

E (m)
7.53

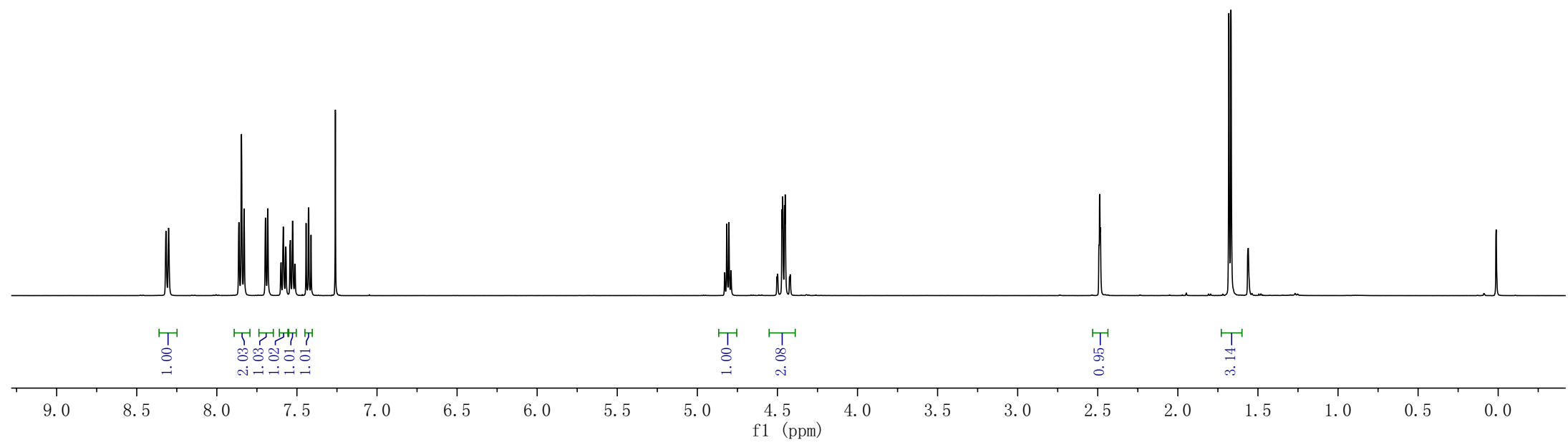
F (dd)
7.43

G (q)
4.81

H (m)
4.46

I (t)
2.49

J (d)
1.67



133.29
133.13
130.69
128.96
128.29
126.84
126.41
125.99
125.13
120.11

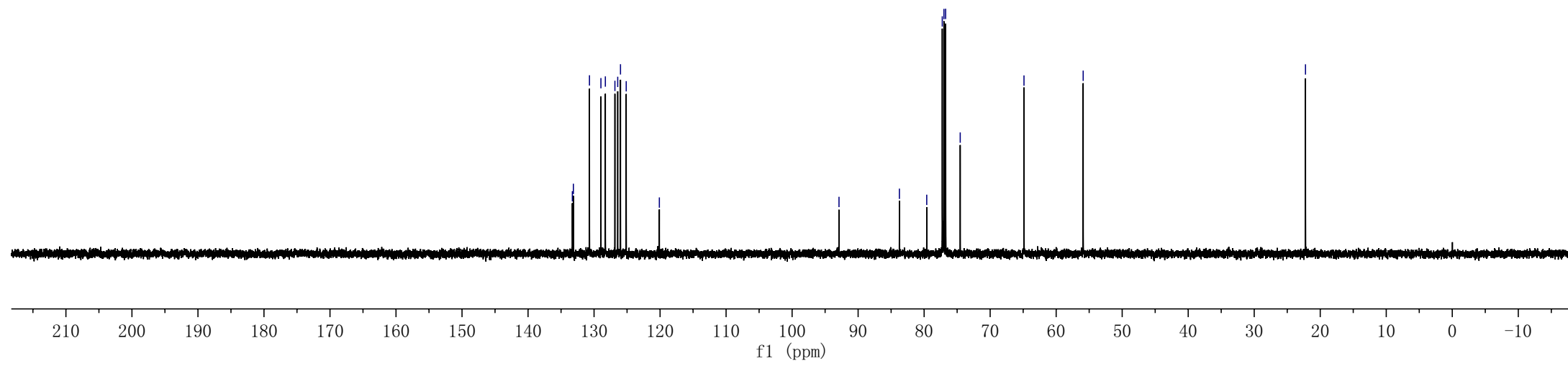
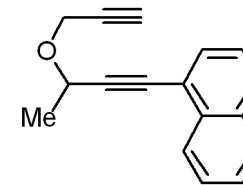
92.90

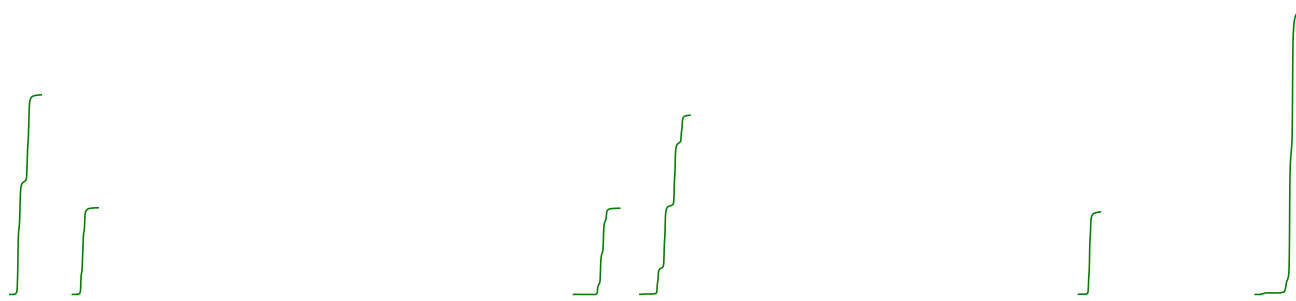
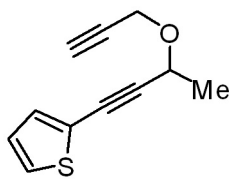
83.75
79.61
77.25
77.00
76.75
74.53

64.87

55.91

22.23





D (dd)
6.97

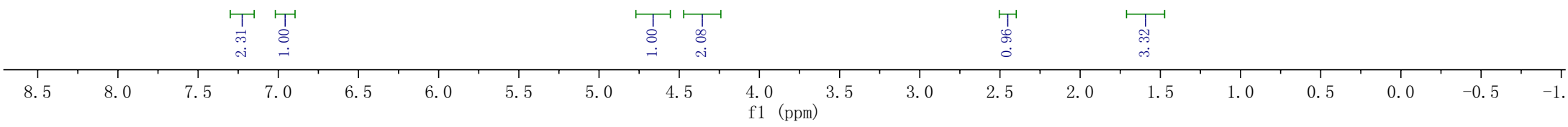
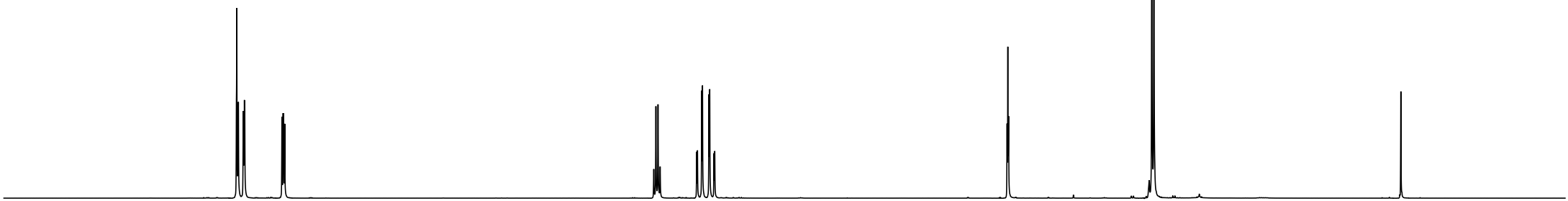
C (m)
7.25

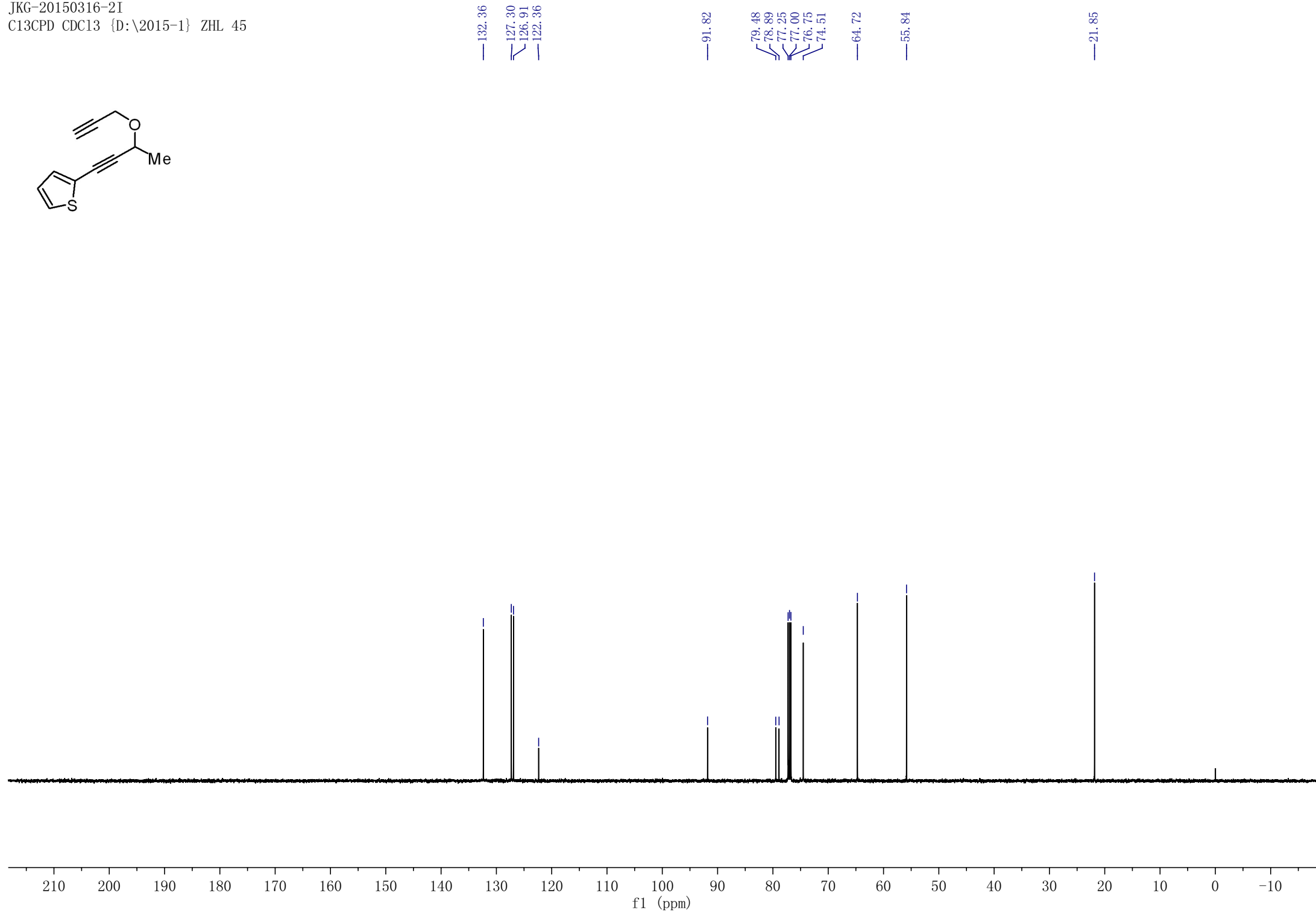
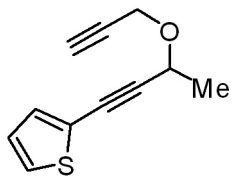
B (ddd)
4.33

A (q)
4.64

E (t)
2.45

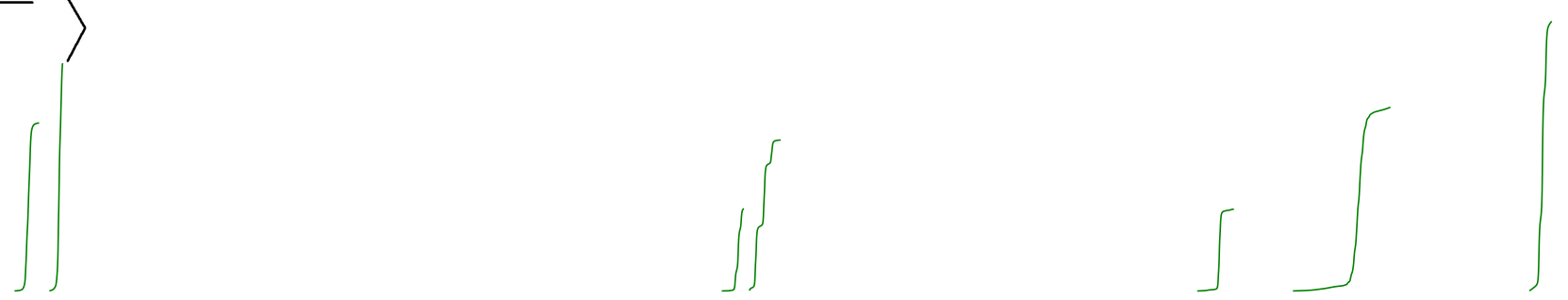
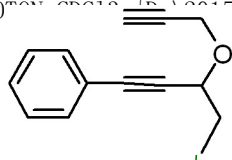
F (t)
1.55





JKG-20150316-1-1S

PROTON NMR (CDCl₃) {ZL 2015-1} ZHL 13



D (m)
7.21

C (m)
7.35

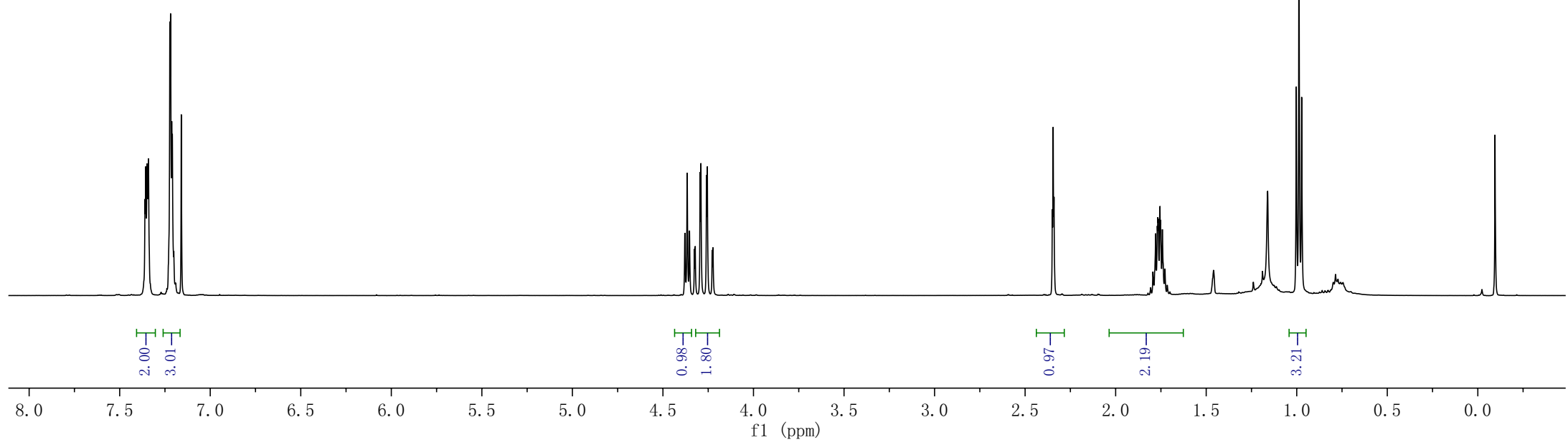
B (qd)
4.27

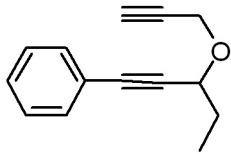
A (dd)
4.36

E (t)
2.35

F (m)
1.76

G (t)
0.99





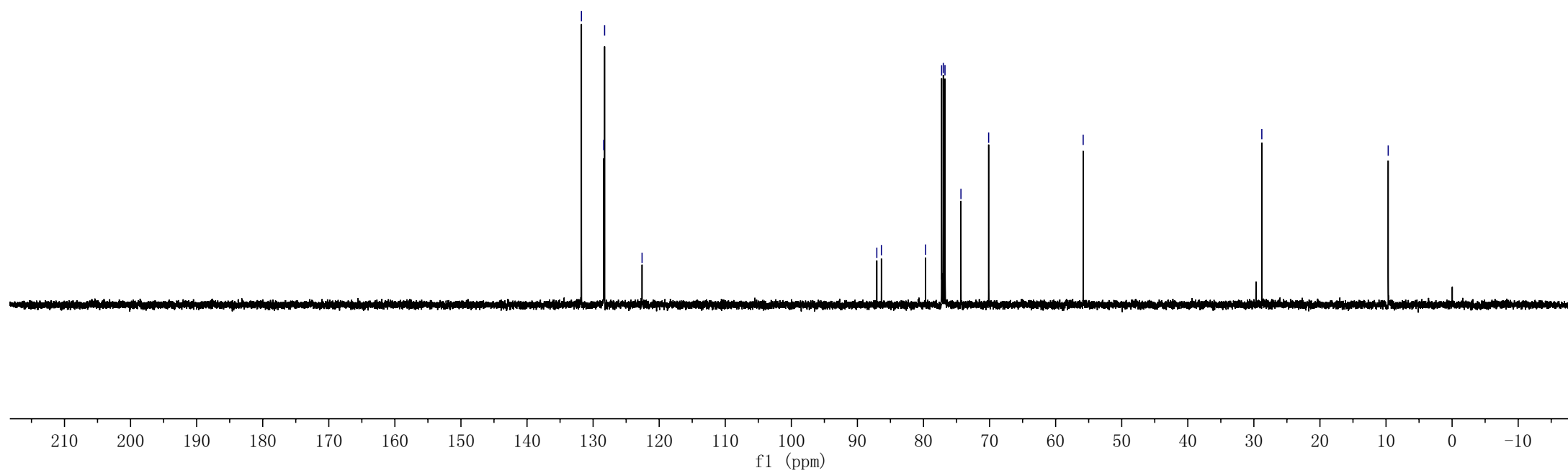
131.77
128.40
128.26
122.59

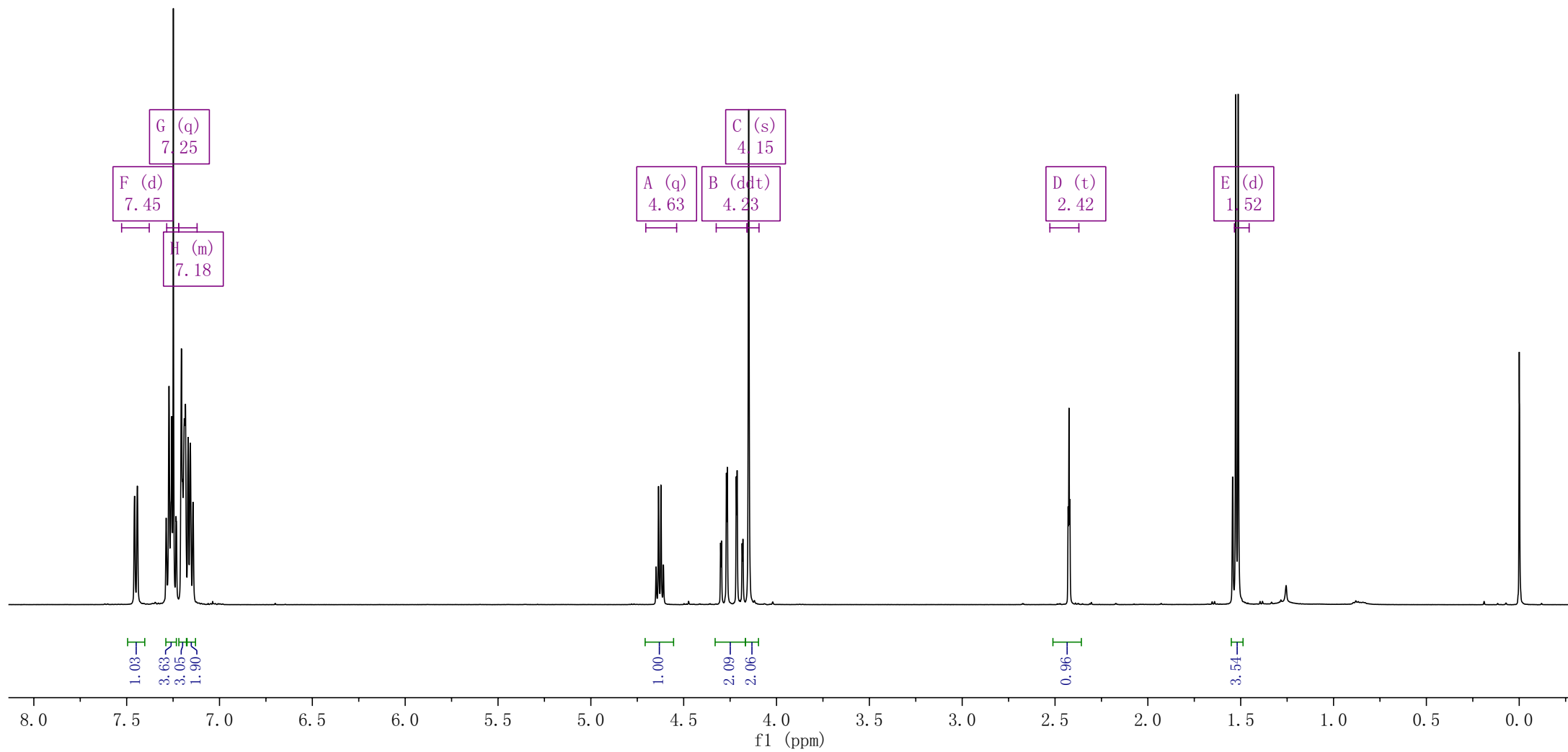
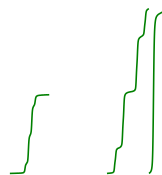
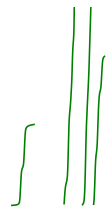
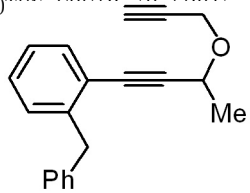
87.06
86.37
79.69
77.25
77.00
76.75
74.33
70.14

55.83

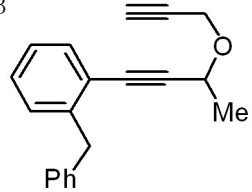
28.80

9.67





JKG-20150320-LX-I-2b
C13 NMR (CDCl₃) {5, 10015 1} ZHL 32



143.01
140.37
132.57
129.49
128.85
128.73
128.38
126.13
126.06
122.23

91.99

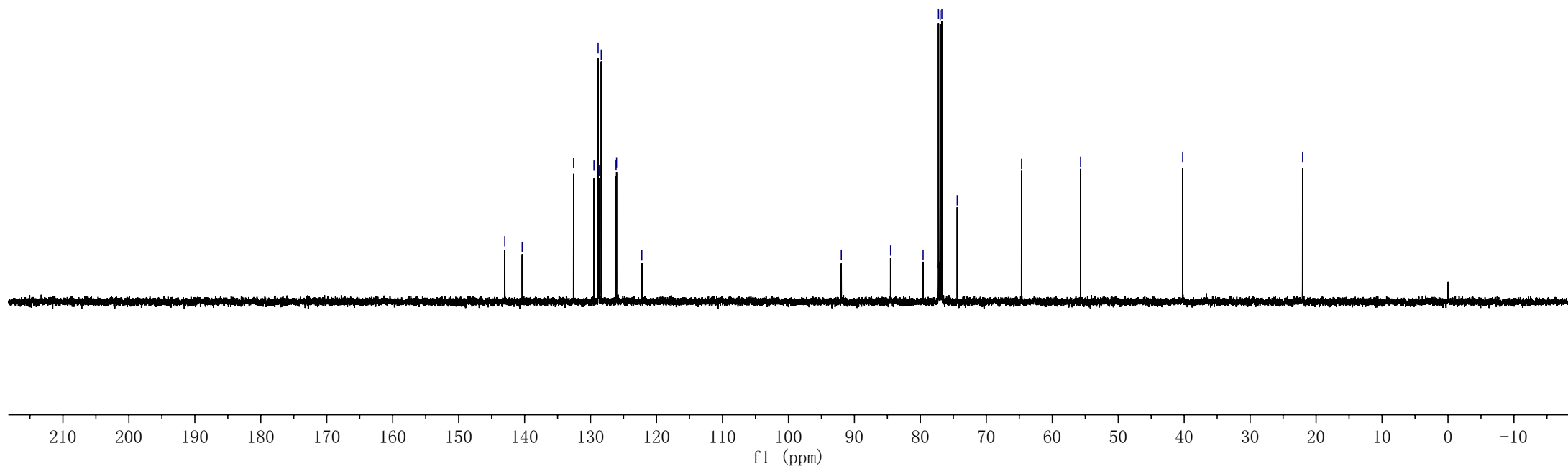
84.52
79.58
77.25
77.00
76.75
74.41

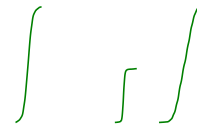
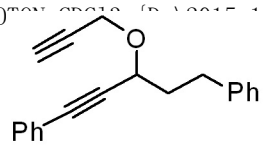
64.66

55.71

40.23

22.04





G (m)
7.28

F (m)
7.46

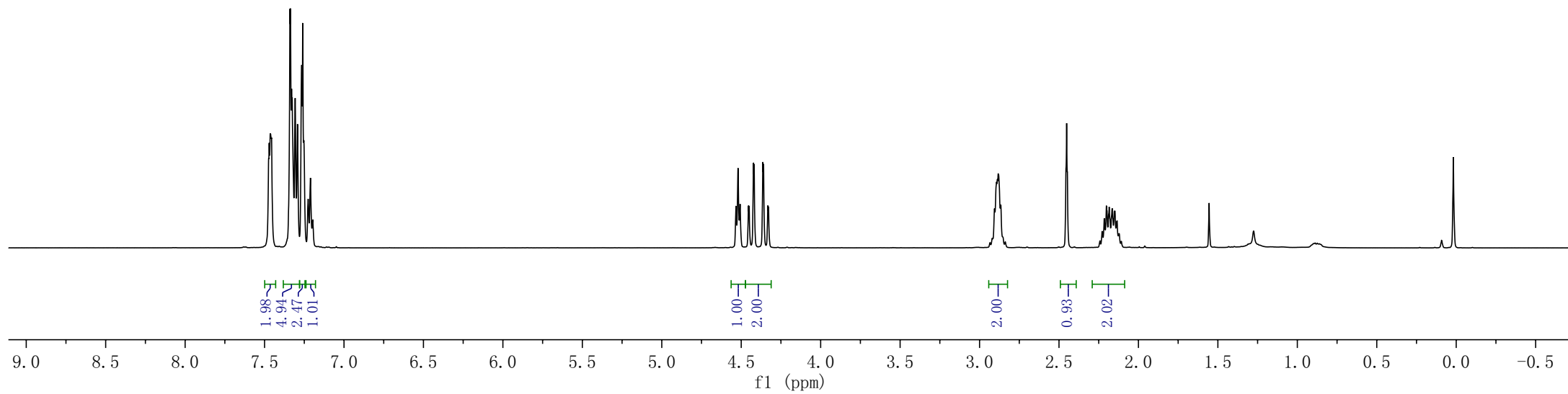
B (ddd)
4.39

A (t)
4.52

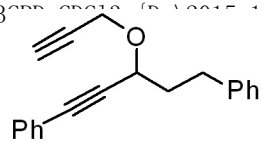
E (m)
2.17

C (m)
2.89

D (d)
2.45



JKG-20150316-1-67C
C13 NMR (CDCl₃) { 2015-1 } ZHL 15



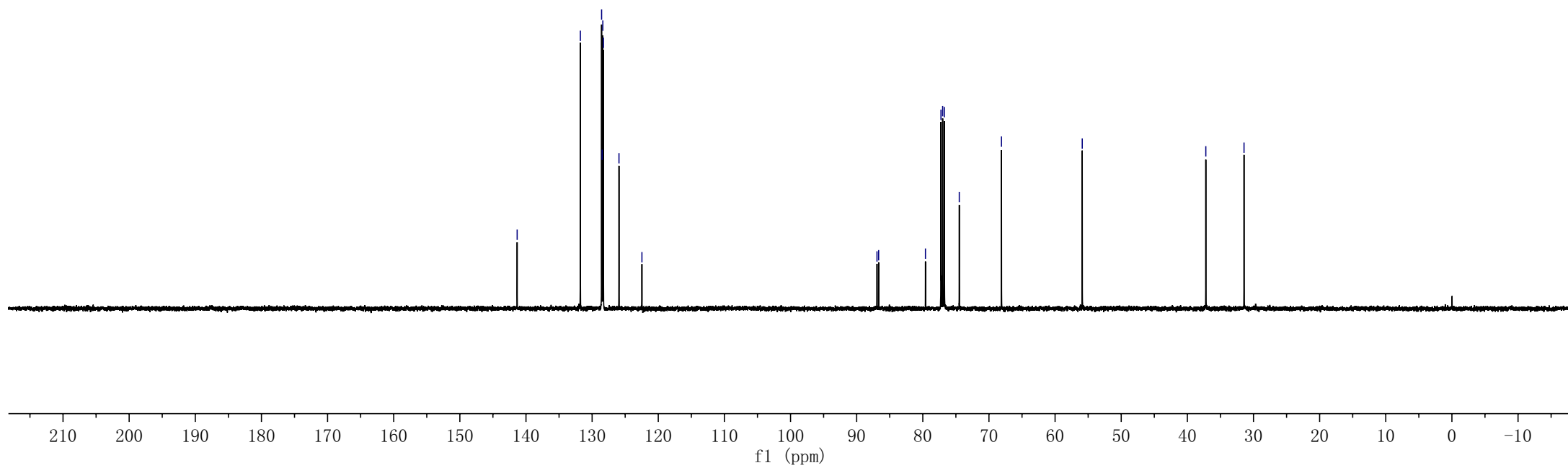
141.33
131.78
128.57
128.49
128.38
128.29
125.94
122.47

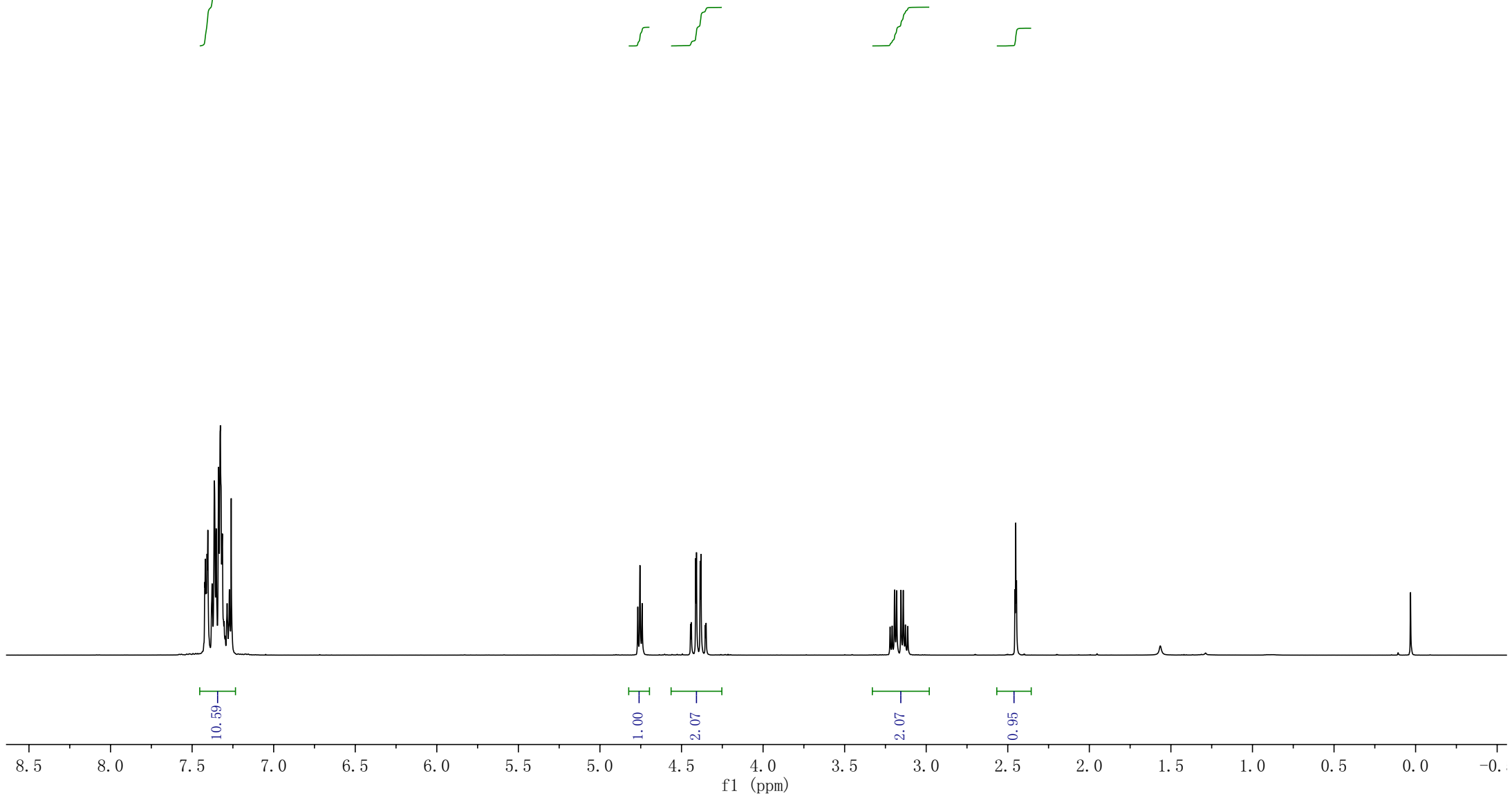
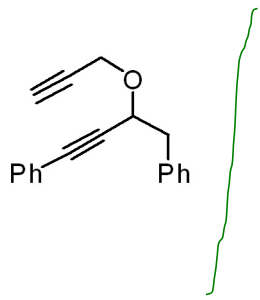
86.93
86.68
79.60
77.25
77.00
76.75
74.49
68.11

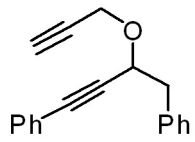
55.89

37.21

31.43





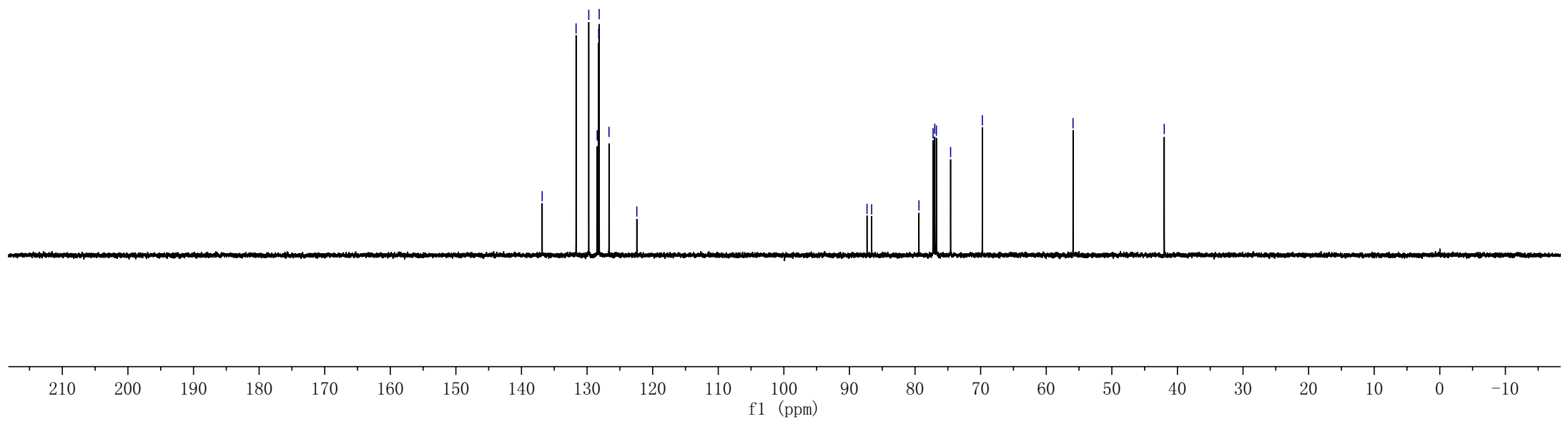


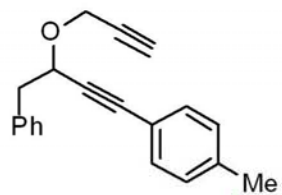
136.85
131.68
129.74
128.46
128.24
128.15
126.66
122.41

87.32
86.62
79.41
77.25
77.00
76.75
74.58
69.74

55.91

42.01





C (m)
7.39

B (d)
7.19

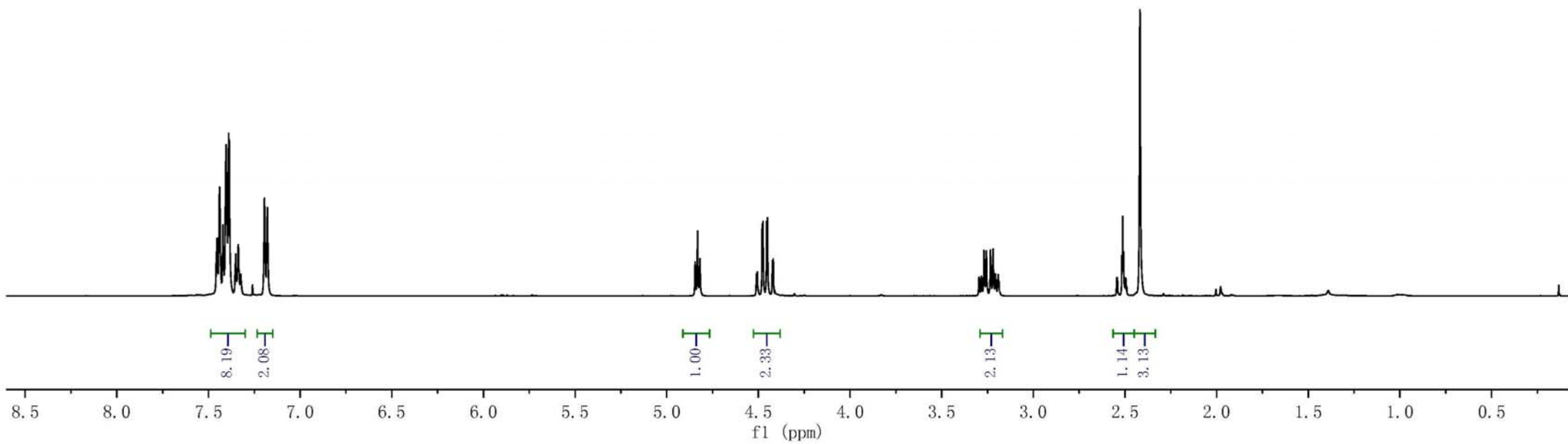
A (t)
4.83

D (qd)
4.46

E (m)
3.24

F (dt)
2.50

G (s)
2.42



138.45
136.81
131.47
129.65
128.90
128.02
126.52
119.24

87.37
85.87

79.38

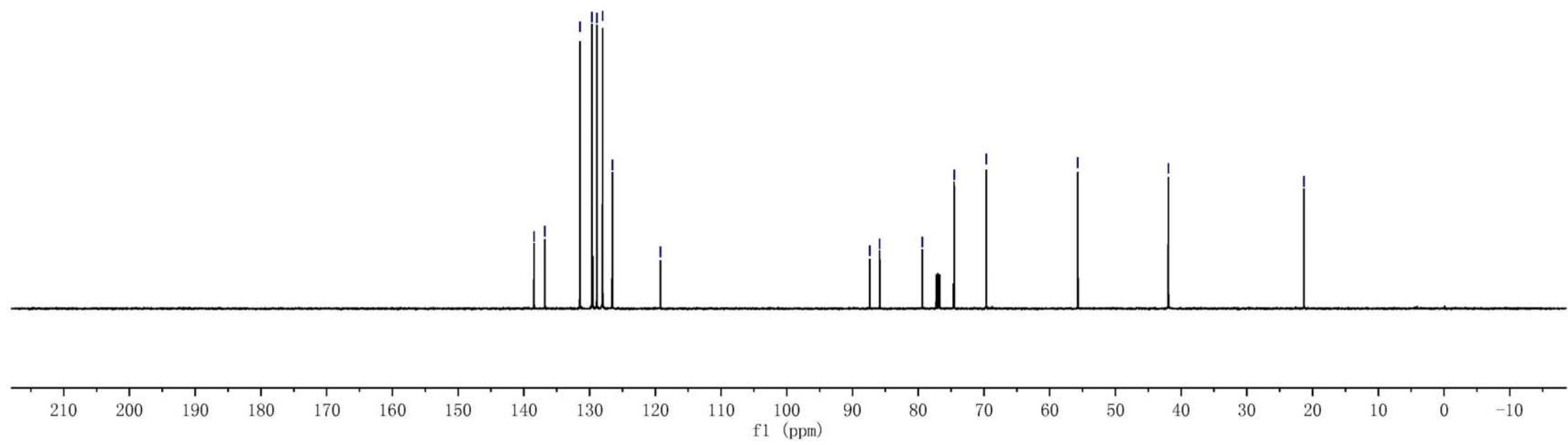
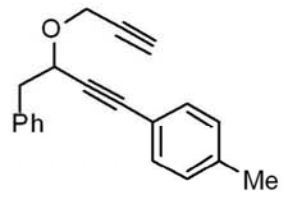
74.53

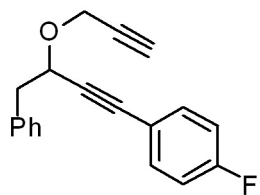
69.64

55.73

41.94

21.32



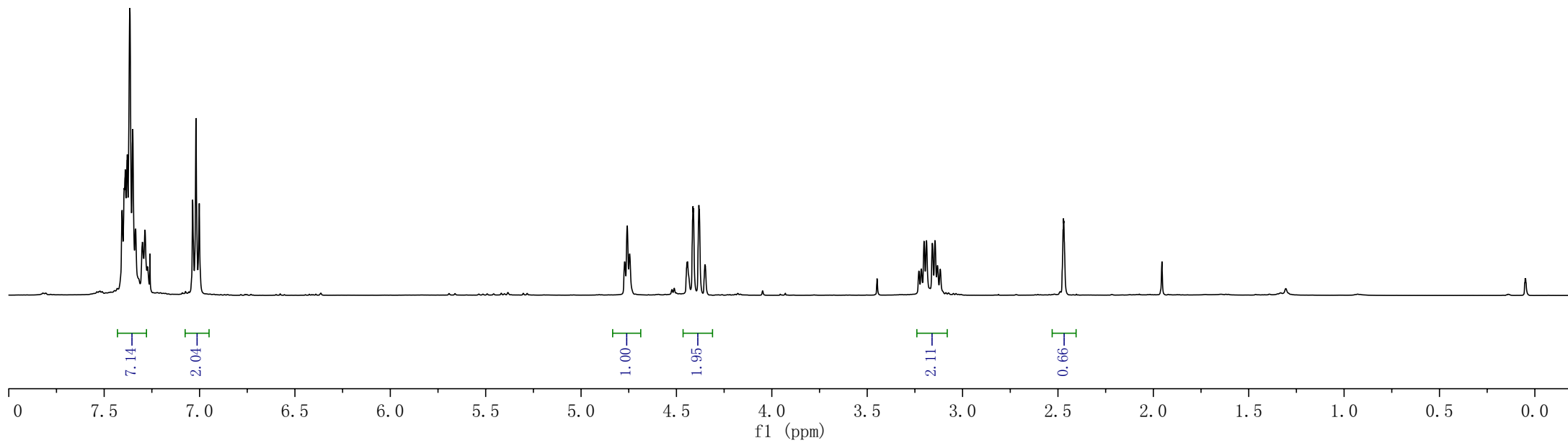


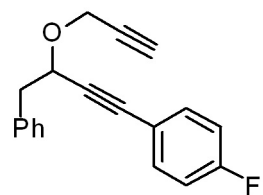
F (m)	E (t)
7.34	7.02

A (t)	B (qd)
4.76	4.40

C (m)
3.16

D (m)
2.48

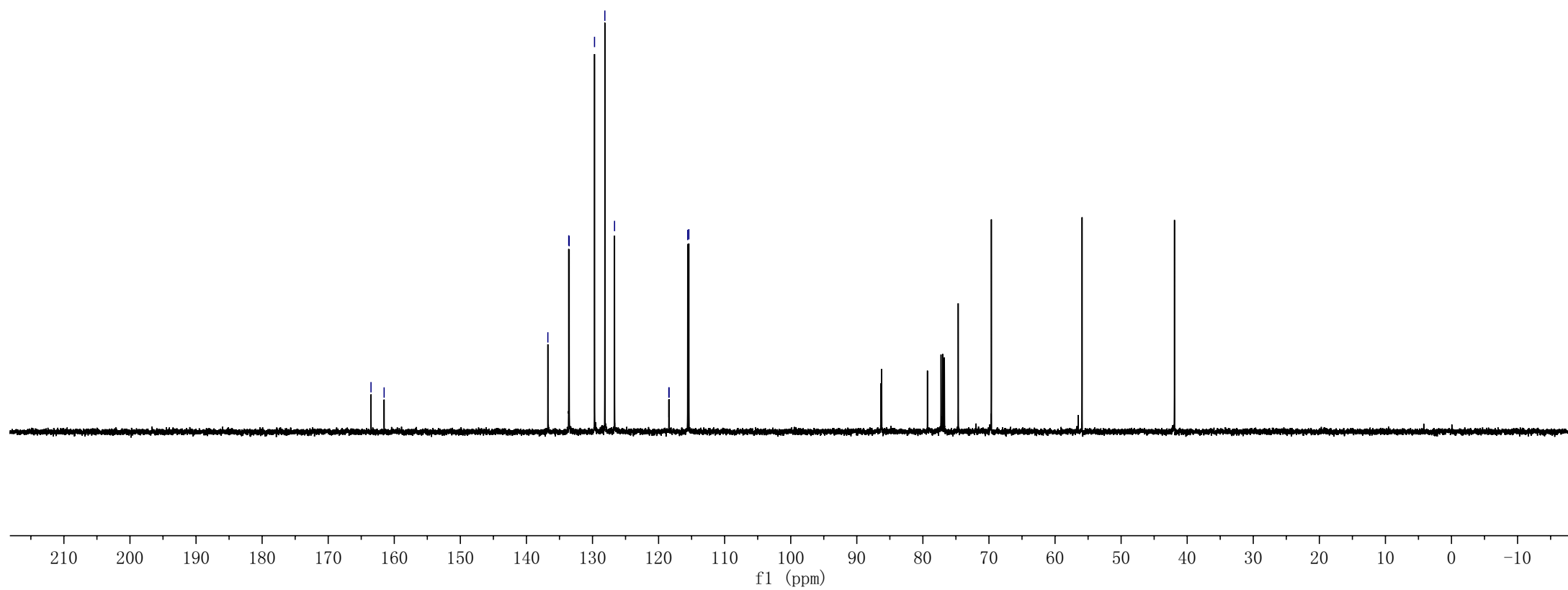


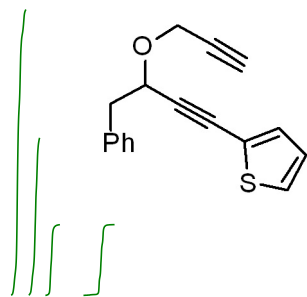


163.52
161.54

136.76
133.60
133.53
129.70
128.13
126.66

118.45
118.42
115.60
115.42





H (m)
7.24

F (dd)
7.17

E (dd)
6.95

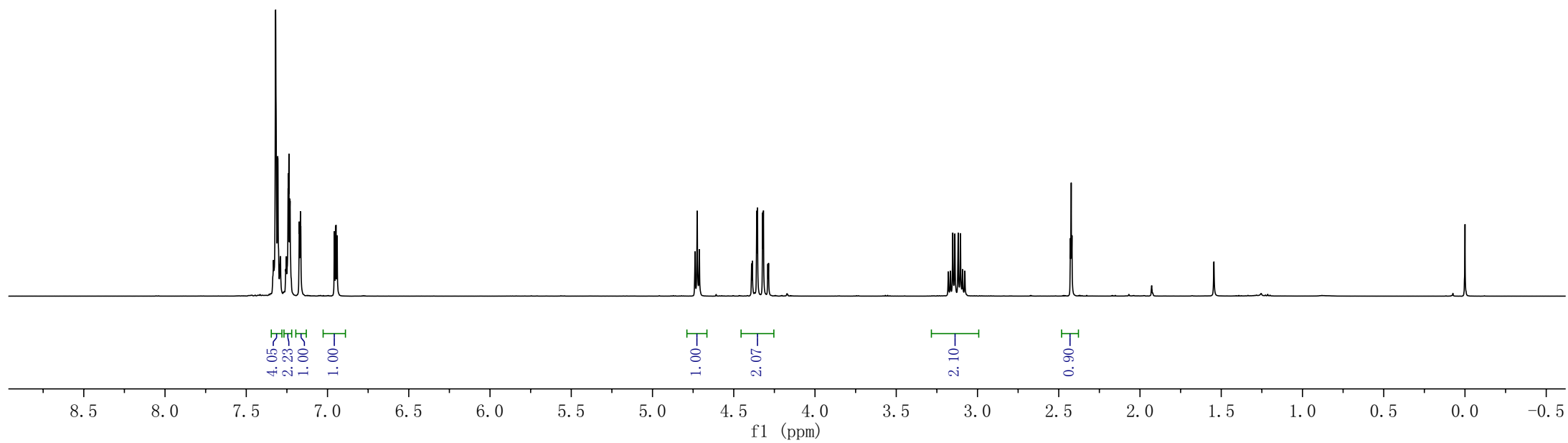
G (m)
7.31

A (t)
4.72

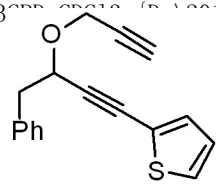
B (m)
4.34

C (qd)
3.13

D (t)
2.42



JKG-20150327-DB-1-6f
C13 NMR (CDCl₃, 125 MHz, 25 °C) ZHL 33



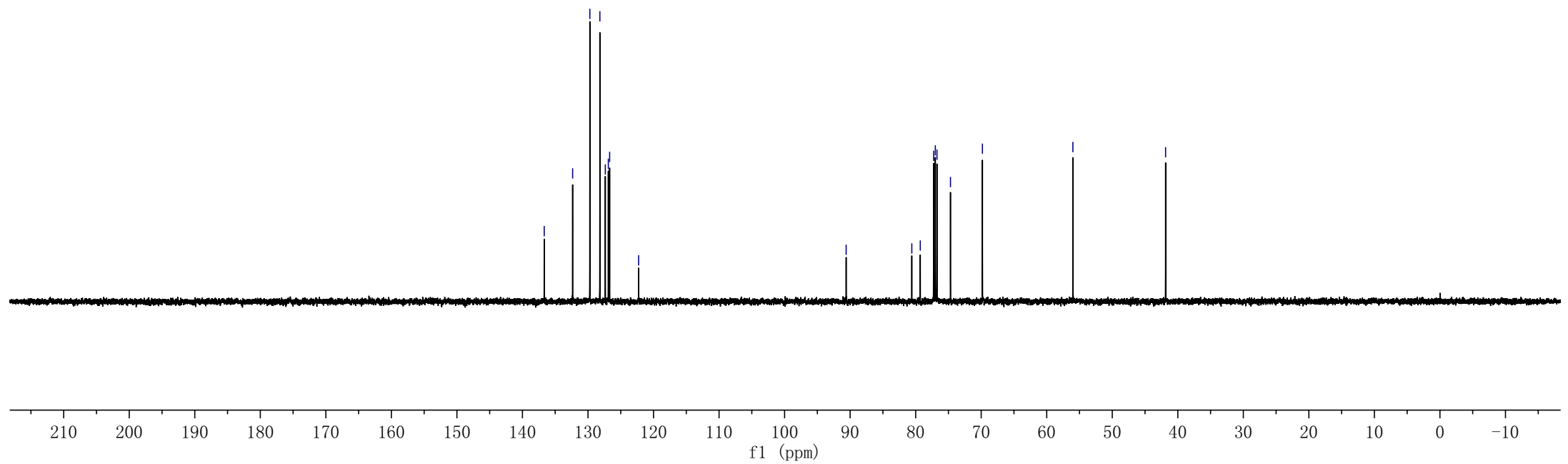
136.68
132.34
129.72
128.19
127.36
126.90
126.69
122.27

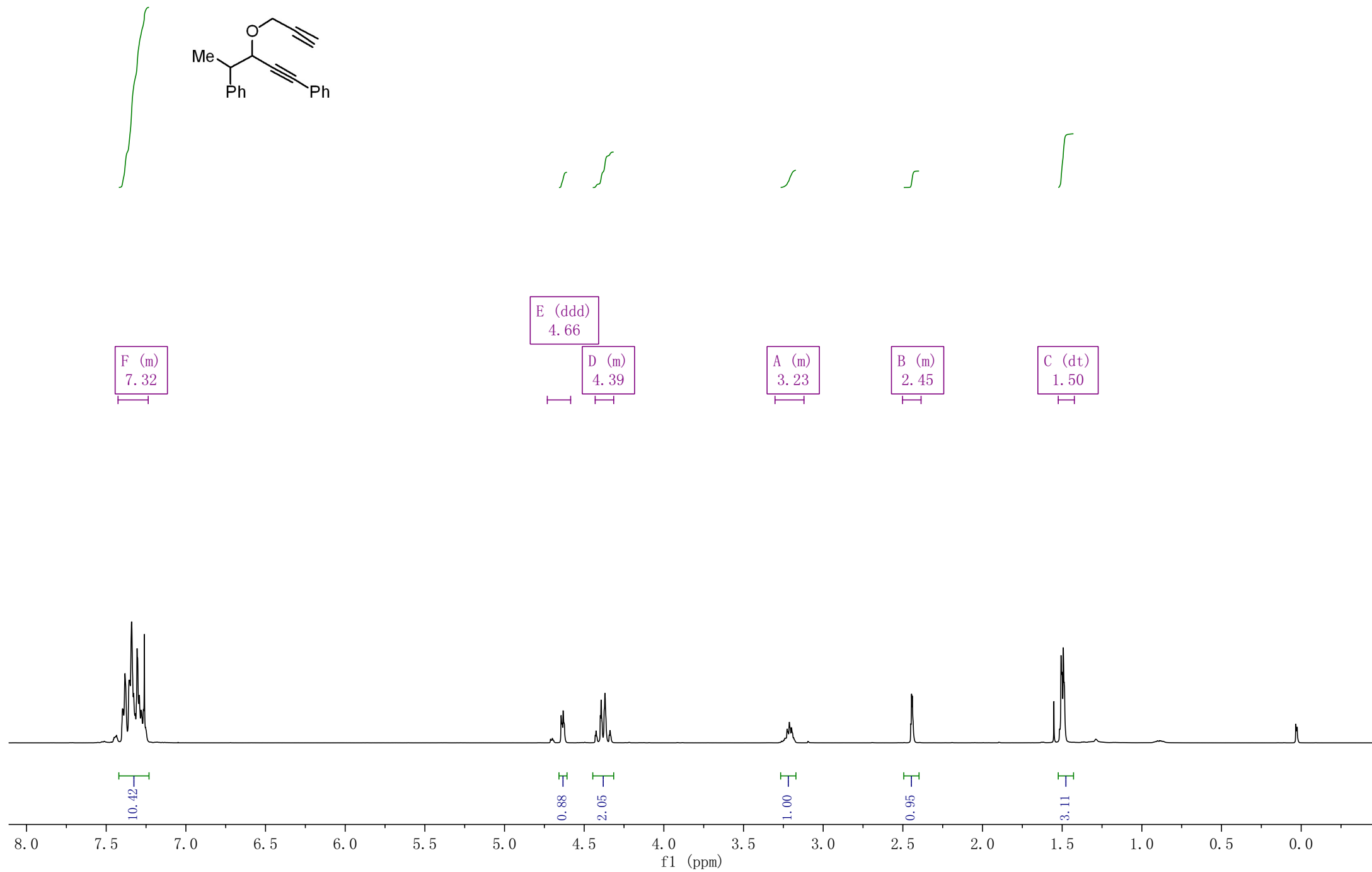
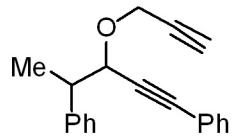
90.60

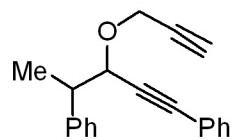
80.59
79.30
77.25
77.00
76.75
74.69
69.81

56.01

41.86







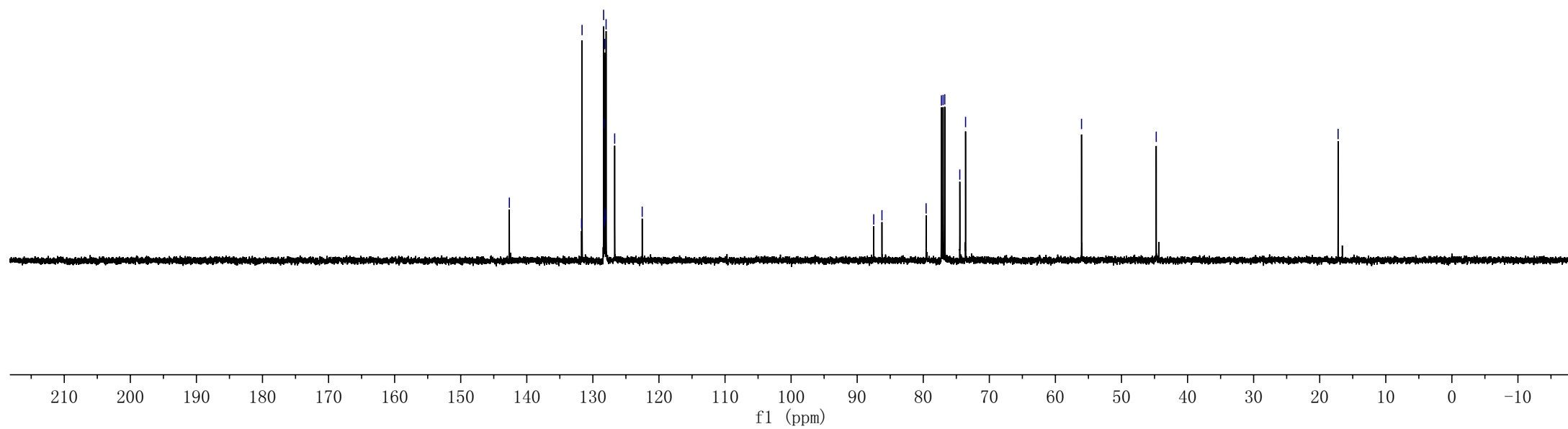
142.64
131.71
131.64
128.38
128.34
128.26
128.19
128.15
128.11
128.00
126.70
122.53

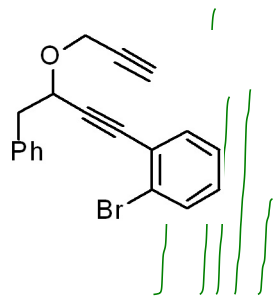
87.50
86.25
79.57
77.25
77.00
76.75
74.47
73.60

56.05

44.74

17.22





H (m)
7.27

F (m)
7.41

E (dd)
7.59

I (td)
7.18

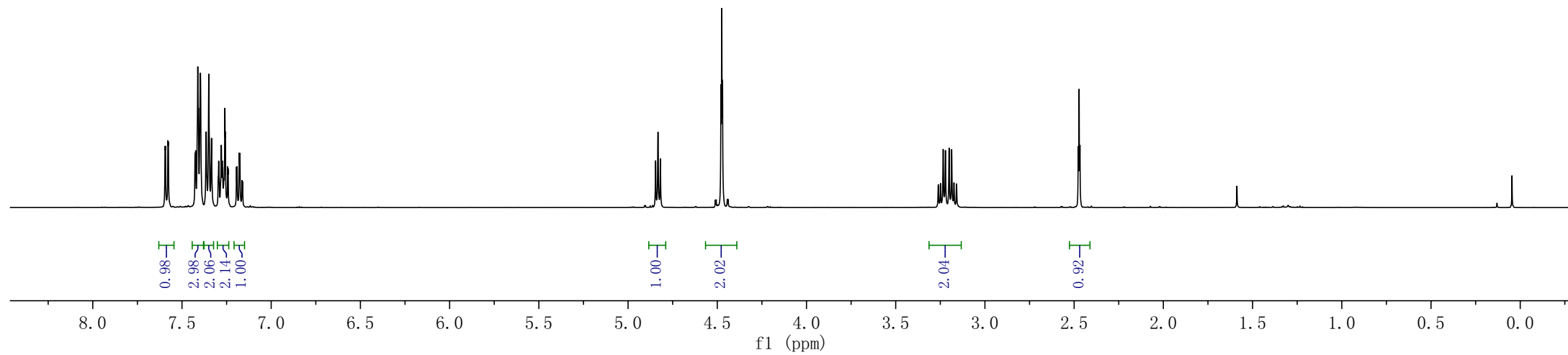
G (dd)
7.35

A (dt)
4.85

B (m)
4.47

C (ddd)
3.21

D (t)
2.47



136.63
133.41
132.30
129.74
129.60
128.16
126.89
126.66
125.42
124.54

91.29

85.76

79.32

77.25

77.00

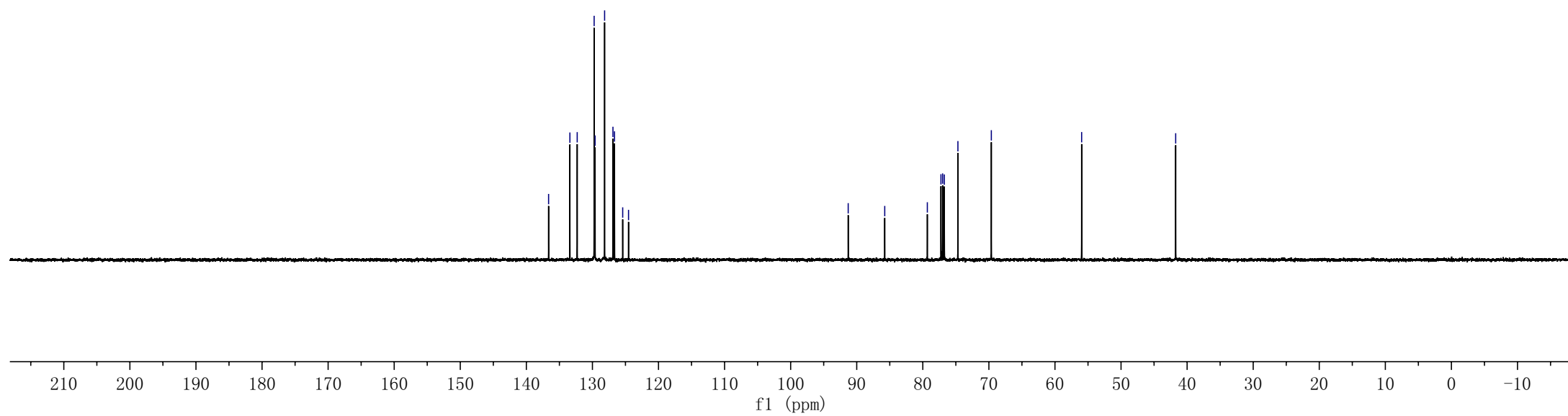
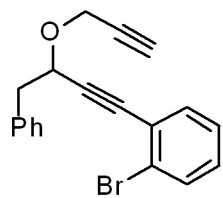
76.75

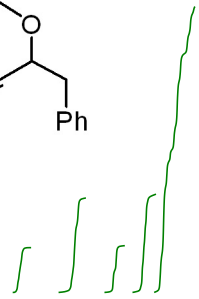
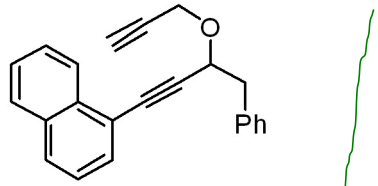
74.69

69.63

55.96

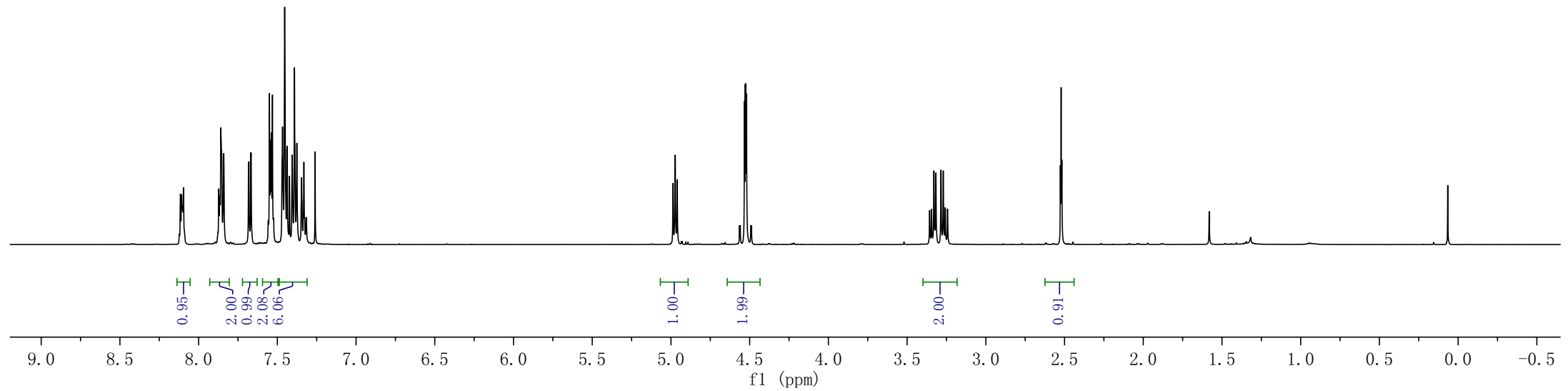
41.73

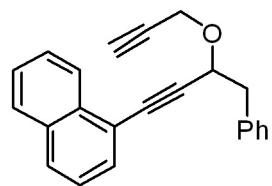




F (m)	I (m)
7.86	7.39
E (m)	G (dd)
8.11	7.67
	H (m)
	7.54

A (m)	B (m)	C (ddd)	D (t)
4.96	4.53	3.30	2.52





136.85
133.18
133.01
130.57
129.82
128.91
128.26
128.16
126.73
126.70
126.35
126.08
125.06
120.01

91.41

85.52

79.41

77.25

77.00

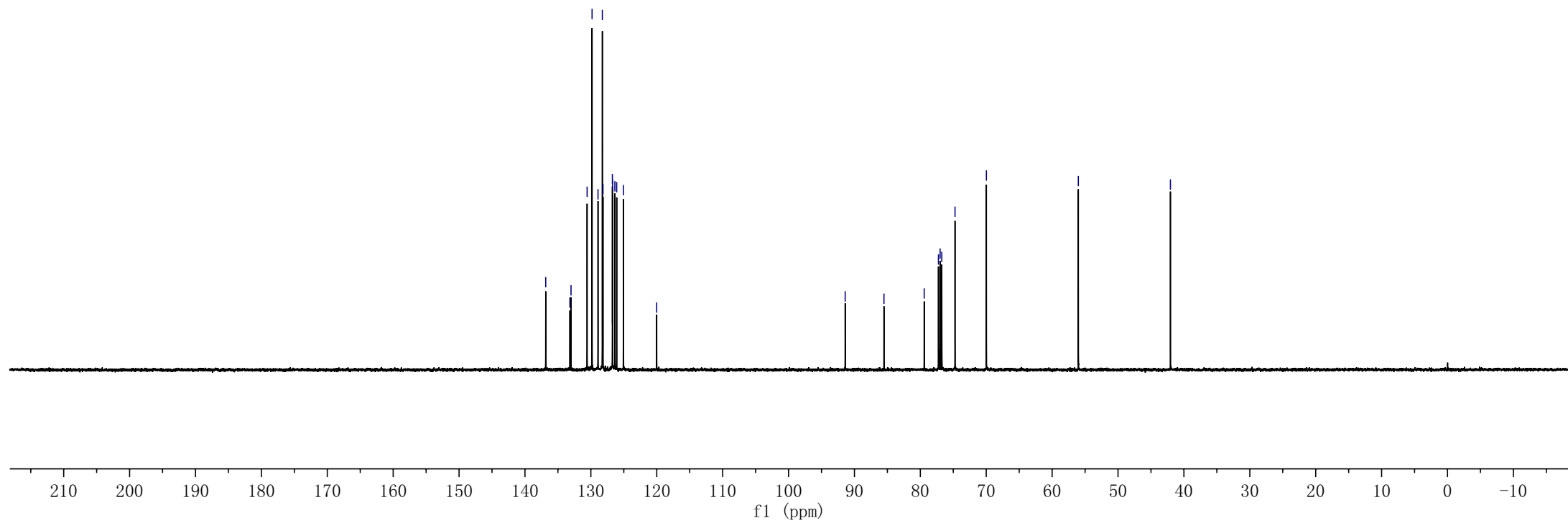
76.75

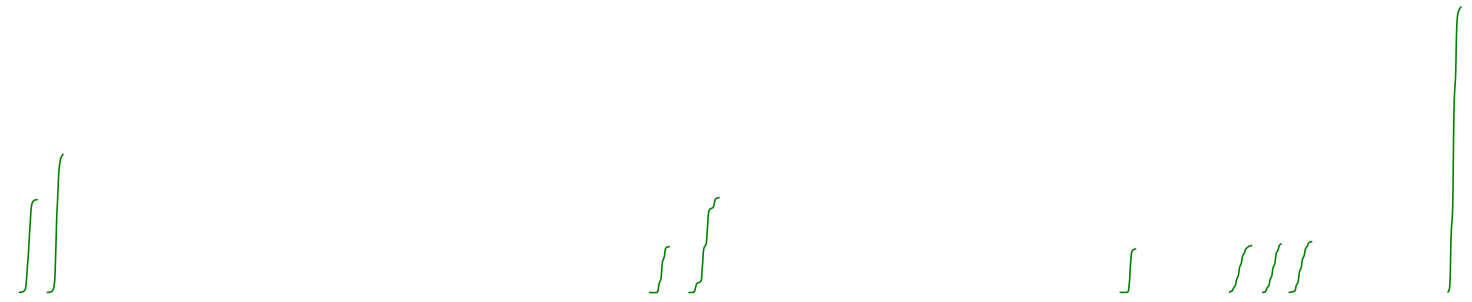
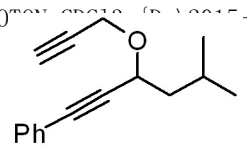
74.74

69.98

56.02

42.05





D (m)
7.31
C (dd)
7.44

B (qd)
4.37
A (t)
4.57

G (dt)
1.80
E (t)
2.45
F (tt)
1.94
H (dt)
1.67

I (t)
0.98

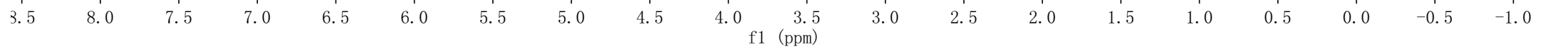
2.00
2.98

0.99
2.04

0.94

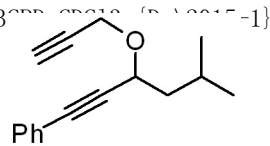
1.01
1.05
1.10

6.15



JKG-20150316-1-68A

C13 NMR (CDCl₃) {J=125.1 Hz}



138.74

128.38

128.26

122.61

87.51

86.13

79.70

77.25

77.00

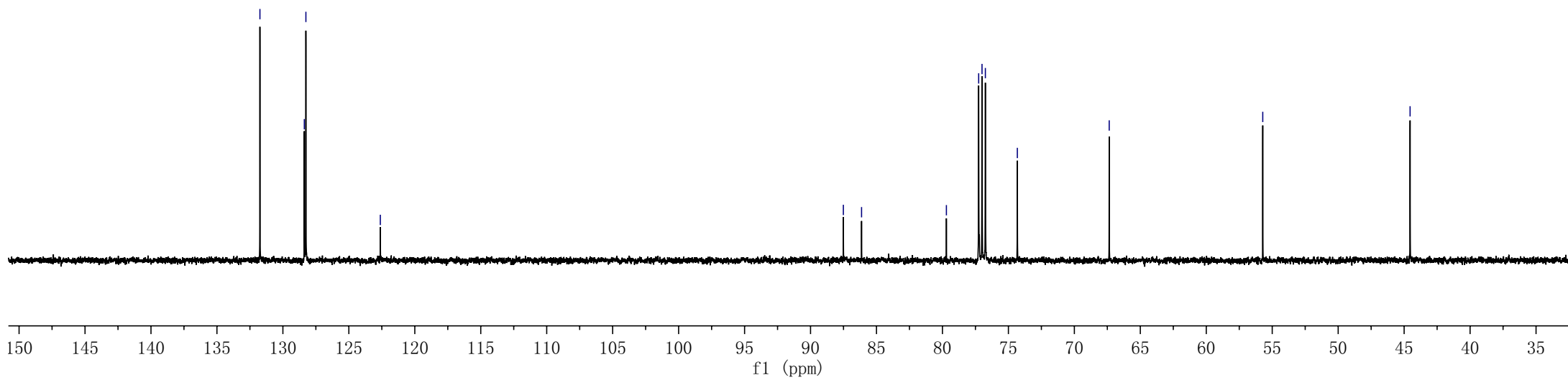
76.75

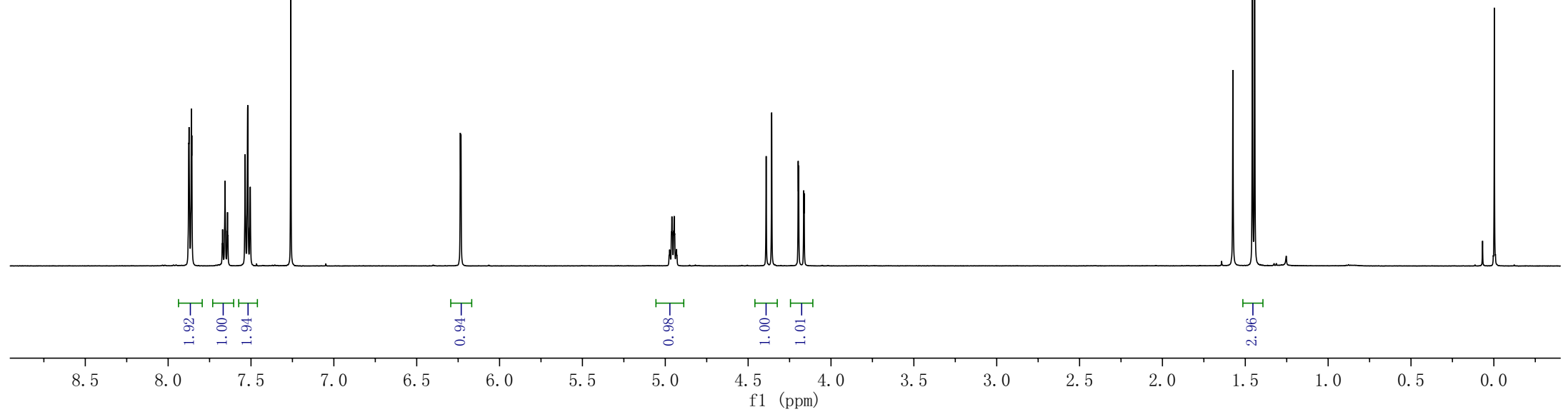
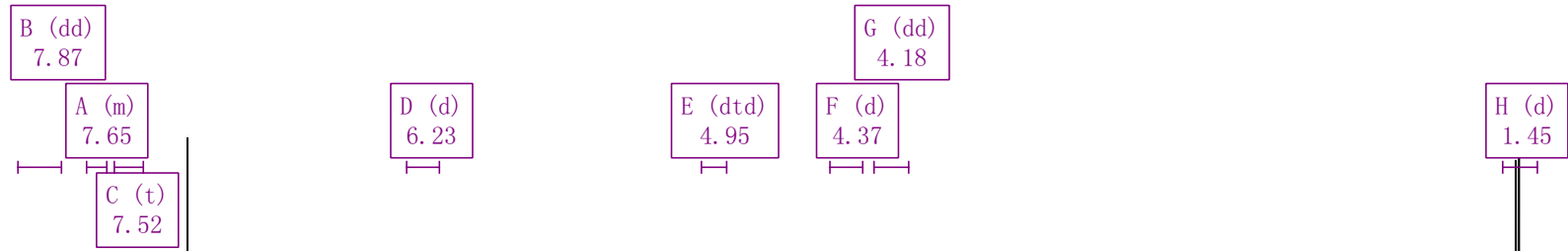
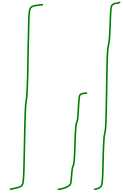
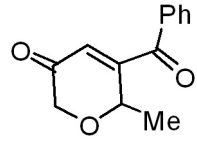
74.32

67.36

55.72

44.55





JKG-20150508-LX-118D
C13CPD CDC13 {DMSO-d6-15-1} ZHL 4

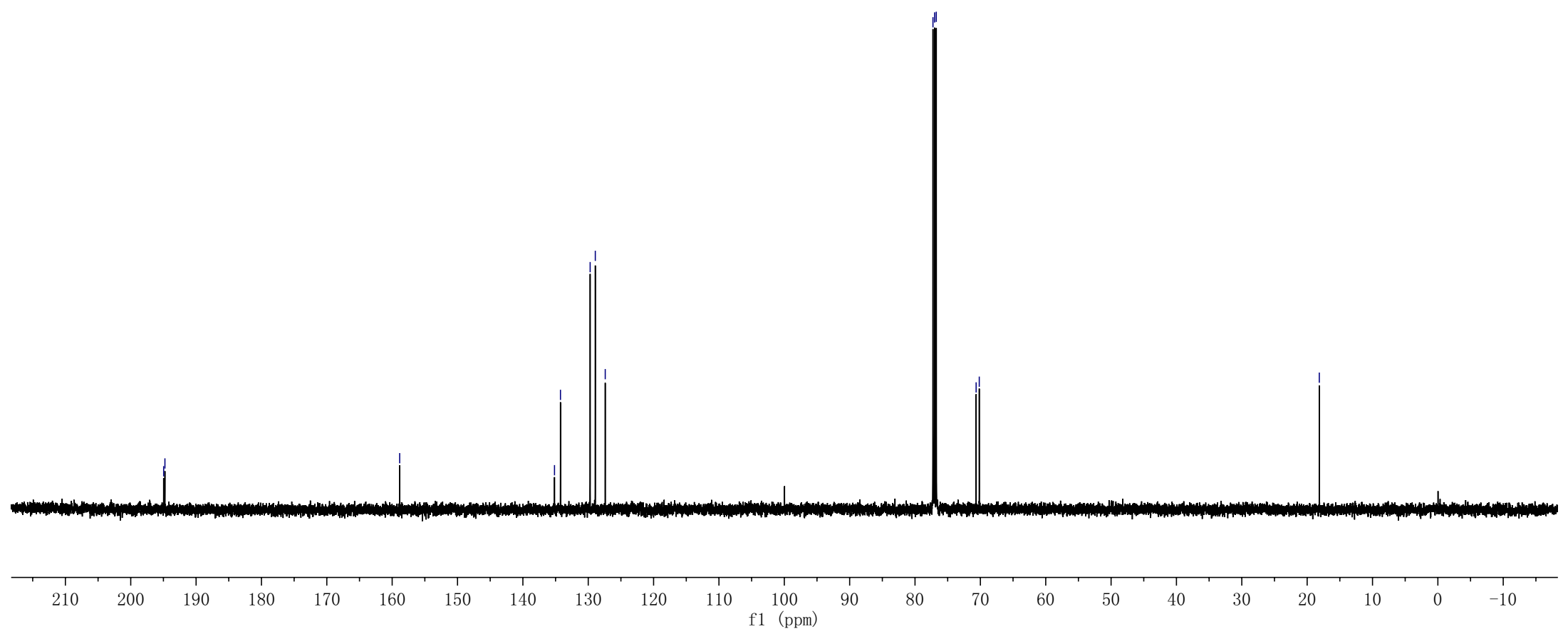
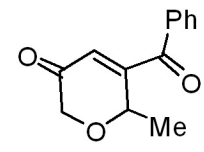
197.94
195.77

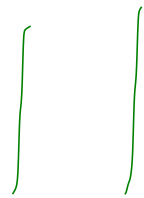
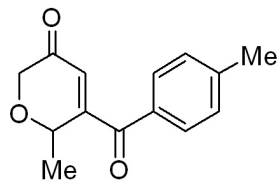
158.85

135.16
134.25
129.71
128.92
127.40

77.25
77.00
76.75
70.65
70.17

18.14





F (d)
7.83

E (d)
7.36

D (s)
6.26

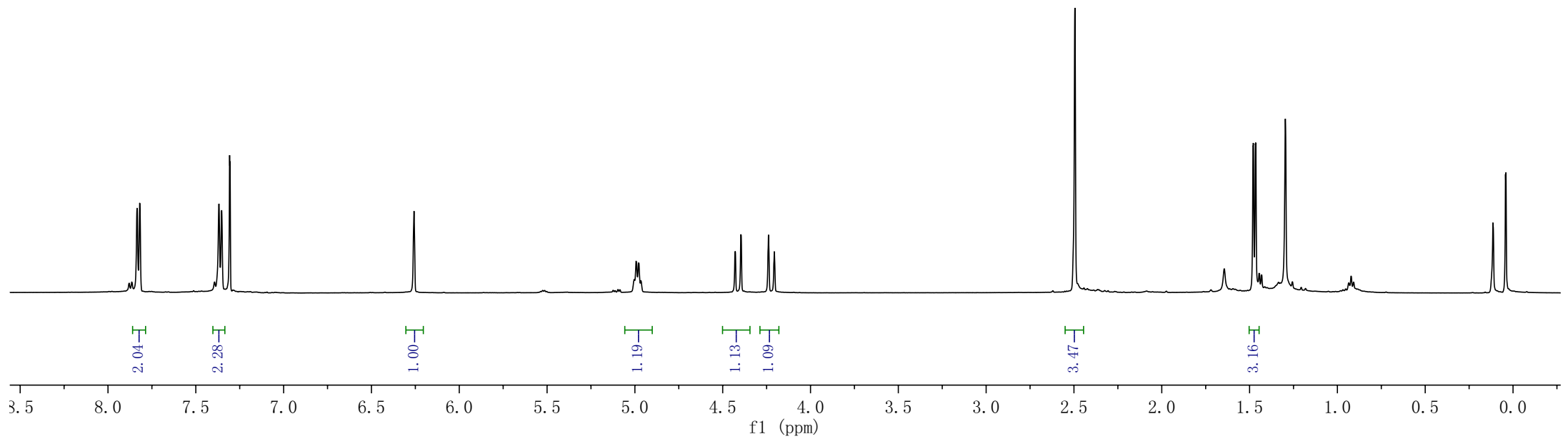
A (dd)
4.99

B (d)
4.41

C (d)
4.22

G (s)
2.49

H (m)
1.47



191.86
190.39

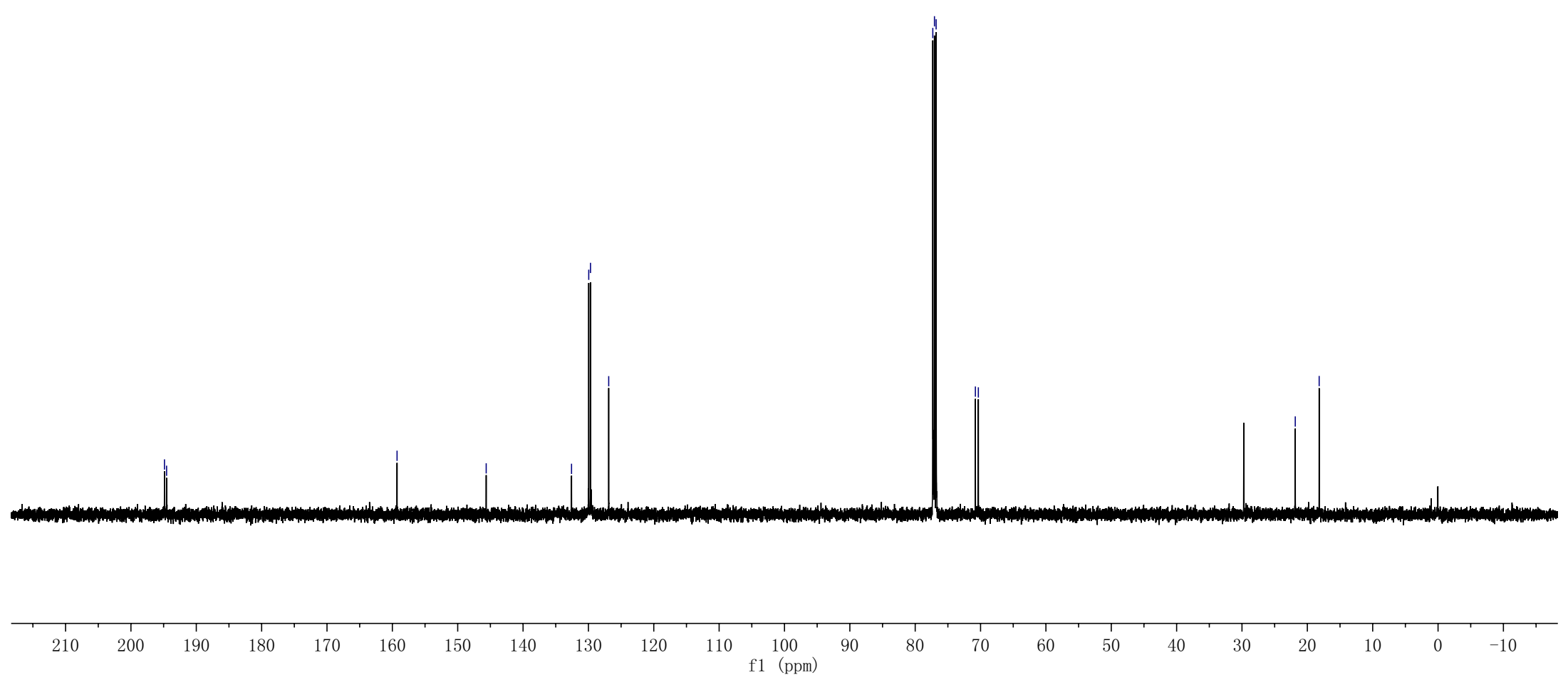
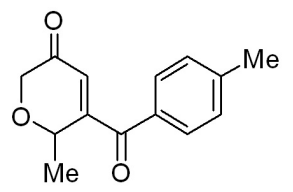
159.28

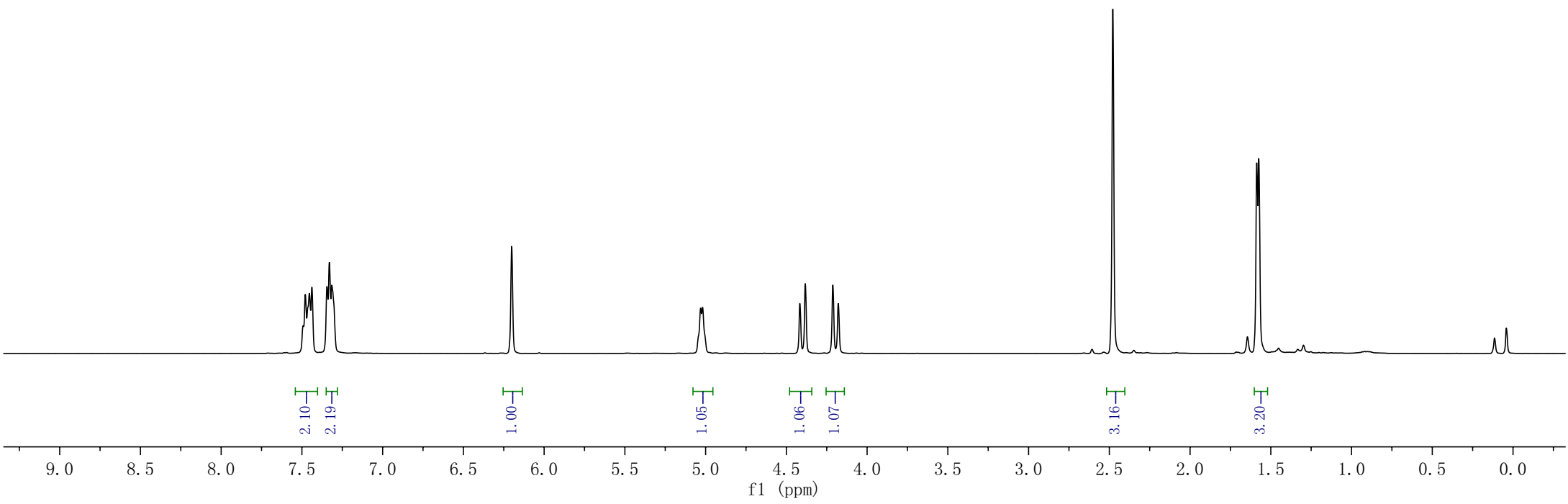
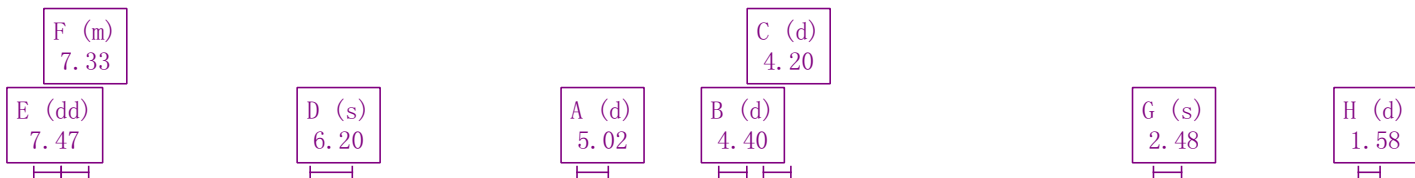
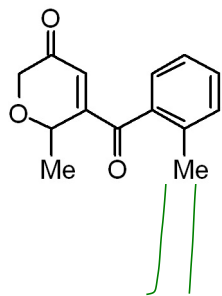
145.64

132.58
129.95
129.68
126.90

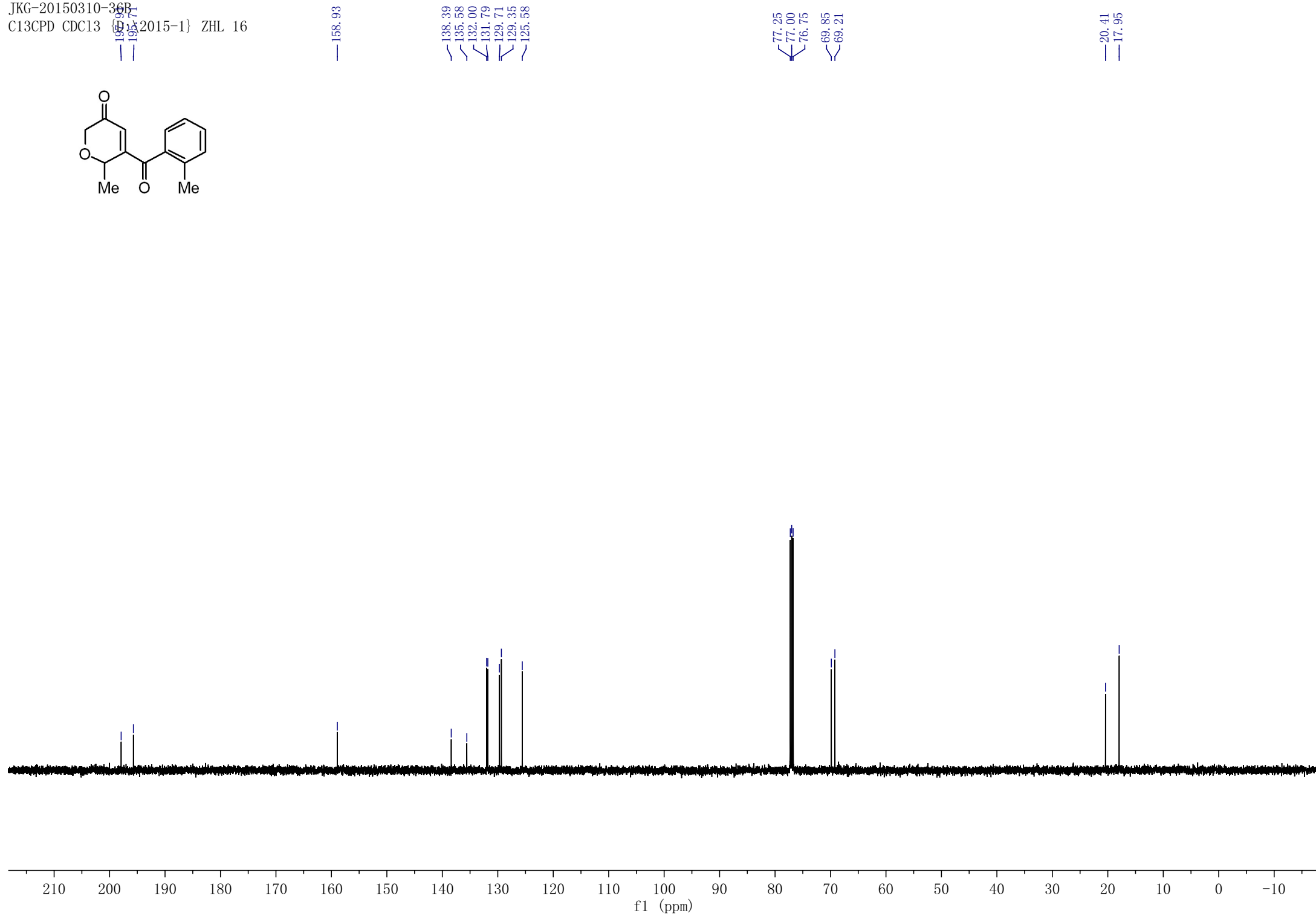
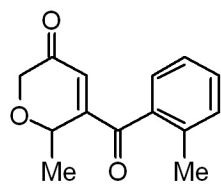
77.31
77.05
76.80
70.79
70.34

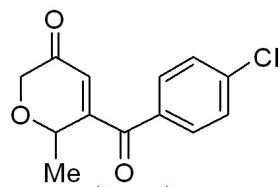
21.85
18.19





JKG-20150310-36P
C13CPD CDC13 (QNP 101) 2015-1} ZHL 16





D (m)
7.86

C (m)
7.55

B (d)
6.26

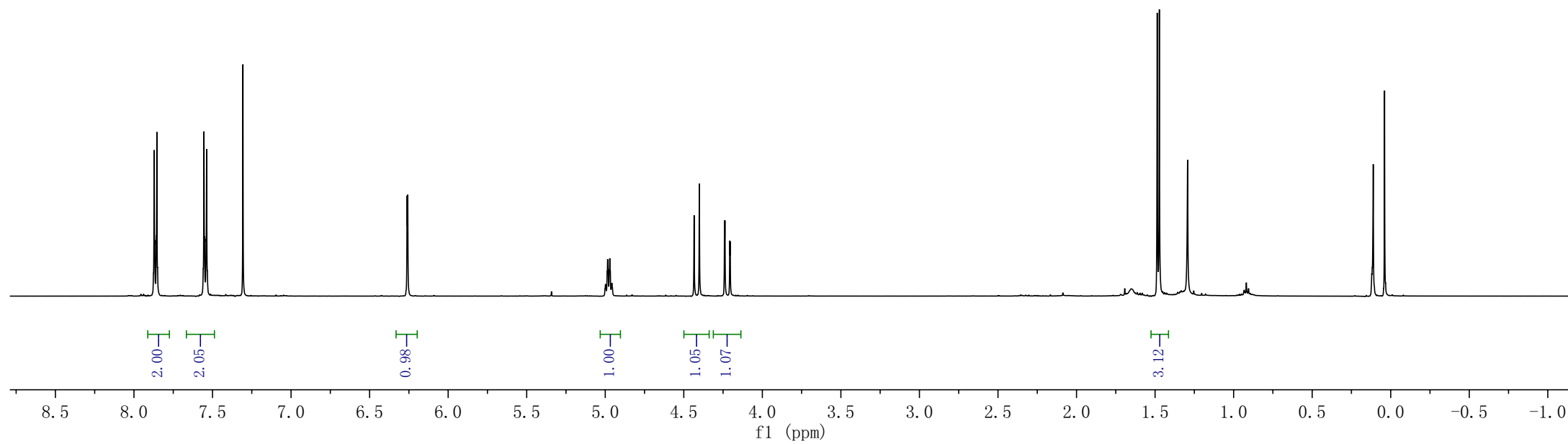
E (m)
4.98

A (m)
4.98

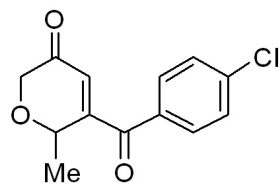
G (dd)
4.22

F (d)
4.42

H (d)
1.48



JKG-20150311-I-36B
C13CPD CDC13 {D:2015-1} ZHL 15



194.88
194.80

158.36

141.03

133.37

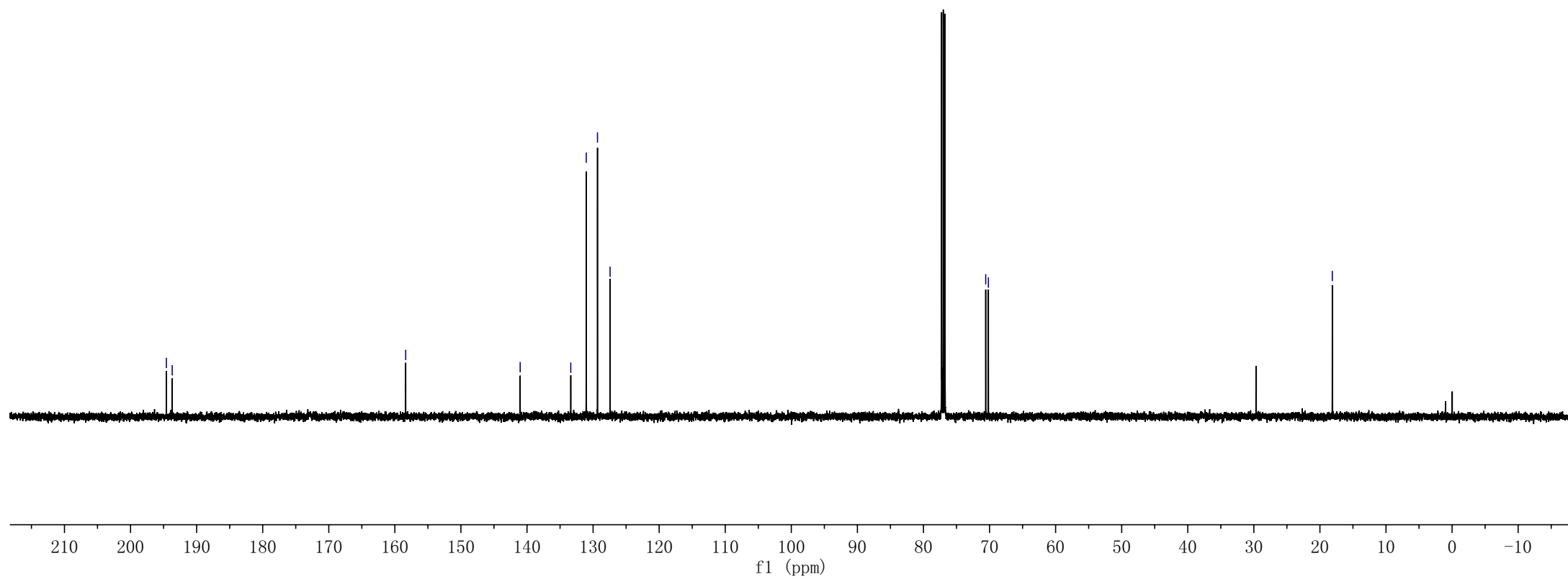
131.03

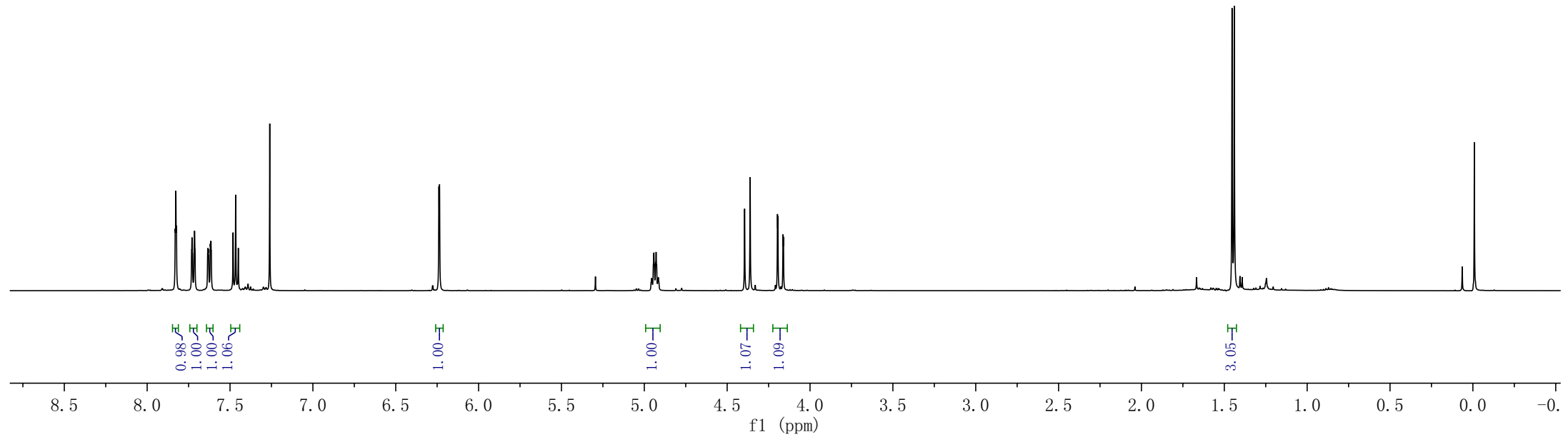
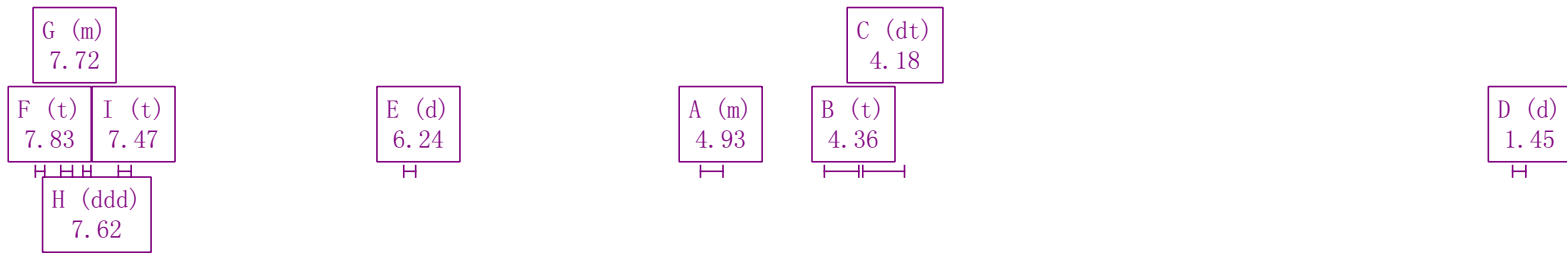
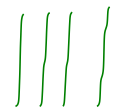
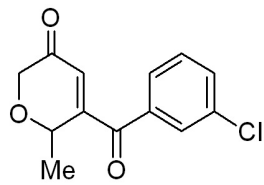
129.33

127.43

70.58
70.17

18.13





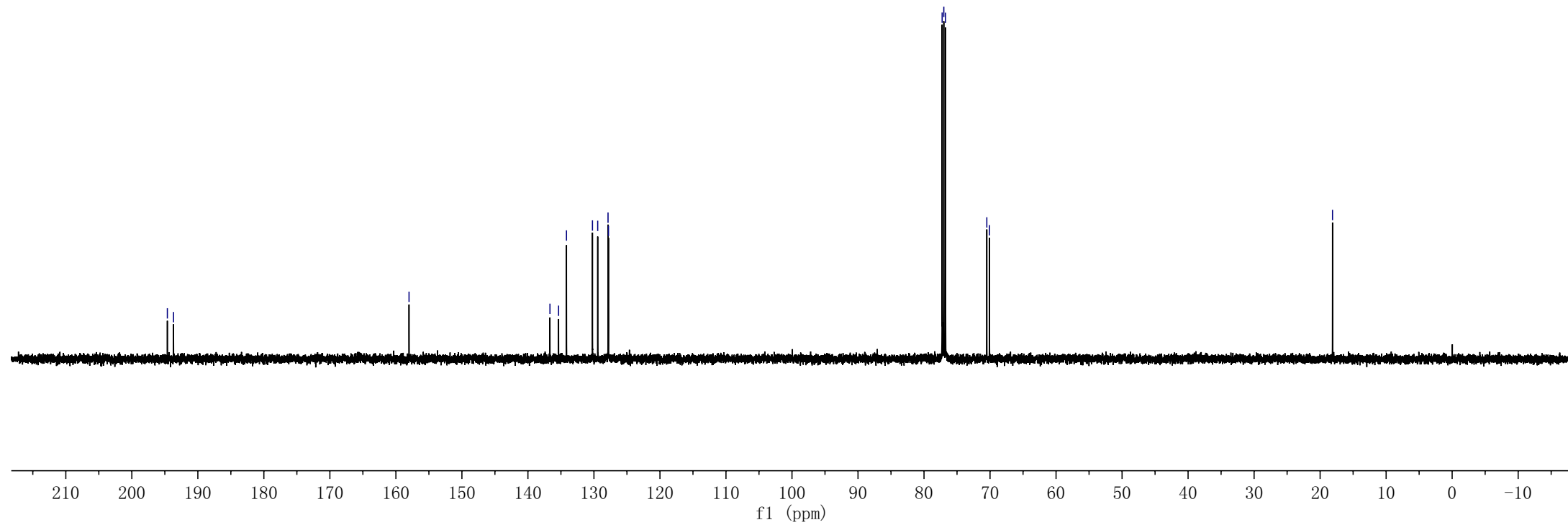
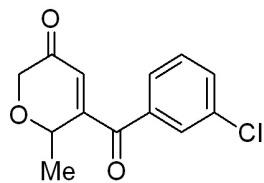
194.63
192.67

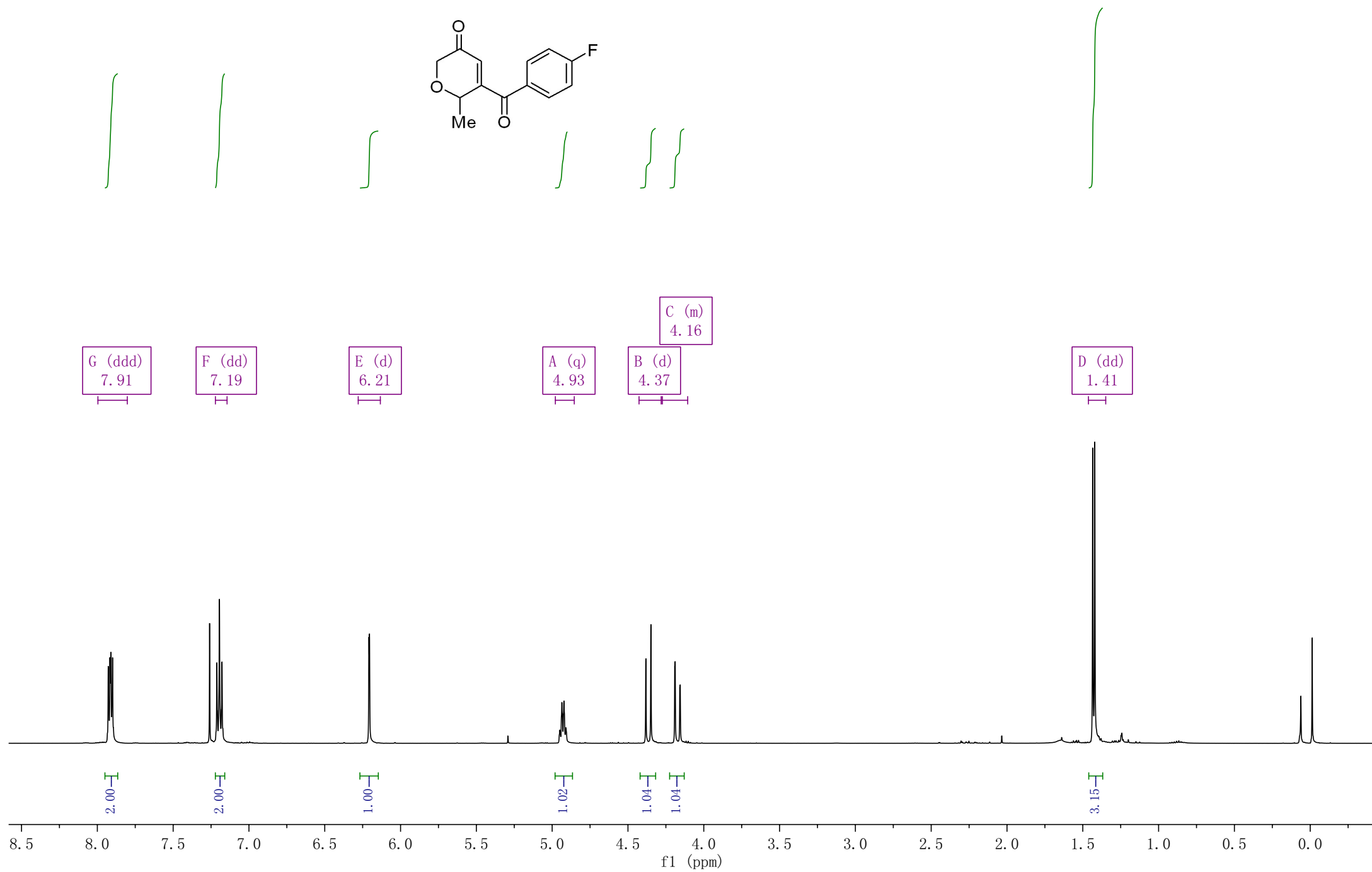
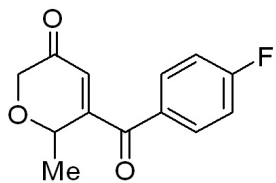
158.01

136.66
135.36
134.16
130.22
129.43
127.86
127.80

77.25
77.00
76.75
70.49
70.09

18.12





JKG-20150311-I-38B
C13CPD CDC13 {D:\2015-1} ZHL 12

194.88
194.82

167.46
165.41

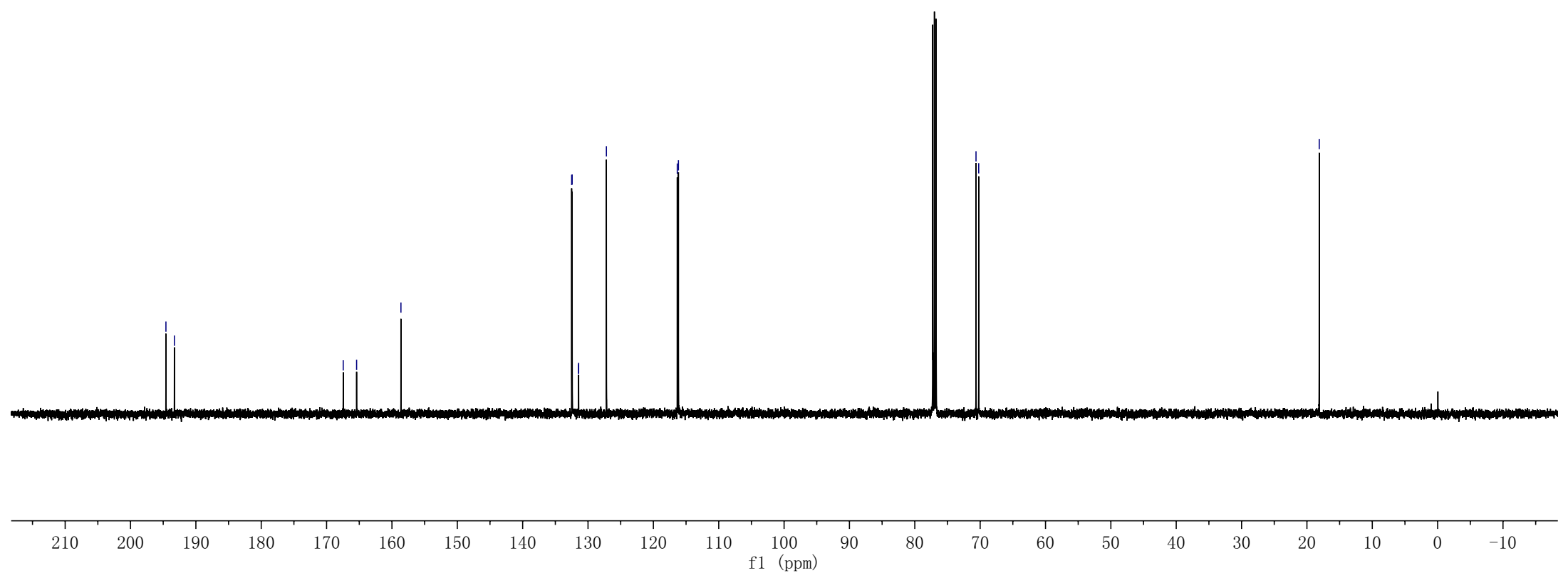
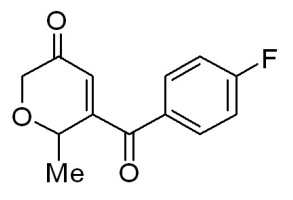
158.62

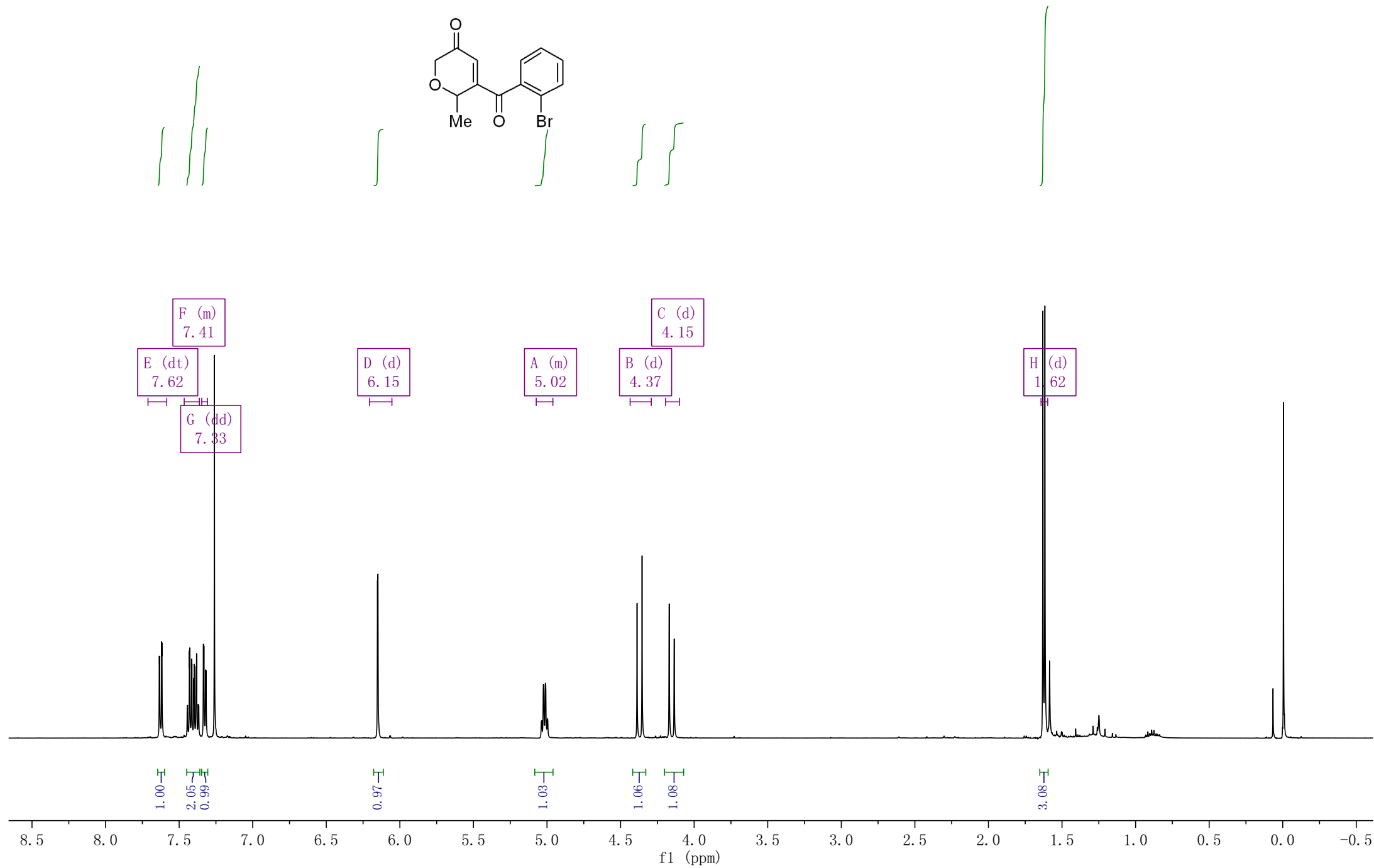
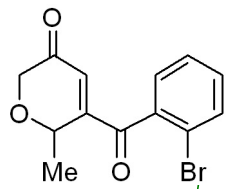
132.50
132.43
131.46
131.43
127.19

116.34
116.17

70.63
70.22

18.12





196.34
194.66

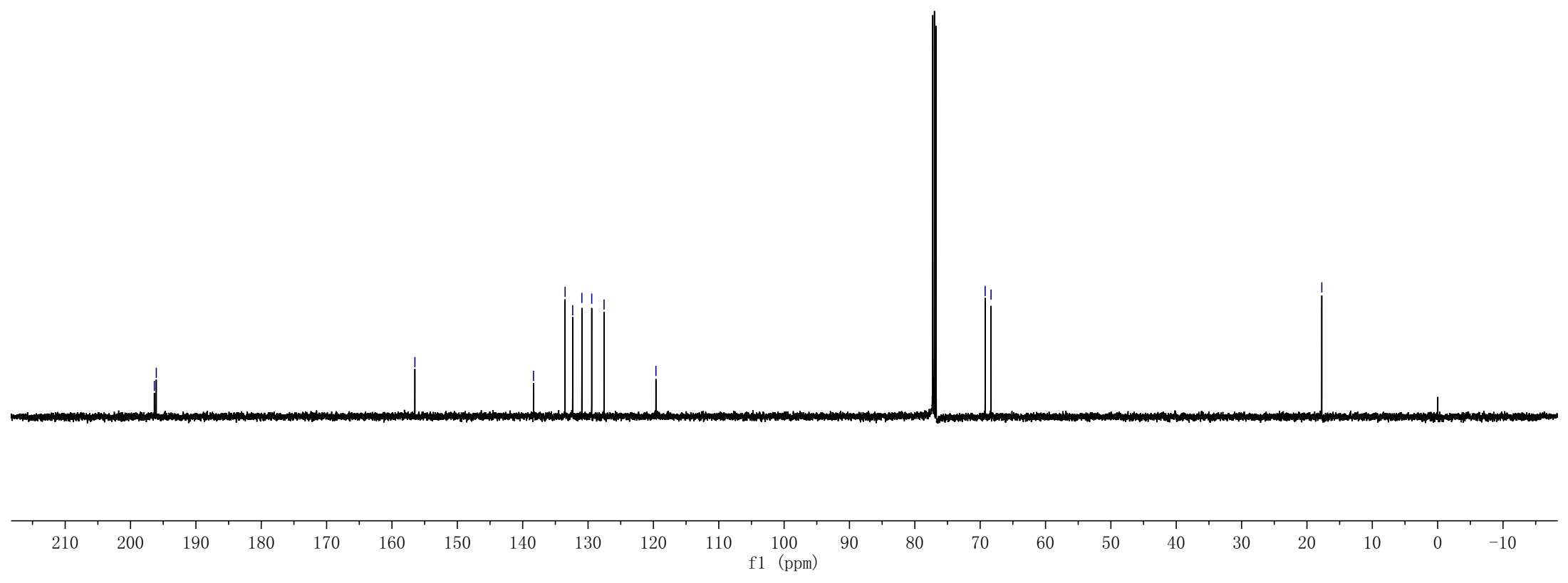
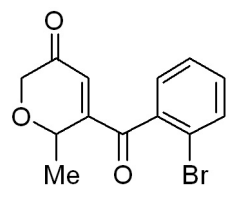
156.49

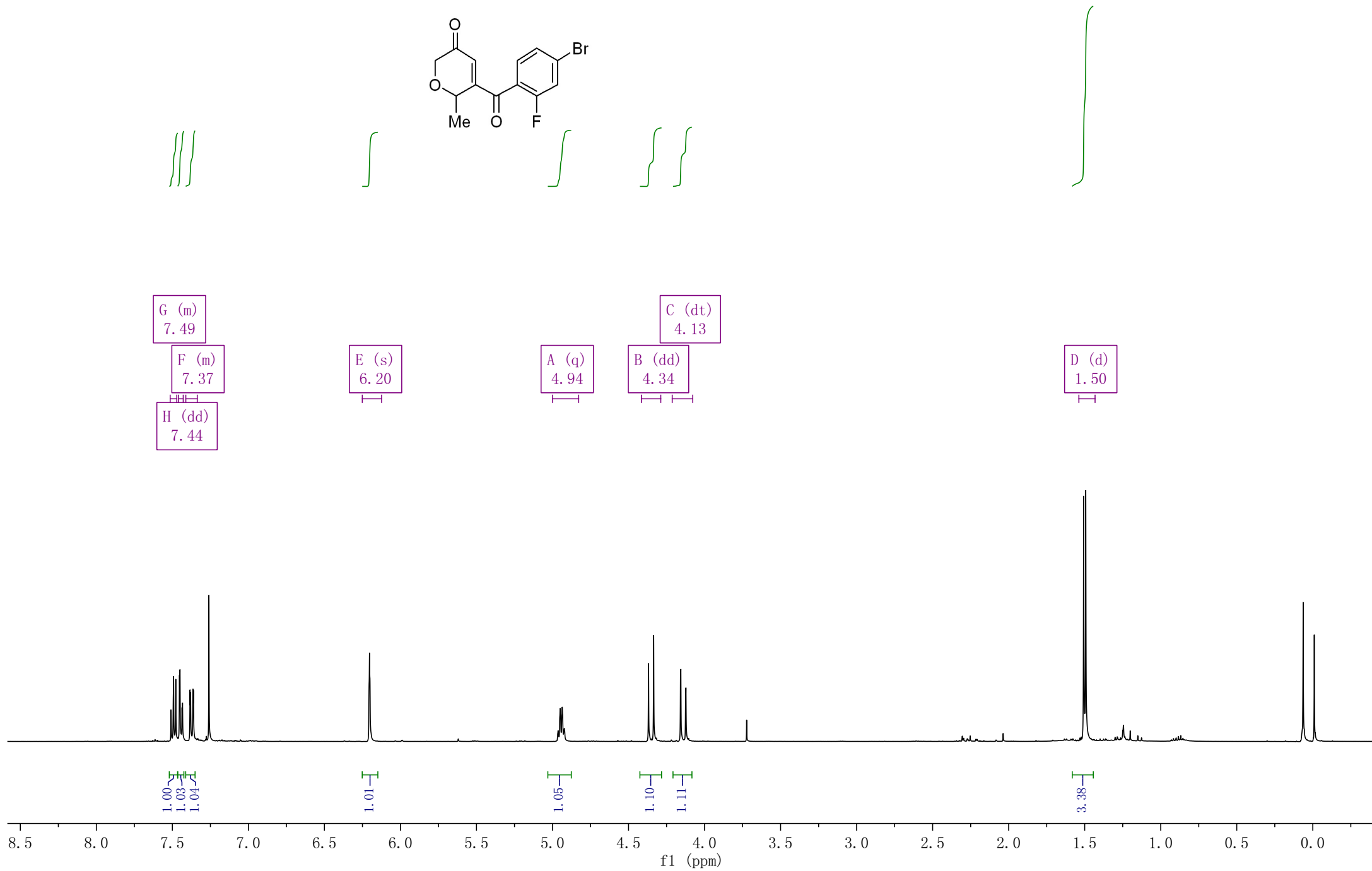
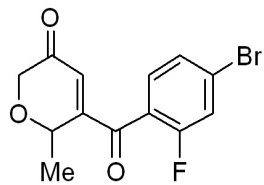
138.35
133.51
132.35
130.94
129.44
127.55

119.61

69.24
68.34

17.73





JKG-20150311-I-48A
C13CPD CDC13 {D:2015-1} ZHL 10

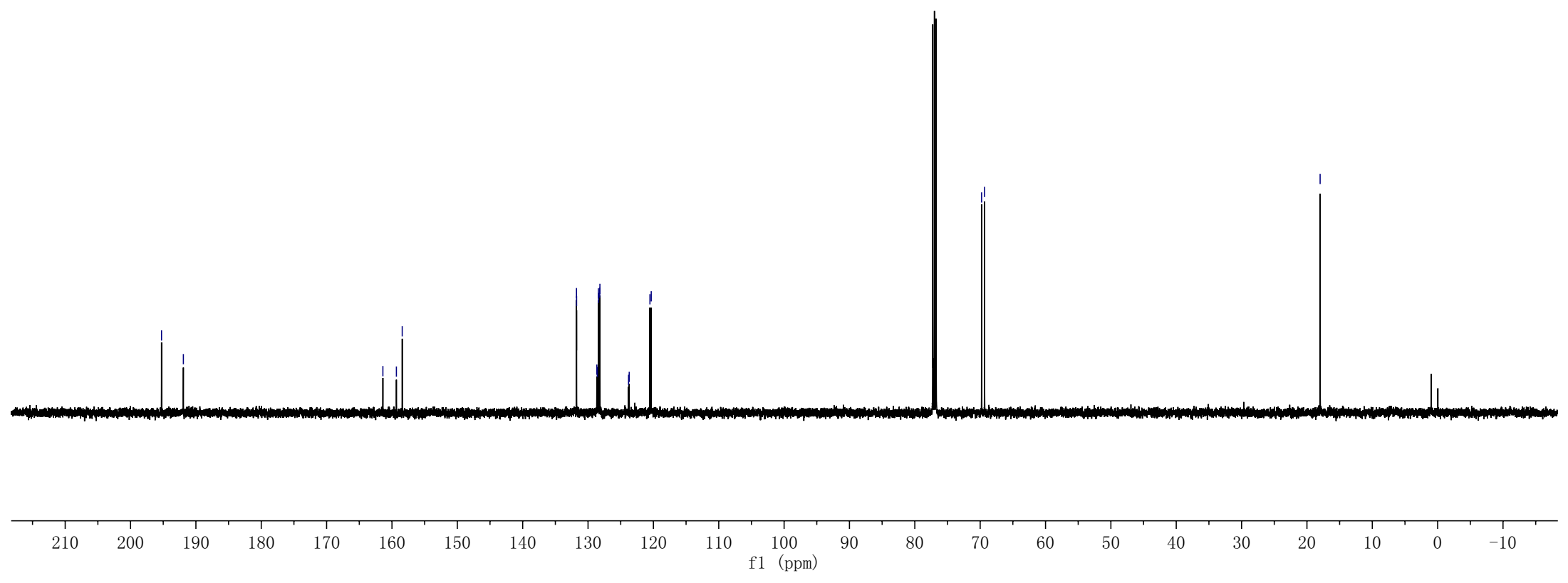
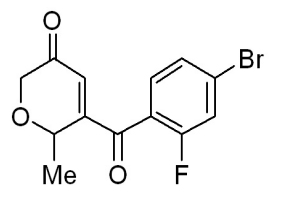
195.26
194.32

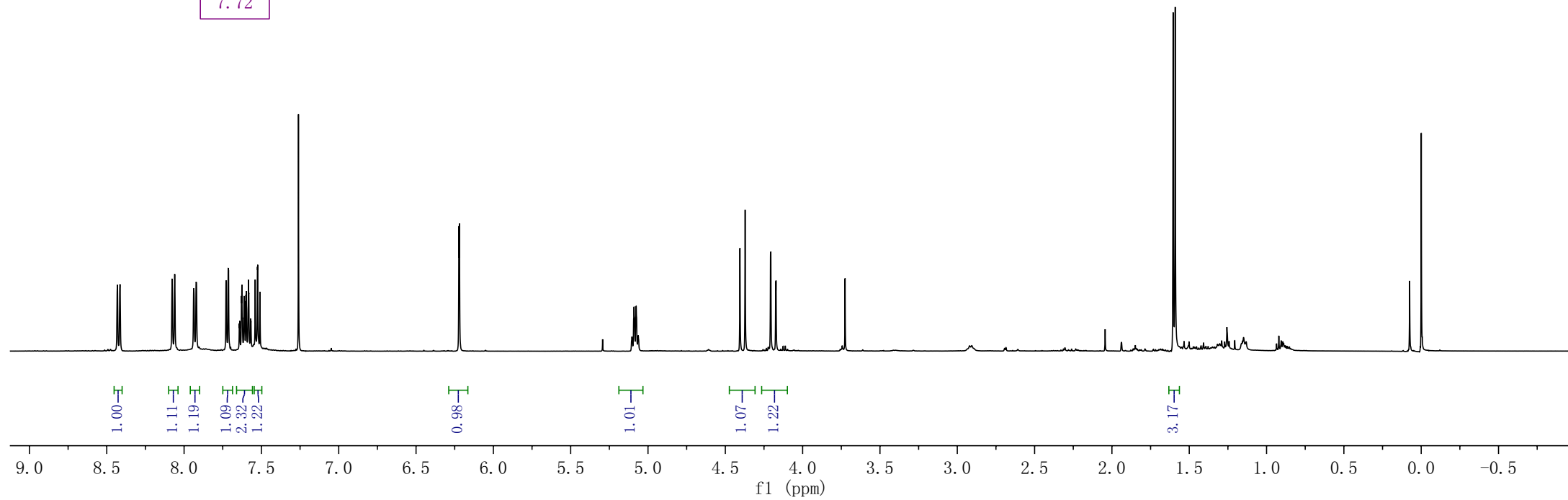
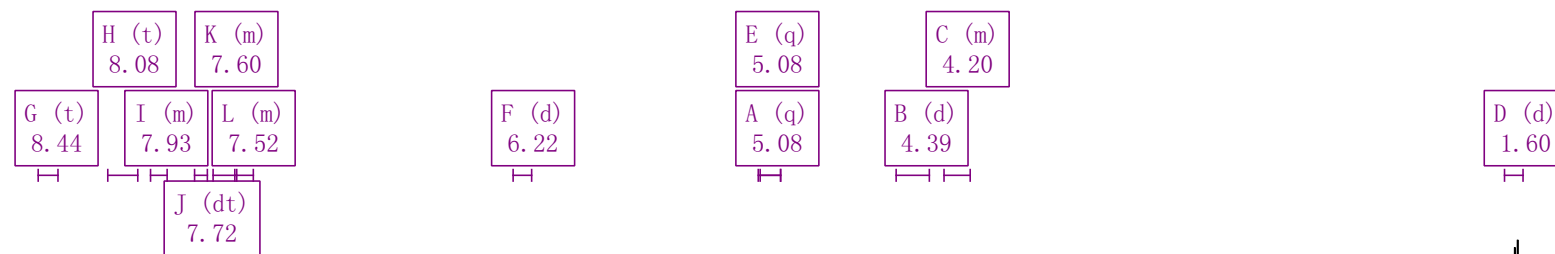
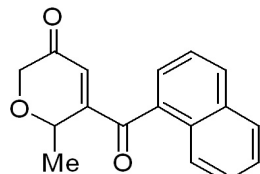
161.39
159.32
158.43

131.77
131.75
128.66
128.58
128.42
128.39
128.21
128.18
123.80
123.70
120.53
120.33

69.78
69.33

17.98





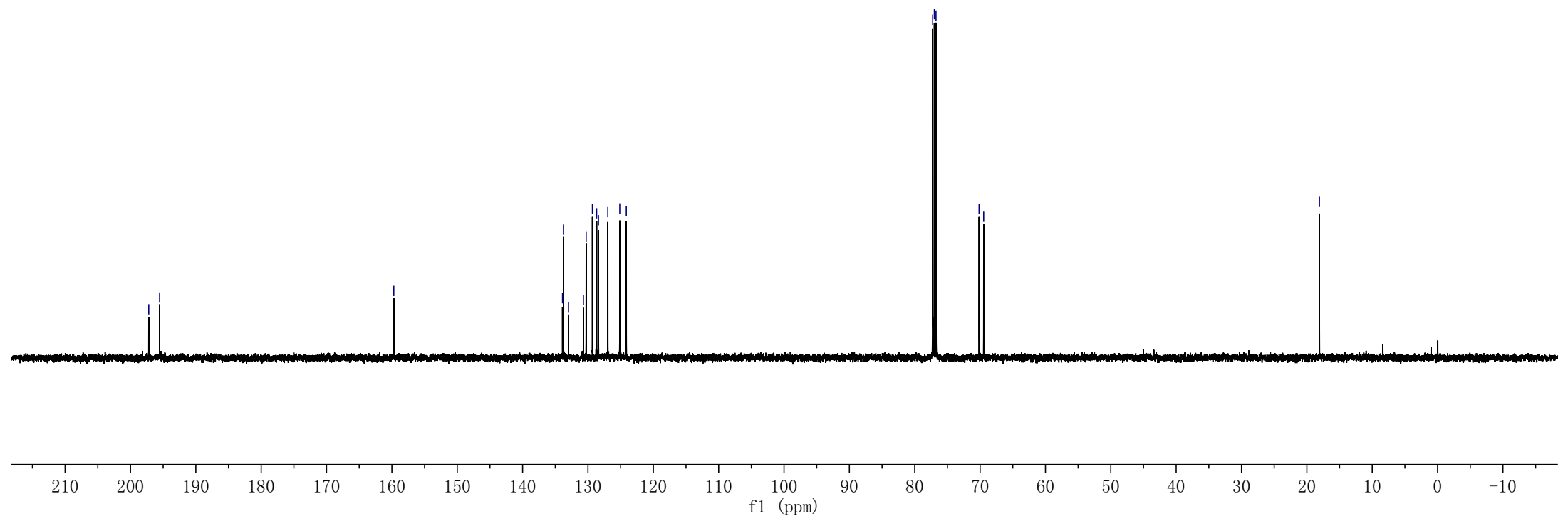
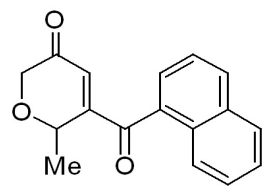
197.90
196.84

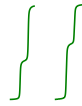
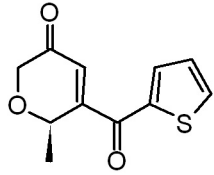
159.71

133.90
133.75
132.98
130.70
130.27
129.32
128.67
128.40
126.96
125.13
124.13

77.25
77.00
76.75
70.16
69.45

18.08





A (m)
7.83

C (m)
7.21

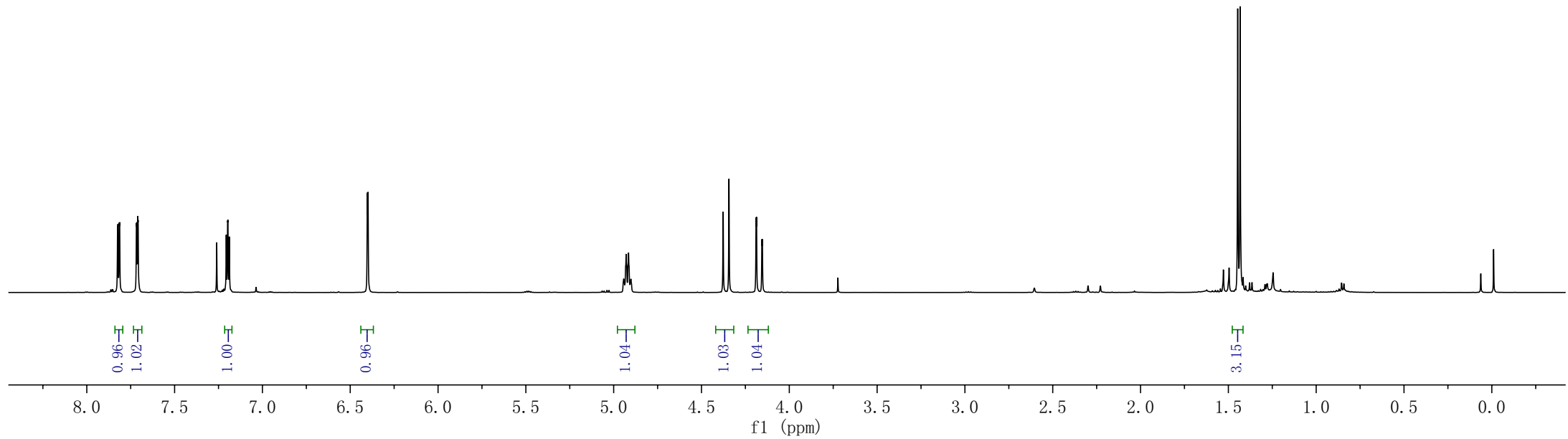
D (d)
6.40

E (q)
4.92

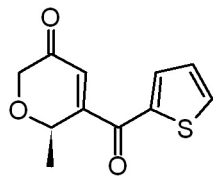
F (d)
4.36

G (dd)
4.17

H (d)
1.44



JKG-20141229-J-45A



194.75

186.28

158.88

142.06

136.60

135.32

128.61

126.48

77.25

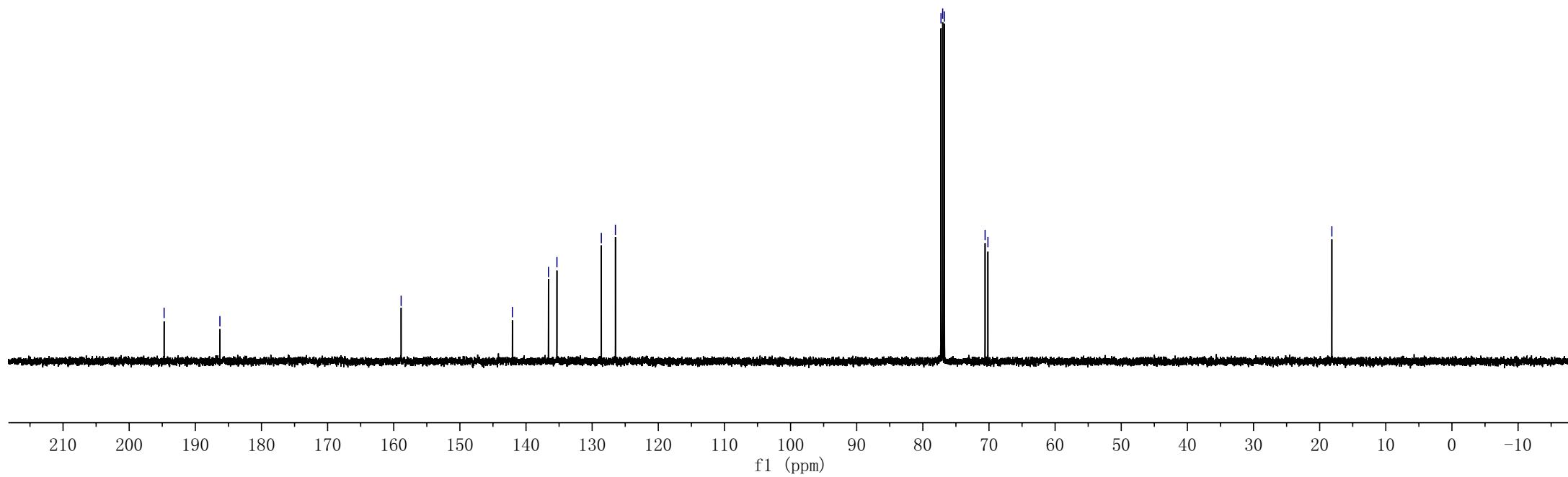
77.00

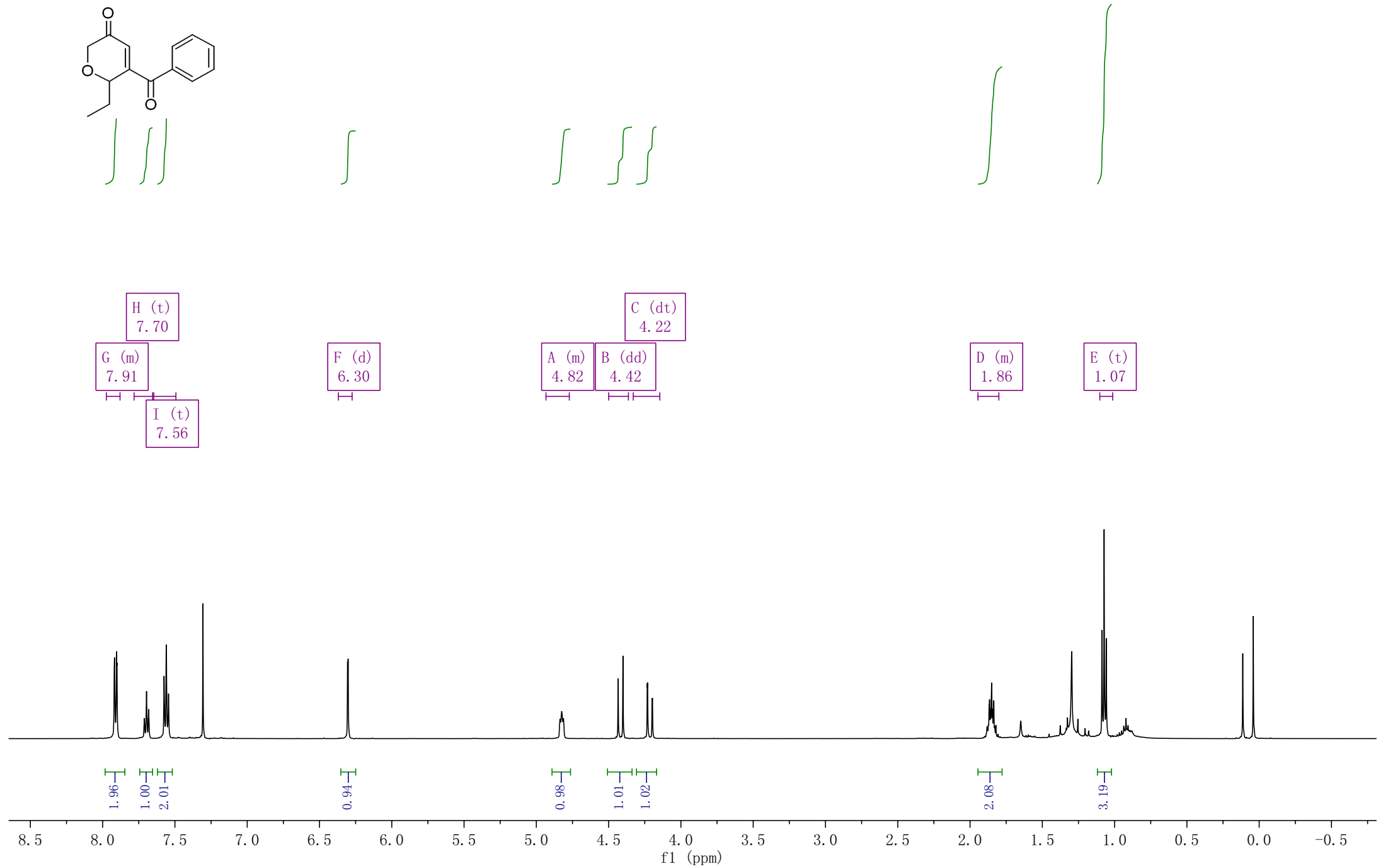
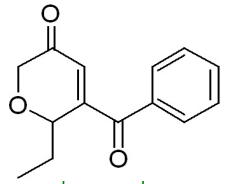
76.75

70.59

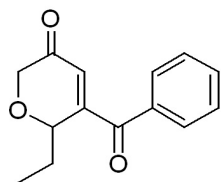
70.16

18.16





JKG-20150311-I-36A
C13CPD CDC13 {DMSO-2015-1} ZHL 9



195.85
194.84

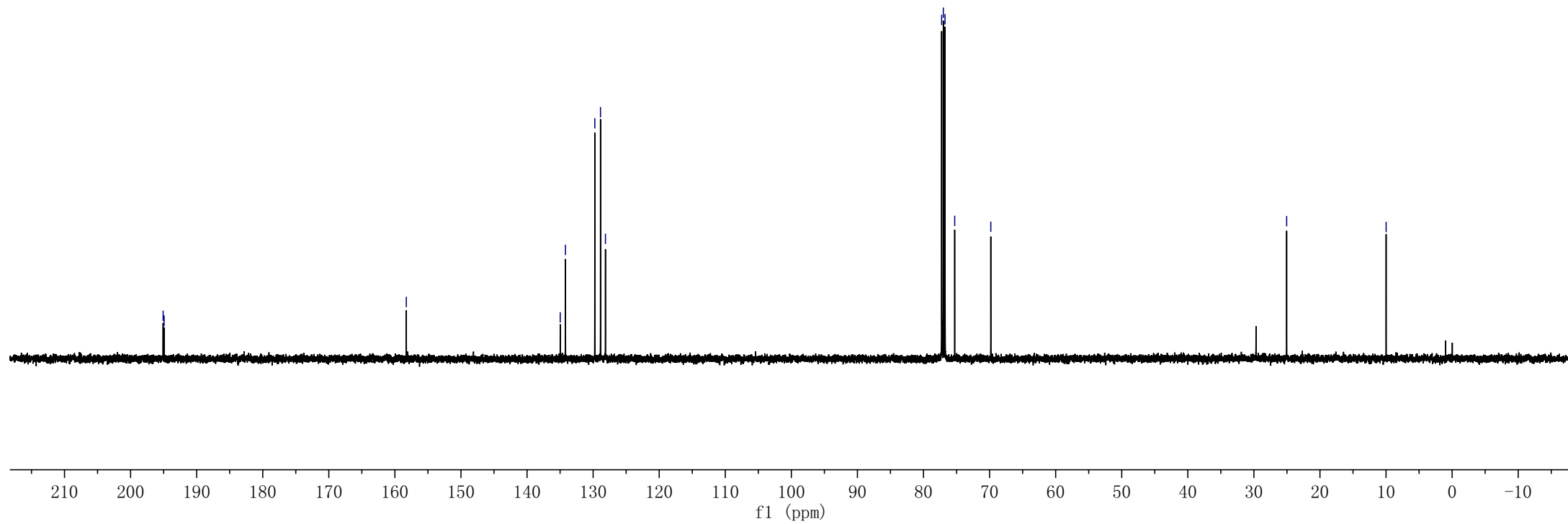
158.27

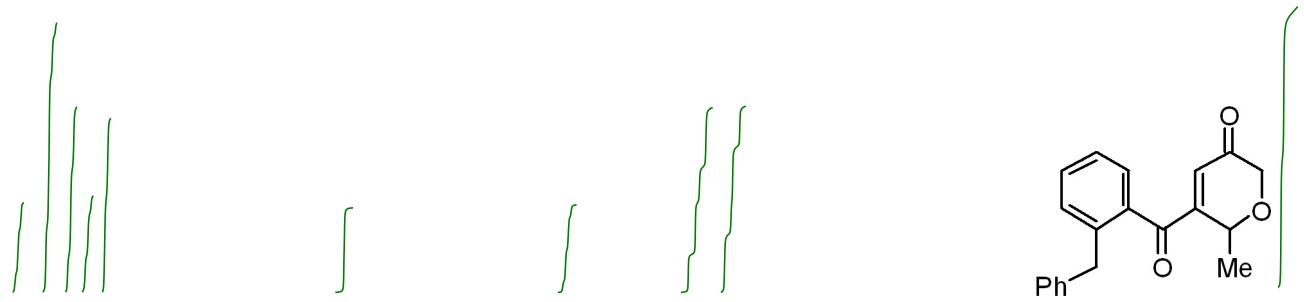
134.98
134.19
129.74
128.88
128.13

77.25
77.00
76.75
75.28
69.82

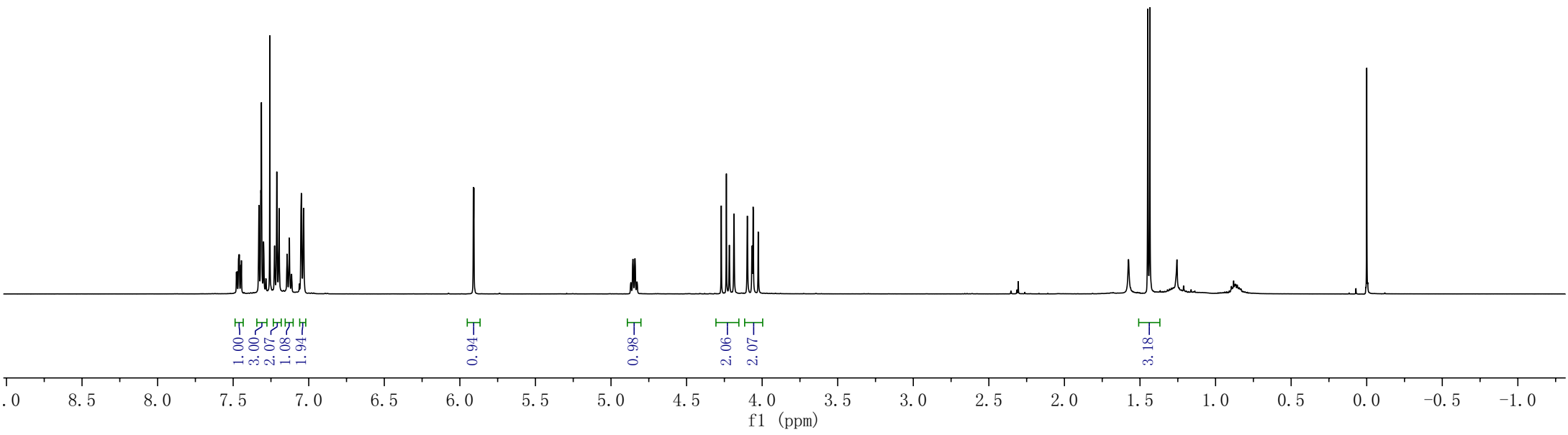
25.04

9.99

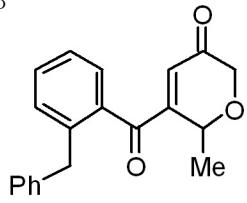




Label	Multiplicity	Chemical Shift (ppm)
I	(m)	7.31
G	(t)	7.13
J	(m)	7.46
F	(t)	7.05
H	(t)	7.21
E	(d)	5.91
A	(q)	4.85
B	(dd)	4.23
C	(m)	4.06
D	(d)	1.44



JKG-20150320-LX-I-2a
C13 NMR (CDCl₃) 125 MHz, 300 K, 1} ZHL 31



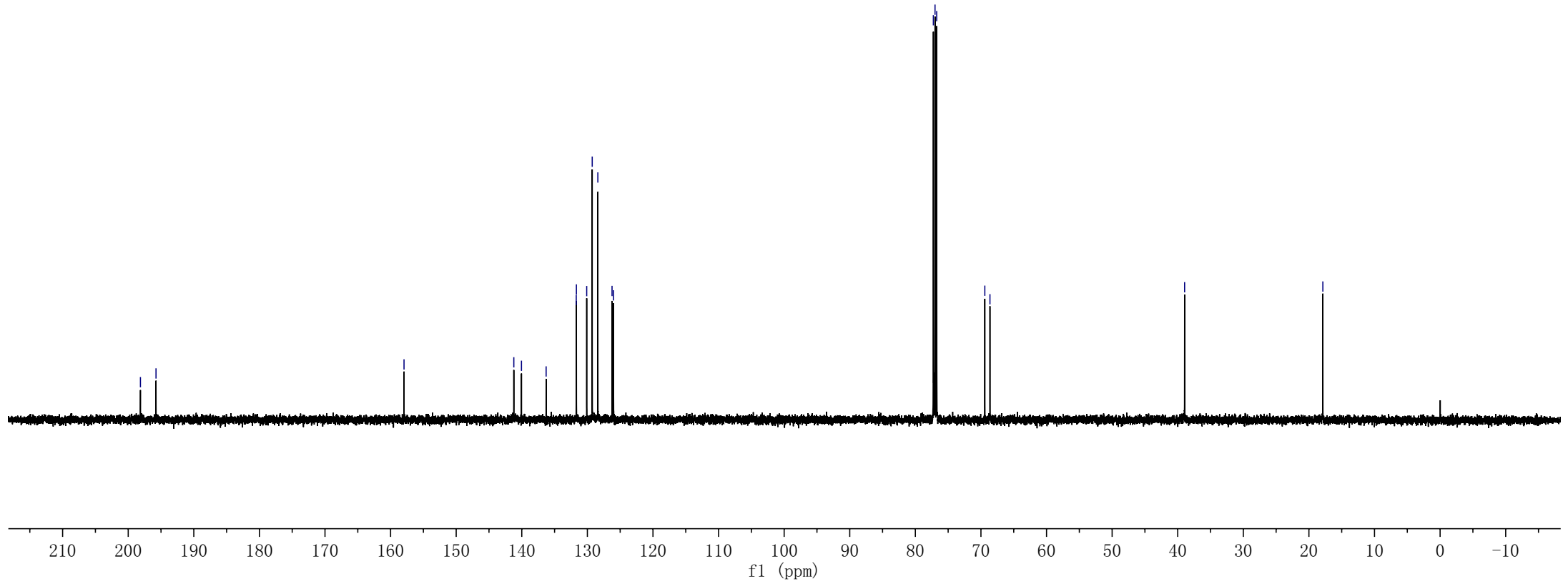
157.95

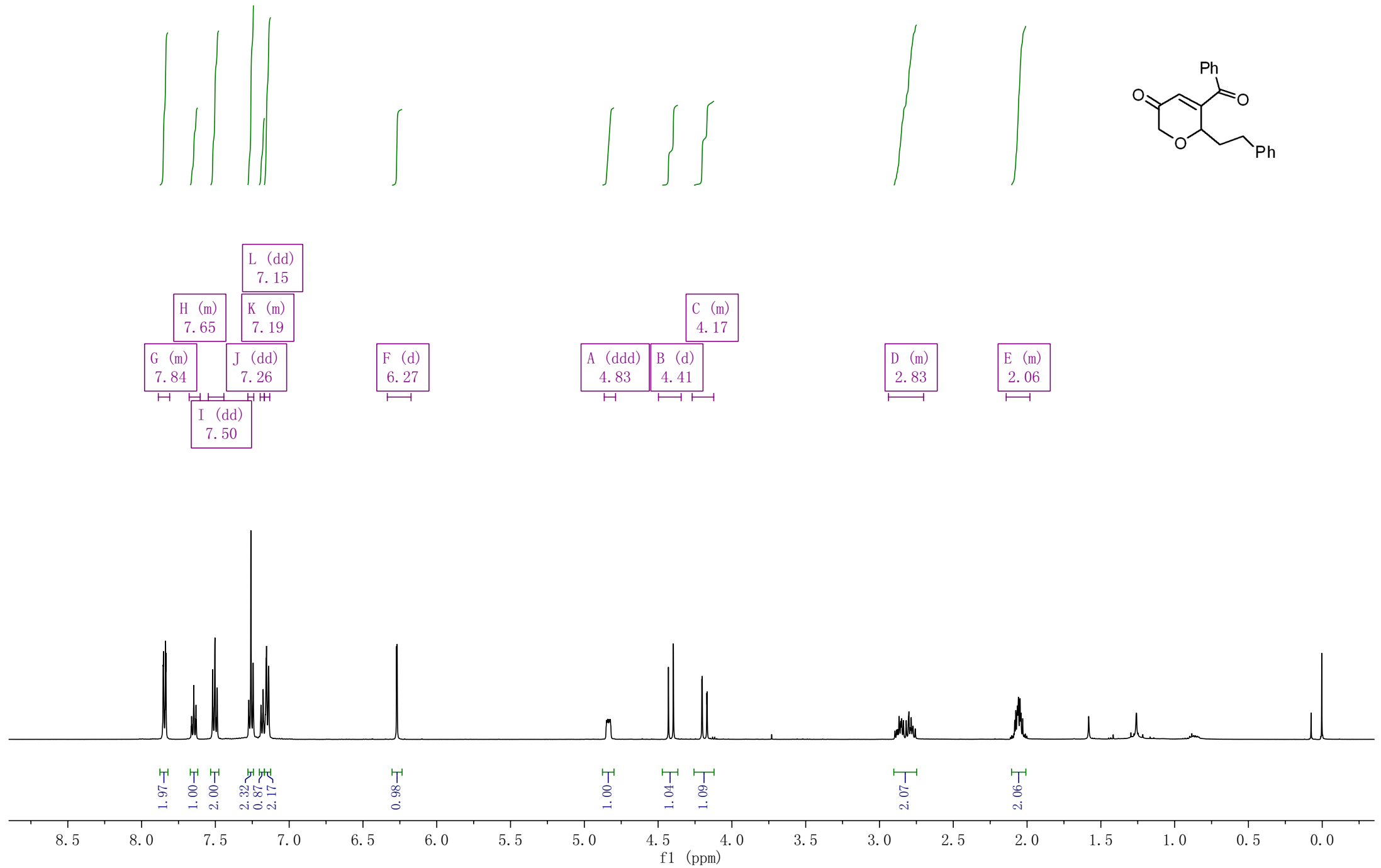
141.21
140.05
136.29
131.70
131.67
130.10
129.26
128.40
126.24
126.01

77.25
77.00
76.75
69.41
68.63

38.95

17.87





JKG-20150309-69B-3
C13CPD CDC13 {DMSO-d6-15-1} ZHL 13

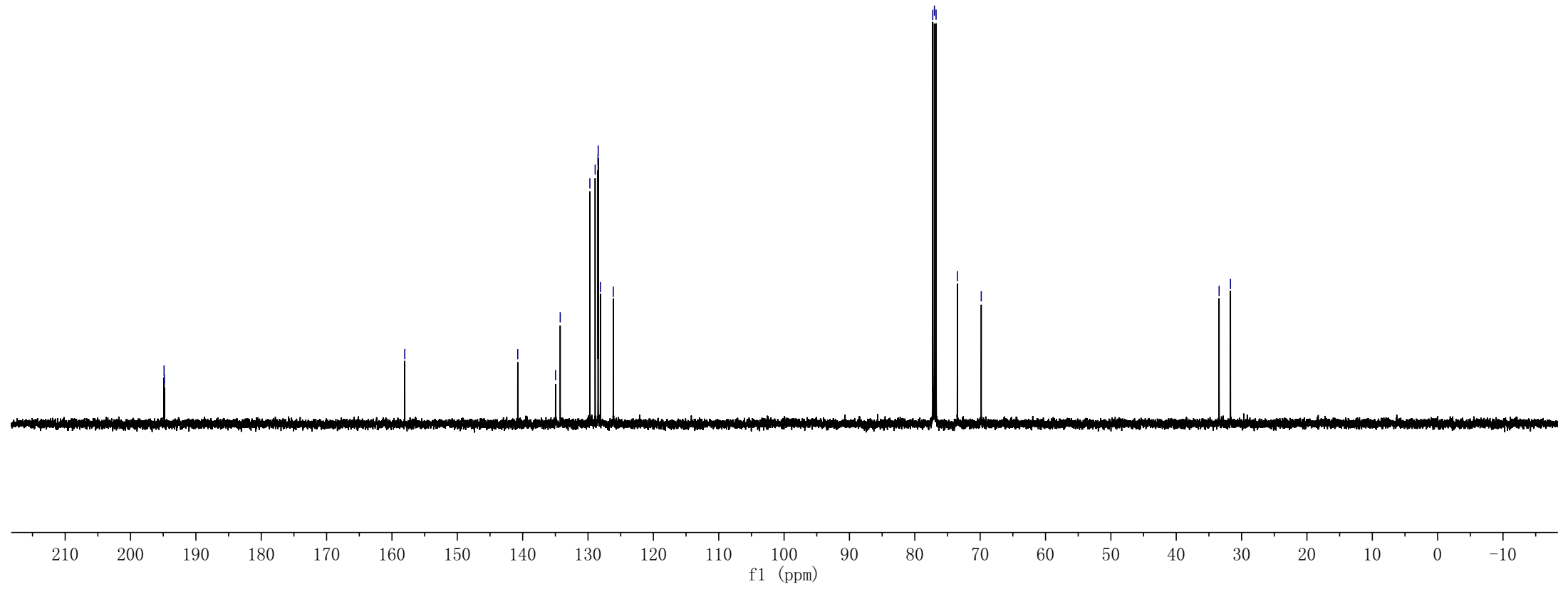
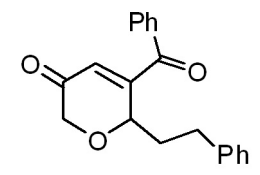
197.81
196.83

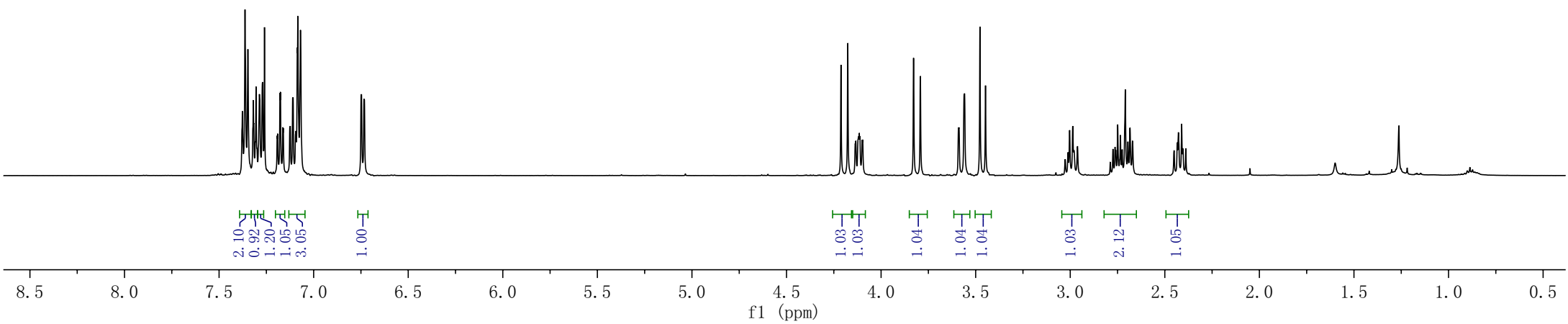
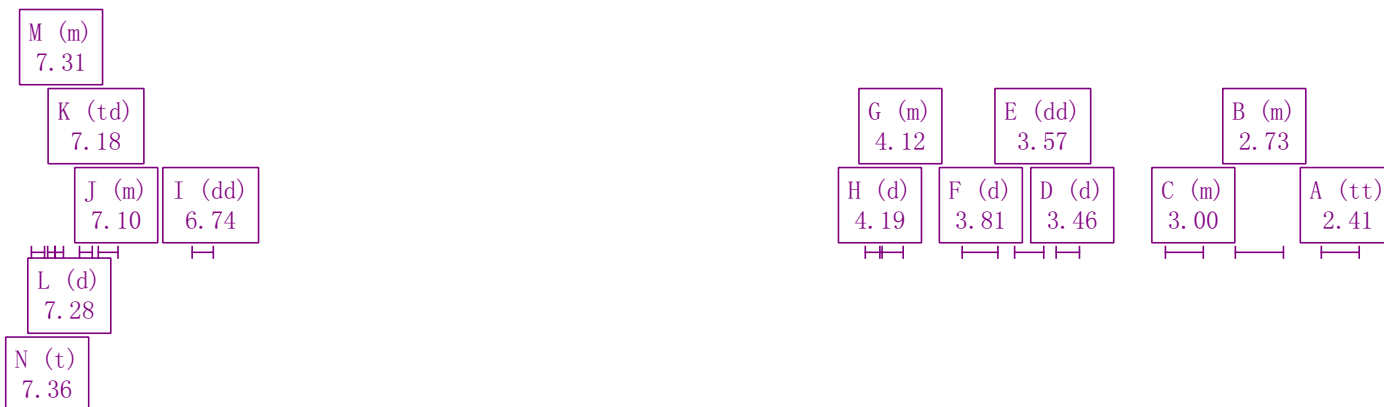
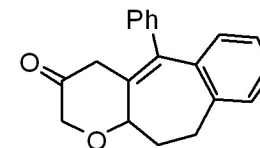
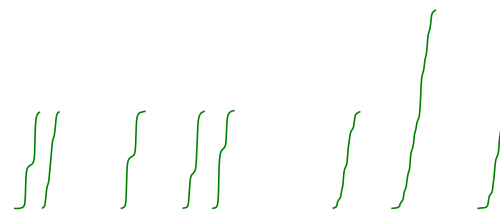
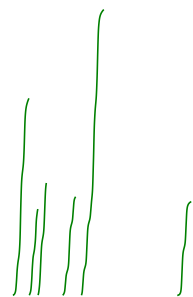
158.04

140.75
134.97
134.26
129.72
128.91
128.47
128.44
128.11
126.14

77.25
77.00
76.75
73.49
69.83

33.44
31.70





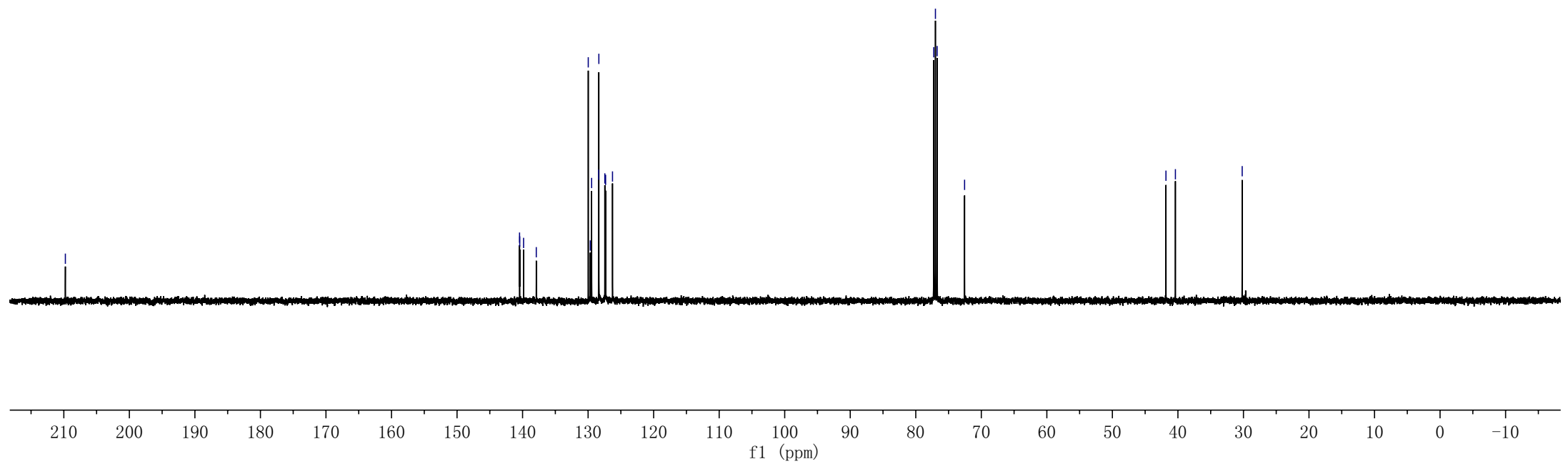
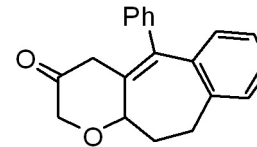
JKG-20150309-69B-1
C13CPD: CDC13 {D:\2015-1} ZHL 12

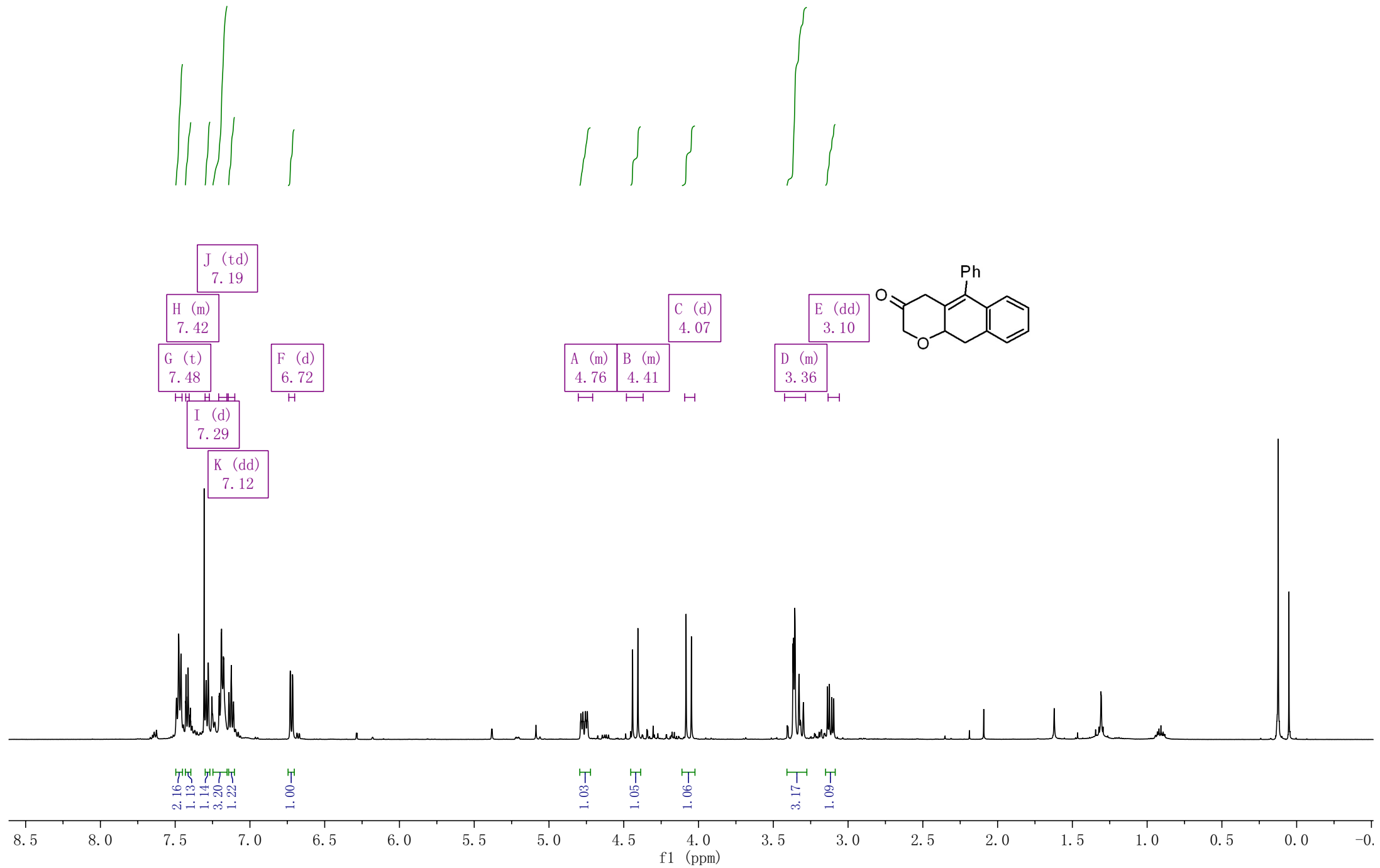
140.46
140.43
139.85
137.91
129.98
129.66
129.46
128.40
128.36
127.45
127.33
126.28

77.25
77.00
76.74
72.55

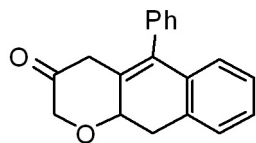
41.83
40.38

30.19





JKG-20150109-61-B
C13CPD CDC13 {D:\2015-1} ZHL 26

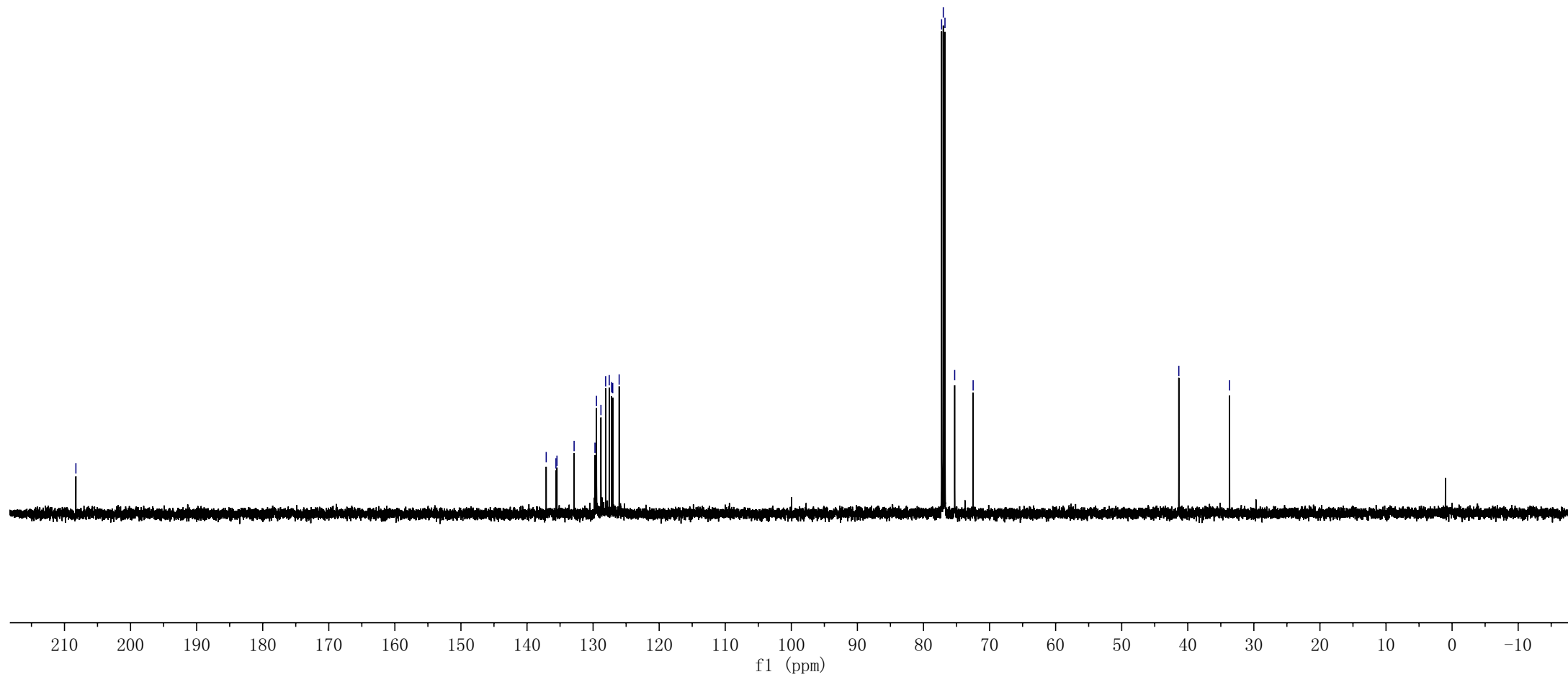


137.10
135.62
135.47
132.87
129.72
129.49
128.81
128.10
127.56
127.20
127.03
126.06

77.25
77.00
76.75
75.28
72.48

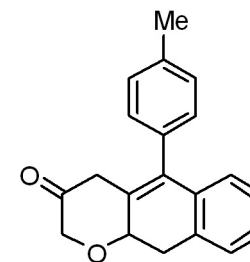
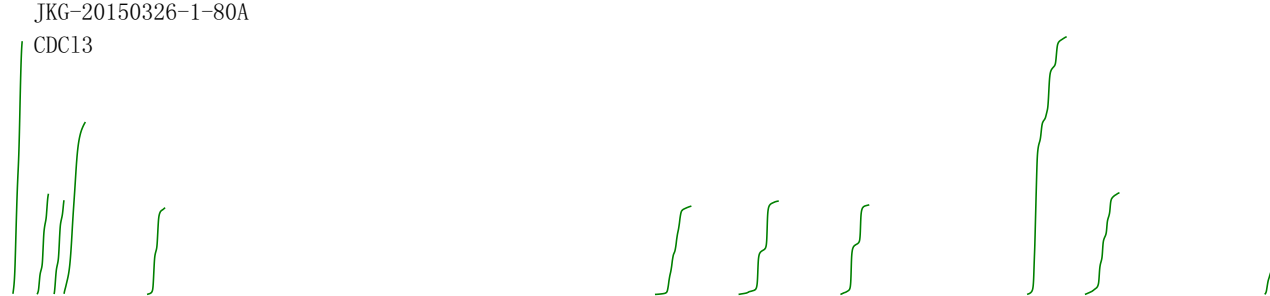
41.36

33.68

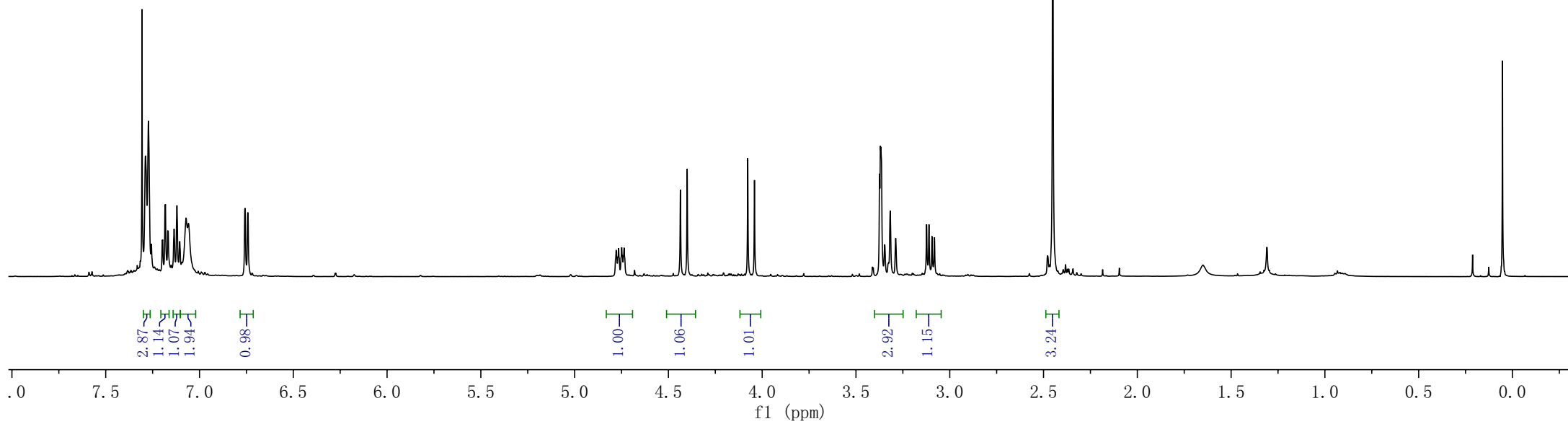


Parameters

Parameter Value
 Data File Name D:/ 文章/ paper-1-NMR/ NMR/ jkg-03-26/ JKG-20150326-1-80A/ 10/ fid
 Title JKG-20150326-1-80A
 Solvent CDCl3



I (m) 7.27	H (m) 7.14	G (t) 6.74	A (td) 4.74	B (d) 4.42	C (m) 4.13	D (m) 3.34	E (m) 3.11	F (m) 2.45
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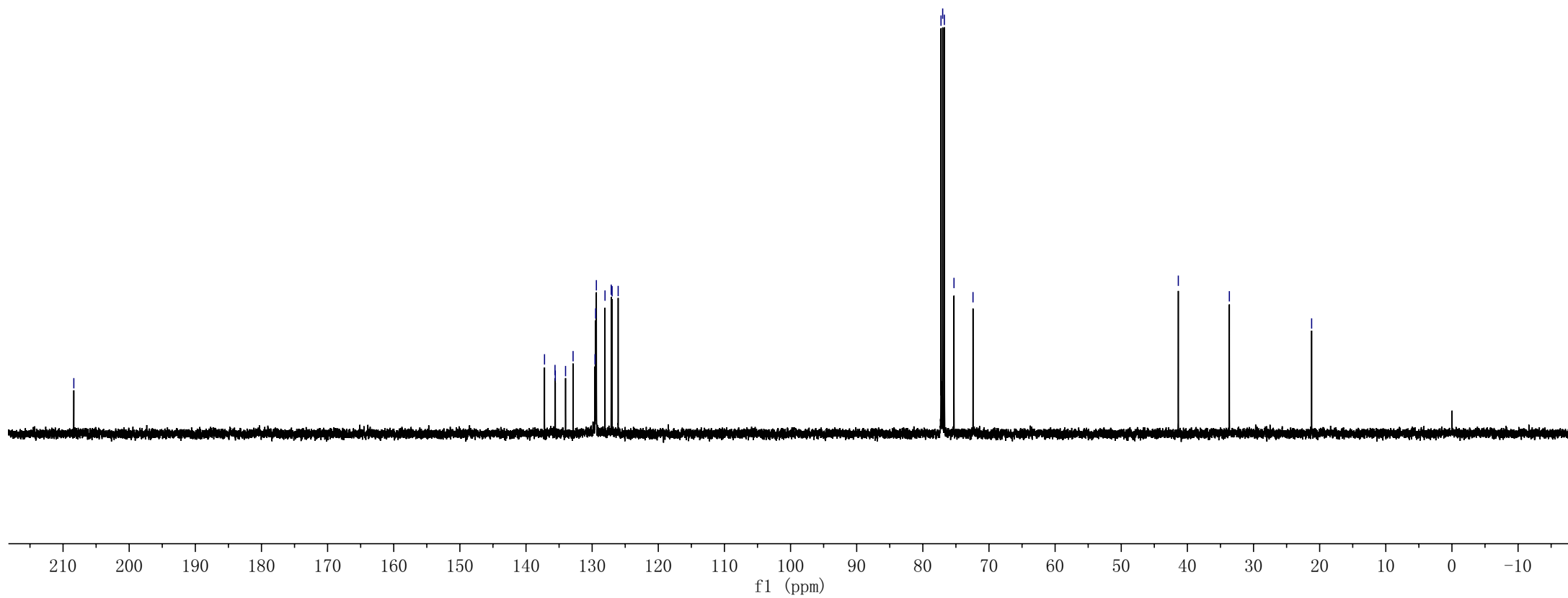
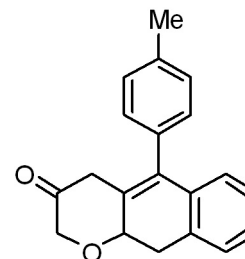
Parameter 208.37
Data File Name D:/ 文章/ paper-1-NMR/ NMR/ jkg-03-26/ JKG-20150326-1-80A/ 10/ fid
Title JKG-20150326-1-80A
Solvent CDCl3

Parameters Value
137.20
135.62
135.57
134.02
132.88
129.57
129.47
129.36
128.05
127.12
126.98
126.07

77.25
77.00
76.75
75.29
72.41

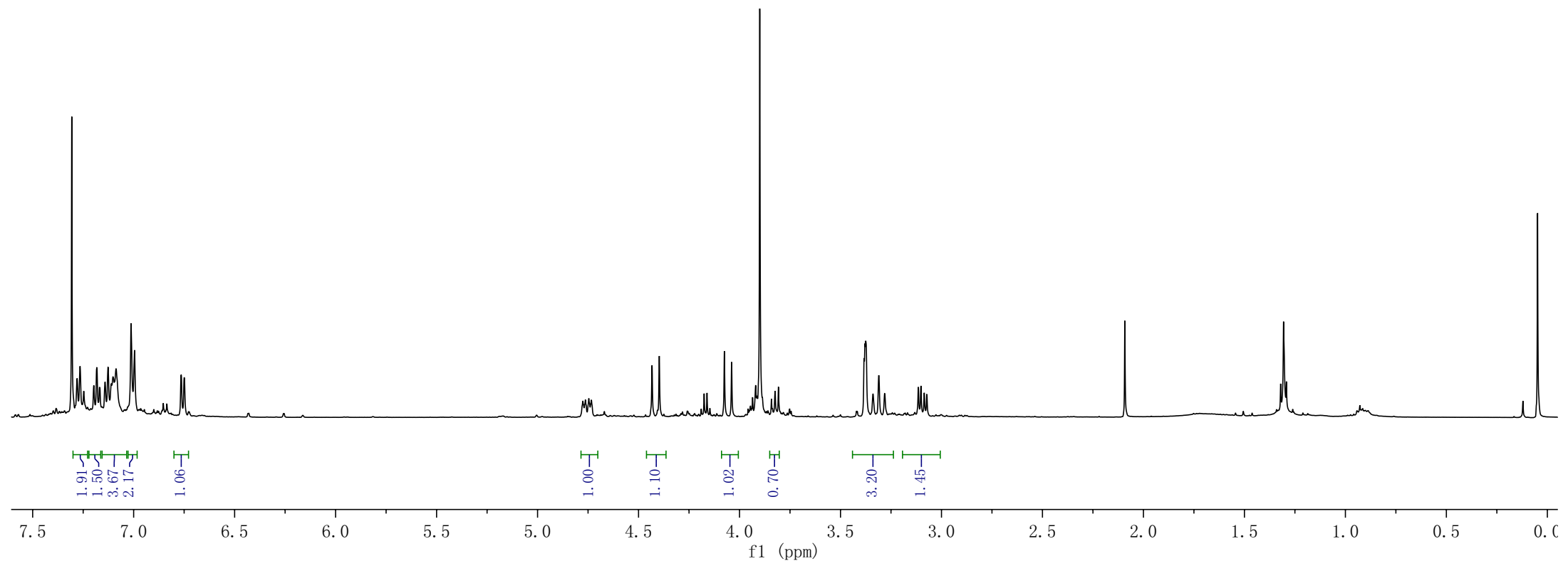
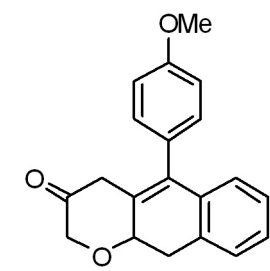
41.37
33.65

21.21



Parameters

Parameter Value
Data File Name D:/ 文章/ paper-1-NMR/ NMR/ jkg-03-26/ JKG-20150326-1-80A/ 10/ fid
Title JKG-20150326-1-80A
Solvent CDCl3



Parameter Value
Data File Name D:/ 文章/ paper-1-NMR/ NMR/ jkg-03-26/ JKG-20150326-1-80A/ 10/ fid
Title JKG-20150326-1-80A
Solvent CDC13

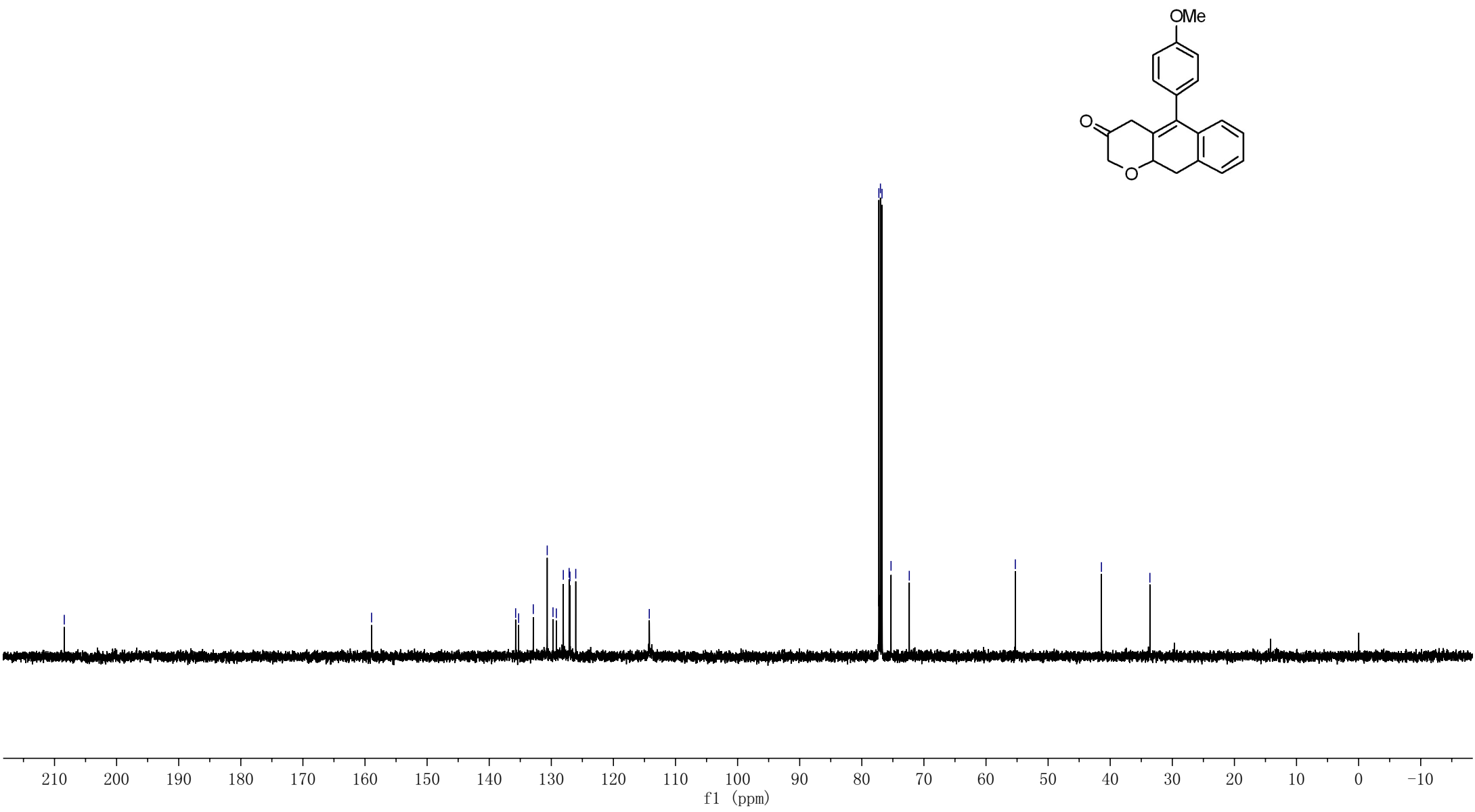
Parameters Value
158.94
135.74
135.26
132.90
130.66
129.73
129.19
128.07
127.13
127.00
126.06
114.22

77.25
77.00
76.75
75.29
72.35

55.28

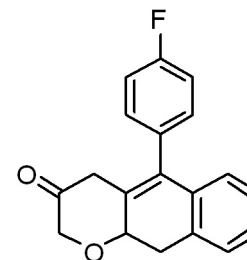
41.41

33.61

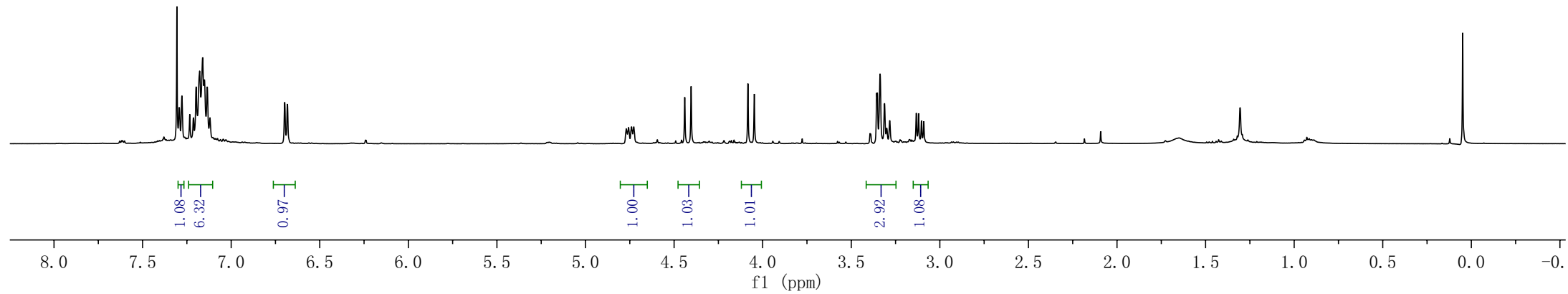


Parameters

Parameter Value
 Data File Name D:/ 文章/ paper-1-NMR/ NMR/ jkg-03-26/ JKG-20150326-1-80A/ 10/ fid
 Title JKG-20150326-1-80A
 Solvent CDCl3



H (m) 7.17	B (m) 4.40	E (m) 3.13
G (m) 7.29	A (dt) 4.73	D (m) 3.33
F (d) 6.69	C (m) 4.08	



—208.02

163.18
161.22

135.33
134.64
132.92
132.90
132.87
131.25
131.19
130.34
128.19
127.36
127.08
125.89
115.97
115.80

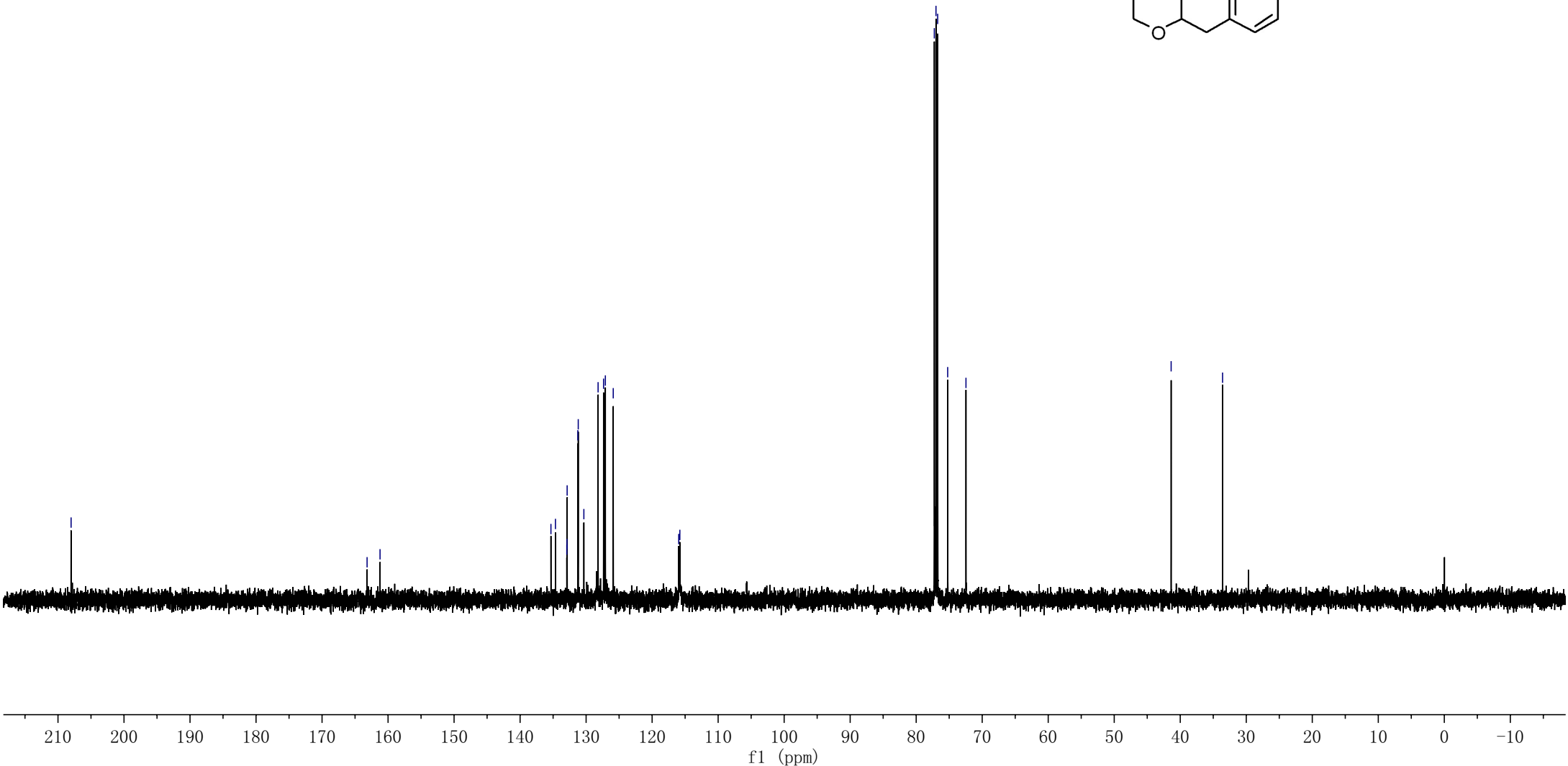
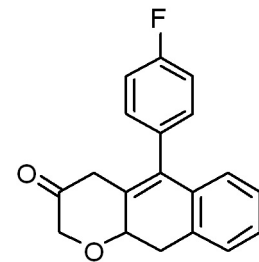
77.25
77.00
76.75
75.23
72.46

—41.38

—33.59

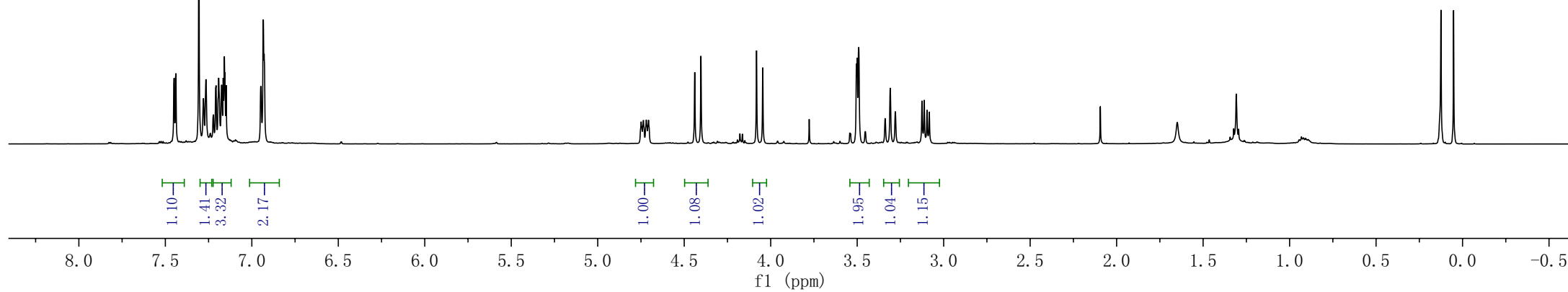
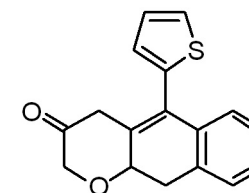
Parameters

Parameter	Value
Data File Name	D:/ 文章/ paper-1-NMR/ NMR/ jkg-03-26/ JKG-20150326-1-80A/ 10/ fid
Title	JKG-20150326-1-80A
Solvent	CDC13



Parameters

Parameter	Value
Data File Name	D:/ 文章/ paper-1-NMR/ NMR/ jkg-03-26/ JKG-20150326-1-74A/ 10/ fid
Title	JKG-20150326-1-74A
Solvent	CDC13
Spectrometer Frequency	500.13
Spectral Size	65536



—207.73

137.14
135.33
133.86
132.46
128.42
128.03
127.77
127.48
127.28
127.19
126.21
125.83

77.25
77.00
76.75
75.34
72.54

—41.60

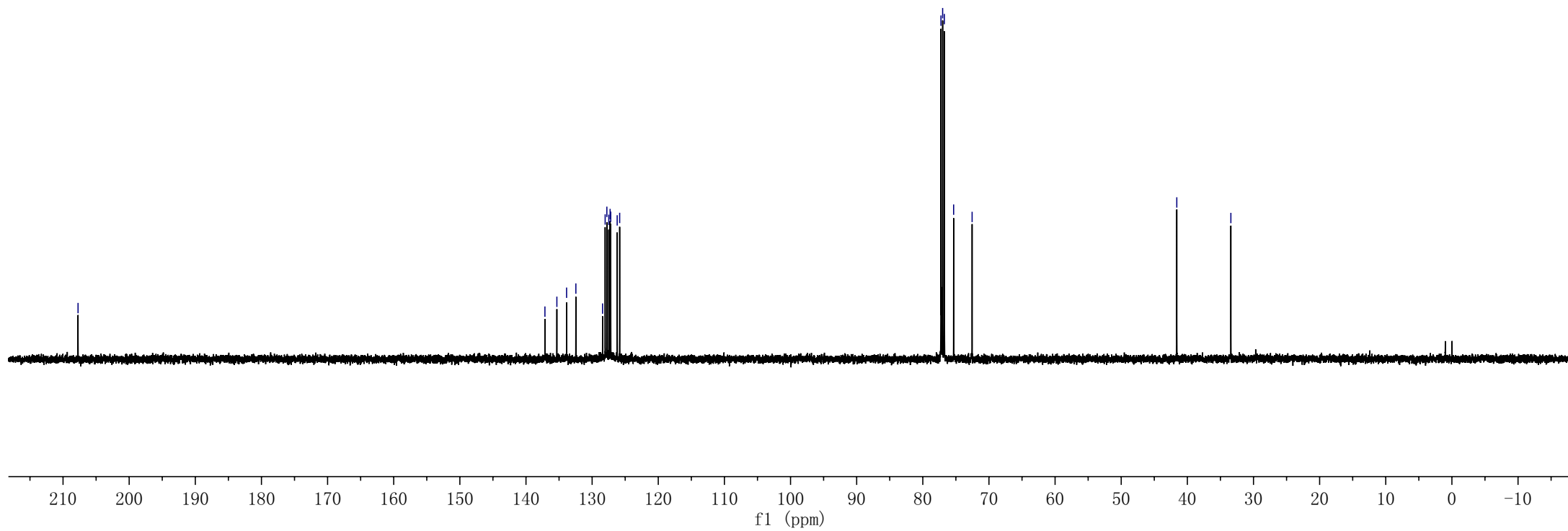
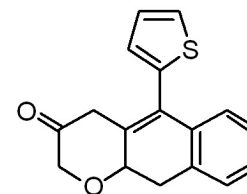
—33.42

Parameters

Parameter Value

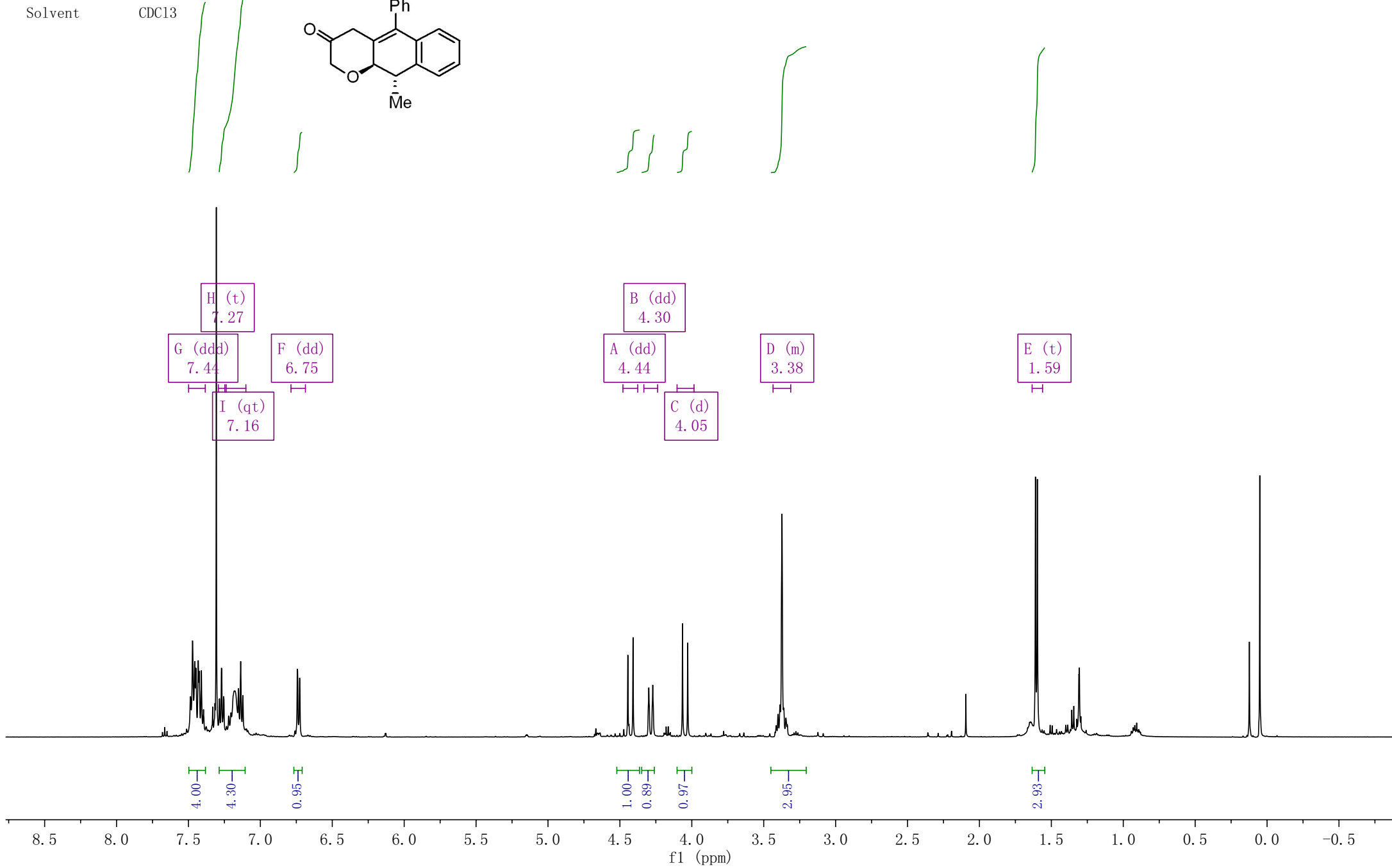
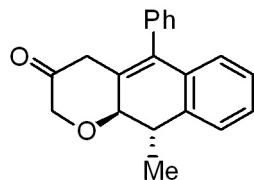
Data File Name D:/ 文章/ paper-1-NMR/ NMR/ jkg-03-26/ JKG-20150326-1-74A/ 11/ fid

Title JKG-20150326-1-74A



Parameters

Parameter Value
Data File Name D:/ 文章/ paper-1-NMR/ NMR/ jkg-03-26/ JKG-20150326-1-73B/ 10/ fid
Title JKG-20150326-1-73B
Solvent CDCl3



208.70

Parameters

137.40
137.24
135.54
135.32
129.68
129.60
128.77
127.53
127.45
126.67
126.06
124.97
122.85

80.03
77.25
77.00
76.74
72.05

41.55

36.04

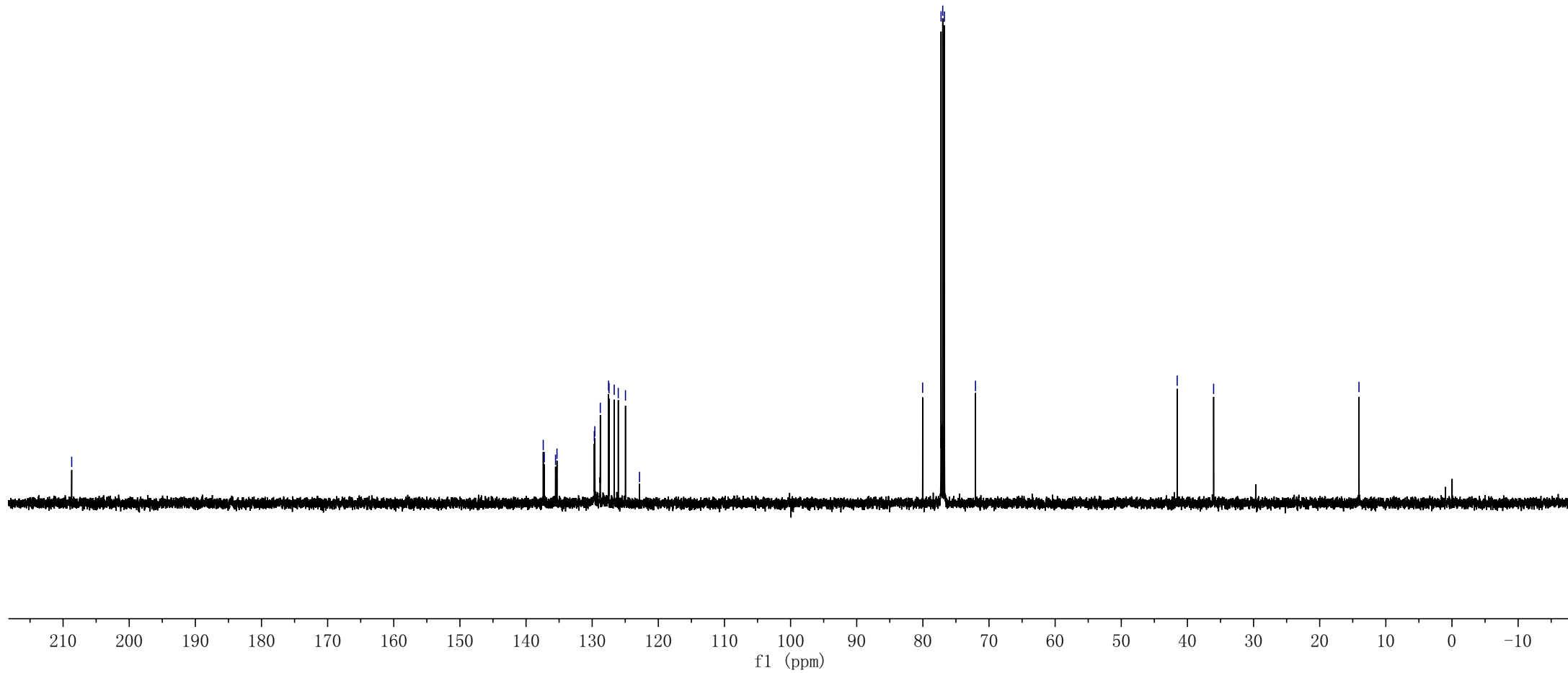
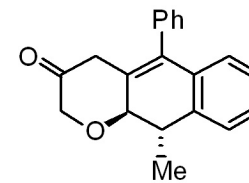
14.06

Parameter Value

Data File Name D:/ 文章/ paper-1-NMR/ NMR/ jkg-03-26/ JKG-20150326-1-73B/ 10/ fid

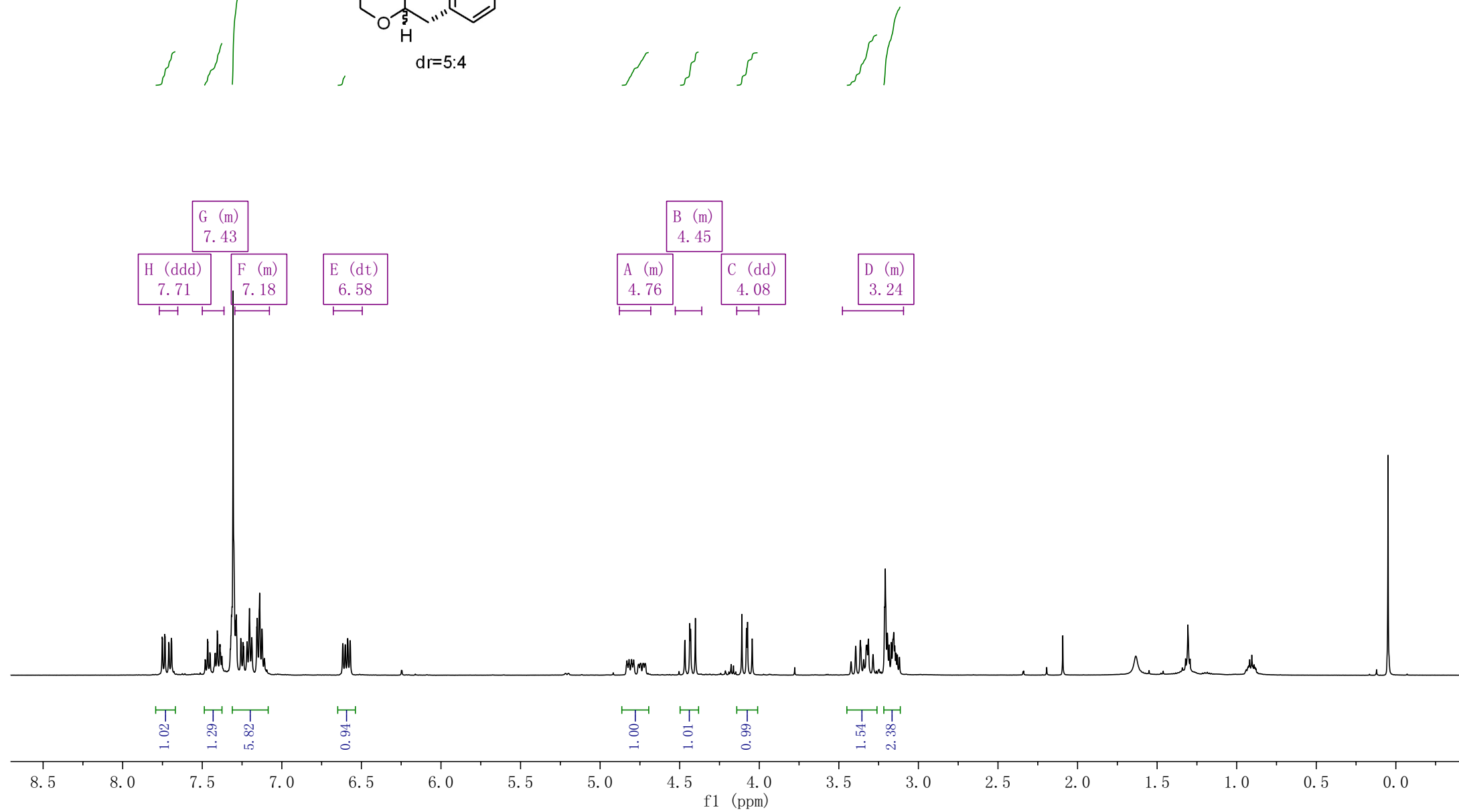
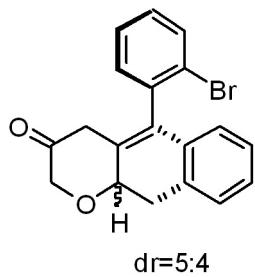
Title JKG-20150326-1-73B

Solvent CDC13



Parameters

Parameter Value
 Data File Name D:/ 文章/ paper-1-NMR/ NMR/ jkg-03-26/ JKG-20150326-1-73B/ 11/ fid
 Title JKG-20150326-1-73B
 Solvent CDCl3



207.89
207.43

Parameters
137.93
137.49
134.59
134.35
134.04
133.32
133.01
132.87
132.66
131.38
131.15
131.07
130.76
129.45
129.42
128.21
128.18
128.05
127.75
127.37
127.35
127.20
127.13
125.57
124.82
124.21
124.01

75.13
75.10
72.78
72.72

41.38
41.06
33.71
33.59

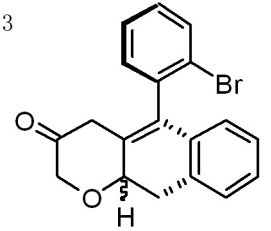
Parameter

Value

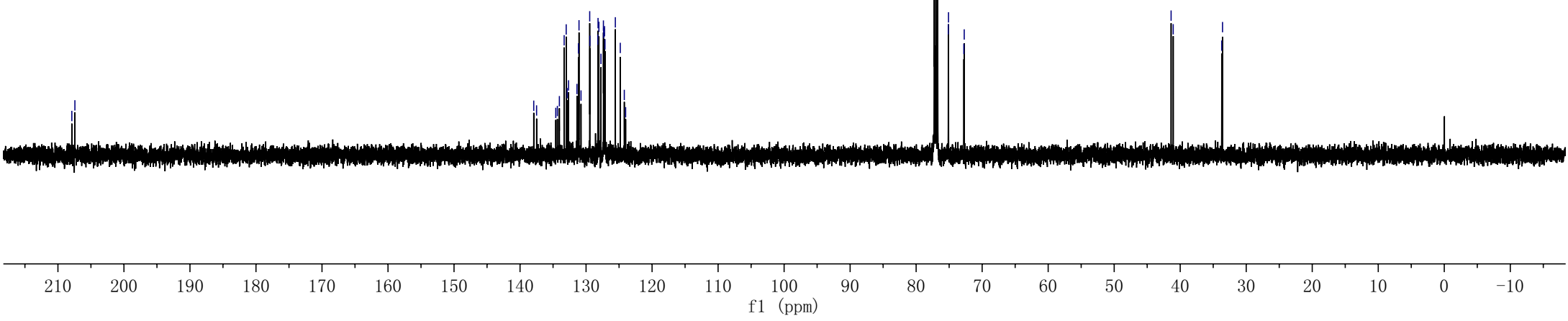
Data File Name D:/ 文章/ paper-1-NMR/ NMR/ jkg-03-26/ JKG-20150326-1-75A/ 10/ fid

Title JKG-20150326-1-75A

Solvent CDC13

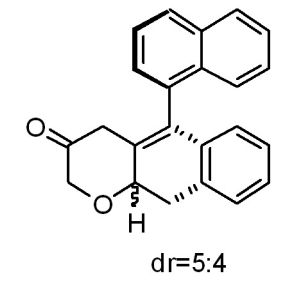


dr=5:4

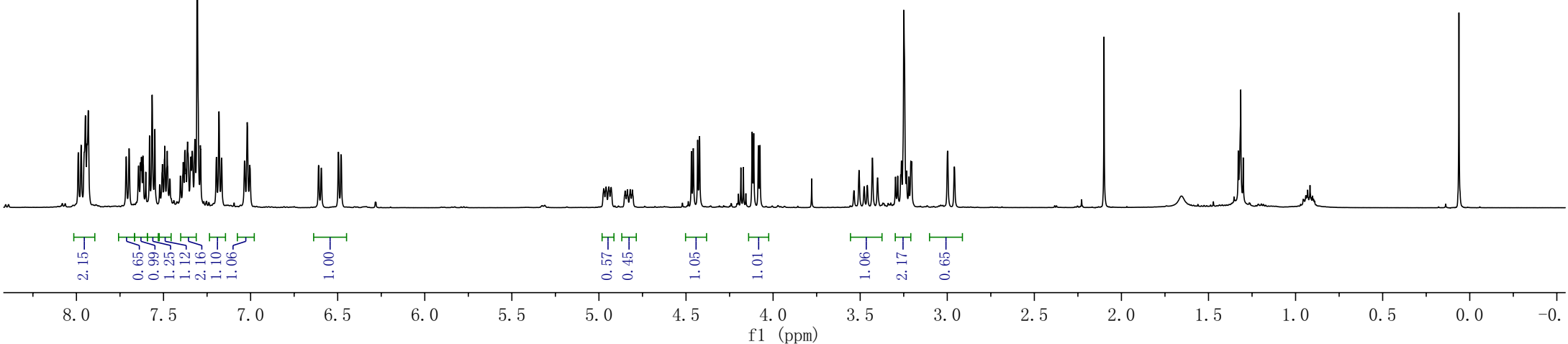


Parameters

Parameter Value
 Data File Name D:/ 文章/ paper-1-NMR/ NMR/ jkg-03-26/ JKG-20150326-1-75A/ 11/ fid
 Title JKG-20150326-1-75A
 Solvent CDCl3



K (m) 7.63	I (m) 7.18	C (dd) 4.10	E (m) 3.26
J (m) 7.96	L (m) 7.49	A (m) 4.90	D (m) 3.45
H (m) 7.03	G (dd) 6.54	B (m) 4.46	F (m) 3.02
M (m) 7.35			

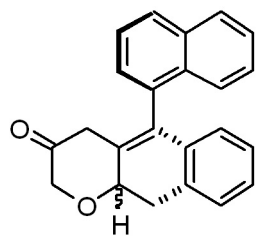


Parameter
Data File Name D:/ 文章/ paper-1-NMR/ NMR/ jkg-03-26/ JKG-20150326-1-75A/ 11/ fid
Title JKG-20150326-1-75A
Solvent CDCl3

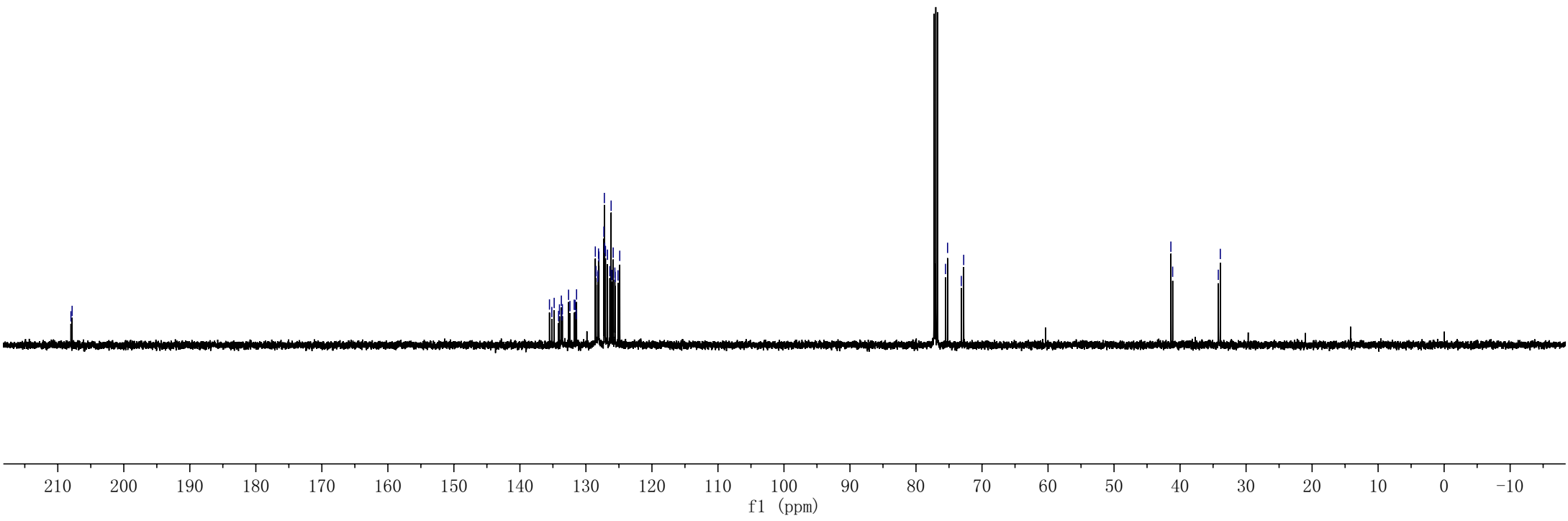
208.01
207.83
135.52
134.16
133.81
133.14
133.01
133.72
133.65
133.56
132.63
132.42
131.78
131.63
131.48
131.42
128.58
128.48
128.21
128.16
128.09
128.03
127.28
127.21
127.16
127.04
126.73
126.37
126.18
126.06
125.87
125.62
125.57
125.14
124.88

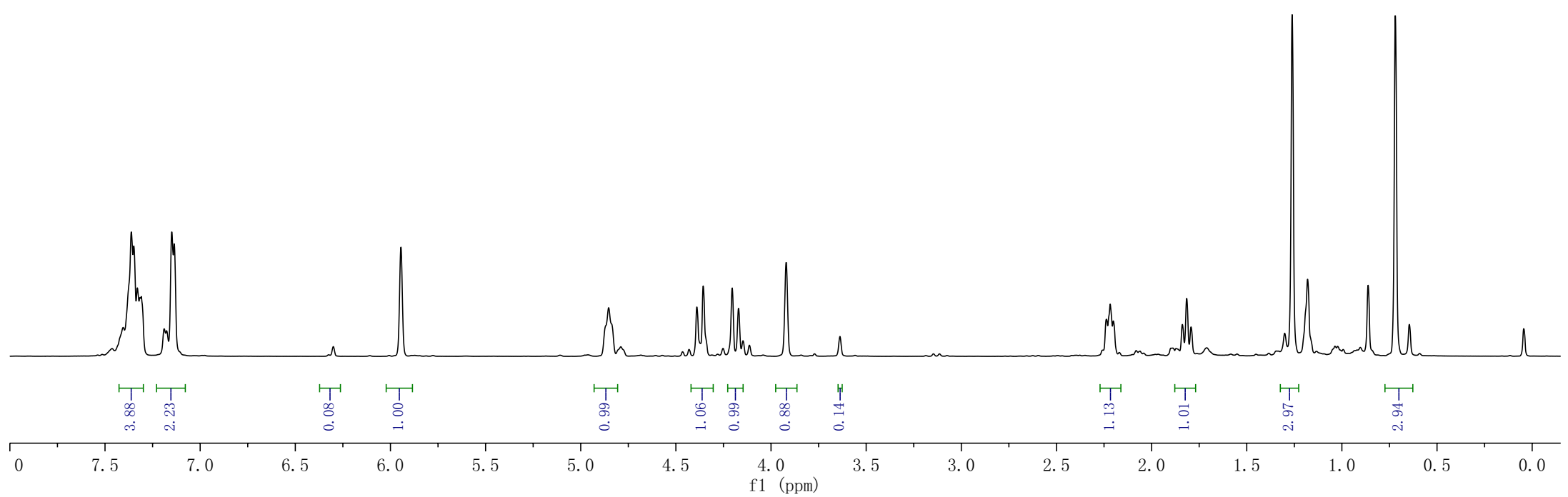
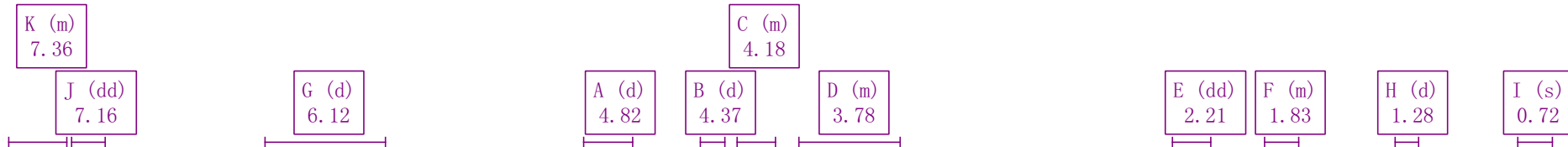
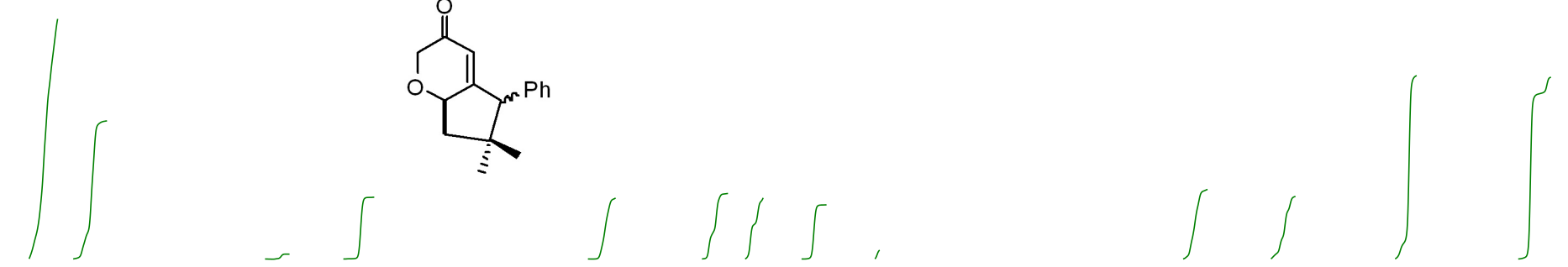
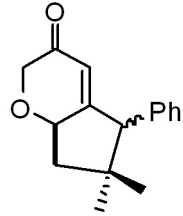
75.53
75.22
73.13
72.77

41.39
41.12
34.21
33.90

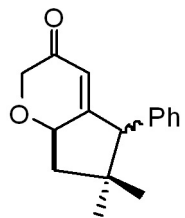


dr=5:4





JKG-20150310-I-69P
C13CPD CDC13 {D:2015-1} ZHL 17



195.09
174.17

137.67
129.13
128.34
127.12
122.30

77.98
77.25
77.00
76.75
72.87

60.08

44.73
41.30

28.62
24.42

