Electronic Supplementary Information

Gold(III)-Catalyzed Bicyclizations of Alkylidenecyclopropane-tethered Ynones for Divergent Synthesis of Indene and Naphthalenone-Based Polycycles

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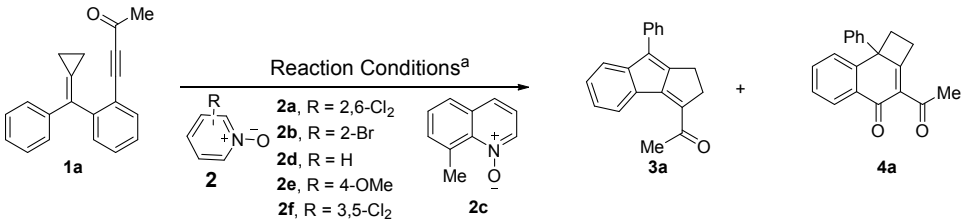
1. **Supplementary Notes**

Dry tetrahydrofuran (THF) and toluene were distilled over sodium under N_2 for at least 3 h prior to use. Anhydrous 1,2-dicloroethane, PhCl and PhF were bought from Energy Chemical, and were used as received from commercial source. Dry DCM was distilled from calcium hydride under the atmosphere of nitrogen and collected fresh immediately before use. All reactions sensitive to air or moisture were conducted under nitrogen atmosphere in dry solvents. All glassware and stir bars were washed with aquaregia prior to use. Ampicillin sodium, bisBenzimide H 33342 trihydrochloride (Hoechst 33342) and Propidium iodide (PI) were bought from Tansoole, and were used without further purification.

^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker Advance spectrometer at 500 MHz and 125 MHz in $CDCl_3$, *d*-Acetone or *d*-DMSO with reference to residual solvents signals [^{1}H NMR $CDCl_3$ (7.26), *d*-Acetone (2.05), *d*-DMSO (2.50); ^{13}C NMR $CDCl_3$ (77.16), *d*-Acetone (29.84), *d*-DMSO (39.52)]. Chemical shift values were given in δ (ppm) and coupling constants were mentioned in Hz. Proton multiplicity is reported as a singlet (s), a broad singlet (br), a doublet (d), a triplet (t), a triplet double (td) or a multiplet (m). High resolution mass spectrometry (HRMS) was performed with a Thermo Scientific LTQ Orbitrap XL unless otherwise noted. The bacterias (*B.c*: *Bacillus cereus*, CGMCC 1.1846; *B.s*: *Bacillus subtilis*, CGMCC 1.821; *R.s*: *Ralstonia solanacearum*, CGMCC 1.12711; *MRSA*: *Methicillin-resistant Staphylococcus aureus*, ATCC 43300; *S.a*: *Staphylococcus aureus* CGMCC 1.8721) were provided by the College of Plant Protection, Northwest A&F University.

2. **Supplementary Table 1.** Screening conditions.

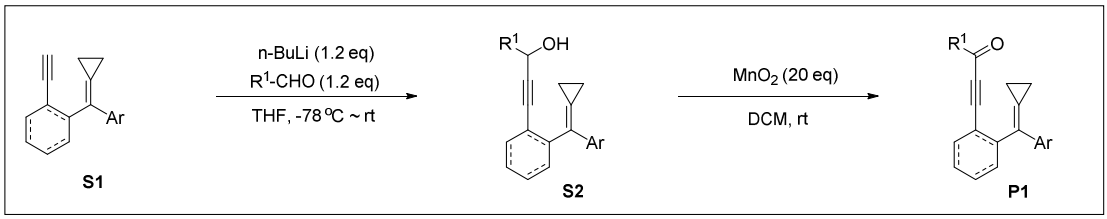


Entry	Catalysts (10 mol %)	Solvents	Oxidants (1.5 eq)	Temperatures (^oC)	Time (h)	Yields (%)[b]	
						3a	**4a**
1	$Ph_3PAuNTf_2$[c]	PhCl	**2a**	40	24	<1	<1
2	$IPrAuNTf_2$[c]	PhCl	**2a**	40	24	<1	<1
3	$XPhosAuNTf_2$[c]	PhCl	**2a**	40	24	<1	<1
4	$^TMetBuXPhosAuNTf_2$[c]	PhCl	**2a**	40	24	<1	<1
5	$(2,4\text{-}^tBuO)_3PAuNTf_2$[c]	PhCl	**2a**	40	24	<1	<1
6	$PicAuCl_2$	PhCl	**2a**	40	24	64	<1
7	$PicAuCl_2$	$PhCH_3$	**2a**	40	24	49	<1
8	$PicAuCl_2$	$PhCF_3$	**2a**	40	24	40	<1
9	$PicAuCl_2$	DCE	**2a**	40	24	10	<1
10	$PicAuCl_2$	DCM	**2a**	40	24	55	<1
11	$PicAuCl_2$	PhCl	**2b**	40	24	<1	41
12	$PicAuCl_2$	PhCl	**2c**	40	24	<1	57
13	$PicAuCl_2$	PhCl	**2d**	40	24	<1	<10
14	$PicAuCl_2$	PhCl	**2e**	40	24	<1	<10
15	$PicAuCl_2$	PhCl	**2f**	40	24	<1	<10
16	$PicAuCl_2$[e]	PhCl	**2a**[d]	40	36	62	<1
17	$PicAuCl_2 + Cu(OTf)_2$[f]	PhCl	**2a**[d]	40	24	71	<1
18	$PicAuCl_2 + Zn(OTf)_2$[f]	PhCl	**2a**[d]	40	24	65	<1
19	$PicAuCl_2 + Sc(OTf)_2$[f]	PhCl	**2a**[d]	40	24	56	<1
20	$PicAuCl_2$	PhCl	**2c**[d]	60	8	<1	79
21	$PicAuCl_2$	PhCl	**2c**[d]	70	8	<1	71
22	$PicAuCl_2$[e]	PhCl	**2c**[d]	60	8	<1	73
23	$Cu(OTf)_2$	PhCl	**2a**[d]	40	24	0	0
24	$FeCl_3$	PhCl	**2c**[d]	60	8	<5	N.D.
25[g]	Lewis acids	PhCl	**2c**[d]	60	8	Messy	Messy

[a] All reactions were carried out in 4 mL PhCl in the presence of **1a** (0.2 mmol). [b] isolated yields are reported. [c] 5 mol % catalyst was used. [d] 1.2 eq of oxidant was used. [e] 5 mol % gold catalyst was used. [f] 5 mol % gold catalyst and 10 mol % Lewis acid were used. g Lewis acids = $BF_3•Et_2O$, $AlCl_3$, $TiCl_4$.

3. Experimental procedures:[1]

3.1 Procedure 1.

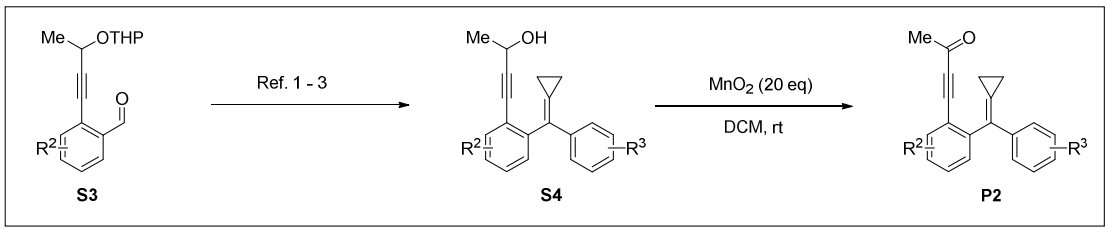


Supplementary Figure 1. Synthetic route of substrate I

To a solution of **S1**[1-3] (1.0 eq) in THF at -78 °C was added *n*-BuLi (1.2 eq) dropwise under a nitrogen atmosphere. After stirring at -78 °C for 1 h, the substituted aldehydes (1.2 eq) dissolved in 5 mL THF were added to the above mixture dropwise. After addition, the mixture was allowed to warm up to rt and stirred for another 1 h. Upon completion, the mixture was quenched with saturated NH_4Cl solution, extracted with EtOAc, washed with brine, dried over Na_2SO_4, filtered and concentrated to get the crude product which was purified by chromatography on silica gel to get the desired compound **S2**.

To a solution of **S2** (1.0 eq) in dry CH_2Cl_2 was added MnO_2 (20 eq) in one portion at rt and then the mixture was stirred at rt for 3 h. Upon completion, the mixture was filtered through a celite plug, concentrated to give the crude product and the residue was purified by chromatography on silica gel to get the desired substrate **P1**.

3.2 Procedure 2.



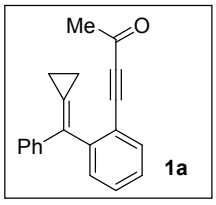
Supplementary Figure 2. Synthetic route of substrate II

To a solution of **S4**[1-3] (1.0 eq) in dry CH_2Cl_2 was added MnO_2 (20 eq) in one portion at rt and then the mixture was stirred at rt for 5 h. Upon completion, the

mixture was filtered through a celite plug, concentrated to give the crude product and the residue was purified by chromatography on silica gel to get the desired substrate **P2**.

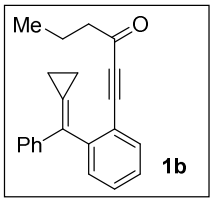
3.3 Data of substrates

4-(2-(cyclopropylidene(phenyl)methyl)phenyl)but-3-yn-2-one, **1a**, the title



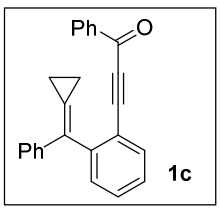
compound was synthesized according to procedure 1, overall yield 49%, 1.02 g, yellow oil. (R_f = 0.66, hexane/ethyl acetate = 15:1) **^{1}H NMR (500 MHz, *d*-Acetone):** δ = 7.68 (d, *J* = 7.5 Hz, 1H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.45 - 7.43 (m, 4H), 7.34 (t, *J* = 6.5 Hz, 2H), 7.26 - 7.23 (m, 1H), 2.01 (s, 3H), 1.65 (t, *J* = 7.5 Hz, 2H), 1.25 (t, *J* = 8.0 Hz, 2H); **^{13}C NMR (125 MHz, *d*-Acetone):** δ = 184.1, 146.5, 141.1, 134.7, 131.6, 131.4, 129.2, 129.1, 128.3, 127.9, 127.8, 127.7, 120.7, 91.8, 89.9, 32.6, 5.6, 2.6; HRMS (ESI) m/z calcd for $C_{20}H_{17}O^+$ $(M+H)^+$: 273.1274, found: 273.1276.

1-(2-(cyclopropylidene(phenyl)methyl)phenyl)hex-1-yn-3-one, 1b, the title



compound was synthesized according to procedure 1, overall yield 43%, 0.56 g, yellow oil, (R_f = 0.63, hexane/ethyl acetate = 15:1). **^{1}H NMR (500 MHz, *d*-Acetone):** δ = 7.68 (d, *J* = 7.5 Hz, 1H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.47 - 7.42 (m, 4H), 7.34 (t, *J* = 7.0 Hz, 2H), 7.25 (t, *J* = 7.0 Hz, 1H), 2.22 (t, *J* = 7.0 Hz, 2H), 1.66 (t, *J* = 7.5 Hz, 2H), 1.47 - 1.42 (m, 2H), 1.23 (t, *J* = 7.5 Hz, 2H), 0.80 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (125 MHz, *d*-Acetone):** δ = 187.5, 146.5, 140.9, 134.7, 131.6, 131.4, 129.3, 129.1, 128.4, 127.8, 127.7, 127.6, 120.9, 91.4, 90.2, 47.7, 18.1, 13.7, 5.7, 2.4; **HRMS** (ESI) m/z calcd for $C_{22}H_{21}O^+$ $(M+H)^+$: 301.1587, found: 301.1588.

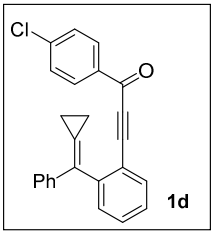
3-(2-(cyclopropylidene(phenyl)methyl)phenyl)-1-phenylprop-2-yn-1-one, **1c**, the



title compound was synthesized according to procedure 1, overall yield 52%, 0.66 g, yellow oil, (R_f = 0.58, hexane/ethyl acetate = 15:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 7.80 - 7.79 (m, 3H), 7.52

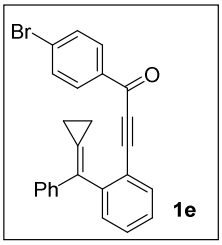
- 7.49 (m, 4H), 7.43 - 7.39 (m, 1H), 7.38 - 7.33 (m, 3H), 7.30 - 7.24 (m, 3H), 1.62 - 1.58 (m, 2H), 1.22 - 1.19 (m, 2H); **^{13}C NMR (125 MHz, $CDCl_3$):** (*two carbons merged to others*) δ = 178.1, 146.0, 139.8, 137.0, 134.5, 133.8, 130.8, 130.5, 129.7, 128.5, 127.4, 127.2, 127.2, 127.0, 120.6, 93.1, 89.6, 5.9, 2.1; **HRMS** (ESI) m/z calcd for $C_{25}H_{19}O^+$ $(M+H)^+$: 335.1430, found: 335.1433.

1-(4-chlorophenyl)-3-(2-(cyclopropylidene(phenyl)methyl)phenyl)prop-2-yn-1-on



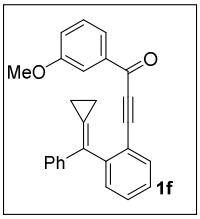
e, **1d**, the title compound was synthesized according to procedure 1, overall yield 41%, 0.50 g, yellow oil, (R_f = 0.67, hexane/ethyl acetate = 15:1). **^{1}H NMR (500 MHz, *d*-Acetone):** δ = 7.85 (d, *J* = 8.0 Hz, 1H), 7.76 (d, *J* = 8.5 Hz, 2H), 7.64 (t, *J* = 8.0 Hz, 1H), 7.53 - 7.51 (m, 3H), 7.46 - 7.41 (m, 3H), 7.38 (t, *J* = 8.0 Hz, 2H), 7.27 (t, *J* = 7.0 Hz, 1H), 1.69 - 1.65 (m, 2H), 1.22 - 1.19 (m, 2H); **^{13}C NMR (125 MHz, *d*-Acetone):** δ = 176.4, 146.7, 140.6, 140.5, 136.3, 135.2, 132.2, 131.5, 131.4, 129.7, 129.3, 129.2, 128.6, 128.0, 127.9, 127.5, 120.7, 93.5, 89.8, 6.1, 2.2; **HRMS** (ESI) m/z calcd for $C_{25}H_{18}ClO^+$ $(M+H)^+$: 369.1041, found: 369.1042.

1-(4-bromophenyl)-3-(2-(cyclopropylidene(phenyl)methyl)phenyl)prop-2-yn-1-on



e, **1e**, the title compound was synthesized according to procedure 1, overall yield 43%, 0.71 g, yellow oil, (R_f = 0.68, hexane/ethyl acetate = 15:1). **^{1}H NMR (500 MHz, *d*-Acetone):** δ = 7.85 (d, *J* = 7.5 Hz, 1H), 7.68 - 7.62 (m, 3H), 7.58 - 7.57 (m, 2H), 7.53 - 7.51 (m, 3H), 7.45 (d, *J* = 7.5 Hz, 1H), 7.37 (t, *J* = 7.0 Hz, 2H), 7.27 (t, *J* = 7.0 Hz, 1H), 1.67 (t, *J* = 7.0 Hz, 2H), 1.20 (t, *J* = 7.5 Hz, 2H); **^{13}C NMR (125 MHz, *d*-Acetone):** δ = 176.6, 146.7, 140.4, 136.6, 135.1, 132.7, 132.1, 131.6, 131.4, 129.5, 129.3, 129.1, 128.5, 128.0, 127.9, 127.5, 120.7, 93.5, 89.7, 6.1, 2.2; **HRMS** (ESI) m/z calcd for $C_{25}H_{18}BrO^+$ $(M+H)^+$: 413.0536, found: 413.0539.

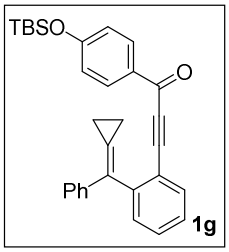
3-(2-(cyclopropylidene(phenyl)methyl)phenyl)-1-(3-methoxyphenyl)prop-2-yn-1-



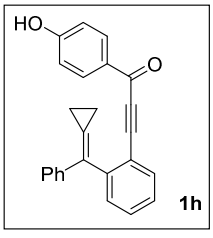
one, 1f, the title compound was synthesized according to procedure

1, overall yield 55%, 0.81 g, yellow oil, (R_f = 0.48, hexane/ethyl acetate = 15:1). **^{1}H NMR (500 MHz, *d*-Acetone):** δ = 7.84 (d, *J* = 7.5 Hz, 1H), 7.60 (t, *J* = 7.0 Hz, 1H), 7.51 - 7.49 (m, 3H), 7.44 - 7.39 (m, 3H), 7.35 - 7.28 (m, 3H), 7.23 (t, *J* = 7.0 Hz, 1H), 7.17 - 7.16 (m, 1H), 3.76 (s, 3H), 1.66 (t, *J* = 7.5 Hz, 2H), 1.21 (t, *J* = 7.5 Hz, 2H); **^{13}C NMR (125 MHz, *d*-Acetone):** δ = 177.4, 160.8, 146.8, 140.7, 139.1, 135.1, 131.9, 131.3, 130.7, 129.3, 129.2, 128.5, 127.9, 127.8, 127.7, 123.2, 121.2, 121.0, 113.5, 92.8, 90.1, 55.8, 6.0, 2.4; **HRMS** (ESI) m/z calcd for $C_{26}H_{21}O_2^+$ $(M+H)^+$: 365.1536, found: 365.1539.

1-(4-((tert-butyldimethylsilyl)oxy)phenyl)-3-(2-(cyclopropylidene(phenyl)methyl) phenyl)prop-2-yn-1-one, **1g**, the title compound was synthesized according to procedure 1, overall yield 38%, 0.88 g, yellow oil, (R_f = 0.53, hexane/ethyl acetate = 15:1). **^{1}H NMR (500 MHz, *d*-Acetone):** δ = 7.82 (d, *J* = 7.5 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 2H), 7.60 (t, *J* = 6.0 Hz, 1H), 7.53 - 7.51 (m, 3H), 7.42 (d, *J* = 7.5 Hz, 1H), 7.37 (t, *J* = 7.5 Hz, 2H), 7.27 (t, *J* = 7.5 Hz, 1H), 6.83 (d, *J* = 8.5 Hz, 2H), 1.64 (t, *J* = 7.5 Hz, 2H), 1.20 (t, *J* = 7.5 Hz, 2H), 1.01 (s, 9H), 0.28 (s, 6H); **^{13}C NMR (125 MHz, *d*-Acetone):** (*one carbon merged to others*) δ = 176.3, 161.9, 146.6, 140.6, 134.9, 132.4, 131.8, 131.7, 131.3, 129.3, 128.5, 127.9, 127.8, 127.6, 121.2, 120.8, 92.1, 90.1, 26.0, 18.9, 6.1, 2.2, -4.2; **HRMS** (ESI) m/z calcd for $C_{31}H_{33}O_2Si^+$ $(M+H)^+$: 465.2244, found: 465.2245.

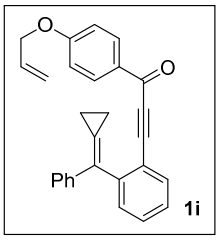


3-(2-(cyclopropylidene(phenyl)methyl)phenyl)-1-(4-hydroxyphenyl)prop-2-yn-1-one, 1h, the title compound was synthesized according to procedure 1, overall yield 31%, 0.36 g, light yellow oil, (R_f = 0.14, hexane/ethyl acetate = 8:1). **^{1}H NMR (500 MHz, *d*-Acetone):** δ = 9.42 (s, 1H), 7.81 (dd, *J* = 7.5, 2.0 Hz, 1H), 7.73 - 7.70 (m, 2H), 7.58 (td, *J* = 8.0, 1.5 Hz, 1H), 7.52 - 7.46 (m, 3H), 7.41 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.37 - 7.34 (m, 2H), 7.25 (tt, *J* = 8.0, 1.5 Hz, 1H), 6.84 - 6.81 (m, 2H), 1.65 - 1.62 (m, 2H), 1.20 - 1.17 (m, 2H); **^{13}C NMR (125 MHz, *d*-Acetone):** δ = 176.2, 163.6, 146.4, 140.5,

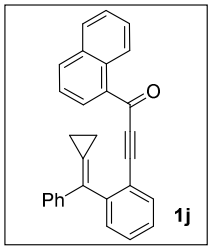


134.9, 132.6, 131.6, 131.2, 130.2, 129.2, 129.2, 128.4, 127.8, 127.6, 127.5, 121.2, 116.2, 91.7, 90.1, 6.0, 2.2; **HRMS** (ESI) m/z calcd for $C_{25}H_{19}O_2^+$ $(M+H)^+$: 351.1380, found: 351.1481.

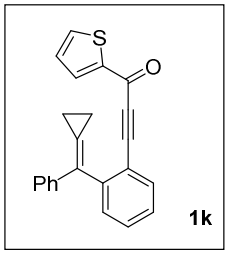
1-(4-(allyloxy)phenyl)-3-(2-(cyclopropylidene(phenyl)methyl)phenyl)prop-2-yn-1-one, **1i**, the title compound was synthesized according to procedure 1, overall yield 36%, 0.53 g, light yellow oil, (R_f = 0.40, hexane/ethyl acetate = 15:1). **^{1}H NMR (500 MHz, *d*-Acetone):** δ = 7.83 (d, *J* = 7.5 Hz, 1H), 7.75 (d, *J* = 7.5 Hz, 2H), 7.62 - 7.59 (m, 1H), 7.52 - 7.48 (m, 3H), 7.42 (d, *J* = 7.5 Hz, 1H), 7.37 (t, *J* = 7.5 Hz, 2H), 7.27 (t, *J* = 7.5 Hz, 1H), 6.91 (d, *J* = 8.5 Hz, 2H), 6.12 - 6.04 (m, 1H), 5.44 (d, *J* = 19.0 Hz, 1H), 5.30 (d, *J* = 10.5 Hz, 1H), 4.68 - 4.67 (m, 2H), 1.65 (t, *J* = 7.5 Hz, 2H), 1.20 (t, *J* = 7.5 Hz, 2H); **^{13}C NMR (125 MHz, *d*-Acetone):** δ = 176.2, 164.2, 146.5, 140.6, 135.0, 133.9, 132.3, 131.7, 131.3, 131.1, 129.3, 128.5, 128.0, 127.7, 127.6, 121.2, 118.2, 118.1, 115.4, 92.0, 90.2, 69.7, 6.1, 2.2; **HRMS** (ESI) m/z calcd for $C_{28}H_{23}O_2^+$ $(M+H)^+$: 391.1693, found: 391.1695.



3-(2-(cyclopropylidene(phenyl)methyl)phenyl)-1-(naphthalen-1-yl)prop-2-yn-1-one, 1j, the title compound was synthesized according to procedure 1, overall yield 46%, 0.59 g, yellow oil, (R_f = 0.55, hexane/ethyl acetate = 15:1). **^{1}H NMR (500 MHz, *d*-Acetone):** δ = 9.13 - 9.11 (m, 1H), 8.13 (t, *J* = 7.0 Hz, 1H), 8.07 (d, *J* = 7.0 Hz, 1H), 7.97 (t, *J* = 7.5 Hz, 1H), 7.85 (d, *J* = 7.5 Hz, 1H), 7.63 - 7.58 (m, 3H), 7.51 - 7.50 (m, 3H), 7.44 - 7.39 (m, 2H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.24 (t, *J* = 7.0 Hz, 1H), 1.63 - 1.58 (m, 2H), 1.22 - 1.18 (m, 2H); **^{13}C NMR (125 MHz, *d*-Acetone):** (*one carbon merged to others*) δ = 179.6, 146.6, 140.7, 135.8, 135.6, 134.9, 134.8, 133.3, 131.8, 131.3, 131.3, 129.6, 129.6, 129.3, 129.2, 128.5, 127.9, 127.7, 127.6, 127.6, 126.4, 125.5, 121.2, 91.6, 6.0, 2.3; **HRMS** (ESI) m/z calcd for $C_{29}H_{21}O^+$ $(M+H)^+$: 385.1587, found: 385.1588.

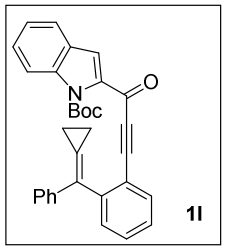


3-(2-(cyclopropylidene(phenyl)methyl)phenyl)-1-(thiophen-2-yl)prop-2-yn-1-one,

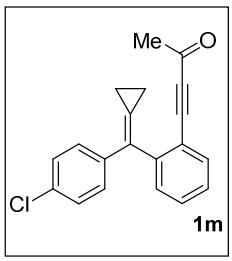


1k, the title compound was synthesized according to procedure 1, overall yield 52%, 0.67 g, light yellow oil. (R_f = 0.49, hexane/ethyl acetate = 15:1) **^{1}H NMR (500 MHz, *d*-Acetone):** δ = 7.88 (s, 1H), 7.83 (d, *J* = 7.0 Hz, 1H), 7.60 (t, *J* = 7.0 Hz, 1H), 7.50 - 7.49 (m, 3H), 7.42 - 7.38 (m, 2H), 7.35 - 7.33 (m, 2H), 7.25 (t, *J* = 7.0 Hz, 1H), 7.08 (s, 1H), 1.65 (t, *J* = 7.5 Hz, 2H), 1.21 (t, *J* = 7.5 Hz, 2H); **^{13}C NMR (125 MHz, *d*-Acetone):** δ = 169.7, 146.6, 145.5, 140.5, 136.5, 136.4, 135.0, 131.9, 131.4, 129.3, 129.2, 129.2, 128.4, 127.9, 127.8, 127.6, 120.7, 91.4, 89.5, 6.1, 2.3; **HRMS** (ESI) m/z calcd for $C_{23}H_{17}OS^+$ $(M+H)^+$: 341.0995, found: 341.0997.

tert-butyl-3-(3-(2-(cyclopropylidene(phenyl)methyl)phenyl)propioloyl)-1H-indole-1-carboxylate, **1l,** the title compound was synthesized according to procedure 1, overall yield 38%, 0.79 g, light yellow oil, (R_f = 0.47, hexane/ethyl acetate = 15:1). **^{1}H NMR (500 MHz, *d*-Acetone):** δ = 8.23 (d, *J* = 7.5 Hz, 1H), 8.18 (s, 1H), 8.12 (d, *J* = 8.0 Hz, 1H), 7.83 (d, *J* = 7.5 Hz, 1H), 7.59 (t, *J* = 7.5 Hz, 1H), 7.51 - 7.48 (m, 3H), 7.43 - 7.38 (m, 2H), 7.32 - 7.27 (m, 3H), 7.17 (t, *J* = 7.5 Hz, 1H), 1.78 - 1.71 (m, 11H), 1.31 (t, *J* = 7.0 Hz, 2H); **^{13}C NMR (125 MHz, *d*-Acetone):** δ = 171.3, 148.7, 145.6, 140.2, 135.7, 135.3, 134.1, 130.6, 130.5, 128.5, 128.2, 127.5, 127.1, 127.1, 126.9, 126.5, 125.7, 124.3, 121.9, 121.3, 120.1, 115.2, 89.9, 88.4, 85.8, 27.3, 4.8, 2.1; **HRMS** (ESI) m/z calcd for $C_{32}H_{28}NO_3^+$ $(M+H)^+$: 474.2064, found: 474.2067.

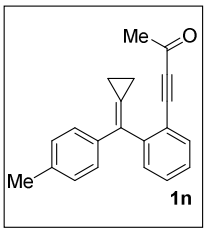


4-(2-((4-chlorophenyl)(cyclopropylidene)methyl)phenyl)but-3-yn-2-one, **1m**, the title compound was synthesized according to procedure 2, overall yield 33%, 0.45 g, light yellow oil, (R_f = 0.67, hexane/ethyl acetate = 15:1). **^{1}H NMR (500 MHz, *d*-Acetone):** δ = 7.70 (d, *J* =

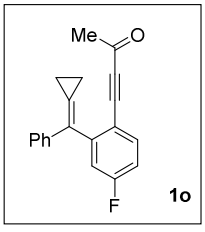


8.0 Hz, 1H), 7.62 - 7.58 (m, 1H), 7.49 - 7.44 (m, 4H), 7.39 - 7.37 (m, 2H), 2.08 (s, 3H), 1.69 - 1.66 (m, 2H), 1.30 - 1.27 (m, 2H); **^{13}C NMR (125 MHz, *d*-Acetone):** δ = 183.9, 145.9, 139.8, 134.7, 133.0, 131.7, 131.3, 129.3, 129.1, 129.0, 128.5, 128.2, 120.6, 92.0, 89.5, 32.5, 5.6, 2.7; **HRMS** (ESI) m/z calcd for $C_{20}H_{16}ClO^+(M+H)^+$: 307.0884, found: 307.0886.

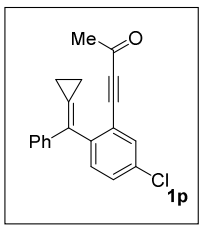
4-(2-(cyclopropylidene(p-tolyl)methyl)phenyl)but-3-yn-2-one, **1n**, the title compound was synthesized according to procedure 2, overall yield 32%, 0.44 g, yellow oil, (R_f = 0.62, hexane/ethyl acetate = 15:1). **^{1}H NMR (500 MHz, *d*-Acetone):** δ = 7.67 (d, *J* = 7.5 Hz, 1H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.45 - 7.41 (m, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.15 (d, *J* = 8.0 Hz, 2H), 2.31 (s, 3H), 2.03 (s, 3H), 1.64 - 1.61 (m, 2H), 1.24 - 1.21 (m, 2H); **^{13}C NMR (125 MHz, *d*-Acetone):** δ = 184.1, 146.7, 138.3, 137.3, 134.7, 131.6, 131.4, 129.7, 129.1, 128.3, 127.7, 126.7, 120.7, 91.7, 90.0, 32.5, 21.1, 5.5, 2.6; **HRMS** (ESI) m/z calcd for $C_{21}H_{19}O^+$ $(M+H)^+$: 287.1430, found: 287.1432.



4-(2-(cyclopropylidene(phenyl)methyl)-4-fluorophenyl)but-3-yn-2-one, **1o**, the title compound was synthesized according to procedure 1, overall yield 35%, 0.50 g, light yellow oil. (R_f = 0.51, hexane/ethyl acetate = 15:1) **^{1}H NMR (500 MHz, *d*-Acetone):** δ = 7.74 (dd, *J* = 7.5, 6.0 Hz, 1H), 7.45 - 7.44 (m, 2H), 7.37 - 7.34 (m, 2H), 7.28 - 7.22 (m, 3H), 2.00 (s, 3H), 1.68 - 1.65 (m, 2H), 1.32 - 1.28 (m, 2H); **^{13}C NMR (125 MHz, *d*-Acetone):** δ = 184.0, 165.6 (J_{CF} = 251.25 Hz), 149.5 (J_{CF} = 8.75 Hz), 140.5, 137.2 (J_{CF} = 8.75 Hz), 129.2, 128.9, 128.5 (J_{CF} =1.25 Hz), 127.9, 127.8, 118.4 (J_{CF} = 22.5 Hz), 117.1 (J_{CF} = 3.75 Hz), 115.8 (J_{CF} = 21.25 Hz), 91.8 (J_{CF} = 1.25 Hz), 88.8, 32.5, 5.7, 2.7; **HRMS** (ESI) m/z calcd for $C_{20}H_{16}FO^+$ $(M+H)^+$: 291.1180, found: 291.1178.

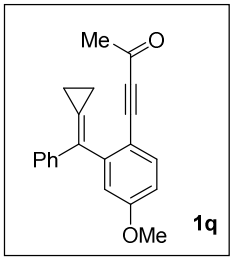


4-(5-chloro-2-(cyclopropylidene(phenyl)methyl)phenyl)but-3-yn-2-one, **1p**, the title compound was synthesized according to procedure 2, overall



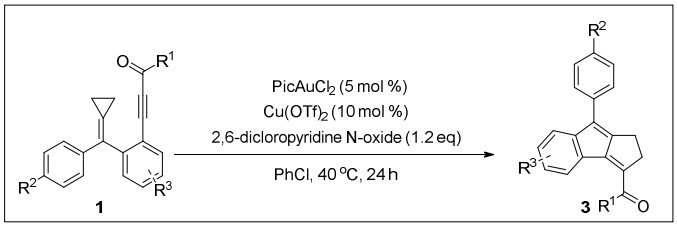
yield 37%, 0.39 g, light yellow oil, (R_f = 0.55, hexane/ethyl acetate = 15:1). **^{1}H NMR (500 MHz, *d*-Acetone):** δ = 7.69 (d, *J* = 8.0 Hz, 1H), 7.61 (td, *J* = 1.5, 8.0 Hz, 1H), 7.50 - 7.46 (m, 2H), 7.42 (s, 1H), 7.38 - 7.34 (m, 2H), 7.29 (dt, *J* = 2.0, 7.0 Hz, 1H), 2.06 (s, 3H), 1.71 - 1.68 (m, 2H), 1.31 - 1.28 (m, 2H); **^{13}C NMR (125 MHz, *d*-Acetone):** δ = 183.1, 147.5, 139.6, 136.3, 135.3, 130.4, 128.3, 128.3, 127.7, 127.4, 127.1, 126.9, 118.7, 91.6, 87.5, 31.7, 4.8, 1.8; **HRMS** (ESI) m/z calcd for $C_{20}H_{16}ClO^+(M+H)^+$: 307.0884, found 307.0888.

4-(2-(cyclopropylidene(phenyl)methyl)-4-methoxyphenyl)but-3-yn-2-one, **1q**, the



title compound was synthesized according to procedure 2, overall yield 28%, 0.42 g, light yellow oil, (R_f = 0.35, hexane/ethyl acetate = 15:1). **^{1}H NMR (500 MHz, *d*-Acetone):** δ = 7.61 (d, *J* = 8.5 Hz, 1H), 7.46 (d, *J* = 7.5 Hz, 2H), 7.33 (t, *J* = 7.5 Hz, 2H), 7.24 (t, *J* = 7.5 Hz, 1H), 7.01 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.98 (d, *J* = 7.5 Hz, 1H), 3.87 (s, 3H), 1.97 (s, 3H), 1.66 - 1.63 (m, 2H), 1.28 - 1.25 (m, 2H); **^{13}C NMR (125 MHz, *d*-Acetone):** δ = 184.0, 162.6, 148.7, 140.8, 136.7, 129.2, 129.0, 127.7, 127.7, 127.6, 116.9, 114.2, 112.6, 91.5, 91.0, 56.0, 32.5, 5.7, 2.6; **HRMS** (ESI) m/z calcd for $C_{21}H_{19}O_2^+$ $(M+H)^+$: 303.1380, found: 303.1378.

4. General procedure of the gold(III)-catalyzed tandem annulation



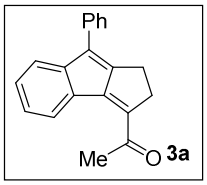
Supplementary Figure 3. Procedure of the gold(III)-catalyzed tandem annulation

To a dry Schlenk tube, 2, 6-dichloropyridine *N*-oxide (1.2 eq, 0.24 mmol, 39.3 mg), $PicAuCl_2$ (5 mol %, 0.01 mmol, 3.9 mg), $Cu(OTf)_2$ (10 mol %, 0.02, 7.2 mg), PhCl (3 mL) were added successively at rt and then a ynone (0.2 mmol) dissolved in PhCl (1 mL) was added to the above mixture. Then the vial was capped with

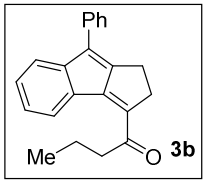
Teflon-coated cap, and the resulting solution was stirred at rt for 5 min, and then was heated at 40 ^{o}C until the reaction was complete, as monitored by thin layer chromatography. And then the reaction mixture was purified by chromatography to get the desired compound **3**.

Data of 3a-3q

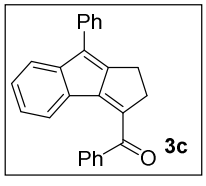
1-(8-phenyl-1,2-dihydrocyclopenta[a]inden-3-yl)ethan-1-one, **3a**, yield 71%. 38.7 mg, red solid, (R_f = 0.38, hexane/ethyl acetate = 30:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.44 (d, *J* = 7.5 Hz, 1H), 7.62 - 7.60 (m, 2H), 7.48 - 7.44 (m, 3H), 7.37 - 7.30 (m, 2H), 7.21 (t, *J* = 7.5 Hz, 1H), 3.35 - 3.34 (m, 2H), 2.91 - 2.89 (m, 2H), 2.47 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$):** (*one carbon merged to others*) δ = 197.5, 153.9, 151.0, 150.2, 140.2, 135.1, 134.1, 130.0, 128.8, 127.9, 127.6, 127.0, 125.5, 120.1, 39.3, 30.3, 23.1; **HRMS** (ESI) m/z calcd for $C_{20}H_{17}O^+$ $(M+H)^+$: 273.1274, found: 273.1276.



1-(8-phenyl-1,2-dihydrocyclopenta[a]inden-3-yl)butan-1-one, **3b**, yield 66%. 39.5 mg, red solid, (R_f = 0.45, hexane/ethyl acetate = 30:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.48 (d, *J* = 7.0 Hz, 1H), 7.61 (d, *J* = 7.5 Hz, 2H), 7.48 - 7.44 (m, 3H), 7.36 - 7.29 (m, 2H), 7.21 (t, *J* = 7.5 Hz, 1H), 3.38 - 3.36 (m, 2H), 2.93 - 2.91 (m, 2H), 2.74 (t, *J* = 7.0 Hz, 2H), 1.81 - 1.74 (m, 2H), 1.02 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 200.0, 153.8, 150.9, 150.2, 140.4, 135.2, 133.9, 130.1, 129.9, 128.8, 127.9, 127.6, 127.0, 125.4, 120.1, 44.4, 38.8, 23.1, 17.2, 14.0; **HRMS** (ESI) m/z calcd for $C_{22}H_{21}O^+$ $(M+H)^+$: 301.1587, found: 301.1589.

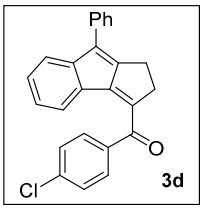


phenyl(8-phenyl-1,2-dihydrocyclopenta[a]inden-3-yl)methanone, **3c**, yield 67%. 44.7 mg, red oil, (R_f = 0.52, hexane/ethyl acetate = 30:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.00 (d, *J* = 7.5 Hz, 2H), 7.67 - 7.63 (m, 3H), 7.52 - 7.46 (m, 5H), 7.37 (t, *J* = 7.5 Hz, 1H), 7.21 (t, *J* = 7.5 Hz, 1H), 6.86 (t, *J* = 7.5 Hz, 1H), 6.62 (d, *J* = 7.5 Hz, 1H), 3.55 - 3.53 (m, 2H), 3.02 -3.00

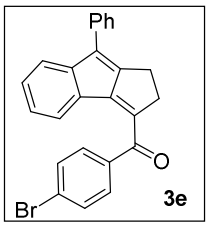


(m, 2H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 195.4, 151.8, 151.2, 150.2, 142.0, 138.2, 135.1, 133.5, 132.4, 129.6, 129.4, 129.0, 129.0, 128.8, 127.9, 127.5, 125.6, 124.2, 120.0, 40.7, 23.2; **HRMS** (ESI) m/z calcd for $C_{25}H_{19}O^+(M+H)^+$: 335.1430, found: 335.1433.

(4-chlorophenyl)(8-phenyl-1,2-dihydrocyclopenta[a]inden-3-yl)methanone, **3d**,

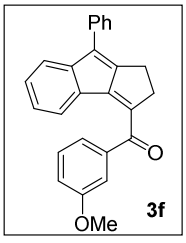


yield 75%. 55.3 mg, red solid, (R_f = 0.47, hexane/ethyl acetate = 30:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 7.94 (d, *J* = 7.5 Hz, 2H), 7.65 (d, *J* = 7.0 Hz, 2H), 7.50 - 7.47 (m, 5H), 7.37 (t, *J* = 7.0 Hz, 1H), 7.22 (t, *J* = 7.0 Hz, 1H), 6.90 (t, *J* = 7.5 Hz, 1H), 6.69 (d, *J* = 7.5 Hz, 1H), 3.51 - 3.50 (m, 2H), 3.01 - 2.99 (m, 2H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 194.0, 151.7, 151.4, 150.2, 141.3, 140.0, 136.4, 135.0, 132.7, 130.9, 129.5, 129.3, 129.2, 128.8, 127.9, 127.6, 125.5, 124.4, 120.2, 40.7, 23.2; **HRMS** (ESI) m/z calcd for $C_{25}H_{18}ClO^+$ $(M+H)^+$: 369.1041, found: 369.1041.



(4-bromophenyl)(8-phenyl-1,2-dihydrocyclopenta[a]inden-3-yl) methanone, **3e**, yield 85%. 70.1 mg, red solid, (R_f = 0.45, hexane/ethyl acetate = 30:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 7.86 (d, *J* = 8.0 Hz, 2H), 7.65 - 7.63 (m, 4H), 7.50 - 7.45 (m, 3H), 7.37 (t, *J* = 7.0 Hz, 1H), 7.22 (t, *J* = 7.0 Hz, 1H), 6.91 (t, *J* = 7.5 Hz, 1H), 6.70 (d, *J* = 7.5 Hz, 1H), 3.51 - 3.50 (m, 2H), 3.00 - 2.99 (m, 2H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 194.2, 151.7, 151.5, 150.2, 141.2, 136.8, 135.0, 132.8, 132.3, 131.0, 129.5, 129.2, 128.8, 128.7, 127.8, 127.6, 125.5, 124.4, 120.2, 40.7, 23.2; **HRMS** (ESI) m/z calcd for $C_{25}H_{18}BrO^+$ $(M+H)^+$: 413.0536, found: 413.0537.

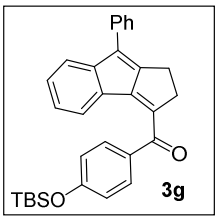
(3-methoxyphenyl)(8-phenyl-1,2-dihydrocyclopenta[a]inden-3-yl)methanone, **3f**,



yield 85%, 57.6 mg, red solid, (R_f = 0.32, hexane/ethyl acetate = 30:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 7.65 (d, *J* = 7.0 Hz, 2H), 7.57 - 7.45 (m, 5H), 7.39 - 7.35 (m, 2H), 7.22 - 7.18 (m, 2H), 6.88 (t,

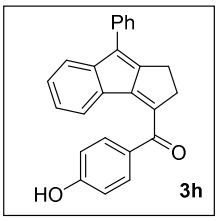
J = 7.5 Hz, 1H), 6.72 (d, *J* = 7.5 Hz, 1H), 3.86 (s, 3H), 3.54 - 3.52 (m, 2H), 3.01 - 3.00 (m, 2H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 195.1, 160.2, 151.8, 151.3, 150.2, 142.0, 139.5, 135.2, 132.5, 130.0, 129.7, 129.0, 128.8, 127.9, 127.5, 125.6, 124.3, 122.6, 120.3, 120.0, 113.0, 55.7, 40.8, 23.2; **HRMS** (ESI) m/z calcd for $C_{26}H_{21}O_2^+$ $(M+H)^+$: 365.1536, found: 365.1538.

(4-((tert-butyldimethylsilyl)oxy)phenyl)(8-phenyl-1,2-dihydrocyclopenta[a]inden



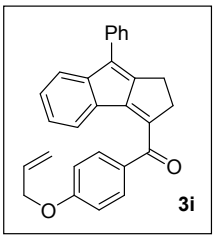
-3-yl)methanone, **3g**, yield 76%. 70.1 mg, red oil, (R_f = 0.53, hexane/ethyl acetate = 30:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 7.95 (d, *J* = 8.0 Hz, 2H), 7.66 - 7.64 (m, 2H), 7.50 - 7.47 (m, 3H), 7.36 (t, *J* = 7.0 Hz, 1H), 7.21 (t, *J* = 7.5 Hz, 1H), 6.93 - 6.92 (m, 2H), 6.86 (t, *J* = 7.5 Hz, 1H), 6.68 (d, *J* = 7.0 Hz, 1H), 3.53 - 3.52 (m, 2H), 3.01 - 3.00 (m, 2H), 1.01 (s, 9H), 0.26 (s, 6H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 194.1, 161.0, 152.0, 150.1, 150.0, 142.8, 135.3, 132.0, 131.9, 131.4, 129.7, 128.8, 128.8, 127.9, 127.4, 125.4, 124.0, 120.6, 119.9, 40.9, 25.8, 23.3, 18.5, -4.2; **HRMS** (ESI) m/z calcd for $C_{31}H_{33}O_2Si^+$ $(M+H)^+$: 465.2244, found: 465.2244.

(4-hydroxyphenyl)(8-phenyl-1,2-dihydrocyclopenta[a]inden-3-yl)methanone, **3h**,



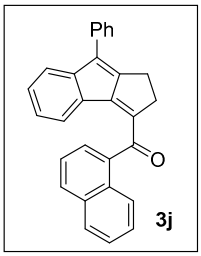
yield 62%, 43.5 mg, red wax like solid, (R_f = 0.13, hexane/ethyl acetate = 8:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 9.45 (s, 1H), 7.93 (d, *J* = 9.0 Hz, 2H), 7.70 (d, *J* = 7.5 Hz, 2H), 7.52 - 7.49 (m, 3H), 7.36 (t, *J* = 7.5 Hz, 1H), 7.24 (t, *J* = 7.5 Hz, 1H), 6.99 (d, *J* = 7.5 Hz, 2H), 6.93 (t, *J* = 7.5 Hz, 1H), 6.84 (d, *J* = 7.5 Hz, 1H), 3.51 - 3.50 (m, 2H), 3.04 - 3.03 (m, 2H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 193.8, 163.5, 152.9, 150.7, 149.4, 144.9, 136.0, 132.8, 131.7, 130.4, 130.4, 129.6, 129.4, 128.5, 128.1, 125.5, 124.7, 120.5, 116.5, 41.6, 23.8; **HRMS** (ESI) m/z calcd for $C_{25}H_{19}O_2^+$ $(M+H)^+$ 351.1379, found 351.1373.

(4-(allyloxy)phenyl)(8-phenyl-1,2-dihydrocyclopenta[a]inden-3-yl)methanone, **3i**,



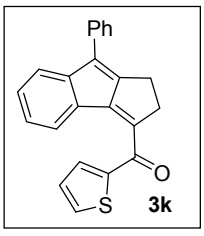
yield 66%, 51.5 mg, red wax like solid, (R_f = 0.21, hexane/ethyl acetate = 30:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.01 (d, *J* = 9.0 Hz, 2H), 7.66 (d, *J* = 7.5 Hz, 2H), 7.50 - 7.47 (m, 3H), 7.36 (t, *J* = 7.5 Hz, 1H), 7.22 (t, *J* = 7.5 Hz, 1H), 6.99 (d, *J* = 8.5 Hz, 2H), 6.89 (t, *J* = 4.5 Hz, 1H), 6.75 (d, *J* = 7.5 Hz, 1H), 6.11 - 6.03 (m, 1H), 5.45 (d, *J* = 17.0 Hz, 1H), 5.34 (d, *J* = 16.0 Hz, 1H), 4.64 (d, *J* = 5.0 Hz, 2H), 3.54 - 3.52 (m, 2H), 3.02 - 3.01 (m, 2H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 193.9, 163.2, 151.9, 150.1, 149.8, 142.8, 135.3, 132.5, 132.1, 131.8, 130.7, 129.7, 128.8, 128.7, 127.9, 127.4, 125.3, 124.1, 119.9, 118.4, 115.0, 69.1, 41.0, 23.3; **HRMS** (ESI) m/z calcd for $C_{28}H_{23}O_2^+$ $(M+H)^+$: 391.1693, found: 391.1694.

naphthalen-1-yl(8-phenyl-1,2-dihydrocyclopenta[a]inden-3-yl)methanone, **3j**, red



solid. yield 69%. 53.1 mg, red oil, (R_f = 0.37, hexane/ethyl acetate = 30:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.42 (d, *J* = 8.0 Hz, 1H), 8.06 (d, *J* = 8.5 Hz, 1H), 7.97 - 7.96 (m, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.64 - 7.58 (m, 4H), 7.51 - 7.47 (m, 3H), 7.42 (d, *J* = 7.5 Hz, 1H), 7.36 (t, *J* = 7.5 Hz, 1H), 7.17 (t, *J* = 7.0 Hz, 1H), 6.78 (t, *J* = 7.5 Hz, 1H), 6.63 (d, *J* = 7.5 Hz, 1H), 3.48 - 3.47 (m, 2H), 2.97 - 2.96 (m, 2H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 196.3, 153.3, 151.9, 150.2, 142.8, 137.3, 135.0, 134.0, 133.7, 132.3, 130.2, 129.7, 129.4, 128.8, 128.6, 128.5, 128.0, 127.9, 127.7, 126.8, 126.2, 125.6, 125.2, 124.7, 120.0, 39.9, 23.0; **HRMS** (ESI) m/z calcd for $C_{29}H_{21}O^+$ $(M+H)^+$: 385.1587, found: 385.1588.

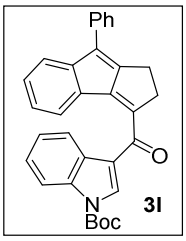
(8-phenyl-1,2-dihydrocyclopenta[a]inden-3-yl)(thiophen-2-yl)methanone, **3k**,



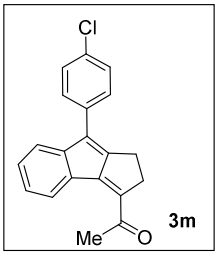
yield 76%, 51.7 mg, red solid, (R_f = 0.38, hexane/ethyl acetate = 30:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 7.84 (d, *J* = 3.5 Hz, 1H), 7.78 (d, *J* = 4.5 Hz, 1H), 7.65 (d, *J* = 7.5 Hz, 2H), 7.50 - 7.47 (m, 3H), 7.38 - 7.35 (m, 2H), 7.27 - 7.24 (m, 1H), 7.14 (t, *J* = 4.5 Hz, 1H), 7.01 (t, *J* = 7.5 Hz, 1H), 3.58 - 3.56 (m, 2H), 3.02 - 3.01 (m, 2H); **^{13}C NMR (125**

MHz, $CDCl_3$): δ = 186.2, 151.9, 151.3, 150.2, 144.4, 141.5, 135.2, 135.1, 134.8, 132.6, 129.8, 129.2, 128.8, 128.5, 127.9, 127.6, 125.8, 124.5, 120.1, 40.6, 23.4; **HRMS** (ESI) m/z calcd for $C_{23}H_{17}OS^+$ $(M+H)^+$: 341.0995, found: 341.0995.

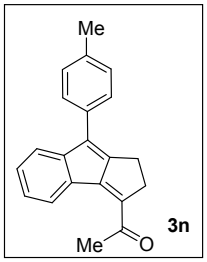
tert-butyl3-(8-phenyl-1,2-dihydrocyclopenta[a]indene-3-carbonyl)-1H-indole-1-carboxylate, **3l**, yield 90%, 85.1 mg, red oil, (R_f = 0.28, hexane/ethyl acetate = 30:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.52 - 8.50 (m, 1H), 8.28 (s, 1H), 8.22 - 8.20 (m, 1H), 7.68 (d, *J* = 6.0 Hz, 2H), 7.52 - 7.42 (m, 6H), 7.37 (t, *J* = 8.0 Hz, 1H), 7.27 - 7.24 (m, 1H), 6.98 (t, *J* = 8.0 Hz, 1H), 3.60 - 3.58 (m, 2H), 3.05 - 3.03 (m, 2H), 1.60 (s, 9H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 189.3, 151.7, 150.2, 150.1, 149.1, 143.2, 135.9, 135.3, 135.0, 132.0, 129.9, 128.9, 128.8, 127.9, 127.6, 127.4, 126.0, 125.5, 124.8, 124.3, 122.9, 120.0, 120.0, 115.2, 85.6, 40.7, 28.1, 23.4; **HRMS** (ESI) m/z calcd for $C_{32}H_{28}NO_3^+$ $(M+H)^+$: 474.2064, found: 474.2064.



1-(8-(4-chlorophenyl)-1,2-dihydrocyclopenta[a]inden-3-yl)ethan-1-one, **3m**, yield 61%, 37.2 mg, red wax like solid, (R_f = 0.30, hexane/ethyl acetate = 30:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.44 (d, *J* = 7.5 Hz, 1H), 7.53 (d, *J* = 8.0 Hz, 2H), 7.43 (d, *J* = 8.5 Hz, 2H), 7.39 (d, *J* = 7.5 Hz, 1H), 7.31 (t, *J* = 7.5 Hz, 1H), 7.22 (t, *J* = 7.5 Hz, 1H), 3.36 - 3.34 (m, 2H), 2.88 - 2.86 (m, 2H), 2.47 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 197.5, 153.6, 151.4, 149.8, 140.6, 133.5, 133.3, 132.9, 130.1, 129.9, 129.1, 129.0, 127.2, 125.6, 119.9, 39.3, 30.3, 23.1; **HRMS** (ESI) m/z calcd for $C_{20}H_{16}ClO^+$ $(M+H)^+$: 307.0884, found: 307.0882.

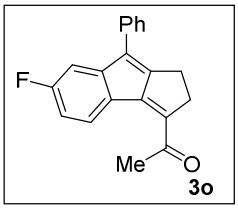


1-(8-(p-tolyl)-1,2-dihydrocyclopenta[a]inden-3-yl)ethan-1-one, **3n**, yield 96%, 55.3 mg, red solid, (R_f = 0.30, hexane/ethyl acetate = 30:1) **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.44 (d, *J* = 7.5 Hz, 1H), 7.51 (d, *J* = 8.0 Hz, 2H), 7.45 (d, *J* = 7.5 Hz, 1H), 7.32 - 7.26 (m, 3H), 7.20 (t, *J* = 7.5 Hz, 1H), 3.33 - 3.31 (m, 2H), 2.88 - 2.87 (m, 2H), 2.45 (s, 3H),



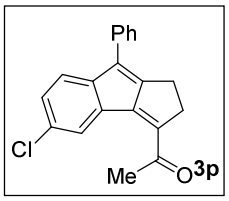
2.42 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 197.5, 154.0, 150.4, 150.3, 139.9, 137.5, 134.1, 132.1, 130.0, 129.9, 129.5, 127.8, 127.0, 125.4, 120.1, 39.2, 30.3, 23.1, 21.5; **HRMS** (ESI) m/z calcd for $C_{21}H_{19}O^+$ $(M+H)^+$: 287.1430, found: 287.1431.

1-(6-fluoro-8-phenyl-1,2-dihydrocyclopenta[a]inden-3-yl)ethan-1-one, **3o**, yield



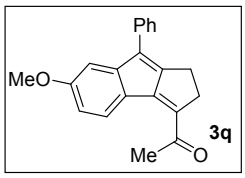
49%, 28.4 mg, red oil, (R_f = 0.30, hexane/ethyl acetate = 30:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.44 - 8.41 (m, 1H), 7.57 (d, *J* = 7.5 Hz, 2H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.36 (t, *J* = 7.5 Hz, 1H), 7.13 (dd, *J* = 9.5, 2.5 Hz, 1H), 6.86 (td, *J* = 9.0, 2.5 Hz, 1H), 3.37 - 3.35 (m, 2H), 2.94 - 2.92 (m, 2H), 2.46 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 197.5, 164.4 (J_{CF} = 246.25 Hz), 152.9 (J_{CF} = 8.75 Hz), 152.8, 152.7, 139.9, 134.6, 133.3, 128.9, 128.4 (J_{CF} = 10.0 Hz), 127.9, 127.7, 125.9 (J_{CF} = 3.75 Hz), 111.3 (J_{CF} = 22.5 Hz), 108.27 (J_{CF} = 25.0 Hz), 39.2, 30.2, 23.2; **^{19}F NMR** (470 MHz, $CDCl_3$) δ = -109.6; **HRMS** (ESI) m/z calcd for $C_{20}H_{16}FO^+$ $(M+H)^+$ 291.1180, found 291.1181.

1-(5-chloro-8-phenyl-1,2-dihydrocyclopenta[a]inden-3-yl)ethan-1-one, **3p**, yield



49%, 29.7 mg, red oil, (R_f = 0.25, hexane/ethyl acetate = 30:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.44 (d, *J* = 7.5 Hz, 1H), 7.57 (t, *J* = 1.5 Hz, 1H), 7.48 - 7.47 (m, 1H), 7.41 - 7.37 (m, 2H), 7.33 (t, *J* = 7.5 Hz, 2H), 7.22 (t, *J* = 7.5 Hz, 1H), 3.38 - 3.36 (m, 2H), 2.91 - 2.89 (m, 2H), 2.48 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 197.5, 153.5, 151.9, 149.6, 140.9, 136.9, 134.7, 132.7, 130.1, 130.0, 129.8, 127.8, 127.6, 127.2, 126.0, 125.7, 119.9, 39.3, 30.3, 23.1; **HRMS** (ESI) m/z calcd for $C_{20}H_{16}ClO^+$ $(M+H)^+$: 307.0884, found 307.0887.

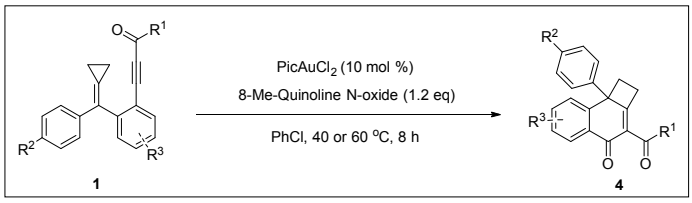
1-(6-methoxy-8-phenyl-1,2-dihydrocyclopenta[a]inden-3-yl)ethan-1-one, **3q**, yield



53%, 31.8 mg, red oil, (R_f = 0.20, hexane/ethyl acetate = 30:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.39 (d, *J* = 8.5 Hz, 1H), 7.58 (d, *J* = 7.0 Hz, 2H), 7.46 (t, *J* = 7.5 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.00 (d, *J* = 2.5 Hz, 1H), 6.67 (dd, *J* = 8.5, 2.5 Hz, 1H), 3.85 (s, 3H), 3.33 - 3.31 (m, 2H), 2.90 - 2.88 (m, 2H), 2.45 (s, 3H); **^{13}C NMR (125**

MHz, $CDCl_3$): δ = 197.5, 161.8, 153.4, 152.8, 152.5, 137.9, 135.0, 133.5, 128.8, 128.4, 127.8, 127.6, 122.8, 108.4, 108.2, 55.7, 38.9, 30.2, 23.1; **HRMS** (ESI) m/z calcd for $C_{21}H_{19}O_2^+$ $(M+H)^+$: 303.1380, found: 303.1379.

5. General procedure of the gold(III)-catalyzed oxidative cyclization

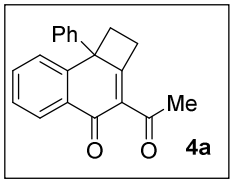


Supplementary Figure 4. Procedure of the gold(III)-catalyzed oxidative cyclization

To a dry Schlenk tube, 8-Me-Quinoline *N*-oxide (1.2 eq, 0.24 mmol, 38.2 mg), $PicAuCl_2$ (10 mol %, 0.02 mmol, 7.8 mg), PhCl (3 mL) were added successively at rt and then a ynone (0.2 mmol) dissolved in PhCl (1 mL) was added to the above mixture. Then the vial was capped with Teflon-coated cap, the resulting solution was stirred at rt for 5 min, and then was heated until the reaction was complete, as monitored by thin layer chromatography. The reaction mixture was purified by chromatography to get the desired compound **4**.

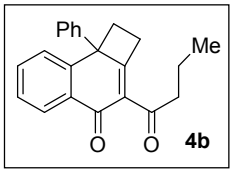
Data of 4a-4q

3-acetyl-8b-phenyl-1,8b-dihydrocyclobuta[a]naphthalen-4(2H)-one, **4a**, yield 79%.



45.6 mg, light yellow oil, (R_f = 0.54, hexane/ethyl acetate = 8:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.08 (d, *J* = 8.0 Hz, 1H), 7.44 - 7.41 (m, 1H), 7.38 - 7.28 (m, 6H), 7.21 (t, *J* = 7.5 Hz, 1H), 3.42 - 3.35 (m, 1H), 3.33 - 3.28 (m, 1H), 3.22 - 3.18 (m, 1H), 2.58 (s, 3H), 2.55 - 2.50 (m, 1H). **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 197.4, 184.7, 176.0, 147.2, 142.0, 133.0, 132.5, 130.9, 129.3, 127.7, 127.6, 127.3, 126.2, 125.1, 57.9, 34.8, 31.3, 29.5; **HRMS** (ESI) m/z calcd for $C_{20}H_{17}O_2^+$ $(M+H)^+$: 289.1223, found: 289.1226.

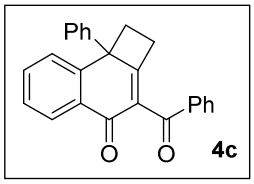
3-butyryl-8b-phenyl-1,8b-dihydrocyclobuta[a]naphthalen-4(2H)-one, **4b**, yield 89%.



55.9 mg, colorless oil, (R_f = 0.57, hexane/ethyl acetate = 8:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.07 (d, *J* = 7.5 Hz, 1H),

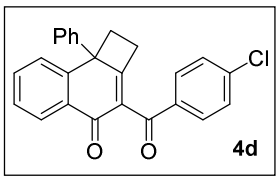
7.42 (td, *J* = 7.0, 1.5 Hz, 1H), 7.38 - 7.36 (m, 2H), 7.34 - 7.26 (m, 4H), 7.21 (t, *J* = 7.5 Hz, 1H), 3.40 - 3.33 (m, 1H), 3.30 - 3.25 (m, 1H), 3.21 - 3.16 (m, 1H), 3.10 - 3.04 (m, 1H), 2.85 - 2.79 (m, 1H), 2.55 - 2.49 (m, 1H), 1.74 - 1.63 (m, 2H), 0.98 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 200.1, 184.7, 175.1, 147.2, 142.1, 133.0, 132.4, 131.1, 129.3, 127.6, 127.5, 127.3, 126.2, 125.1, 57.8, 45.2, 34.5, 29.4, 17.4, 14.0; **HRMS** (ESI) m/z calcd for $C_{22}H_{21}O_2^+$ $(M+H)^+$: 317.1536 found: 317.1537.

3-benzoyl-8b-phenyl-1,8b-dihydrocyclobuta[a]naphthalen-4(2H)-one, **4c**, yield



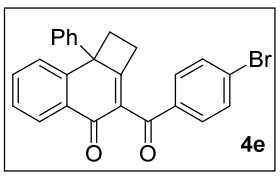
77%. 54.2 mg, white solid, (R_f = 0.33, hexane/ethyl acetate = 8:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.11 (d, *J* = 7.5 Hz, 1H), 7.88 (d, *J* = 7.5 Hz, 2H), 7.57 (t, *J* = 7.0 Hz, 1H), 7.53 - 7.51 (m, 2H), 7.47 - 7.44 (m, 3H), 7.38 - 7.26 (m, 5H), 3.21 - 3.17 (m, 1H), 3.09 - 3.02 (m, 1H), 2.84 - 2.79 (m, 1H), 2.54 - 2.48 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 192.8, 184.1, 169.1, 147.4, 141.9, 137.9, 133.5, 132.6, 132.4, 131.2, 129.4, 129.4, 128.7, 127.9, 127.6, 127.4, 126.3, 125.4, 57.5, 33.2, 29.0; **HRMS** (ESI) m/z calcd for $C_{25}H_{19}O_2^+$ $(M+H)^+$: 351.1380, found: 351.1380.

3-(4-chlorobenzoyl)-8b-phenyl-1,8b-dihydrocyclobuta[a]naphthalen-4(2H)-one,



4d, yield 67%. 51.8 mg, white solid, (R_f = 0.52, hexane/ethyl acetate = 8:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.10 (d, *J* = 8.0 Hz, 1H), 7.81 (d, *J* = 8.5 Hz, 2H), 7.50 (d, *J* = 8.0 Hz, 2H), 7.46 - 7.42 (m, 3H), 7.38 - 7.25 (m, 5H), 3.24 - 3.20 (m, 1H), 3.12 - 3.05 (m, 1H), 2.88 - 2.83 (m, 1H), 2.54 - 2.48 (m, 1H). **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 191.6, 184.0, 169.9, 147.4, 141.7, 140.0, 136.2, 132.7, 132.2, 130.9, 130.8, 129.4, 129.1, 127.9, 127.7, 127.4, 126.2, 125.5, 57.6, 33.3, 28.9; **HRMS** (ESI) m/z calcd for $C_{25}H_{18}ClO_2^+$ $(M+H)^+$: 385.0990, found: 385.0992.

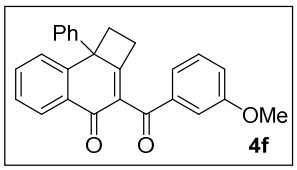
3-(4-bromobenzoyl)-8b-phenyl-1,8b-dihydrocyclobuta[a]naphthalen-4(2H)-one,



4e, yield 72%. 61.9 mg, white solid, (R_f = 0.52, hexane/ethyl acetate = 8:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.10 (d, *J* =

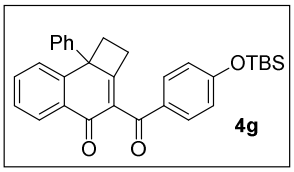
7.5 Hz, 1H), 7.72 (d, *J* = 8.5 Hz, 2H), 7.60 (d, *J* = 8.0 Hz, 2H), 7.50 (d, *J* = 8.0 Hz, 2H), 7.44 (t, *J* = 8.0 Hz, 1H), 7.37 - 7.26 (m, 5H), 3.24 - 3.20 (m, 1H), 3.11 - 3.05 (m, 1H), 2.87 - 2.83 (m, 1H), 2.54 - 2.48 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 191.8, 184.0, 170.0, 147.4, 141.7, 136.6, 132.7, 132.2, 132.0, 130.9, 130.8, 129.4, 128.7, 127.9, 127.7, 127.4, 126.2, 125.5, 57.6, 33.3, 28.9; **HRMS** (ESI) m/z calcd for $C_{25}H_{18}BrO_2^+(M+H)^+$: 429.0485, found: 429.0488.

3-(3-methoxybenzoyl)-8b-phenyl-1,8b-dihydrocyclobuta[a]naphthalen-4(2H)-one,



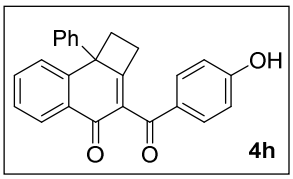
4f, yield 74%, 52.7 mg, white solid, (R_f = 0.23, hexane/ethyl acetate = 8:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.06 (d, *J* = 7.5 Hz, 1H), 7.47 (d, *J* = 7.5 Hz, 2H), 7.40 - 7.37 (m, 3H), 7.32 - 7.24 (m, 5H), 7.21 (t, *J* = 8.0 Hz, 1H), 7.07 (dd, *J* = 8.5, 2.5 Hz, 1H), 3.76 (s, 3H), 3.16 - 3.12 (m, 1H), 3.04 - 2.97 (m, 1H), 2.78 - 2.74 (m, 1H), 2.48 - 2.43 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 192.6, 184.1, 168.8, 159.9, 147.4, 141.9, 139.2, 132.6, 132.3, 131.3, 129.7, 129.4, 127.9, 127.6, 127.4, 126.2, 125.4, 122.4, 120.4, 113.1, 57.4, 55.5, 33.2, 29.0; **HRMS** (ESI) m/z calcd for $C_{26}H_{21}O_3^+$ $(M+H)^+$: 381.1485, found: 381.1488.

3-(4-((tert-butyldimethylsilyl)oxy)benzoyl)-8b-phenyl-1,8b-dihydrocyclobuta[a]n



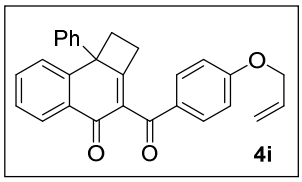
aphthalen-4(2H)-one, **4g**, yield 68%, 65.6 mg, light yellow oil, (R_f = 0.57, hexane/ethyl acetate = 8:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.12 (d, *J* = 7.5 Hz, 1H), 7.84 (d, *J* = 7.5 Hz, 2H), 7.53 - 7.52 (m, 2H), 7.43 (t, *J* = 6.0 Hz, 1H), 7.37 - 7.26 (m, 5H), 6.88 (d, *J* = 7.5 Hz, 2H), 3.20 - 3.17 (m, 1H), 3.07 - 3.01 (m, 1H), 2.85 - 2.81 (m, 1H), 2.53 - 2.48 (m, 1H), 0.99 (s, 9H), 0.24 (s, 6H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 191.3, 184.2, 167.5, 160.9, 147.5, 142.1, 132.5, 132.4, 131.8, 131.5, 131.3, 129.4, 127.9, 127.5, 127.3, 126.3, 125.4, 120.1, 57.4, 33.0, 29.0, 25.7, 18.4, -4.2; **HRMS** (ESI) m/z calcd for $C_{31}H_{33}O_3Si^+$ $(M+H)^+$: 481.2194, found: 481.2191.

3-(4-hydroxybenzoyl)-8b-phenyl-1,8b-dihydrocyclobuta[a]naphthalen-4(2H)-one,



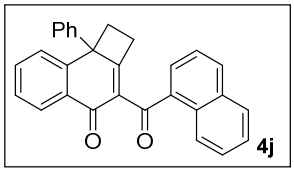
4h, yield 70%, 51.3 mg, white solid, (R_f = 0.12, hexane/ethyl acetate = 4:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 10.56 (s, 1H), 7.92 (d, *J* = 7.5 Hz, 1H), 7.73 - 7.70 (m, 2H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.55 - 7.52 (m, 2H), 7.41 - 7.38 (m, 3H), 7.27 (t, *J* = 7.0 Hz, 1H), 6.88 (d, *J* = 7.5 Hz, 2H), 3.23 - 3.17 (m, 1H), 2.96 - 2.90 (m, 1H), 2.69 - 2.65 (m, 1H), 2.54 - 2.50 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 190.4, 183.5, 166.3, 162.8, 147.9, 142.3, 132.7, 131.7, 131.4, 131.1, 129.3, 128.5, 127.3, 127.3, 126.7, 126.1, 125.9, 115.6, 56.6, 32.2, 28.7; **HRMS** (ESI) m/z calcd for $C_{25}H_{19}O_3^+$ $(M+H)^+$ 367.1329, found 367.1330.

3-(4-(allyloxy)benzoyl)-8b-phenyl-1,8b-dihydrocyclobuta[a]naphthalen-4(2H)-on



e, **4i**, yield 86%, 69.9 mg, light yellow solid, (R_f = 0.21, hexane/ethyl acetate = 8:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.12 (d, *J* = 7.5 Hz, 1H), 7.88 (d, *J* = 9.0 Hz, 2H), 7.52 (d, *J* = 7.5 Hz, 2H), 7.43 (t, *J* = 7.5 Hz, 1H), 7.37 - 7.24 (m, 5H), 6.94 (d, *J* = 9.0 Hz, 2H), 6.08 - 6.00 (m, 1H), 5.42 (d, *J* = 17.0 Hz, 1H), 5.31 (d, *J* = 10.5 Hz, 1H), 4.60 (d, *J* = 5.0 Hz, 2H), 3.21 - 3.17 (m, 1H), 3.08 - 3.01 (m, 1H), 2.86 - 2.81 (m, 1H), 2.53 - 2.48 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 191.2, 184.2, 167.7, 163.0, 147.5, 142.0, 132.6, 132.5, 132.4, 131.9, 131.5, 130.9, 129.4, 127.9, 127.5, 127.3, 126.3, 125.4, 118.3, 114.7, 69.1, 57.4, 33.0, 29.0; **HRMS** (ESI) m/z calcd for $C_{28}H_{23}O_3^+$ $(M+H)^+$: 407.1642, found: 407.1644.

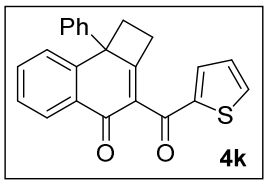
3-(1-naphthoyl)-8b-phenyl-1,8b-dihydrocyclobuta[a]naphthalen-4(2H)-one, **4j**,



yield 69%. 55.5 mg, light yellow solid, (R_f = 0.32, hexane/ethyl acetate = 8:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.63 (d, *J* = 8.5 Hz, 1H), 8.07 (d, *J* = 8.0 Hz, 1H), 7.99 (d, *J* = 8.5 Hz, 1H), 7.90 (d, *J* = 7.5 Hz, 1H), 7.76 (d, *J* = 7.5 Hz, 1H), 7.60 - 7.52 (m, 2H), 7.49 - 7.42 (m, 4H), 7.36 - 7.29 (m, 4H), 7.27 - 7.24 (m, 1H), 3.15 - 3.11 (m, 1H), 2.94 - 2.87 (m, 1H), 2.72 - 2.67 (m, 1H), 2.53 - 2.48 (m, 1H); **^{13}C NMR (125 MHz,**

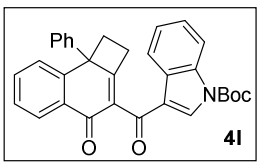
$CDCl_3$): δ = 194.2, 184.0, 171.7, 147.1, 142.0, 136.6, 134.1, 132.9, 132.8, 132.7, 132.5, 130.5, 129.4, 129.3, 128.6, 128.0, 127.9, 127.6, 127.4, 126.6, 126.2, 125.7, 125.2, 124.6, 57.6, 33.4, 29.0; **HRMS** (ESI) m/z calcd for $C_{29}H_{21}O_2^+$ $(M+H)^+$: 401.1536, found: 401.1539.

8b-phenyl-3-(thiophene-2-carbonyl)-1,8b-dihydrocyclobuta[a]naphthalen-4(2H)-



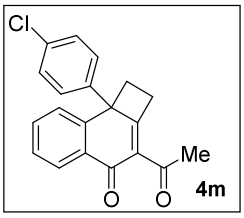
one, **4k**, yield 89%, 63.5 mg, white solid, (R_f = 0.29, hexane/ethyl acetate = 8:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.13 (d, *J* = 7.5 Hz, 1H), 7.69 (dd, *J* = 4.5, 0.5 Hz, 1H), 7.64 (dd, *J* = 4.0, 1.0 Hz, 1H), 7.53 - 7.51 (m, 2H), 7.43 (td, *J* = 7.5, 1.0 Hz, 1H), 7.38 - 7.32 (m, 3H), 7.30 - 7.25 (m, 2H), 7.12 - 7.10 (m, 1H), 3.23 - 3.18 (m, 1H), 3.16 - 3.09 (m, 1H), 2.95 - 2.91 (m, 1H), 2.53 - 2.48 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 184.3, 183.7, 167.9, 147.4, 144.9, 141.9, 135.1, 134.3, 132.6, 132.3, 131.5, 129.4, 128.4, 128.0, 127.6, 127.4, 126.3, 125.4, 57.4, 33.5, 29.1; **HRMS** (ESI) m/z calcd for $C_{23}H_{17}O_2S^+$ $(M+H)^+$: 357.0944, found: 357.0945.

tert-butyl3-(4-oxo-8b-phenyl-1,2,4,8b-tetrahydrocyclobuta[a]naphthalene-3-carb



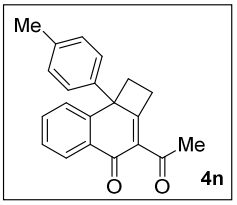
onyl)-1H-indole-1-carboxylate, **4l**, yield 76%, 74.7 mg, light yellow solid, (R_f = 0.23, hexane/ethyl acetate = 8:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.45 (d, *J* = 7.5 Hz, 1H), 8.15 (t, *J* = 8.0 Hz, 2H), 8.06 (s, 1H), 7.55 (d, *J* = 8.0 Hz, 2H), 7.45 - 7.34 (m, 6H), 7.31 - 7.26 (m, 2H), 3.23 - 3.20 (m, 1H), 3.16 - 3.10 (m, 1H), 2.98 - 2.94 (m, 1H), 2.56 - 2.51 (m, 1H), 1.61 (s, 9H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 187.2, 184.3, 166.9, 148.9, 147.4, 142.0, 135.9, 134.6, 132.6, 132.5, 132.4, 129.4, 127.9, 127.5, 127.5, 127.3, 126.2, 125.9, 125.4, 124.7, 122.9, 121.2, 115.1, 85.4, 57.3, 33.4, 29.1, 28.1; **HRMS** (ESI) m/z calcd for $C_{32}H_{28}NO_4^+$ $(M+H)^+$: 490.2013, found: 490.2015.

3-acetyl-8b-(4-chlorophenyl)-1,8b-dihydrocyclobuta[a]naphthalen-4(2H)-one, **4m**,



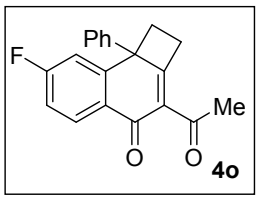
yield 69%, 44.5 mg, light yellow oil, (R_f = 0.37, hexane/ethyl acetate = 8:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.02 (d, *J* = 8.0 Hz, 1H), 7.36 - 7.28 (m, 5H), 7.25 - 7.23 (m, 2H), 3.41 - 3.28 (m, 2H), 3.21 - 3.17 (m, 1H), 2.58 (s, 3H), 2.55 - 2.49 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 197.1, 183.7, 175.8, 148.6, 141.3, 139.0, 131.4, 130.7, 129.5, 129.5, 127.9, 127.9, 126.2, 125.3, 57.5, 34.9, 31.3, 29.4; **HRMS** (ESI) m/z calcd for $C_{20}H_{16}ClO_2^+$ $(M+H)^+$: 323.0833, found: 323.0835.

3-acetyl-8b-(p-tolyl)-1,8b-dihydrocyclobuta[a]naphthalen-4(2H)-one, **4n**, yield



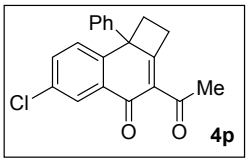
64%, 38.4 mg, light yellow oil, (R_f = 0.48, hexane/ethyl acetate = 8:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.07 (d, *J* = 8.0 Hz, 1H), 7.42 (td, *J* = 7.5, 1.5 Hz, 1H), 7.32 (td, *J* = 7.5, 1.5 Hz, 1H), 7.29 - 7.24 (m, 3H), 7.10 (d, *J* = 8.0 Hz, 2H), 3.42 - 3.35 (m, 1H), 3.31 - 3.27 (m, 1H), 3.19 - 3.15 (m, 1H), 2.58 (s, 3H), 2.53 - 2.47 (m, 1H), 2.28 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 197.4, 184.8, 176.3, 147.4, 139.1, 137.4, 133.0, 132.5, 130.8, 130.0, 127.7, 127.2, 126.1, 125.1, 57.6, 34.8, 31.3, 29.4, 21.1; **HRMS** (ESI) m/z calcd for $C_{21}H_{19}O_2^+$ $(M+H)^+$: 303.1380, found: 303.1382.

3-acetyl-7-fluoro-8b-phenyl-1,8b-dihydrocyclobuta[a]naphthalen-4(2H)-one, **4o**,



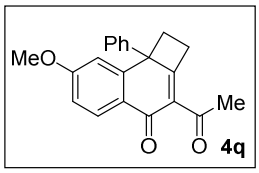
yield 44%, 27.2 mg, light yellow oil, (R_f = 0.50, hexane/ethyl acetate = 8:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.11 - 8.08 (m, 1H), 7.36 - 7.30 (m, 4H), 7.25 - 7.22 (m, 1H), 7.00 (td, *J* = 8.5, 2.5 Hz, 1H), 6.94 (dd, *J* = 8.5, 2.5 Hz, 1H), 3.40 - 3.28 (m, 2H), 3.20 - 3.16 (m, 1H), 2.58 (s, 3H), 2.55 - 2.50 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 197.2, 183.5, 175.6, 165.1 (J_{CF} = 253.75 Hz), 150.0 (J_{CF} = 8.75 Hz), 141.4, 130.9, 130.8 (J_{CF} = 10.0 Hz), 130.8, 129.4, 127.9, 126.2, 115.1 (J_{CF} = 21.25 Hz), 111.9 (J_{CF} = 22.5 Hz), 57.6 (J_{CF} = 2.5 Hz), 34.8, 31.3, 29.4; **^{19}F NMR** (470 MHz, $CDCl_3$) δ = -105.2; **HRMS** (ESI) m/z calcd for $C_{20}H_{16}FO_2^+$ $(M+H)^+$: 307.1129, found: 307.1130.

3-acetyl-6-chloro-8b-phenyl-1,8b-dihydrocyclobuta[a]naphthalen-4(2H)-one, **4p**,



yield 62%, 40.1 mg, light yellow oil, (R_f = 0.37, hexane/ethyl acetate = 8:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.08 (d, *J* = 7.5 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 1H), 7.37 - 7.34 (m, 2H), 7.27 (d, *J* = 7.5 Hz, 1H), 7.22 - 7.20 (m, 3H), 3.41 - 3.28 (m, 2H), 3.17 - 3.13 (m, 1H), 2.58 (s, 3H), 2.56 - 2.51 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 197.3, 184.4, 174.8, 146.3, 144.1, 135.2, 133.0, 132.6, 131.1, 130.5, 127.9, 127.9, 127.7, 126.5, 125.1, 124.5, 57.5, 34.8, 31.3, 29.6; **HRMS** (ESI) m/z calcd for $C_{20}H_{16}ClO_2^+$ $(M+H)^+$: 323.0833, found: 323.0837.

3-acetyl-7-methoxy-8b-phenyl-1,8b-dihydrocyclobuta[a]naphthalen-4(2H)-one,

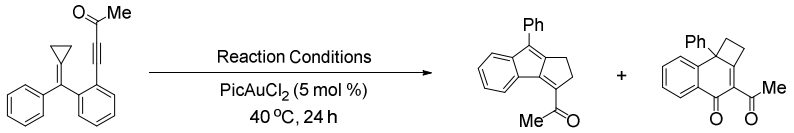


4q, yield 60%, 38.3 mg, light yellow oil, (R_f = 0.30, hexane/ethyl acetate = 8:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.05 (d, *J* = 8.5 Hz, 1H), 7.37 (d, *J* = 7.5 Hz, 2H), 7.29 (t, *J* = 7.0 Hz, 2H), 7.22 (t, *J* = 7.5 Hz, 1H), 6.83 (dd, *J* = 9.0, 2.5 Hz, 1H), 6.71 (d, *J* = 7.5 Hz, 1H), 3.80 (s, 3H), 3.38 - 3.25 (m, 2H), 3.19 - 3.15 (m, 1H), 2.58 (s, 3H), 2.53 - 2.47 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 197.7, 183.9, 175.1, 162.8, 149.6, 142.0, 130.9, 130.1, 129.3, 127.6, 126.4, 126.2, 113.1, 110.0, 57.8, 55.6, 34.8, 31.3, 29.4; **HRMS** (ESI) m/z calcd for $C_{21}H_{19}O_3^+$ $(M+H)^+$: 319.1329, found: 319.1329.

6. Mechanism studies

6.1 Control experimets of the tandem cyclization

Supplementary Table 2. Control experiments[a]



1a **3a** **4a**

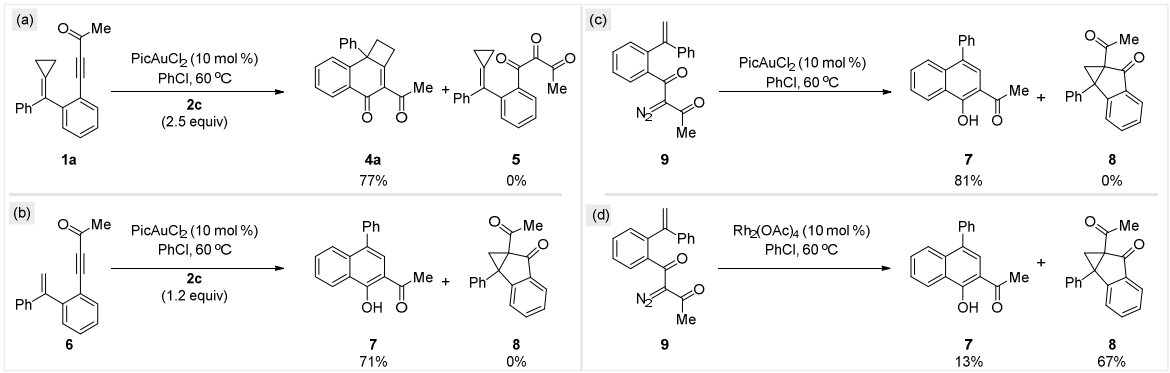
Entry	N-oxide	Additive (10 mol %)	Yield[c] (**3a**/**4a**)
1	-	-	trace/<1
2	-	$Cu(OTf)_2$	trace/<1
3	**2a** (0.1 eq)	$Cu(OTf)_2$	51 (45% Conversion) /<1
4	**2a** (0.2 eq)	$Cu(OTf)_2$	56 (54% Conversion)/<1
5	**2a** (0.4 eq)	$Cu(OTf)_2$	59 (74% Conversion)/<1
6[b]	**2a** (1.2 eq)	$Cu(OTf)_2$	0/0
7[b]	**2a** (1.2 eq)	-	0/0
8	-	2,6-Cl_2-Pyridine	11 (80% **1a** was recovered)/<1
9	-	Lutidine	0/0
10	-	Pyridine	0/0
11	-	TsNa	0/0
12	-	Na_2CO_3	trace/<1
13	-	EDTA-2Na	trace/<1
14	-	Ph_3P	0/0
15	-	18-crown-6	trace/<1
16		2,2'-bipyridien	0/0

[a]All reactions were carried out in 4 mL PhCl in the presence of **1** (0.2 mmol); [b] no catalyst was added; [c] isolated yields are reported.

In order to gain more information concerning about the reaction mechanism, several control experiments were carried out and the results were listed in Supplementary Table 2. According to the results, only trace amount of **3a** was observed in the absence of *N*-oxide **2a** (Supplementary Table 2, entries 1-2). The increase of the loading of **2a** led to different conversions of the substrate **1a**, in a concentration dependent manner, indicating that the higher concentration of poor nucleophilic *N*-oxide **2a** was needed to promote this tandem reaction (Supplementary Table 2, entries 3-5). Moreover, the reactions can not proceed without the gold(III) catalyst (Supplementary Table 2, entries 6-7). And next we want to explore the role of

the *N*-oxide (acts as a base or ligand). First, we screened some bases which involved lewis bases (Supplementary Table 2, entries 8-10) and ionic bases (Supplementary Table 2, entries 11-12), but no promising results were obtained. Second, some ligands were employed in the reactions and only trace amount of **3a** was obtained (Supplementary Table 2, entries 13-16). On the basis of these control experiments and the literature data,[10, 11] we deduced that the *N*-oxide **2a** may act as a coordinative ligand to increase the Lewis acidity of Au(III), which can be efficient activated with ynone.

6.2 Mechanistic studies of the oxidative cyclization

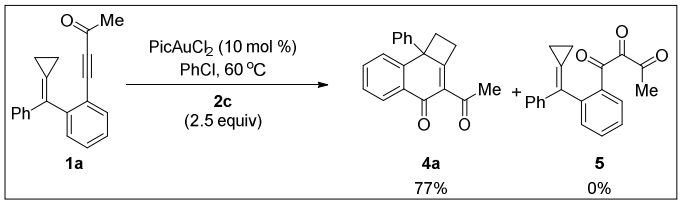


Supplementary Figure 5. Control experiments

In addition, in the presence of excess 8-Me-quinoline *N*-oxide **2c**, double oxidative product **5** was not observed and the product **4a** was obtained in 77% yield (Supplementary Figure 5a). 4-(2-(1-phenylvinyl)phenyl)but-3-yn-2-one, **6**, was also tested under the standard conditions, but no desired gold carbene-cyclopropanation product **8** was isolated (Supplementary Figure 5b). Moreover, the diazo carbonyl species **9** was treated with 10 mol % $PicAuCl_2$ in PhCl at 60 ^oC, generating the naphthol derivative **7** in 81% yield without detecting the cyclopropanation product **8** (Supplementary Figure 5c). Of note, changing the catalyst to a rhodium catalyst, the naphthol derivative **7** and cyclopropanation product **8** was obtained in 13% and 67% yield, respectively (Supplementary Figure 5d). Considering that the diazo compound **9** also does not undergo cyclopropanation under the catalysis of rhodium, we deduce that the gold carbene may involve in the reaction mechanism and this can be interpreted as the gold carbene is more electrophilic than its Rh counterpart. These

control experiments indicated that the mechanism of this oxidative cyclization may go through the *α*-oxo gold carbene intermediate.

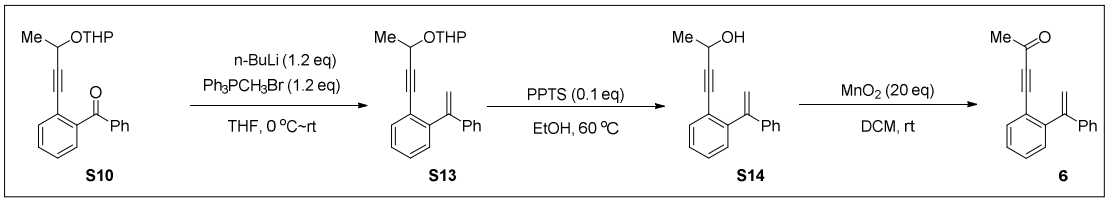
6.2.1 Procedure of the gold(III)-catalyzed oxidative annulation of compound **6**



Supplementary Figure 6. Control experiments of over oxidation

To a dry Schlenk tube, 8-Me-Quinoline *N*-oxide (2.5 eq, 5 mmol, 80 mg), $PicAuCl_2$ (10 mol %, 0.02 mmol, 7.8 mg), PhCl (3 mL) were added successively at rt and then **1a** (0.2 mmol) dissolved in PhCl (1 mL) was added to the above mixture. Then the vial was capped with Teflon-coated cap, and the resulting solution was stirred at rt for 5 min, and then was heated at 60 ^{o}C until the reaction was complete, as monitored by thin layer chromatography. And then the reaction mixture was purified by chromatography to get the desired compound **4a** in 77% yield.

6.2.2 Preparation of compound **6**



Supplementary Figure 7. Synthetic route of compound **6**

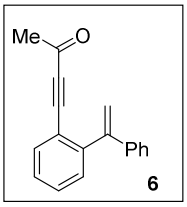
To a stirred suspention of Ph_3CH_3Br (6 mmol, 1.2 eq) in dry THF (20 mL) at 0 ^{o}C was added n-BuLi (2.4 mL, 2.5 M, 1.2 eq) dropwise and stirred at 0 ^{o}C for 0.5 h. **S10** (1.67 g, 1.0 eq) dissolved in dry THF (5 mL) was then added and the resulting mixture was stirred at 0 ^{o}C for 3 h, then at rt for 5 h. Upon completion, the reaction was quenched with saturated NH_4Cl aqueous solution (20 mL). The reaction mixture was extracted with EtOAc three times, and the organic layers were combined, dried over anhydrous Na_2SO_4, concentrated to get the crude product which was purified

with flash column chromatography (PE:EA = 10:1) to get the desired product **S13** (1.35 g, 4.0 mmol, 80%).

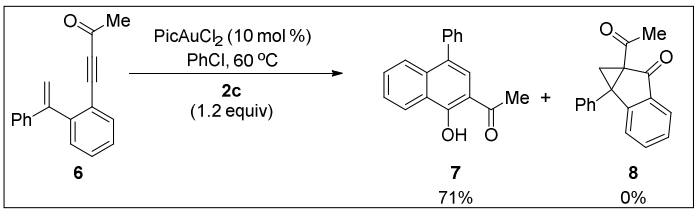
To a solution of **S13** (1.35 g, 4.0 mmol) in EtOH (25 mL) was added PPTS (100 mg, 0.4 mmol, 0.1 eq) in one portion and the reaction mixture was stirred at 60 ^{o}C for 8 h. Upon completion, the reaction was quenched with saturated $NaHCO_3$ aqueous solution, and the mixture was extracted with EtOAc three times. The organic layers were then combined, dried with anhydrous Na_2SO_4, concentrated to get the crude product which was purified with flash column chromatography (PE:EA = 8:1) to yield the desired product **S14** (0.85 g, 3.43 mmol, 86%).

To a solution of **S14** (0.85 g, 3.43 mmol) in anhydrous DCM (20 mL) was added MnO_2 (20 eq) in one portion. After stirred at rt for 5 h, the reaction mixture was filtered through a celite plug and the mixture was then concentrated to get the crude product which was purified by flash column chromatography (PE:EA = 10:1) to obtain the desired product **6** (570 mg, 2.32 mmol, 68%).

4-(2-(1-phenylvinyl)phenyl)but-3-yn-2-one, **6**, overall yield 47%, 0.57 g, light yellow oil. **^{1}H NMR (500 MHz, CDCl$_3$):** δ = 7.60 (d, *J* = 7.5 Hz, 1H), 7.48 (td, *J* = 8.0, 2.0 Hz, 1H), 7.40 - 7.28 (m, 7H), 5.82 (s, 1H), 5.40 (s, 1H), 2.07 (s, 3H); **^{13}C NMR (125 MHz, CDCl$_3$):** δ = 184.6, 148.2, 146.0, 140.6, 134.3, 130.8, 130.4, 128.4, 127.9, 127.8, 127.1, 119.4, 117.0, 91.8, 89.9, 32.5; **HRMS** (ESI) m/z calcd for $C_{18}H_{15}O^{+}$ $(M+H)^{+}$: 247.1117, found: 247.1113.



6.2.3 Procedure of the gold(III)-catalyzed oxidative annulation of compound **6**

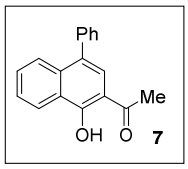


Supplementary Figure 8. Gold(III)-catalyzed oxidative annulation of compound **6**

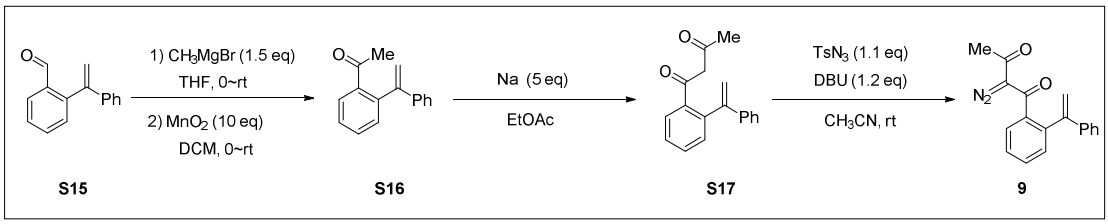
To a dry Schlenk tube, 8-Me-Quinoline *N*-oxide (1.2 eq, 0.24 mmol, 38.2 mg),

$PicAuCl_2$ (10 mol %, 0.02 mmol, 7.8 mg), PhCl (3 mL) were added successively at rt and then compound **6** (0.2 mmol) dissolved in PhCl (1 mL) was added to the above mixture. Then the vial was capped with Teflon-coated cap, and the resulting solution was stirred at rt for 5 min, and then heated at 60 ^{o}C for 8 h. Upon completion, the reaction mixture was purified by chromatography to get the desired compound **7**.

1-(1-hydroxy-4-phenylnaphthalen-2-yl)ethan-1-one, **7**, yield 71%, 37 mg, light yellow solid. **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 14.02 (s, 1H), 8.56 (d, *J* = 9.0 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.60 - 7.44 (m, 8H), 2.70 (s, 3H). The spectral data matched those reported in the literature[4].



6.2.4 Preparation of compound **9**



Supplementary Figure 9. Synthetic route of compound **9**

To a solution of **S15**[5] (1.04 g, 5 mmol) was added CH_3MgBr (6 mmol, 6 mL, 1 M, 1.2 eq) dropwise at 0 ^{o}C. The resulting mixture was strirred at 0 ^{o}C for 1 h under a nitrogen atmosphere. Upon completion, the reaction was quenched with saturated NH_4Cl solution, and the mixture was then extracted with EtOAc, washed with brine, dried over Na_2SO_4 and concentrated to get the crude product which was used directly for the next step.

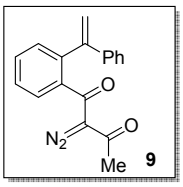
To a solution of the crude product in dry CH_2Cl_2 (25 mL) was added MnO_2 (100 mmol) in one portion at rt and then the mixture was stirred at rt for 5 h. Upon completion, the mixture was filtered through a celite plug, concentrated to give the crude product which was purified by chromatography on silica gel (PE:EA = 9:1) to get the desired substrate **S16** (960 mg, 4.3 mmol, 86%).

To a solution of **S16** (960 mg, 4.3 mmol, 1 eq) in dry EtOAc (15 mL) was added

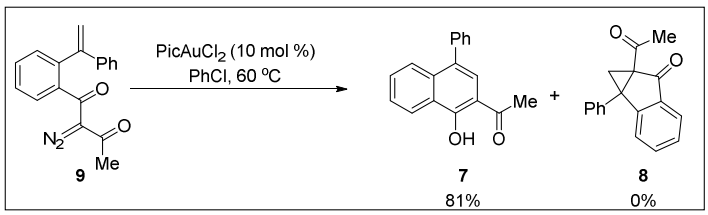
Na (495 mg, 5 eq) at rt, the resulting mixture was stirred at rt for 8 hours. Upon completion, the reaction was quenched with saturated NH_4Cl solution, diluted with water. The mixture was extracted with EtOAc three times, and the organic layers were combined, dried over Na_2SO_4, concentrated to get the crude product which was purified by chromatography on silica gel (PE:EA = 10:1) to get the desired compound **S17** (702 mg, 2.66 mmol, 62%).

To a solution **S17** (702 mg, 2.66 mmol) in dry CH_3CN (20 mL) was added dry DBU (445 mg, 2.93 mmol, 1.1 eq) dropwise at rt. TsN_3 (577 mg, 2.93 mmol, 1.1 eq) dissolved in CH_3CN (5 mL) was then added dropwise to the above mixture. The reaction mixture was stirred at rt for 6 h, upon completion, the reaction was concentrated nearly dry and diluted with water. The mixture was extracted with EtOAc three times, and the organic layers were combined, dried over Na_2SO_4, and then concentrated to get the crude product which was purified by chromatography on silica gel (PE:EA = 8:1) to get the desired compound **9** (557 mg, 1.92 mmol, 72%).

2-diazo-1-(2-(1-phenylvinyl)phenyl)butane-1,3-dione, **9**, overall yield 38%, 557 mg, light yellow oil, (R_f = 0.54, hexane/ethyl acetate = 8:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 7.58 - 7.55 (m, 1H), 7.51 - 7.50 (m, 1H), 7.48 - 7.45 (m, 1H), 7.42 - 7.40 (m, 1H), 7.27 - 7.26 (m, 3H), 7.19 - 7.17 (m, 2H), 5.69 (s, 1H), 5.45 (s, 1H), 2.05 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$):** (*one carbon merged to others*) δ = 190.4, 186.0, 148.3, 140.7, 140.4, 137.6, 131.7, 131.2, 128.7, 128.4, 127.6, 127.4, 117.3, 86.4, 28.6; **HRMS** (ESI) m/z calcd for $C_{18}H_{15}N_2O_2^+$ $(M+H)^+$: 291.1128, found: 291.1129



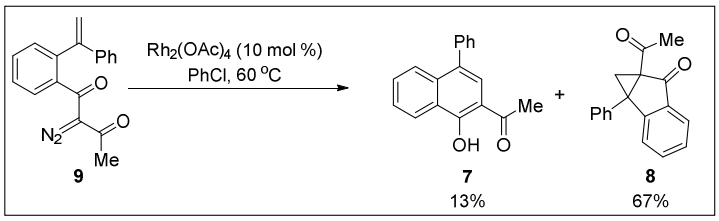
6.2.5 Procedure of the gold(III)-catalyzed annulation of compound **9**



Supplementary Figure 10. Gold(III)-catalyzed annulation of compound **9**

To a dry Schlenk tube, $PicAuCl_2$ (10 mol %, 0.02 mmol, 7.8 mg), PhCl (3 mL) were added successively at rt and then compound **9** (0.2 mmol) dissolved in PhCl (1 mL) was added to the above mixture. Then the vial was capped with Teflon-coated cap, and the resulting solution was stirred at rt for 5 min, then heated at 60 ^{o}C for 8 h. Upon completion, the reaction mixture was purified by chromatography to get the compound **7**.

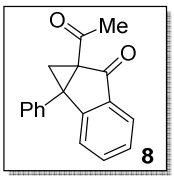
6.2.6 Procedure of the Rhodium-catalyzed annulation of compound **9**



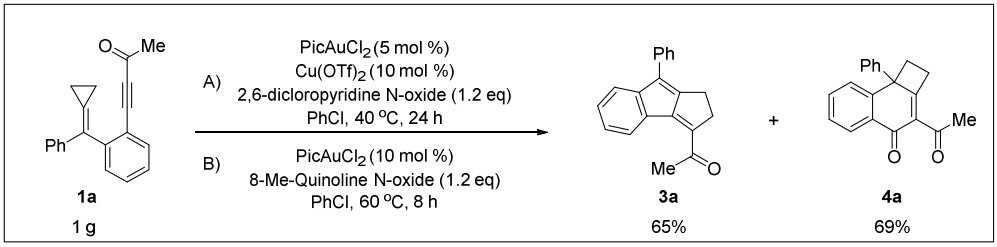
Supplementary Figure 11. Rhodium-catalyzed annulation of compound **9**

To a dry Schlenk tube, $Rh_2(OAc)_4$ (10 mol %, 0.02 mmol, 8.8 mg), PhCl (3 mL) were added successively at rt and then compound **9** (0.2 mmol) dissolved in PhCl (1 mL) was added to the above mixture. Then the vial was capped with Teflon-coated cap, and the resulting solution was stirred at rt for 5 min, then heated at 60 ^{o}C for 8 h. Upon completion, the reaction mixture was purified by chromatography on silica gel to get the compound **7** in 13% yield and compound **8** in 67% yield, respectively.

6-acetyl-1-phenyl-1,6-dihydrocyclopropa[a]inden-6(1H)-one, **8**, yield 67%, 35 mg, light yellow solid, (R_f = 0.67, hexane/ethyl acetate = 8:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 7.78 (d, *J* = 8.0 Hz, 1H), 7.49 (t, *J* = 7.5 Hz, 1H), 7.41 - 7.30 (m, 6H), 7.14 (d, *J* = 7.5 Hz, 1H), 3.09 (d, *J* = 4.0 Hz, 1H), 2.34 (s, 3H), 2.13 (d, *J* = 4.0 Hz, 1H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 198.8, 198.7, 155.4, 134.7, 133.5, 132.9, 129.9, 128.8, 128.5, 128.2, 125.0, 124.8, 54.1, 51.1, 42.2, 30.3; **HRMS** (ESI) m/z calcd for $C_{18}H_{15}O_2^+$ $(M+H)^+$: 263.1067, found: 263.1068.



7. Procedure of gram-scale experiments and synthetic applications



Supplementary Figure 12. Gram-scale experiments of compound **1a**

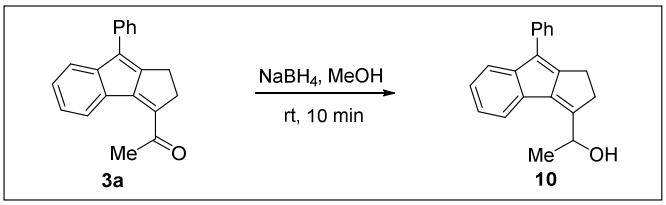
Procedure A:

A dry Schlenk tube was charged with 2, 6-dichloropyridine *N*-oxide (1.2 eq, 4.41 mmol, 723 mg), $PicAuCl_2$ (5 mol %, 0.184 mmol, 71.8 mg), $Cu(OTf)_2$ (10 mol %, 0.368, 133 mg) and then anhydrous PhCl (35 mL) were added successively at rt. To this mixture was added the ynone **1a** (3.68 mmol, 1 g) dissolved in PhCl (5 mL). Then the tube was capped with Teflon-coated cap, and the resulting solution was stirred at rt for 5 min, and then heated at 40 ^{o}C until the reaction was complete, as monitored by thin layer chromatography. And then the reaction mixture was purified by chromatography (PE:EA = 80:1) to get the desired compound **3a** (0.65g, 65%).

Procedure B:

A dry Schlenk tube was charged with 8-Me-Quinoline *N*-oxide (1.2 eq, 4.41 mmol, 702 mg), $PicAuCl_2$ (10 mol %, 0.368 mmol, 143.6 mg), and then anhydrous PhCl (69 mL) were added successively at rt. To this mixture was added the ynone **1a** (3.68 mmol, 1 g) dissolved in PhCl (5 mL). Then the tube was capped with Teflon-coated cap, and the resulting solution was stirred at rt for 5 min, and then heated at 60 ^{o}C until the reaction was complete, as monitored by thin layer chromatography. And then the reaction mixture was purified by chromatography (PE:EA = 8:1) to get the desired compound **4a** (0.73 g, 69%).

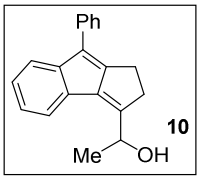
Transformations of product 3a

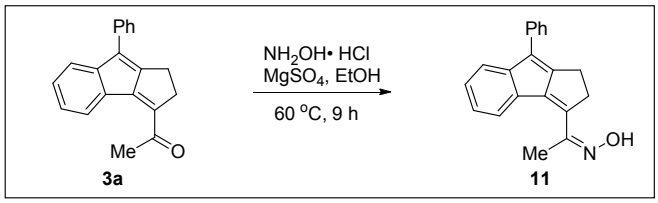


Supplementary Figure 13. Reduction of compound **3a**

To a solution of **3a** (40 mg, 0.15 mmol) in MeOH (5 mL) was added $NaBH_4$ (20 mg, 0.54 mmol) at rt, and the resulting mixture was stirred at this temperature for 20 min. Upon completion, the mixture was quenched with saturated NH_4Cl solution 1 mL, extracted with EtOAc (10 mL thrice). The organic layers were combined, washed with brine, dried over Na_2SO_4, filtered and concentrated to get the crude product. The residue was purified by chromatography on silica gel (PE:EA = 5:1) to get the desired compound **10** as a light yellow solid (39 mg, 95%).

1-(8-phenyl-1,2-dihydrocyclopenta[a]inden-3-yl)ethan-1-ol, **10**, yield 95%. 39 mg, light yellow solid, (R_f = 0.21, hexane/ethyl acetate = 8:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 7.84 (d, *J* = 7.5 Hz, 1H), 7.63 - 7.62 (m, 2H), 7.57 (d, *J* = 7.5 Hz, 1H), 7.47 - 7.44 (m, 2H), 7.33 - 7.28 (m, 2H), 7.17 (d, *J* = 7.5 Hz, 1H), 5.31 (q, *J* = 6.5 Hz, 1H), 3.27 - 3.12 (m, 2H), 2.92 (t, *J* = 5.0 Hz, 2H), 2.01 (s, 1H), 1.56 (d, *J* = 7.0 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 154.6, 152.3, 149.4, 142.9, 136.1, 129.9, 128.7, 128.2, 127.8, 127.5, 126.7, 124.0, 123.4, 119.7, 66.8, 37.9, 23.4, 22.3; **HRMS** (ESI) m/z calcd for $C_{20}H_{19}O^+$ $(M+H)^+$ 275.1430, found 275.1431.



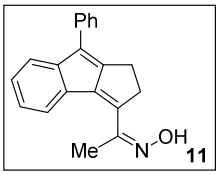


Supplementary Figure 14. Oximation of compound **3a**

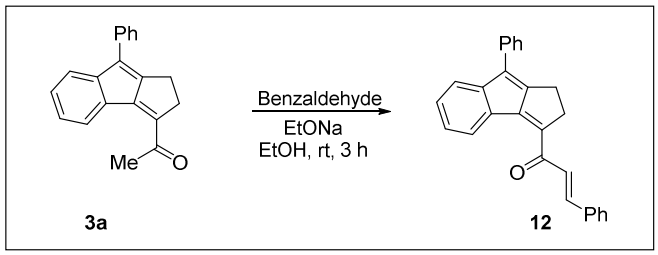
To a solution of **3a** (40 mg, 0.15 mmol) in EtOH (5mL) was added Hydroxylamine hydrochloride (25 mg, 0.36 mmol) and $MgSO_4$ (108 mg, 0.9 mmol) at

rt, and the resulting mixture was allowed to warm up to 60 °C and stirred at this temperature for 9 h. Upon completion, the mixture was filtered and concentrated to get the crude product. The residue was purified by chromatography on silica gel (PE:EA = 5:1) to get the desired compound **11** as a light yellow solid (43 mg, 96%).

1-(8-phenyl-1,2-dihydrocyclopenta[a]inden-3-yl)ethan-1-one oxime, **11**, yield 96%.



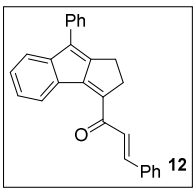
43 mg, light yellow solid, (R_f = 0.43, hexane/ethyl acetate = 8:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.17 (s, 1H), 8.08 (d, *J* = 7.5 Hz, 1H), 7.63 (d, *J* = 7.5 Hz, 2H), 7.53 (d, *J* = 7.5 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 2H), 7.34 - 7.27 (m, 2H), 7.16 (t, *J* = 7.5 Hz, 1H), 3.35 - 3.33 (m, 2H), 2.93 - 2.91 (m, 2H), 2.37 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 155.3, 152.3, 149.8, 146.5, 142.4, 135.7, 130.1, 129.7, 128.7, 128.4, 127.9, 127.0, 125.0, 124.0, 119.8, 40.1, 22.9, 14.1; **HRMS** (ESI) m/z calcd for $C_{20}H_{18}NO^+$ $(M+H)^+$ 288.1383, found 288.1382.



Supplementary Figure 15. Aldol reaction of compound **3a**

To a solution of **3a** (40 mg, 0.15 mmol) in EtOH 2.5 mL was added EtONa (20 mg, 0.3 mmol, fresh prepared) at rt. Then, benzaldehyde (31 mg, 0.3 mmol) was added to the above mixture dropwise at rt, and the resulting mixture was stirred at this temperature for 3 h. Upon completion, the mixture was evaporated to dry to get the crude product. The residue was purified by chromatography on silica gel (PE:EA = 20:1) to get the desired compound **12** as a brown solid (38.7 mg, 71%).

(E)-3-phenyl-1-(8-phenyl-1,2-dihydrocyclopenta[a]inden-3-yl)prop-2-en-1-one,

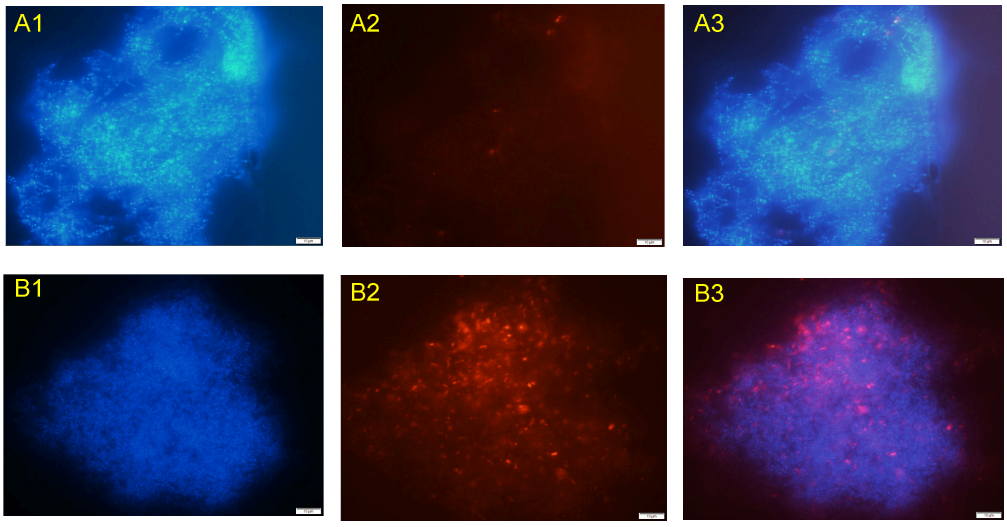


12, yield 71%. 38.7 mg, brown solid, (R_f = 0.69, hexane/ethyl acetate = 8:1). **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 8.32 (d, *J* = 7.5 Hz, 1H), 7.85 (d, *J* = 15.5 Hz, 1H), 7.65 - 7.63 (m, 4H), 7.49 - 7.46 (m,

3H), 7.44 - 7.43 (m, 3H), 7.37 - 7.30 (m, 3H), 7.19 (t, J = 7.5 Hz, 1H), 3.51 - 3.49 (m, 2H), 2.98 - 2.96 (m, 2H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 189.4, 153.8, 151.5, 150.2, 144.6, 142.1, 135.1, 134.9, 133.5, 130.9, 130.1, 129.7, 129.2, 128.8, 127.9, 127.6, 126.9, 125.2, 124.5, 120.2, 39.1, 23.1; **HRMS** (ESI) m/z calcd for $C_{27}H_{21}O^+$ $(M+H)^+$ 361.1587, found 361.1586.

8. Antibacterial activity

The emergence of antibiotics resistance in bacteria is a serious and worsening global public health problem. Thus, to develop a better understanding of hybrids characterized with novel skeletons that show activities against bacterial strains is important.[8, 9] Therefore, the antibacterial activities of all the compounds (**3a-3q**, **4a-4q**) prepared in current study were evaluated against five pathogens: *Bacillus cereus (B. cereus), Bacillus subtilis (B. subtilis)*, *Ralstonia solanacearum (R. solanacearum)*, *Staphylococcus aureus (S. aureus)*, *Methicillin-resistant Staphylococcus aureus (MRSA)*. The results indicated that product **3h** showed promising inhibition against the five pathogens. Further, the minimal inhibitory concentration (MIC) of compound **3h** was tested, showing that the MIC of indene derivative **3h** was 2 μg/mL, which was comparable to the positive control against *R. solanacearum*.



Supplementary Figure 16. Fluorescence micrographs of *R. solanacearum* treated with DMSO or treated with **3h**.[a]

[a] (A1) *R. solanacearum* treated with DMSO, Hoechst stained; (A2) *R. solanacearum* treated with DMSO, PI stained; (A3) *R. solanacearum* treated with DMSO, merged graph; (B1) *R. solanacearum* treated with **3h**, Hoechst stained; (B2) *R. solanacearum* treated with **3h**, PI stained; (B3) *R. solanacearum* treated with **3h**, merged graph.

Moreover, the preliminary antibacterial mechanism was also addressed by using the most potential hybrid **3h** and *R. solanacearum*. Hoechst 33342 and PI (propidium iodide) were used to distinguish the cells with either an intact or a damaged membrane. As illustrated in Supplementary Figure 16, A1, the cells exhibited blue fluorescence treated with DMSO, whereas no fluorescence was observed in the PI channel (Supplementary Figure 16, A2), indicating that the membranes of great majority of the cells were intact. After *R. solanacearum* incubated with **3h** for two hours, the cells exhibited red fluorescence in the PI channel (Supplementary Figure 16, B2) suggesting that the membranes of the cells were damaged, which attributed to that compound **3h** may disrupt processes of cell wall biosynthetic reactions. Therefore, this molecule represents a promising leading compound for seeking potent antibiotics.

8.1 MIC determination

MICs were determined by the broth microdilution method in accordance with the Clinical and Laboratory Standards Institute (CLSI) guidelines[6]. Breifly, the bacterial suspension was adjusted to a concentration of 1×10^6 CFU/mL with Luria-Bertani liquid medium (LB). The tested compound (**3h**) and reference drug (Ampicillin sodium) were dissolved in dimethyl sulfoxide (DMSO) then diluted with LB to prepare the stock solutions. The required concentrations of the compound **3h** and Ampicillin sodium were 128, 64, 32, 16, 8, 4, 2 and 1 μg/mL, respectively (note: the ultimate content of DMSO was less than 0.05%). All the plates were incubated at 37 °C, 140 rpm for 24 h. After incubation, the lowest concentration of the drug that prevented visible growth as determined by OD_{600} nm was recorded as the MIC. The results were listed in Supplementary Table 3.

Supplementary Table 3. MICs of compounds **3h**

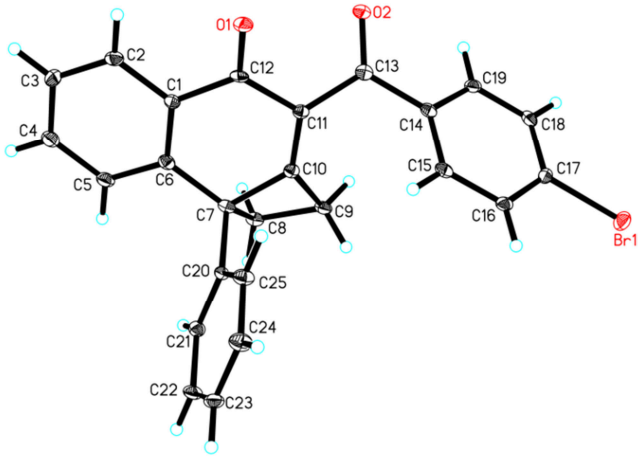
Compounds	MICs (μg/mL)				
	B.c	*B.s*	*R.s*	*MRSA*	*S.a*
3h	32	32	**2**	32	32
3q	32	64	32	64	64
Ampicillin sodium	16	16	**1**	16	8

Note: *B.c*: *Bacillus cereus*, *B.s*: *Bacillus subtilis*, *R.s*: *Ralstonia solanacearum*, *MRSA*: *Methicillin-resistant Staphylococcus aureus*, *S.a*: *Staphylococcus aureus*.

8.2 Fluorescence microscopy assay [7]

Both Hoechst and PI fluorescent dyes were used to determine the ability of the compound **3h** to compromise the membranes of *R. solanacearum*. In brief, bacterial suspension was incubated at 37 °C to the mid-logarithmic phase and then diluted to a concentration of 1×10^6 CFU/mL. Then 2 mL of bacterial suspension was collected with a 5 mL centrifugal tube, followed by incubation with 0.01143 μmol/mL (2 × MIC) of **3h** for 2 h at 37 °C. After centrifuged for 5 min at 3000 × *g*, the cultural supernatant was removed and the cell pellets were washed with phosphate-buffered saline (PBS, 0.1 M, pH 7.2) 2 mL for three times. The cell pellets were resuspended with 2 mL LB liquid medium and incubated with PI and Hoechst 33342 (5 μg/mL) for 20 min on ice in the dark. After centrifuged for 5 min at 3000 × *g*, the cultural supernatant was removed and the cell pellets were washed with phosphate-buffered saline (PBS, 0.1 M, pH 7.2) 2 mL for three times. The cell pellets were resuspended with 1 mL PBS, then the suspension was applied on chamber slides and observed under LECIA DM6 B microscope using 100× oil-immersion objective.

9. X-ray structure of 4e



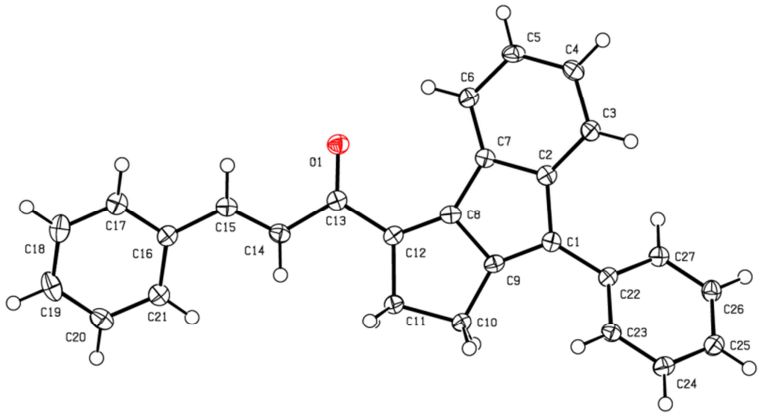
Supplementary Table 4. Crystal data and structure refinement for **4e.**

Identification code	**4e**
Empirical formula	$C_{25}H_{17}BrO_2$
Formula weight	429.29
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	13.3654(9)
b/Å	10.6073(9)
c/Å	13.4584(8)
α/°	90
β/°	90.914(6)
γ/°	90
Volume/Å^3	1907.8(2)
Z	4
ρ_{calc}g/cm^3	1.495
μ/mm^{-1}	2.173
F(000)	872.0
Crystal size/mm^3	0.13 × 0.12 × 0.11
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.89 to 49.992
Index ranges	-12 ≤ h ≤ 15, -12 ≤ k ≤ 11, -15 ≤ l ≤ 16
Reflections collected	7754
Independent reflections	3320 [R_{int} = 0.0461, R_{sigma} = 0.0661]
Data/restraints/parameters	3320/0/253
Goodness-of-fit on F^2	1.052
Final R indexes [I>=2σ (I)]	R_1 = 0.0429, wR_2 = 0.0915

Final R indexes [all data] $R_1 = 0.0575$, $wR_2 = 0.0993$

Largest diff. peak/hole / e $Å^{-3}$ 0.71/-0.33

10. X-ray structure of 12



Supplementary Table 5. Crystal data and structure refinement for **12**.

Identification code	**12**
Empirical formula	$C_{27}H_{20}O$
Formula weight	360.43
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	16.9512(17)
b/Å	7.3838(4)
c/Å	16.2147(15)
α/°	90
β/°	116.035(12)
γ/°	90
Volume/$Å^3$	1823.6(3)
Z	4
$\rho_{calc}g/cm^3$	1.313
μ/mm^{-1}	0.602

F(000)	760.0
Crystal size/mm^3	0.12 × 0.11 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/	5.802 to 146.89
Index ranges	-20 ≤ h ≤ 15, -6 ≤ k ≤ 9, -20 ≤ l ≤ 18
Reflections collected	6306
Independent reflections	3545 [R_{int} = 0.0525, R_{sigma} = 0.0752]
Data/restraints/parameters	3545/0/269
Goodness-of-fit on F^2	1.061
Final R indexes [I>=2σ (I)]	R_1 = 0.0676, wR_2 = 0.1753
Final R indexes [all data]	R_1 = 0.0952, wR_2 = 0.1882
Largest diff. peak/hole / e $Å^{-3}$	0.31/-0.33

11. Supplementary References:

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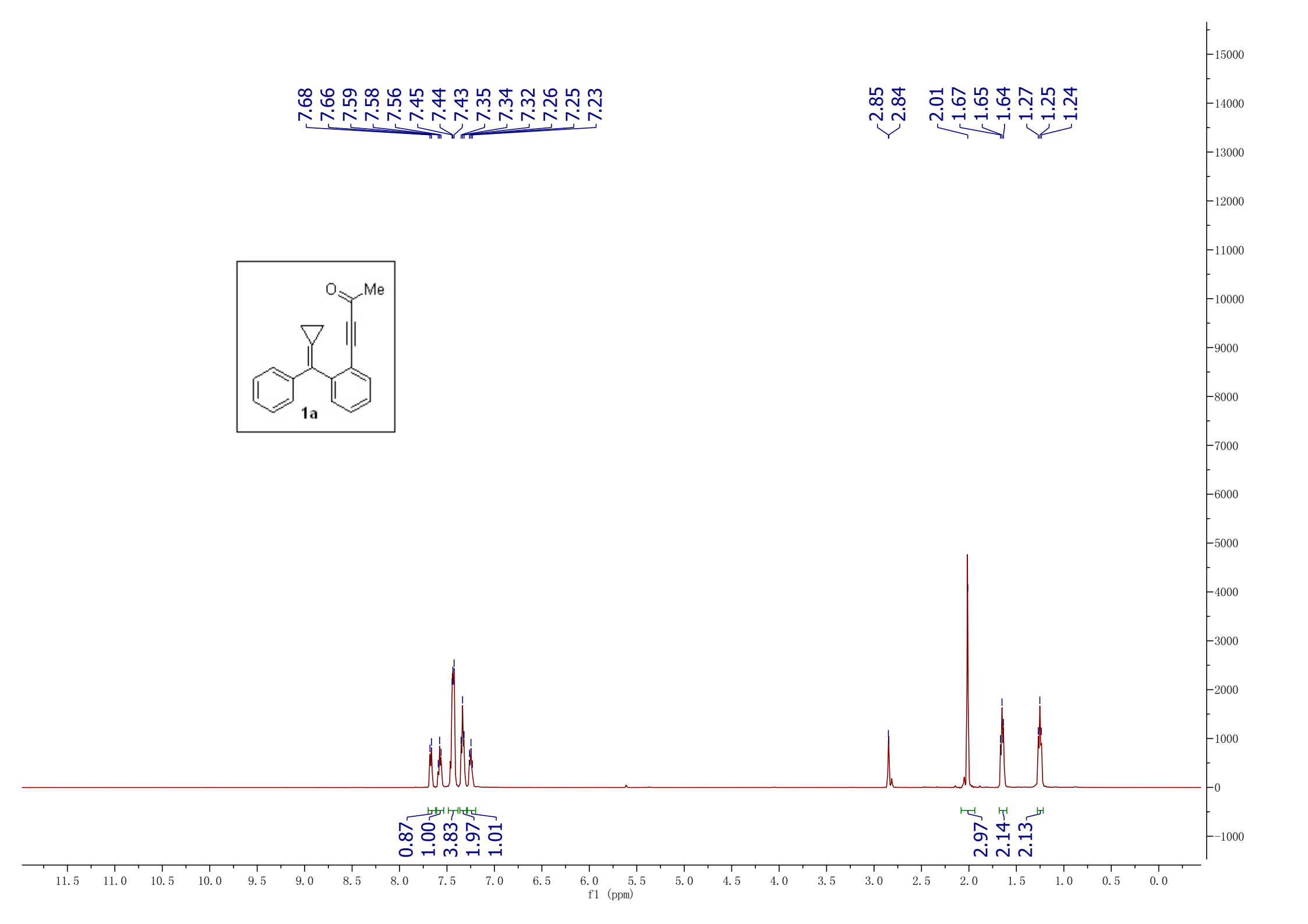
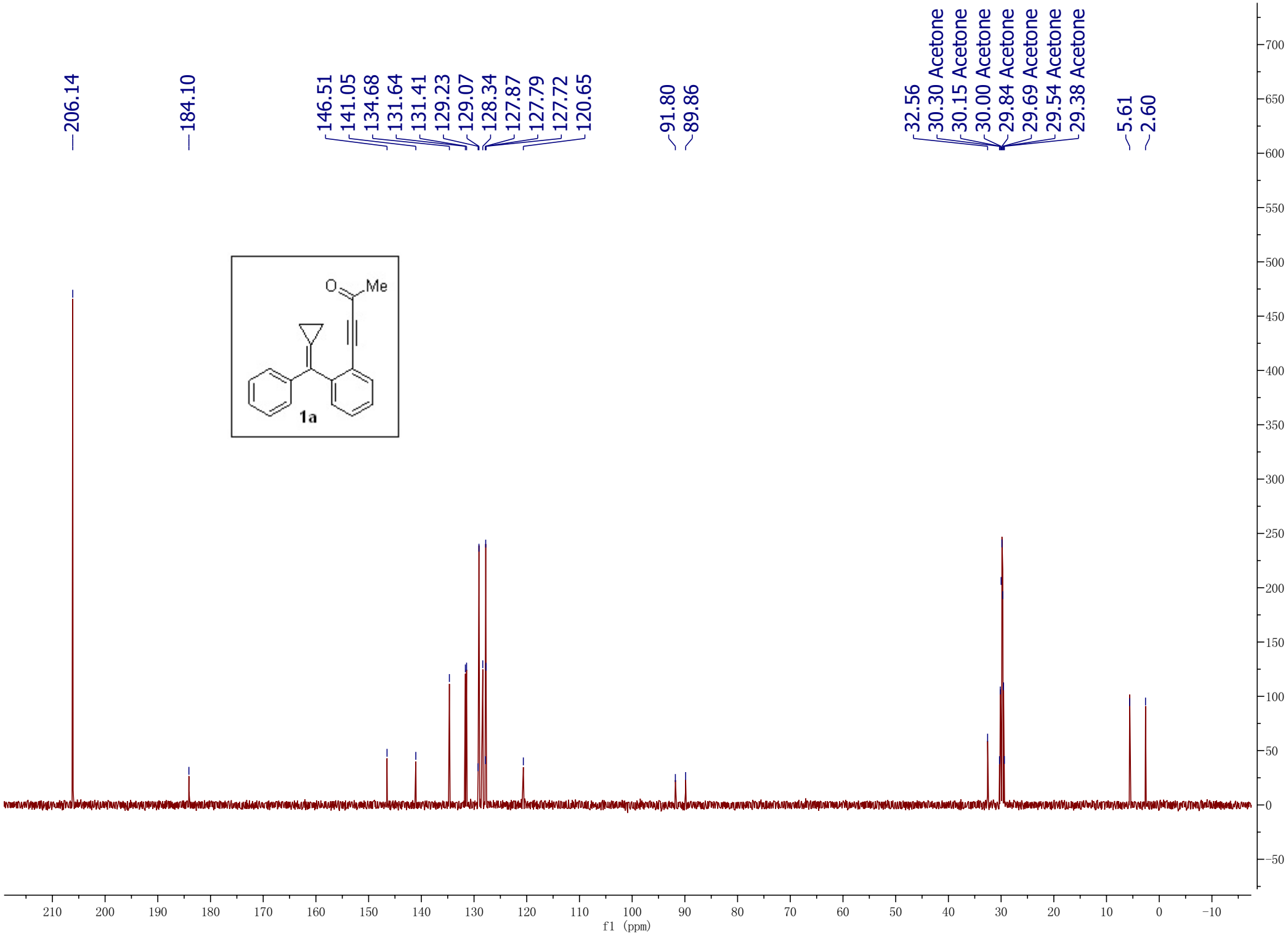

7.68
7.66
7.59
7.58
7.56
7.45
7.44
7.43
7.35
7.34
7.32
7.26
7.25
7.23
2.85
2.84
2.01
1.67
1.65
1.64
1.27
1.25
1.24
O
Me
1a
0.87
1.00
3.83
1.97
1.01
2.97
2.14
2.13
f1 (ppm)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146.51
141.05
134.68
131.64
131.41
129.23
129.07
128.34
127.87
127.79
127.72
120.65
91.80
89.86
32.56
30.30 Acetone
30.15 Acetone
30.00 Acetone
29.84 Acetone
29.69 Acetone
29.54 Acetone
29.38 Acetone
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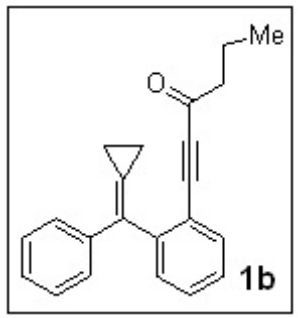
2.60
O
Me
1a
f1 (ppm)

232-P7/10
PROTON Acetone {D:\2018-1} ZHL 51

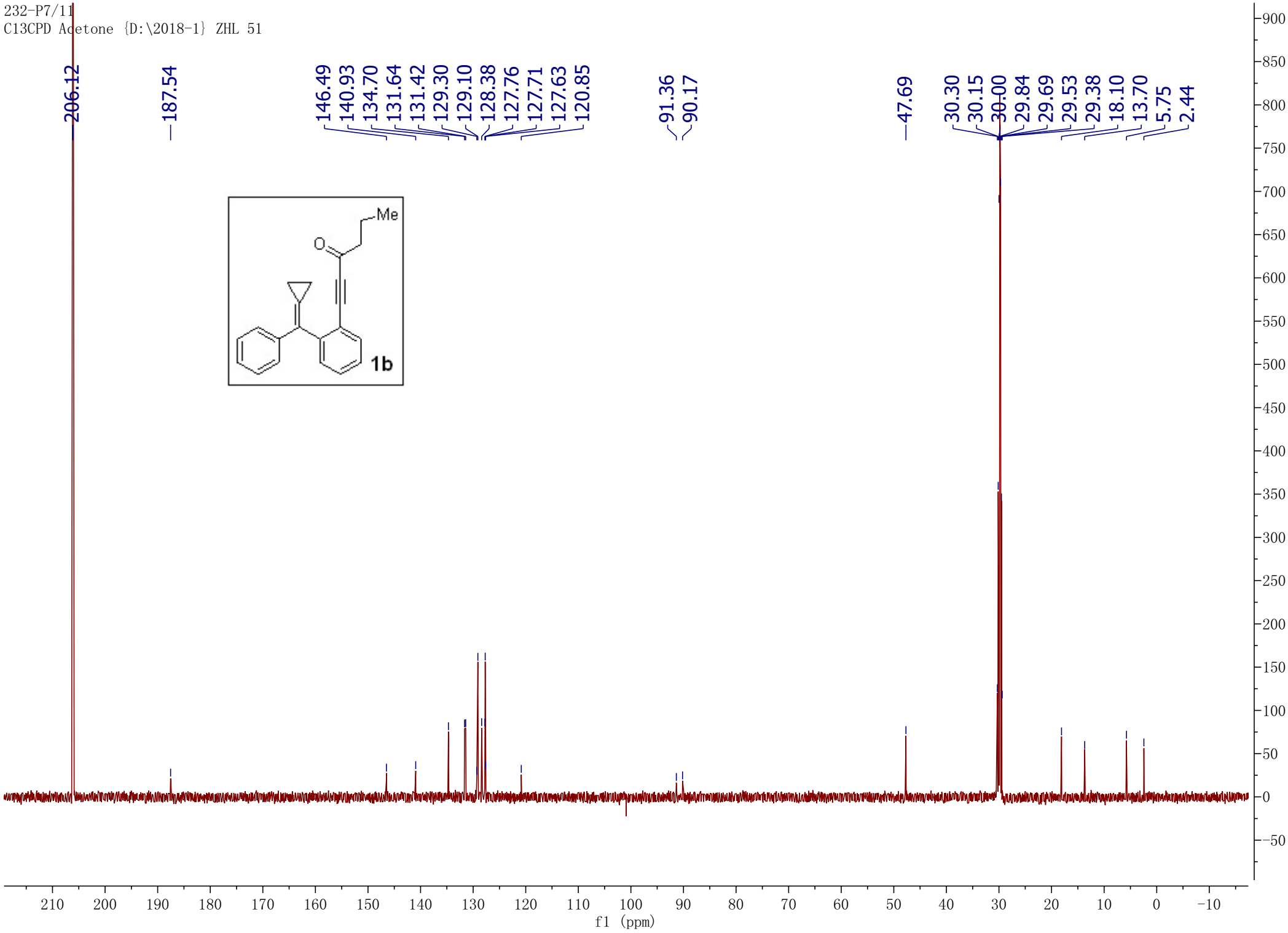


7.69 7.67 7.60 7.58 7.57 7.47 7.42 7.35 7.34 7.32 7.26 7.25 7.24

2.23 2.22 2.20 2.05 1.67 1.66 1.64 1.47 1.46 1.45 1.45 1.44 1.43 1.42 1.25 1.23 1.22 0.81 0.80 0.78

0.95 1.00 4.02 2.03 1.04 1.94 2.10 2.02 2.05 3.02

f1 (ppm)


232-P7/11
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129.30
129.10
128.38
127.76
127.71
127.63
120.85
91.36
90.17
47.69
30.30
30.15
30.00
29.84
29.69
29.53
29.38
18.10
13.70
5.75
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Me
O
1b
f1 (ppm)

JKG-20180329-219-P6/10
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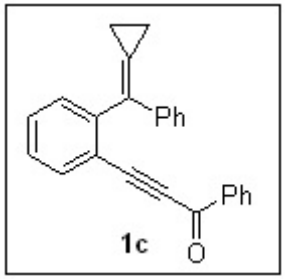

JKG-20180329-219-P6/11
C13CPD CDCl3 {D:\2018-1} ZHL 2

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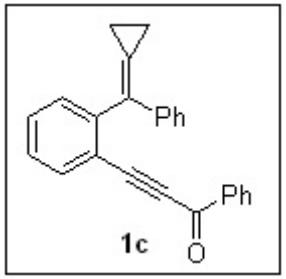
139.76
137.00
134.52
133.83
130.83
130.47
129.65
128.51
127.45
127.22
127.16
126.97
120.55
93.13
89.61
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
5.87
2.15



f1 (ppm)

232-P5/10
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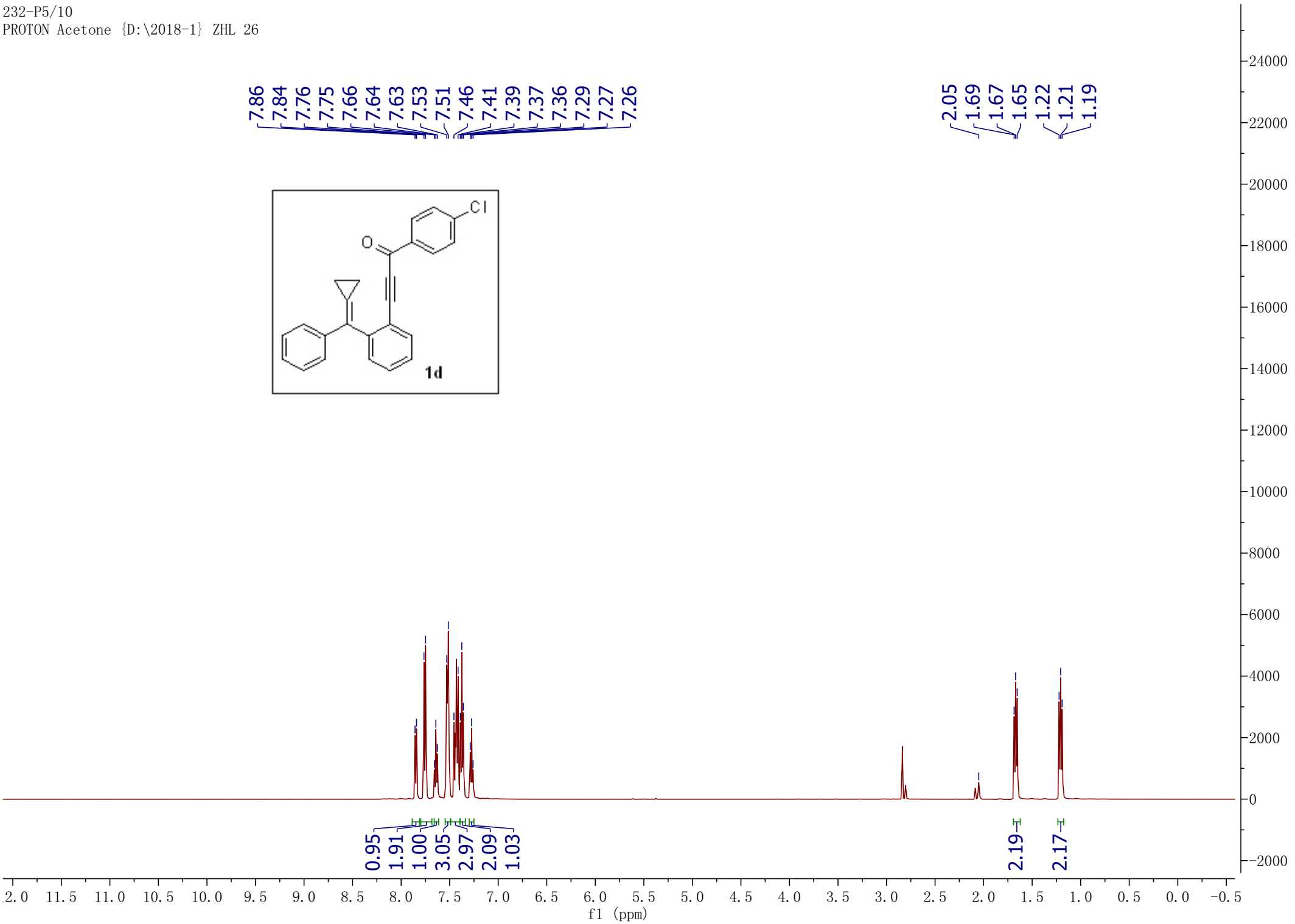

232-P5/11
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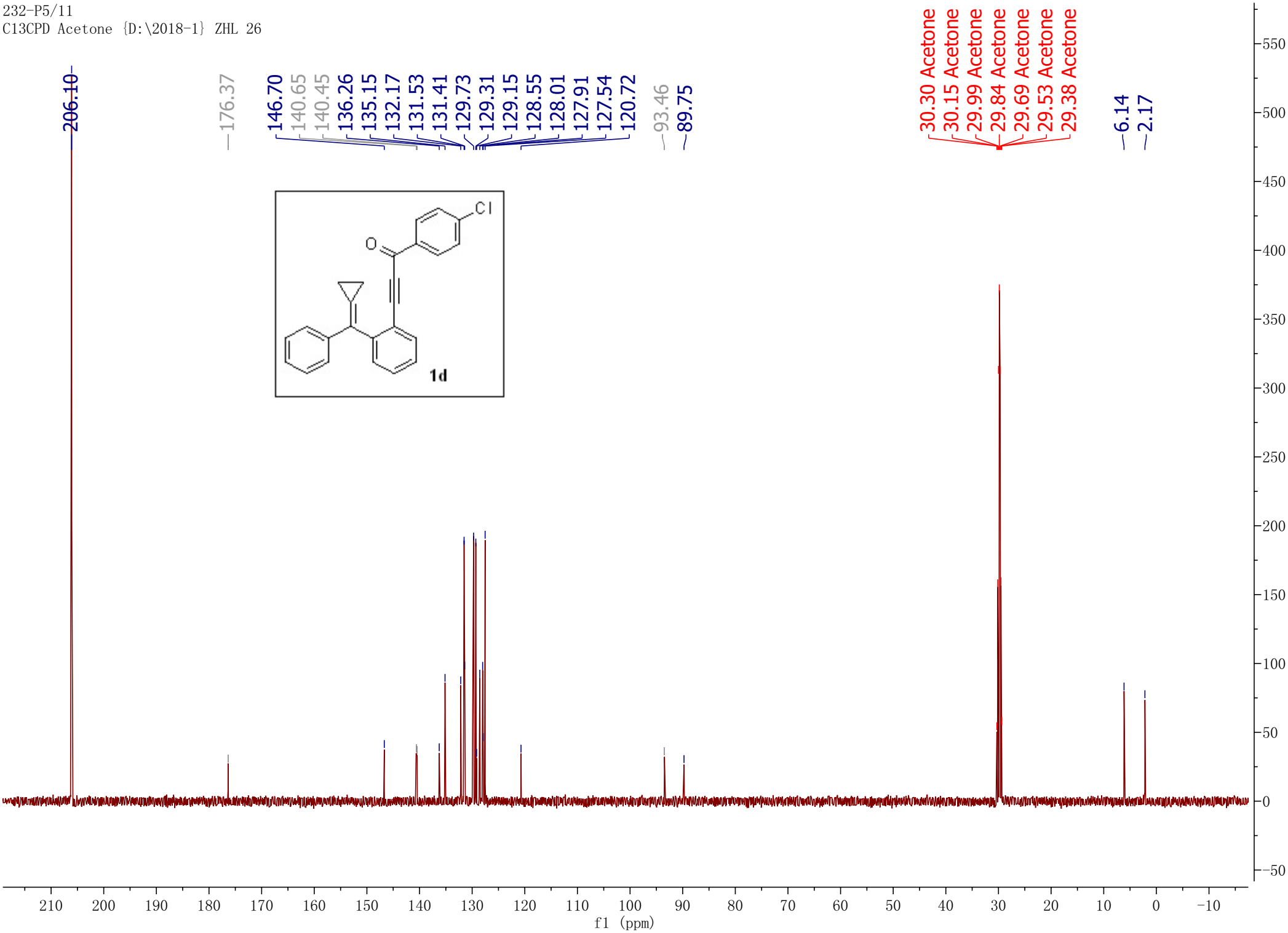

232-P6/10
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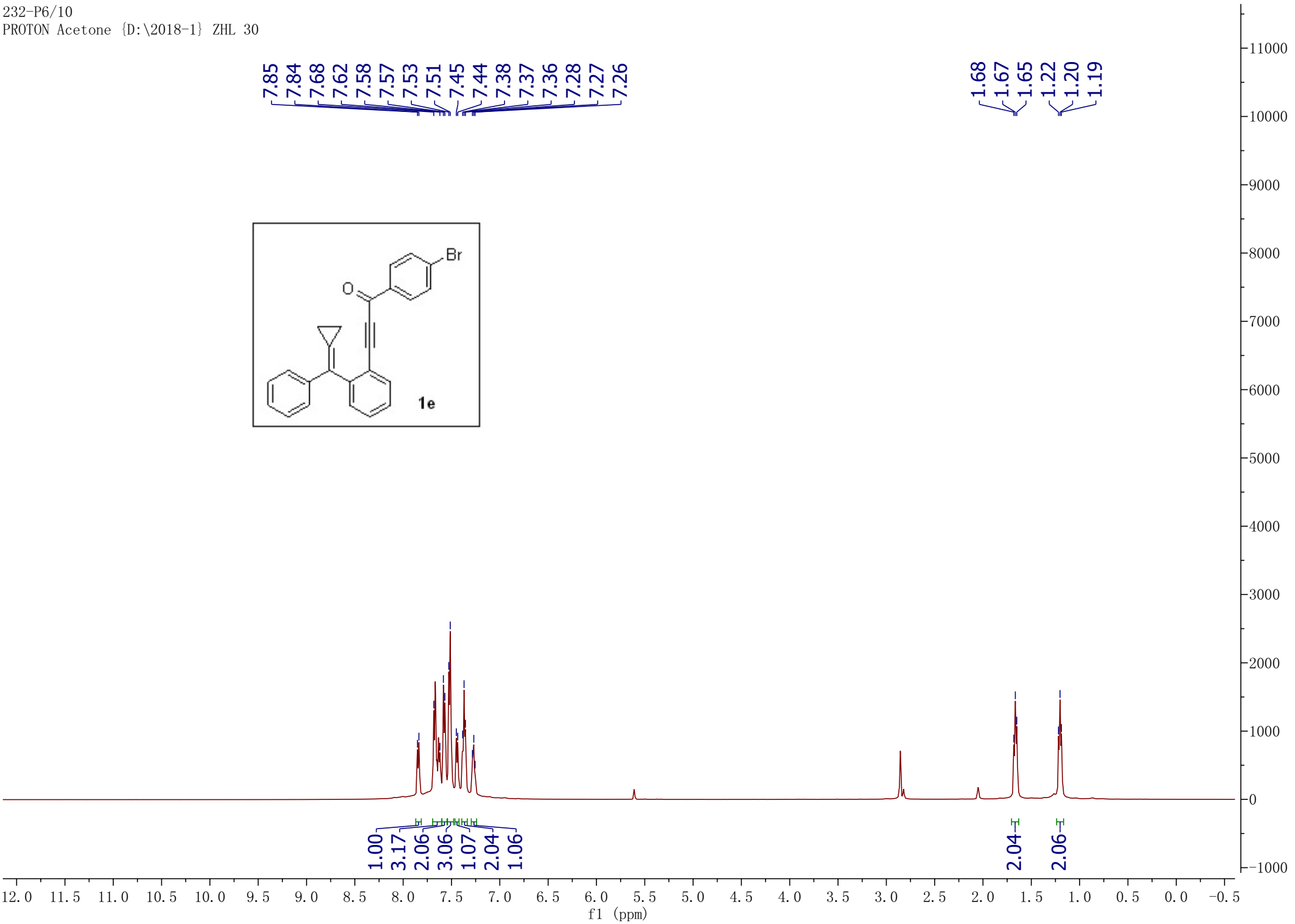

232-P6/11
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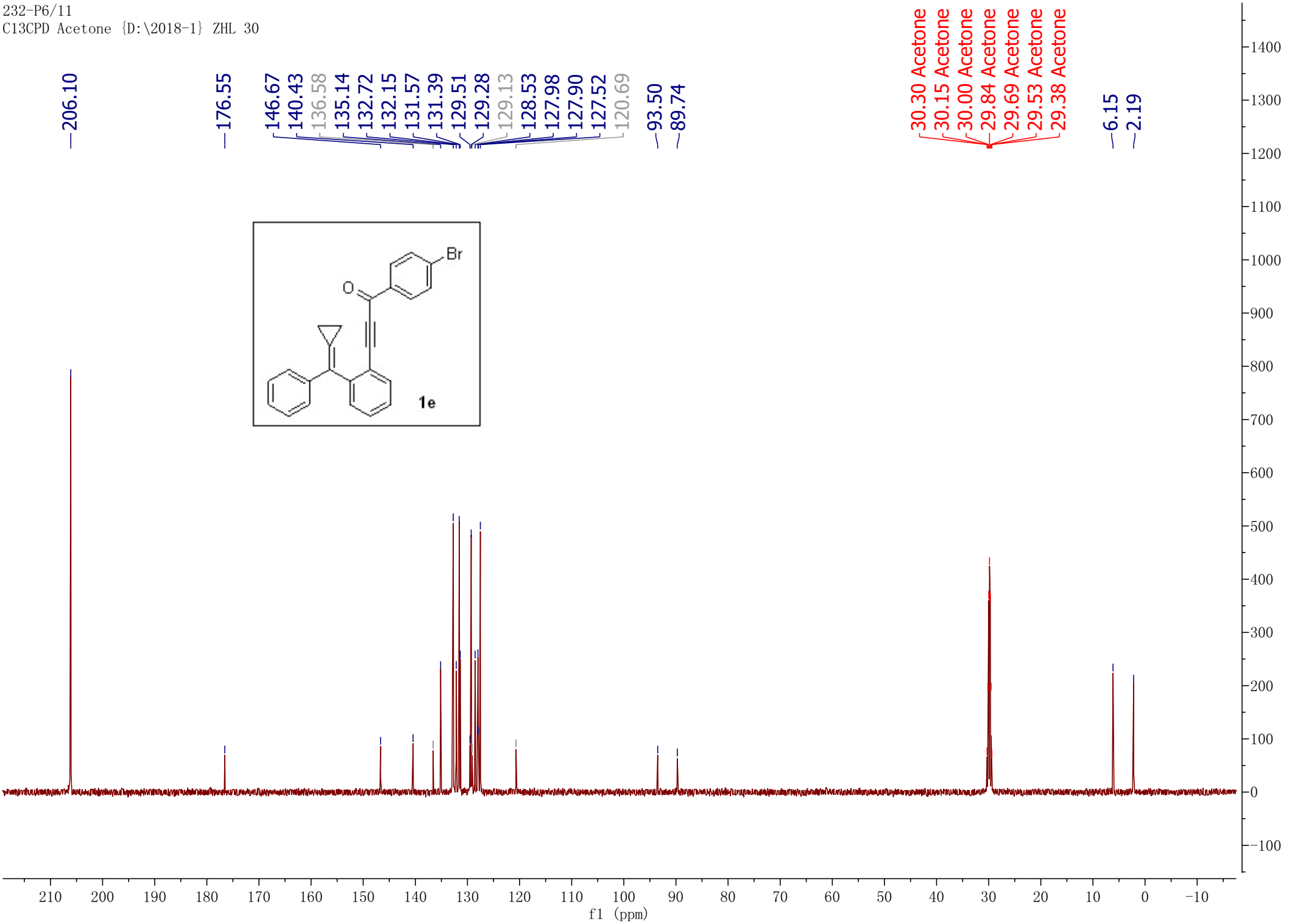

236-P1/10
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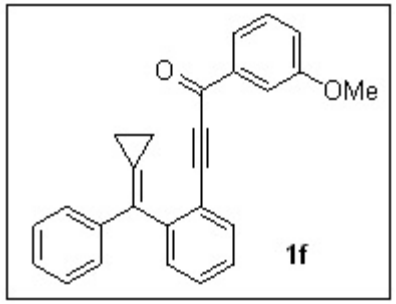

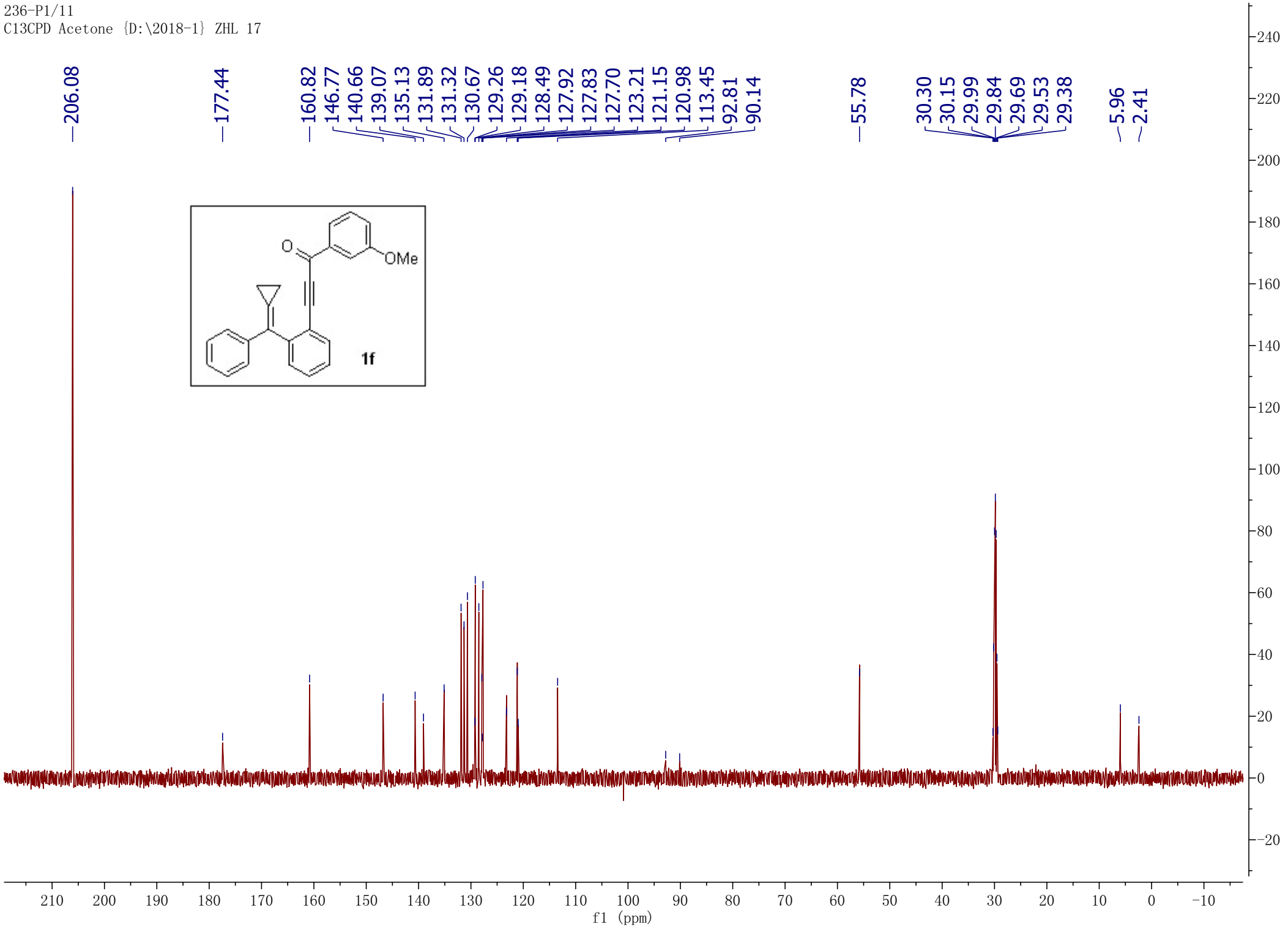
236-P1/11
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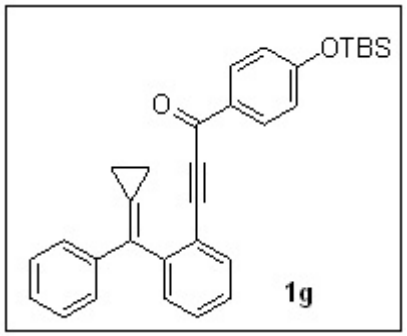
140.66
139.07
135.13
131.89
131.32
130.67
129.26
129.18
128.49
127.92
127.83
127.70
123.21
121.15
120.98
113.45
92.81
90.14
55.78
30.30
30.15
29.99
29.84
29.69
29.53
29.38
5.96
2.41
O
OMe
1f
f1 (ppm)

236-P2/10
PROTON Acetone {D:\2018-1} ZHL 18



f1 (ppm)

236-P2/11
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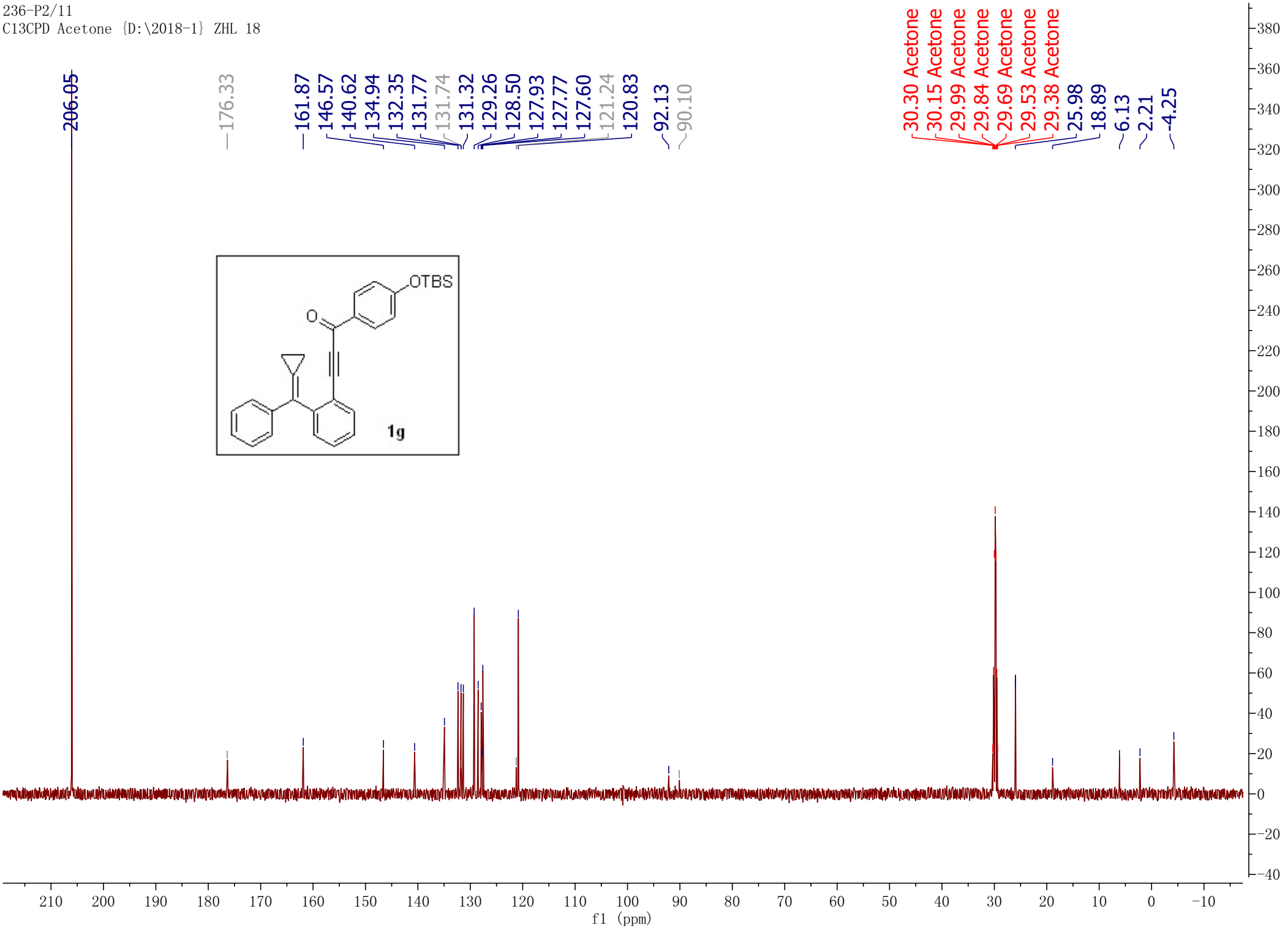

JKG-20181128-250-P6/10
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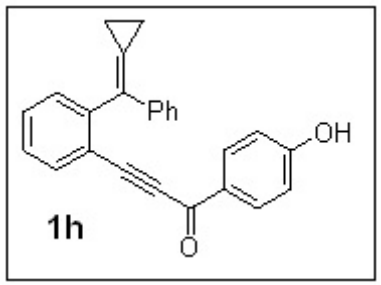

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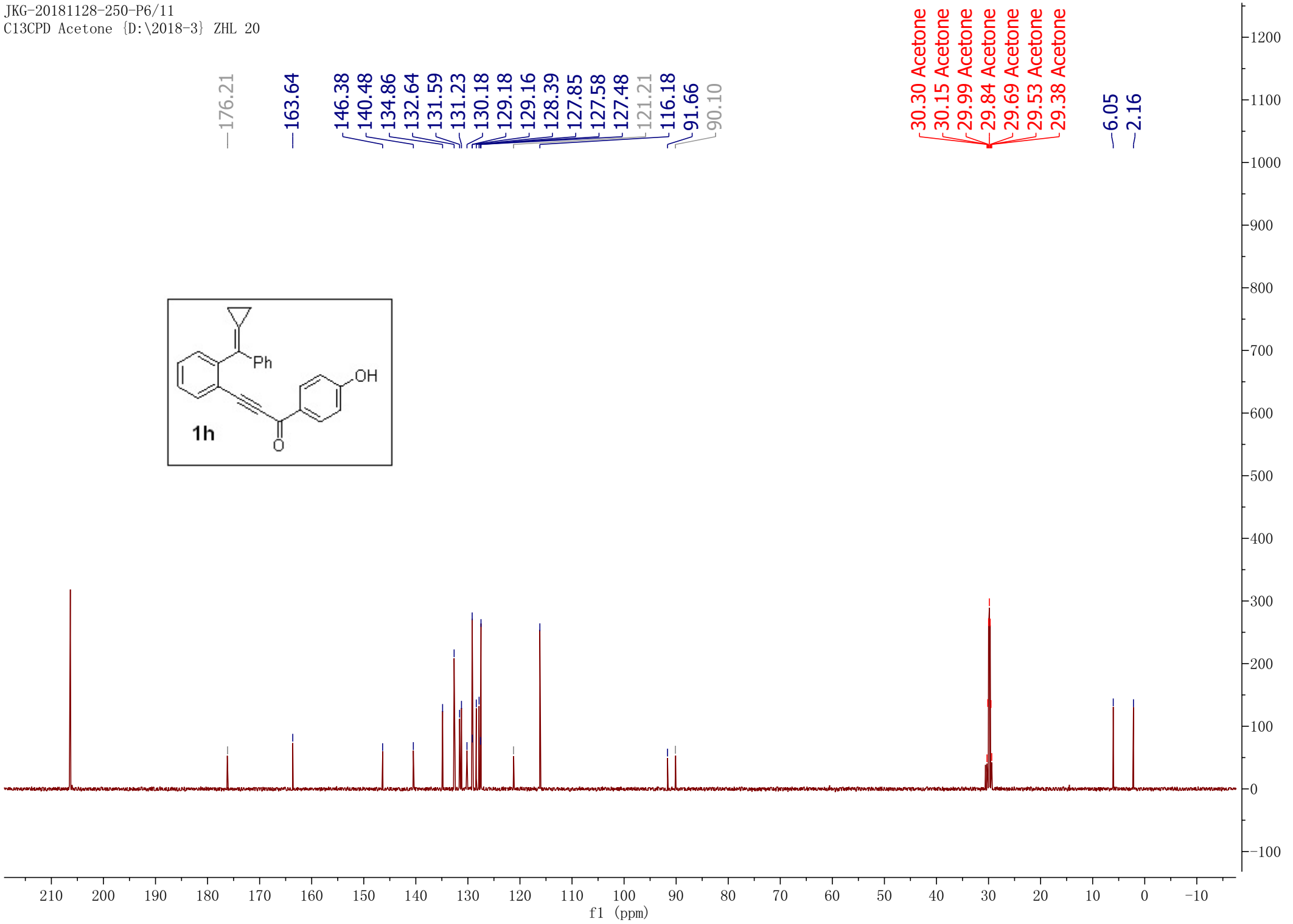

237-P3/10
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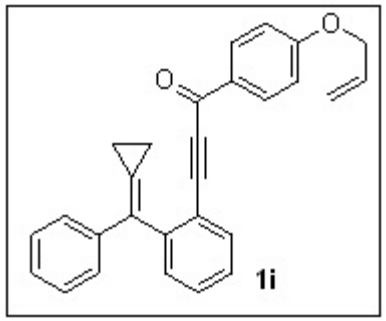

237-P3/11
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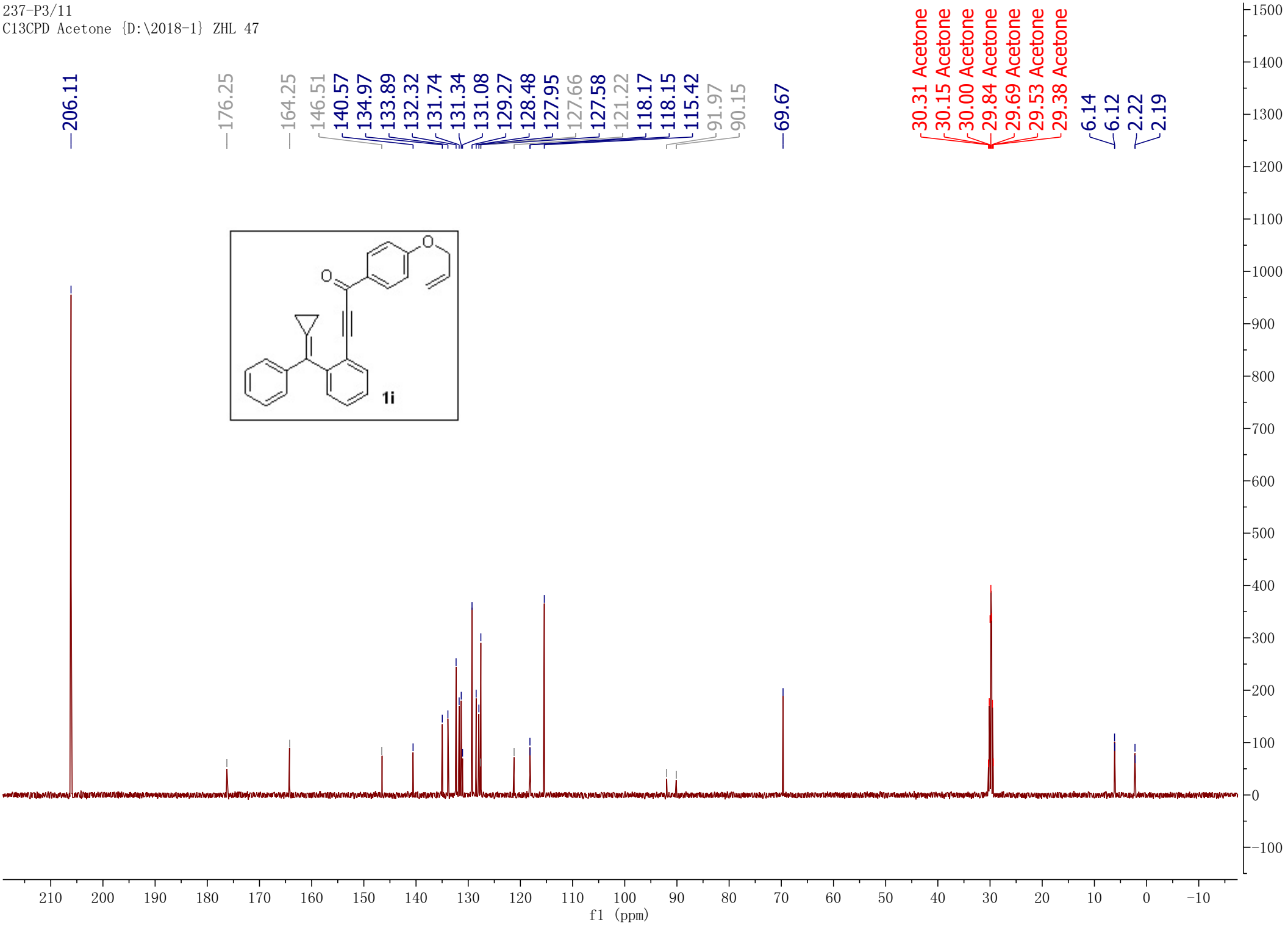

234-P9/10
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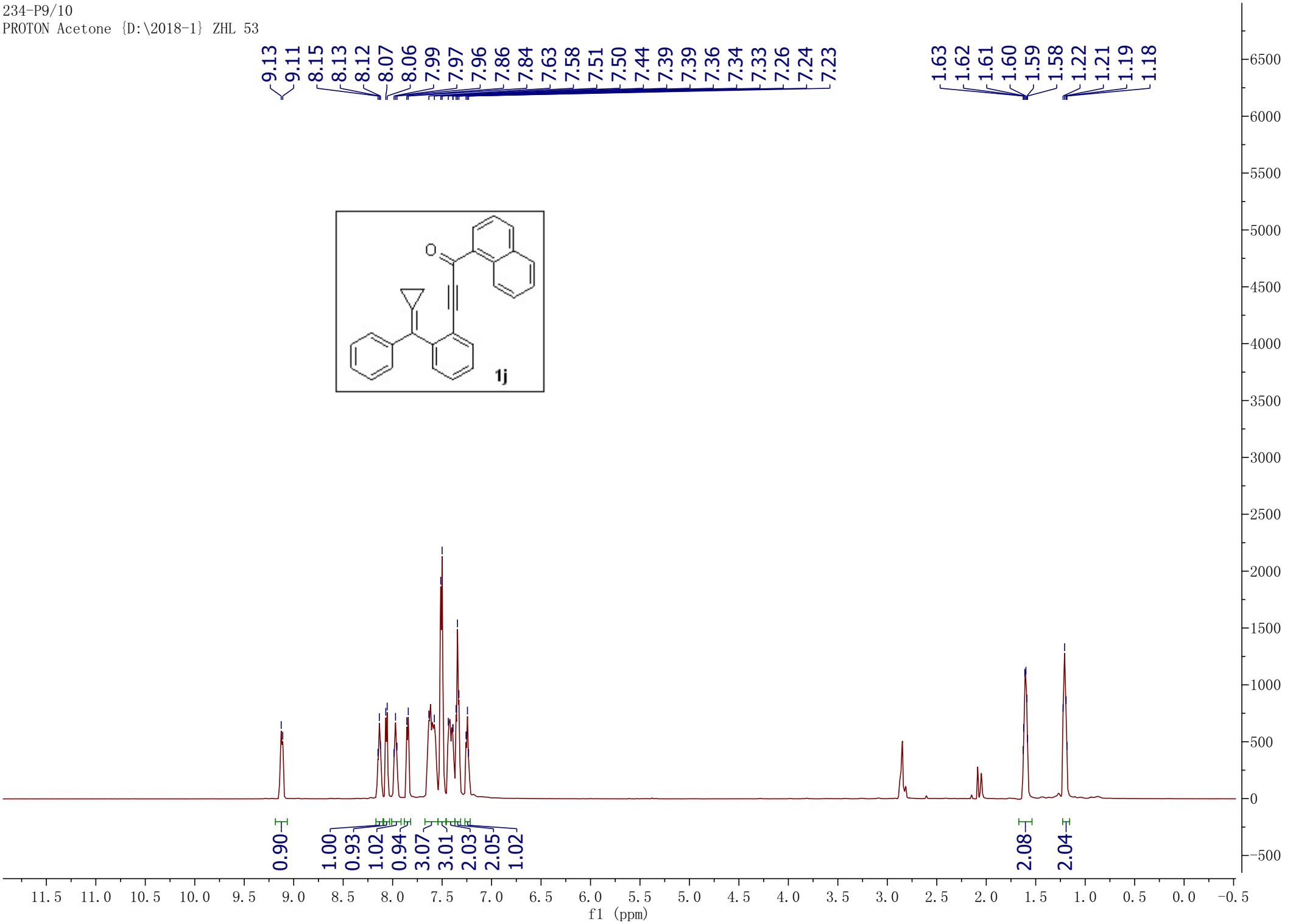

234-P9/11
C13CPD Acetone {D:\2018-1} ZHL 53

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131.34
131.29
129.62
129.59
129.28
129.23
128.49
127.91
127.73
127.62
127.57
126.37
125.55
121.16
91.61
30.30 Acetone
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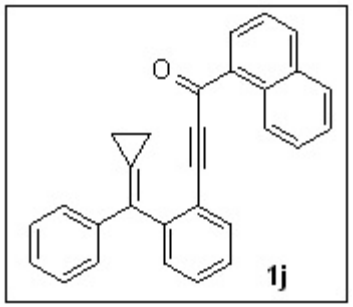
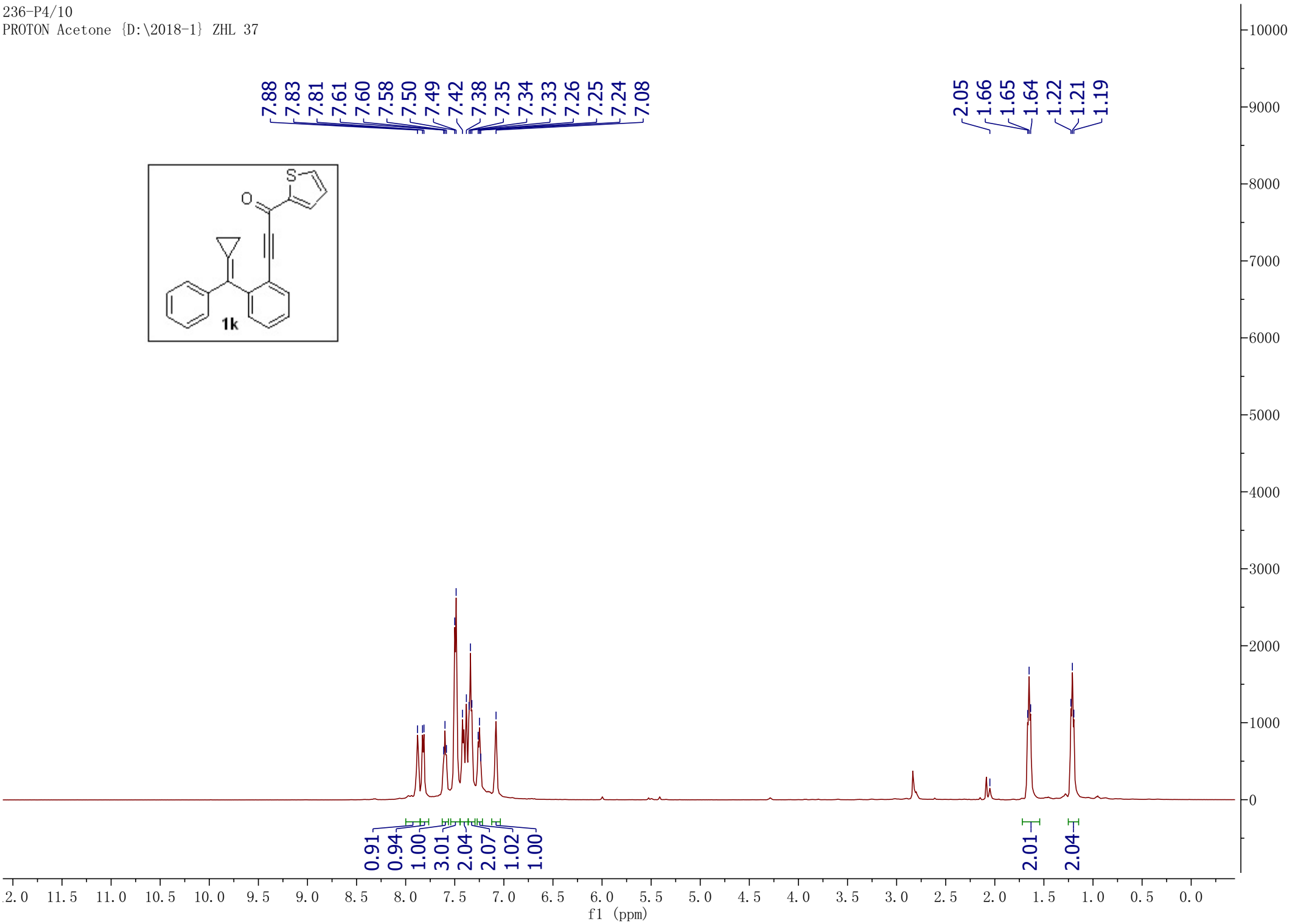
6.01
2.27

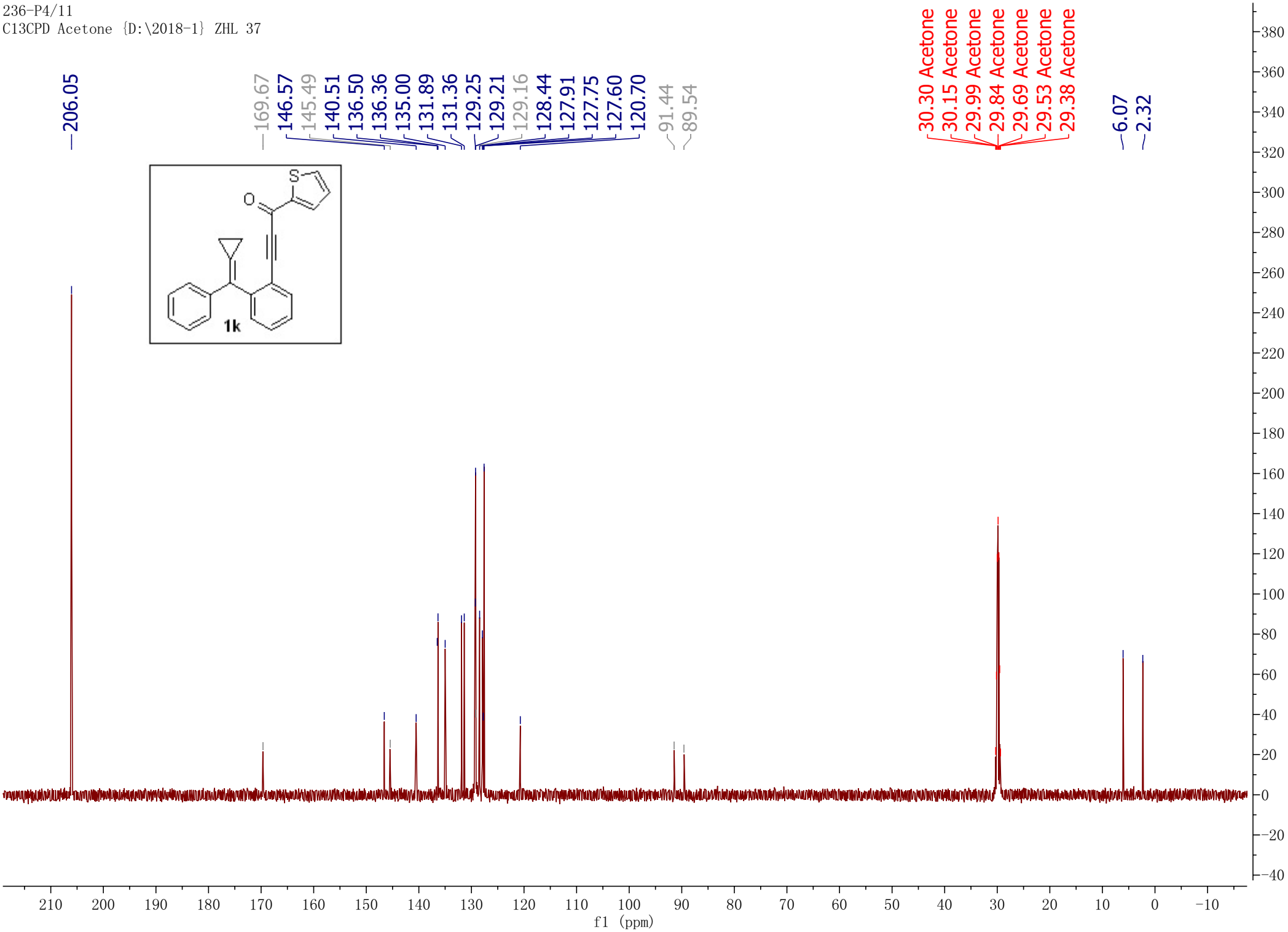


f1 (ppm)

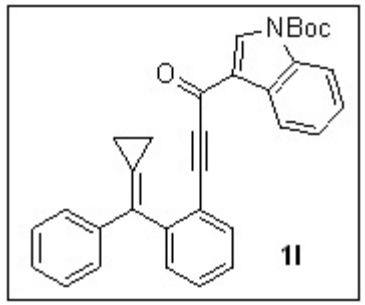
236-P4/10
PROTON Acetone {D:\2018-1} ZHL 37



236-P4/11
C13CPD Acetone {D:\2018-1} ZHL 37

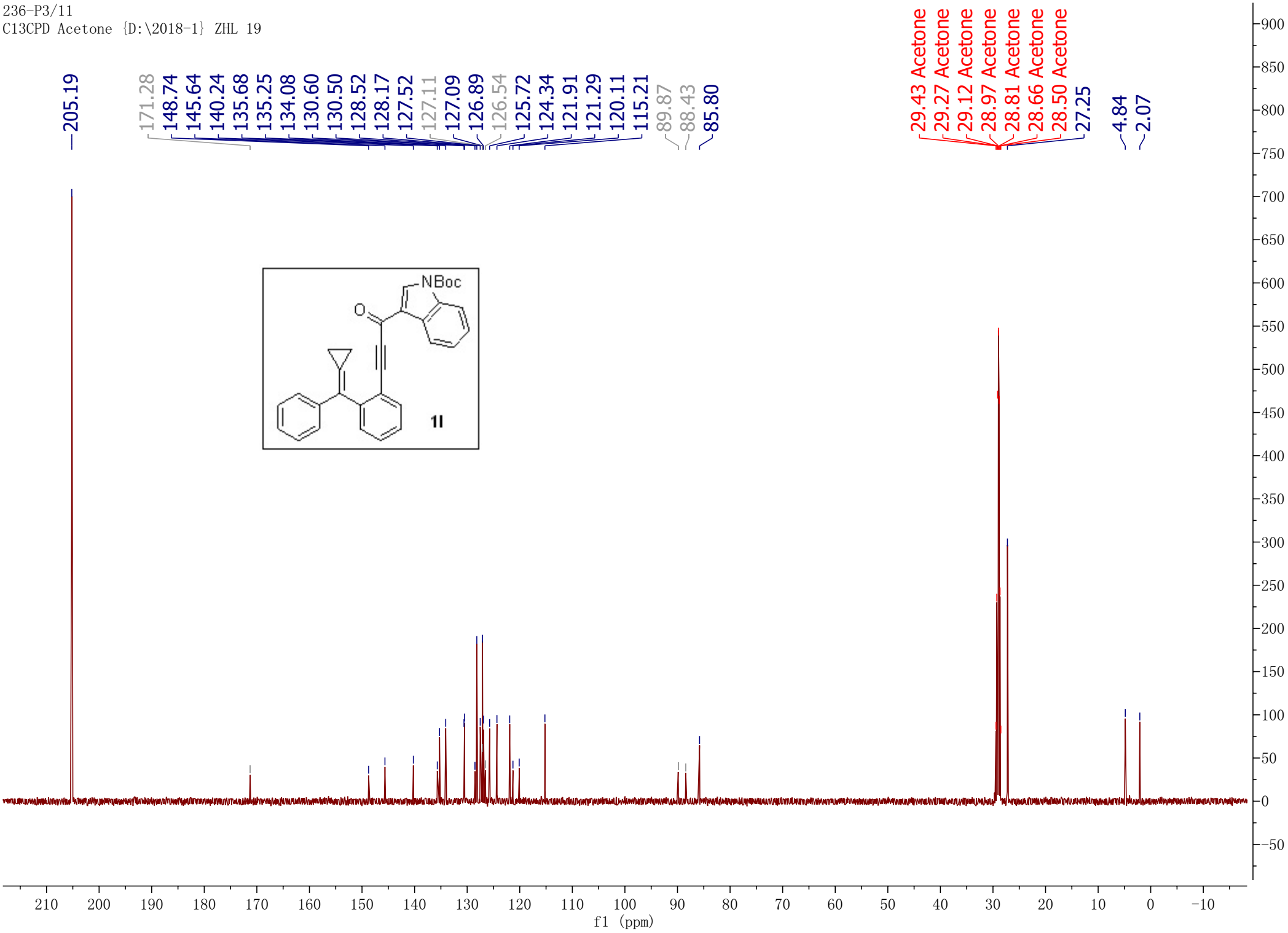


236-P3/10
PROTON Acetone {D:\2018-1} ZHL 19

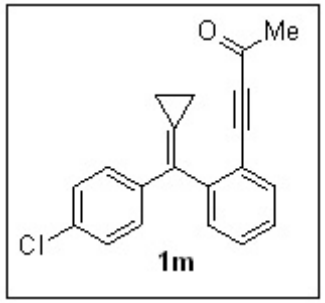


f1 (ppm)

236-P3/11
C13CPD Acetone {D:\2018-1} ZHL 19



242-P2/10
PROTON Acetone {D:\2018-1} ZHL 35



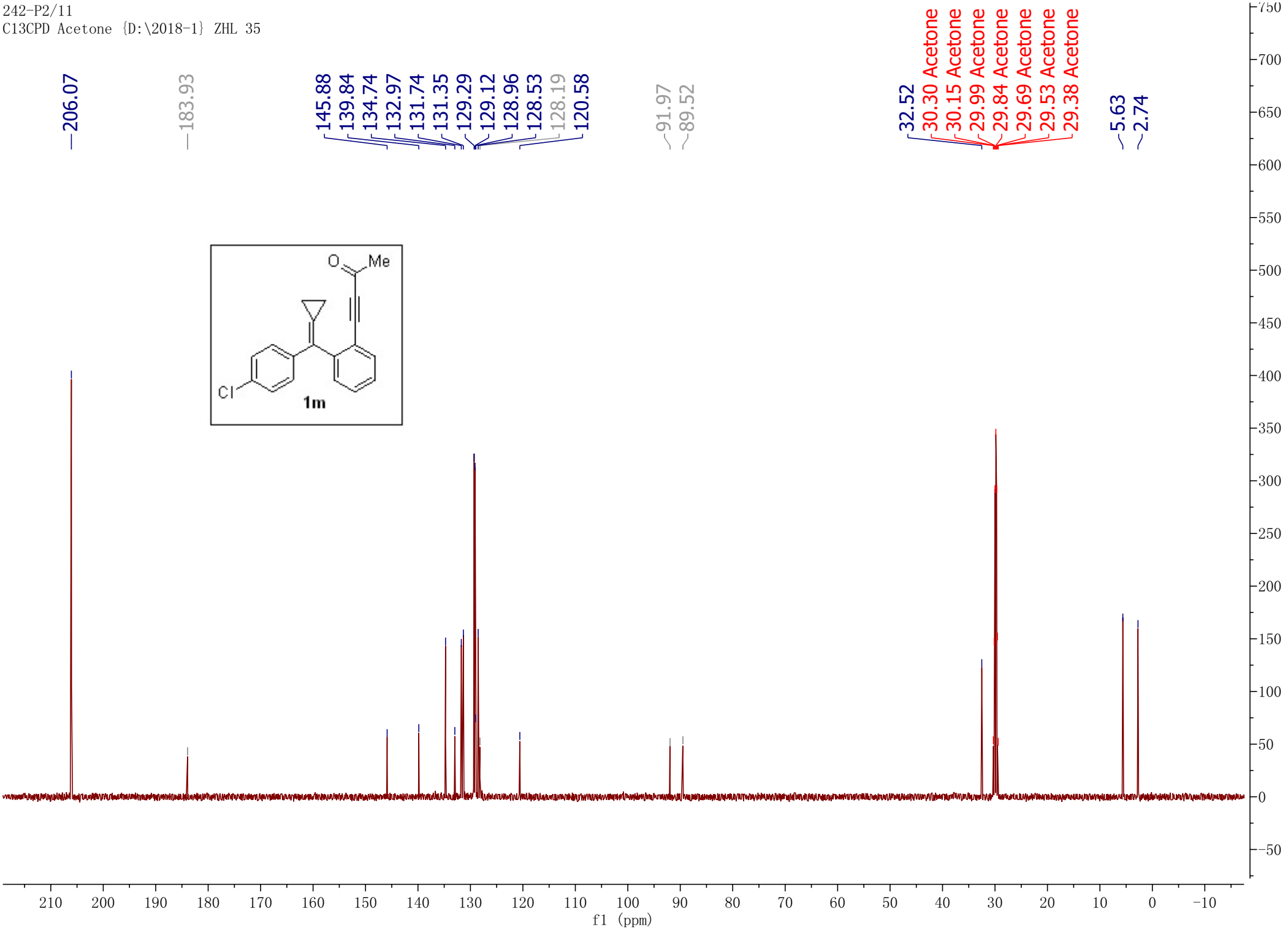
7.70 7.69 7.62 7.60 7.58 7.49 7.44 7.39 7.37

2.08 1.69 1.67 1.66 1.30 1.28 1.27

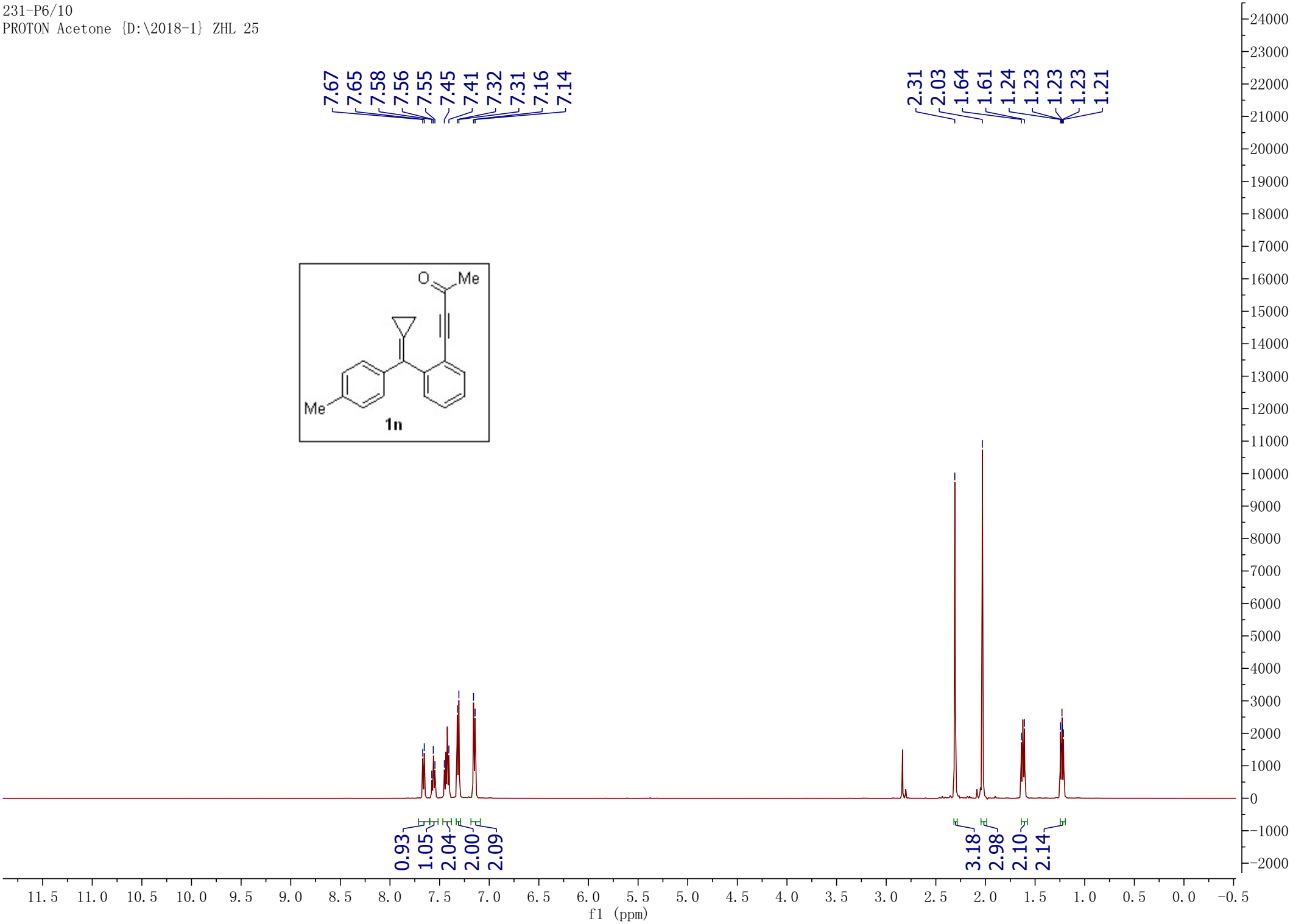
0.93 1.00 3.98 2.01 2.94 2.05 2.05

f1 (ppm)

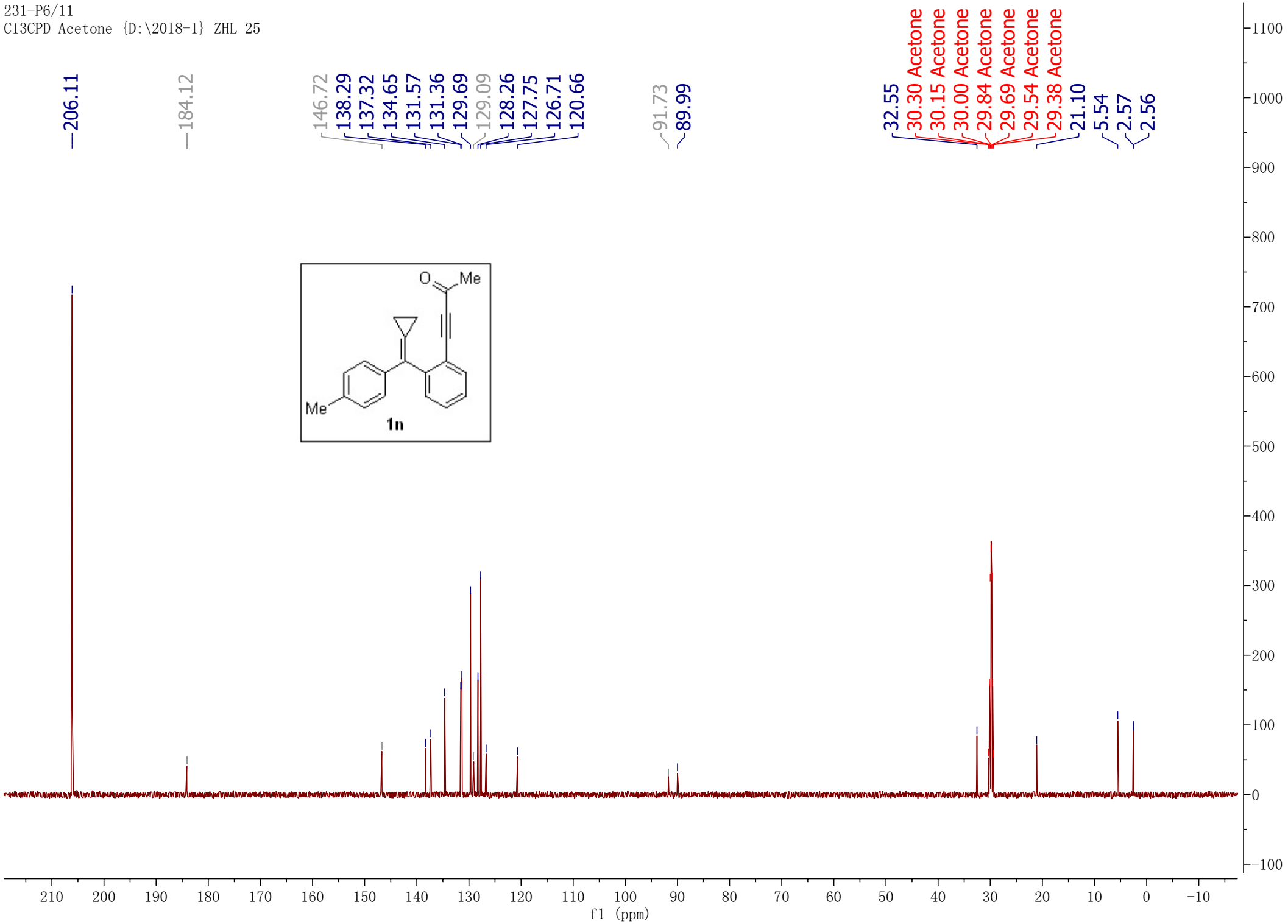
242-P2/11
C13CPD Acetone {D:\2018-1} ZHL 35



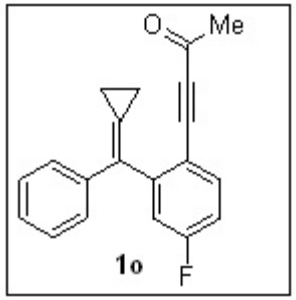
231-P6/10
PROTON Acetone {D:\2018-1} ZHL 25



231-P6/11
C13CPD Acetone {D:\2018-1} ZHL 25



244-P2/10
PROTON Acetone {D:\2018-1} ZHL 9



1o

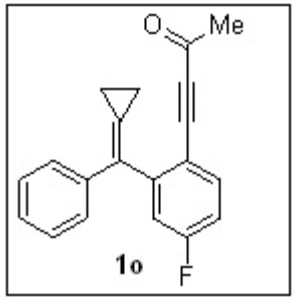
7.75 7.74 7.73 7.72 7.45 7.45 7.44 7.37 7.33 7.28 7.22

2.00 1.68 1.65 1.32 1.28

0.92 2.00 2.00 3.01 2.94 2.09 2.11

f1 (ppm)

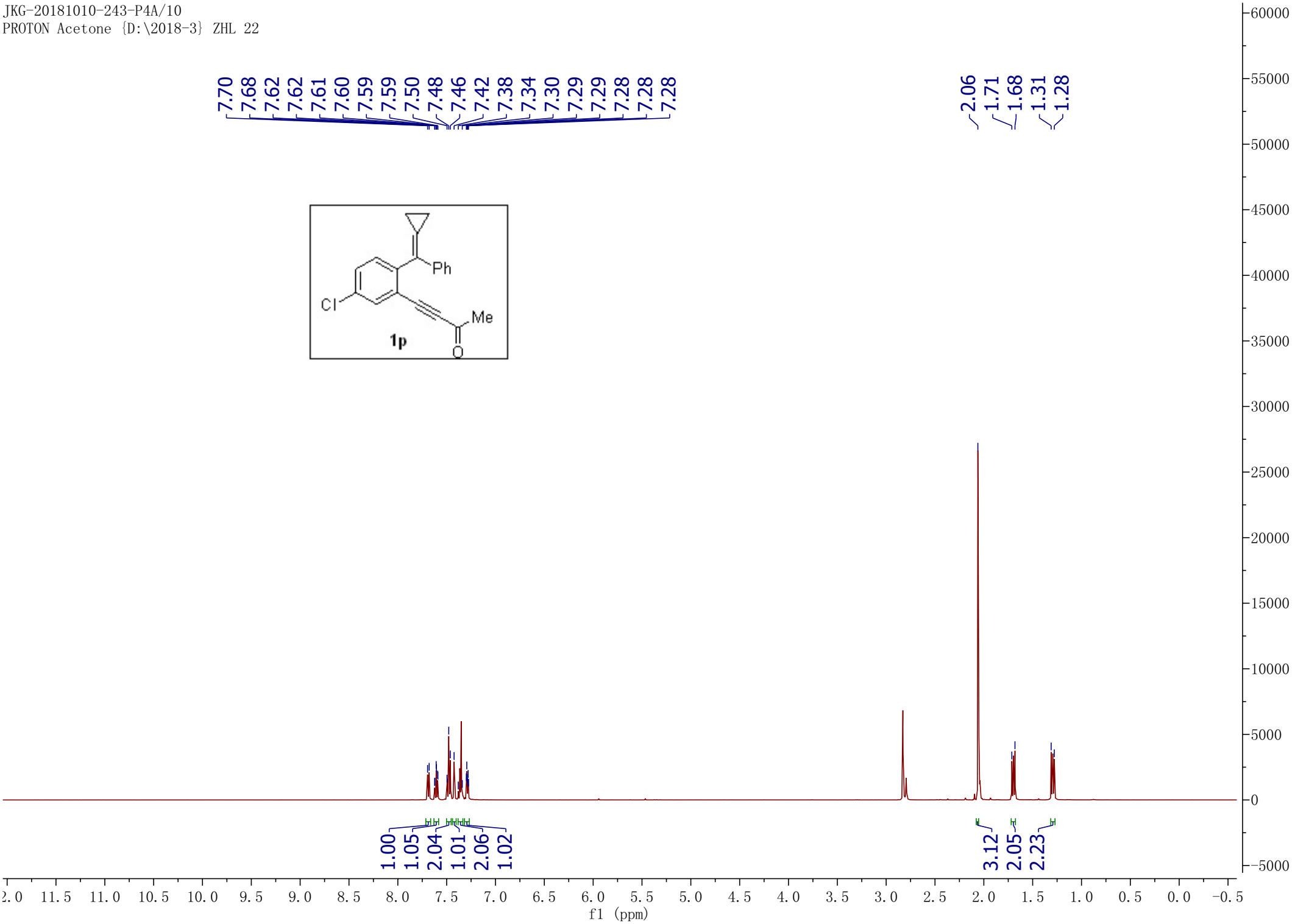
244-P2/11
C13CPD Acetone {D:\2018-1} ZHL 9



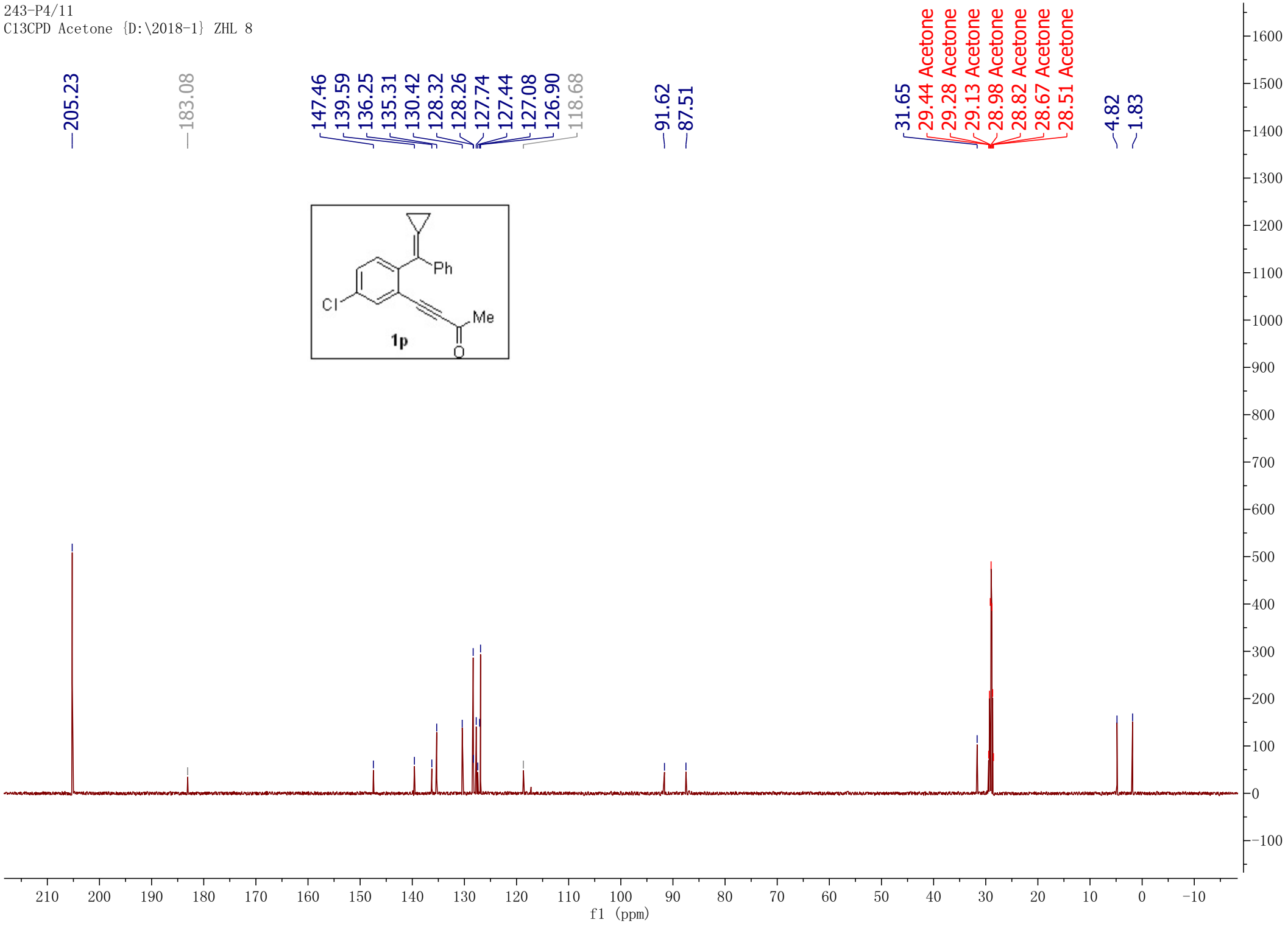
206.10
183.98
165.56
163.55
149.51
149.44
140.46
137.23
137.16
129.17
128.93
128.51
128.50
127.91
127.75
118.48
118.30
117.12
117.09
115.84
115.67
91.79
91.78
88.79
32.50
30.30 Acetone
30.15 Acetone
29.99 Acetone
29.84 Acetone
29.69 Acetone
29.53 Acetone
29.38 Acetone
5.67
2.66

f1 (ppm)

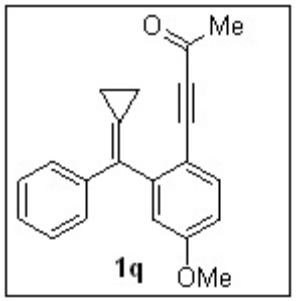
JKG-20181010-243-P4A/10
PROTON Acetone {D:\2018-3} ZHL 22



243-P4/11
C13CPD Acetone {D:\2018-1} ZHL 8



243-P2/10
PROTON Acetone {D:\2018-1} ZHL 7



7.62 7.60 7.46 7.45 7.35 7.33 7.32 7.26 7.24 7.23 7.03 7.02 7.01 7.00 6.98 6.98

3.87

1.97 1.66 1.63 1.28 1.25

0.94 1.96 2.01 1.00 1.02 0.98

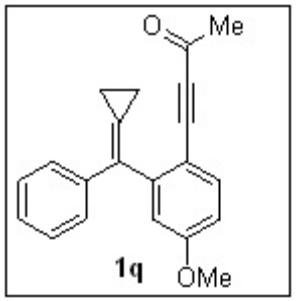
3.12

2.97 2.02 2.04

f1 (ppm)

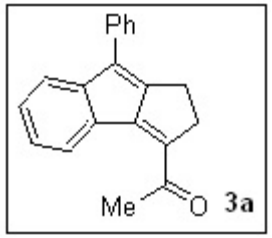
243-P2/11
C13CPD Acetone {D:\2018-1} ZHL 7

206.11
183.97
162.59
148.72
140.82
136.69
129.24
129.04
127.73
127.69
127.64
116.93
114.22
112.55
91.54
91.02
55.98
32.45
30.30 Acetone
30.15 Acetone
29.99 Acetone
29.84 Acetone
29.69 Acetone
29.53 Acetone
29.38 Acetone
5.67
2.57



f1 (ppm)

JKG-20180905-218-P6/10
PROTON CDCl3 {D:\2018-3} ZHL 12



8.45 8.43 7.62 7.61 7.60 7.48 7.44 7.37 7.36 7.30 7.26 7.23 7.21 7.20

3.35 3.34 2.91 2.89 2.47

0.94 1.97 3.07 2.07 1.04 2.00 2.00 3.00

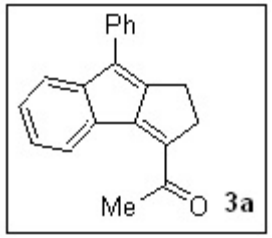
25000 20000 15000 10000 5000 0

11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

f1 (ppm)

JKG-20180905-218-P6/11
C13CPD CDCl3 {D:\2018-3} ZHL 12

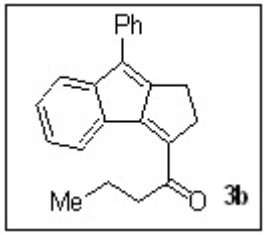
197.52
153.88
150.96
150.18
140.21
135.09
134.11
129.98
128.76
127.87
127.61
127.05
125.46
120.11
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
39.26
30.29
23.08



3a

f1 (ppm)

JKG-20180907-234-P8C/10
PROTON CDCl3 {D:\2018-3} ZHL 13

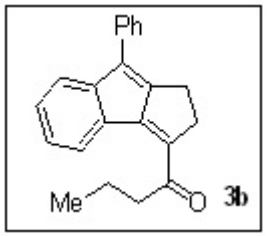


8.48 8.47 7.62 7.60 7.48 7.44 7.36 7.29 7.26 7.22 7.21 7.19 3.38 3.36 2.93 2.91 2.75 2.74 2.72 1.81 1.74 1.04 1.02 1.01

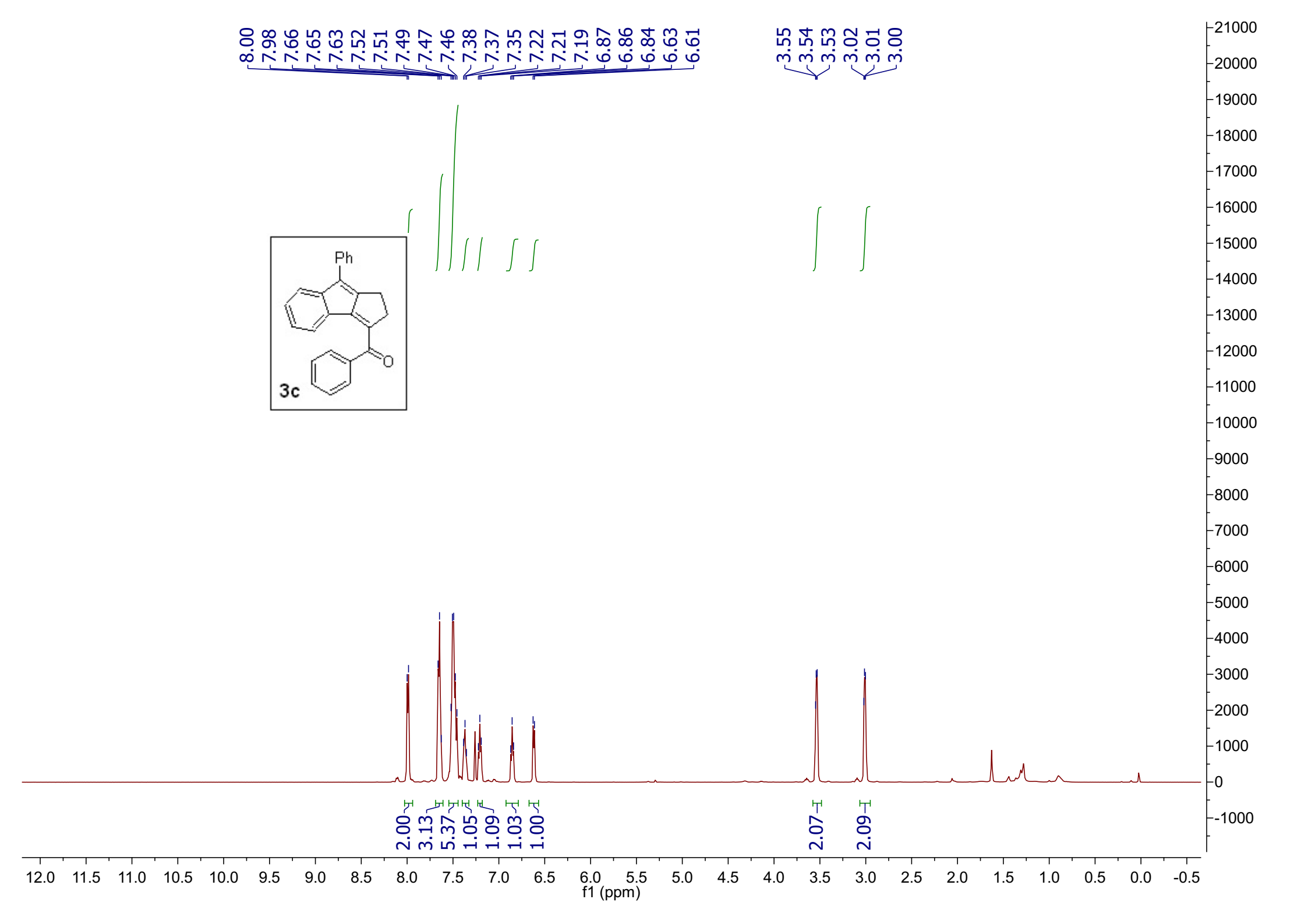
0.98 2.00 3.05 2.04 1.02 2.00 2.00 2.02 2.00 3.04

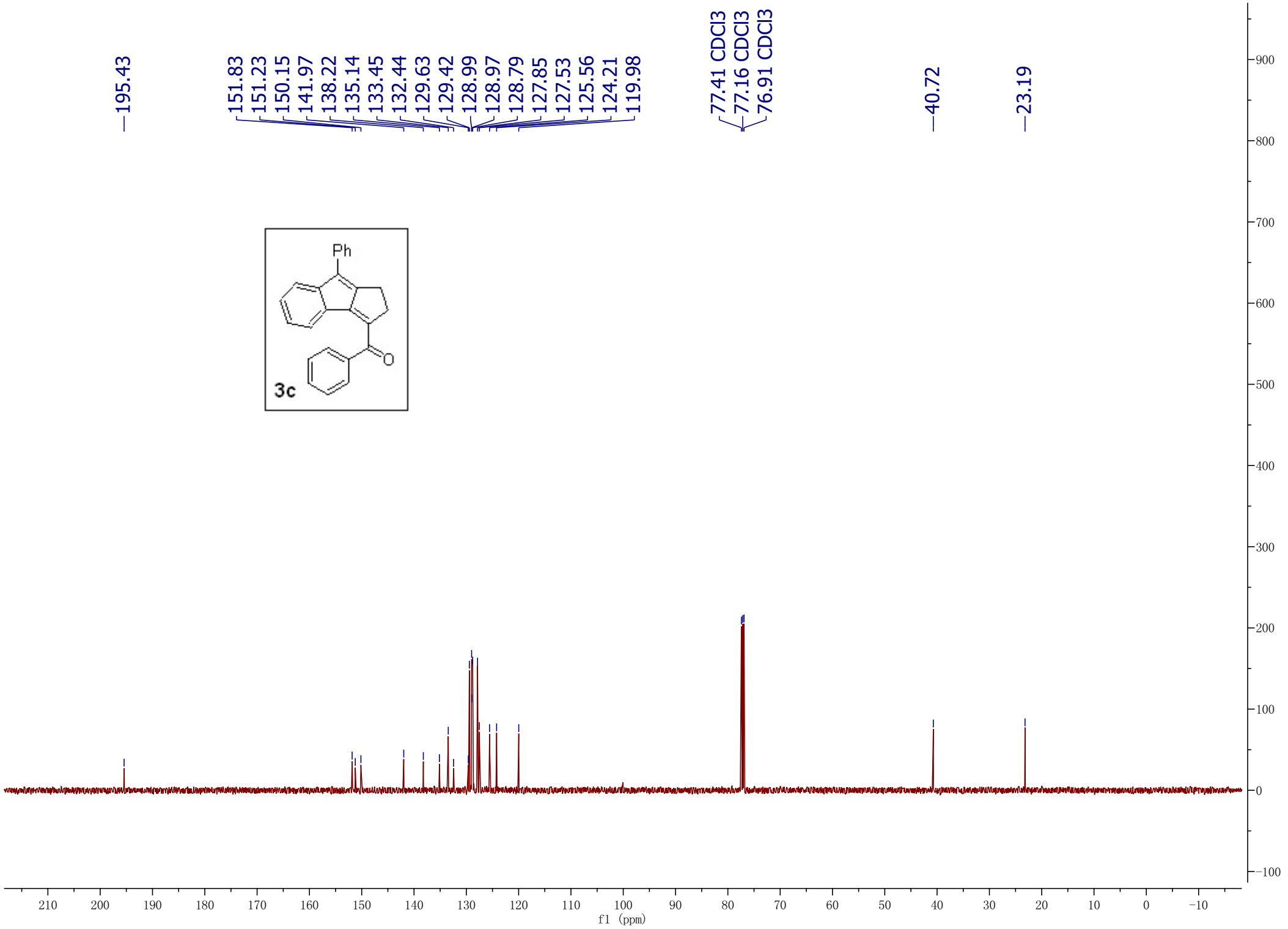
f1 (ppm)

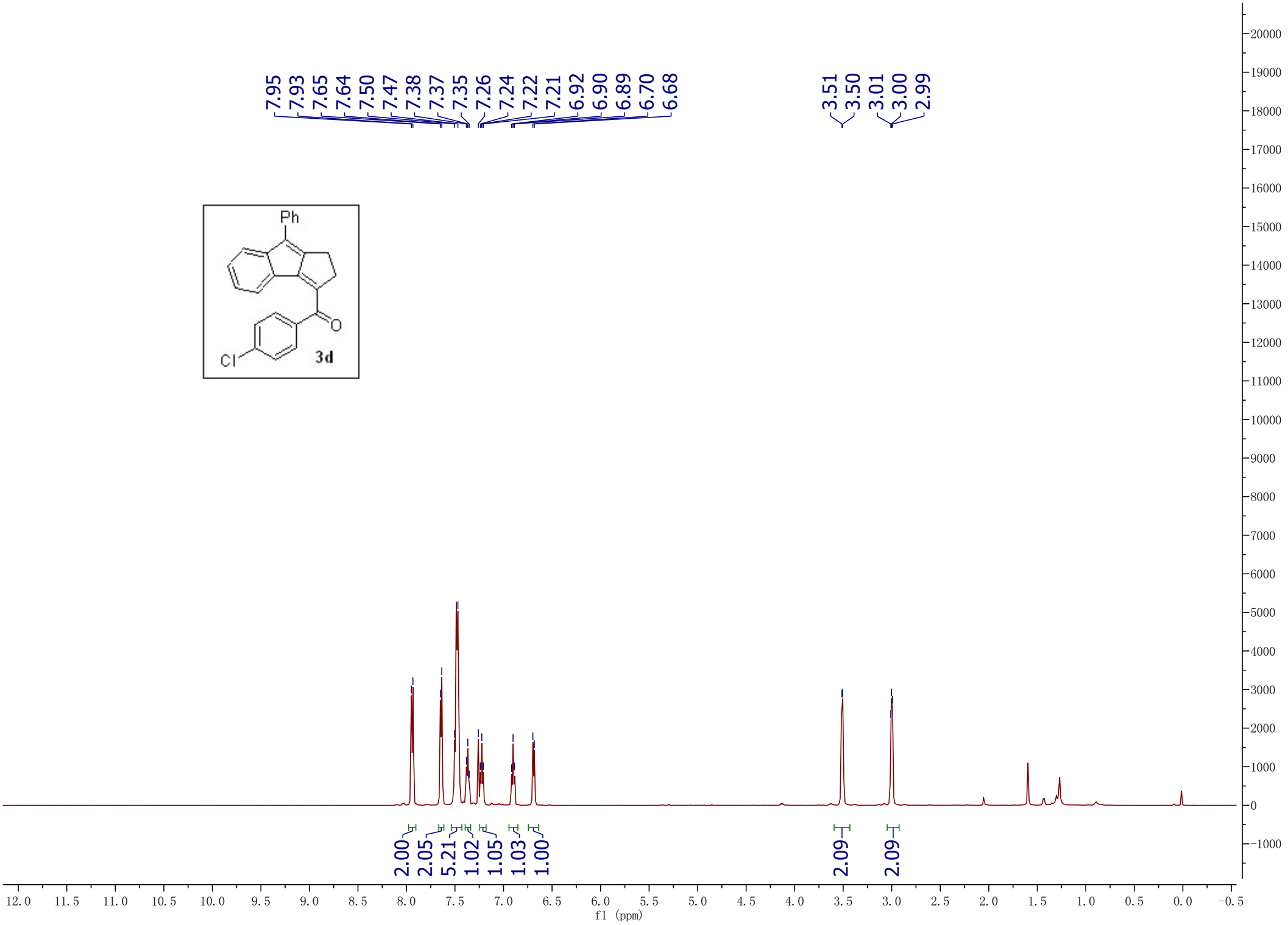
JKG-20180907-234-P8C/12
C13CPD CDCl3 {D:\2018-3} ZHL 13

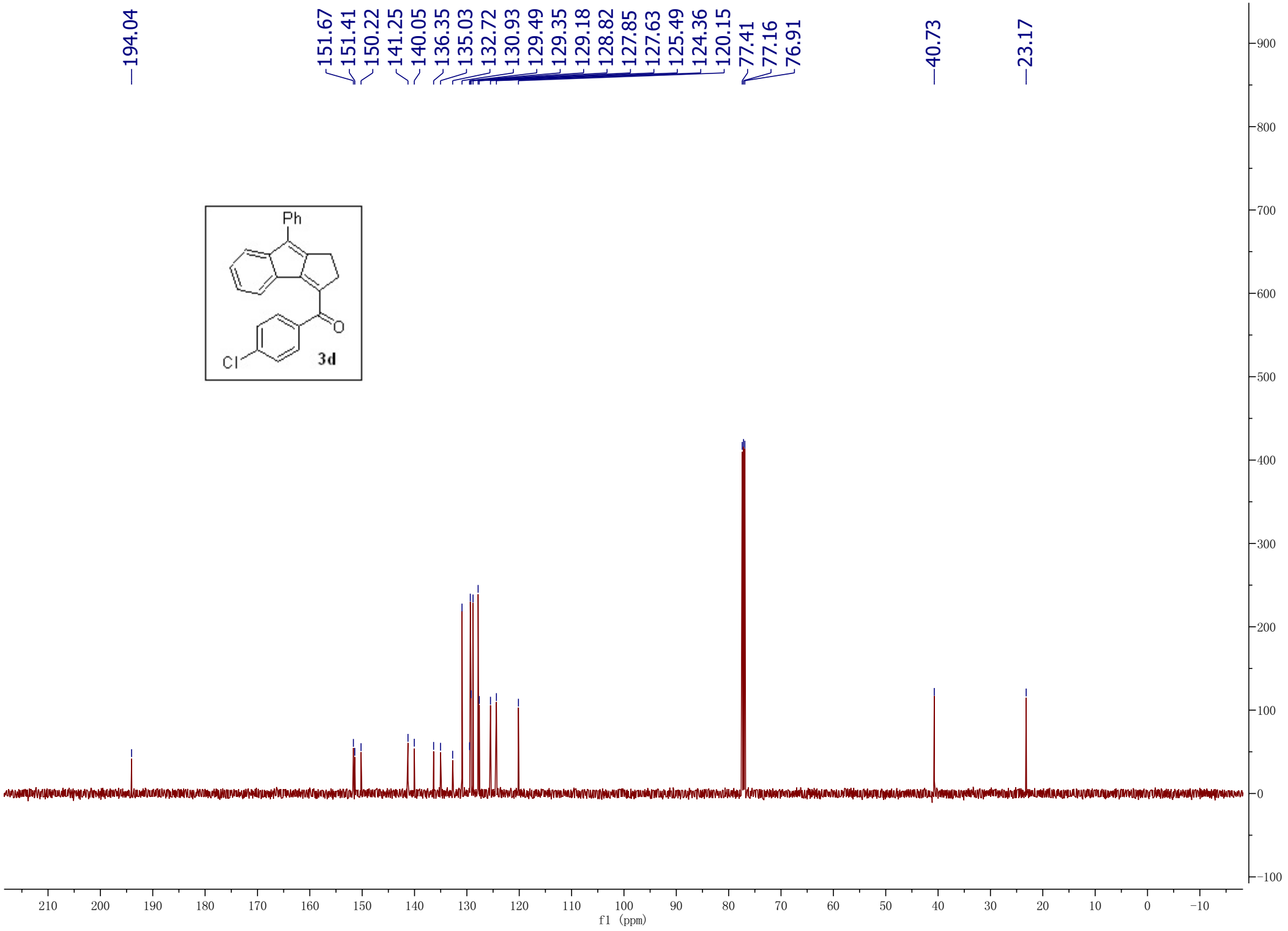


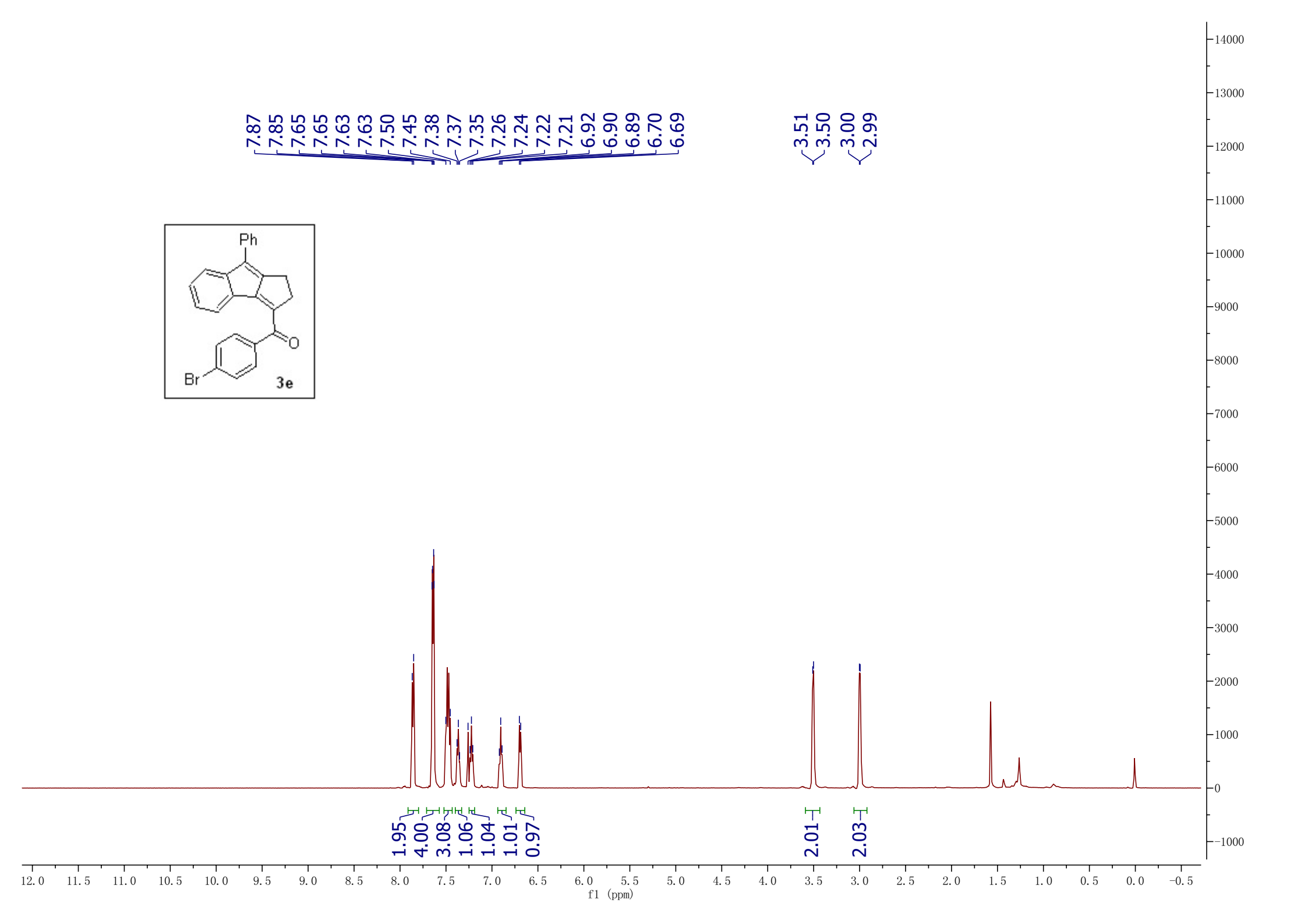
f1 (ppm)

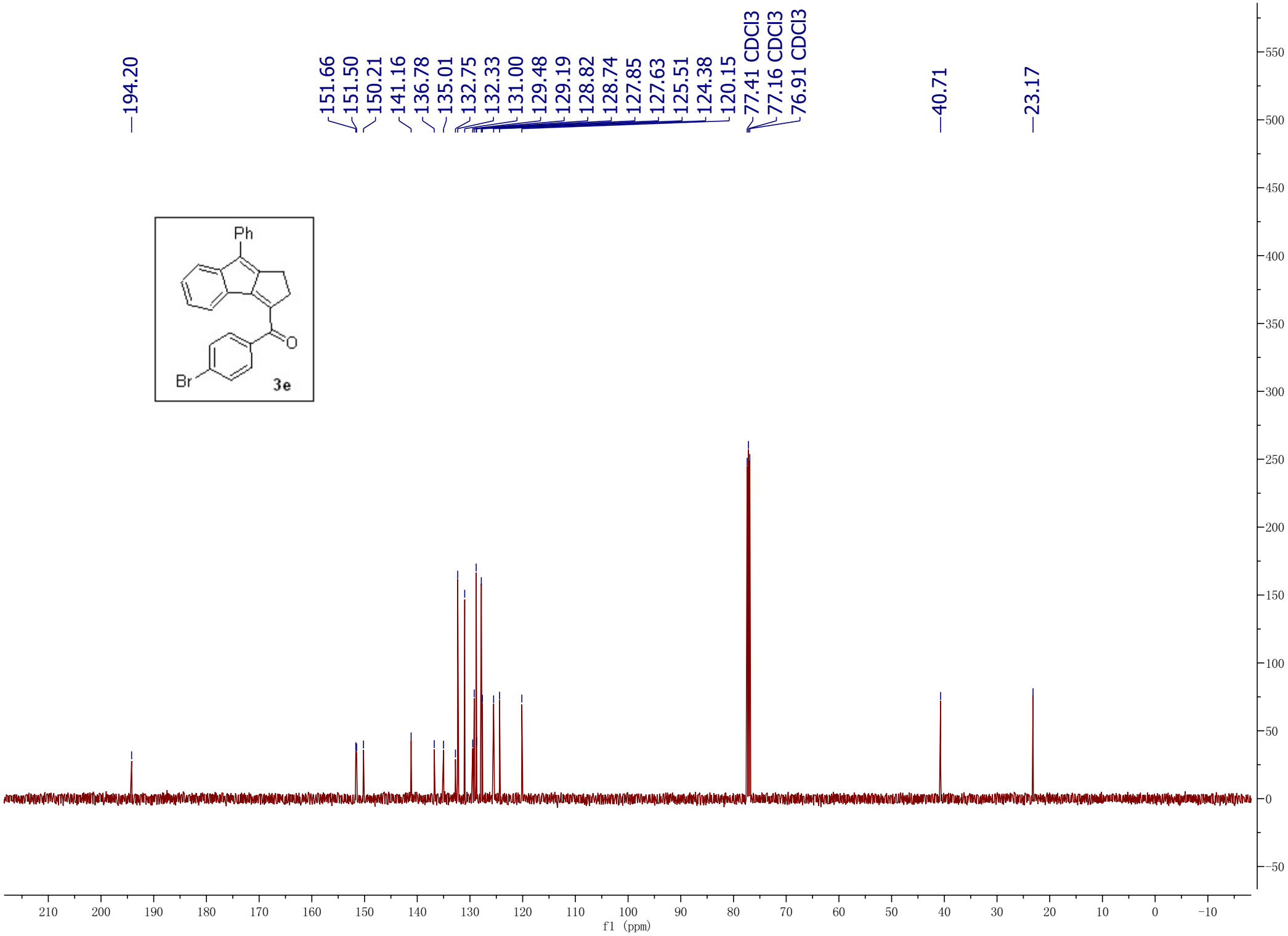

8.00
7.98
7.66
7.65
7.63
7.52
7.51
7.49
7.47
7.46
7.38
7.37
7.35
7.22
7.21
7.19
6.87
6.86
6.84
6.63
6.61
3.55
3.54
3.53
3.02
3.01
3.00
Ph
O
3c
2.00
3.13
5.37
1.05
1.09
1.03
1.00
2.07
2.09
f1 (ppm)


195.43
151.83
151.23
150.15
141.97
138.22
135.14
133.45
132.44
129.63
129.42
128.99
128.97
128.79
127.85
127.53
125.56
124.21
119.98
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
40.72
23.19
Ph
O
3c
f1 (ppm)

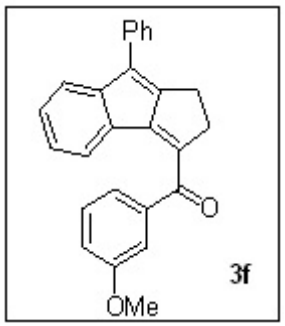

7.95
7.93
7.65
7.64
7.50
7.47
7.38
7.37
7.35
7.26
7.24
7.22
7.21
6.92
6.90
6.89
6.70
6.68
3.51
3.50
3.01
3.00
2.99
Ph
O
Cl
3d
2.00
2.05
5.21
1.02
1.05
1.03
1.00
2.09
2.09
f1 (ppm)


194.04
151.67
151.41
150.22
141.25
140.05
136.35
135.03
132.72
130.93
129.49
129.35
129.18
128.82
127.85
127.63
125.49
124.36
120.15
77.41
77.16
76.91
40.73
23.17
Ph
O
Cl
3d
f1 (ppm)


7.87
7.85
7.65
7.65
7.63
7.63
7.50
7.45
7.38
7.37
7.35
7.26
7.24
7.22
7.21
6.92
6.90
6.89
6.70
6.69
3.51
3.50
3.00
2.99
Ph
O
Br
3e
1.95
4.00
3.08
1.06
1.04
1.01
0.97
2.01
2.03
f1 (ppm)


194.20
151.66
151.50
150.21
141.16
136.78
135.01
132.75
132.33
131.00
129.48
129.19
128.82
128.74
127.85
127.63
125.51
124.38
120.15
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
40.71
23.17
Ph
O
Br
3e
f1 (ppm)

JKG-20180913-240-P2/10
PROTON CDCl3 {D:\2018-3} ZHL 41



7.66 7.64 7.57 7.45 7.39 7.35 7.26 7.22 7.18 6.90 6.88 6.87 6.73 6.71

3.86 3.54 3.52 3.01 3.00

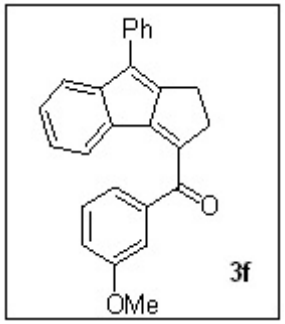
2.08 5.19 2.08 2.12 1.04 1.00

3.11 2.06 2.05

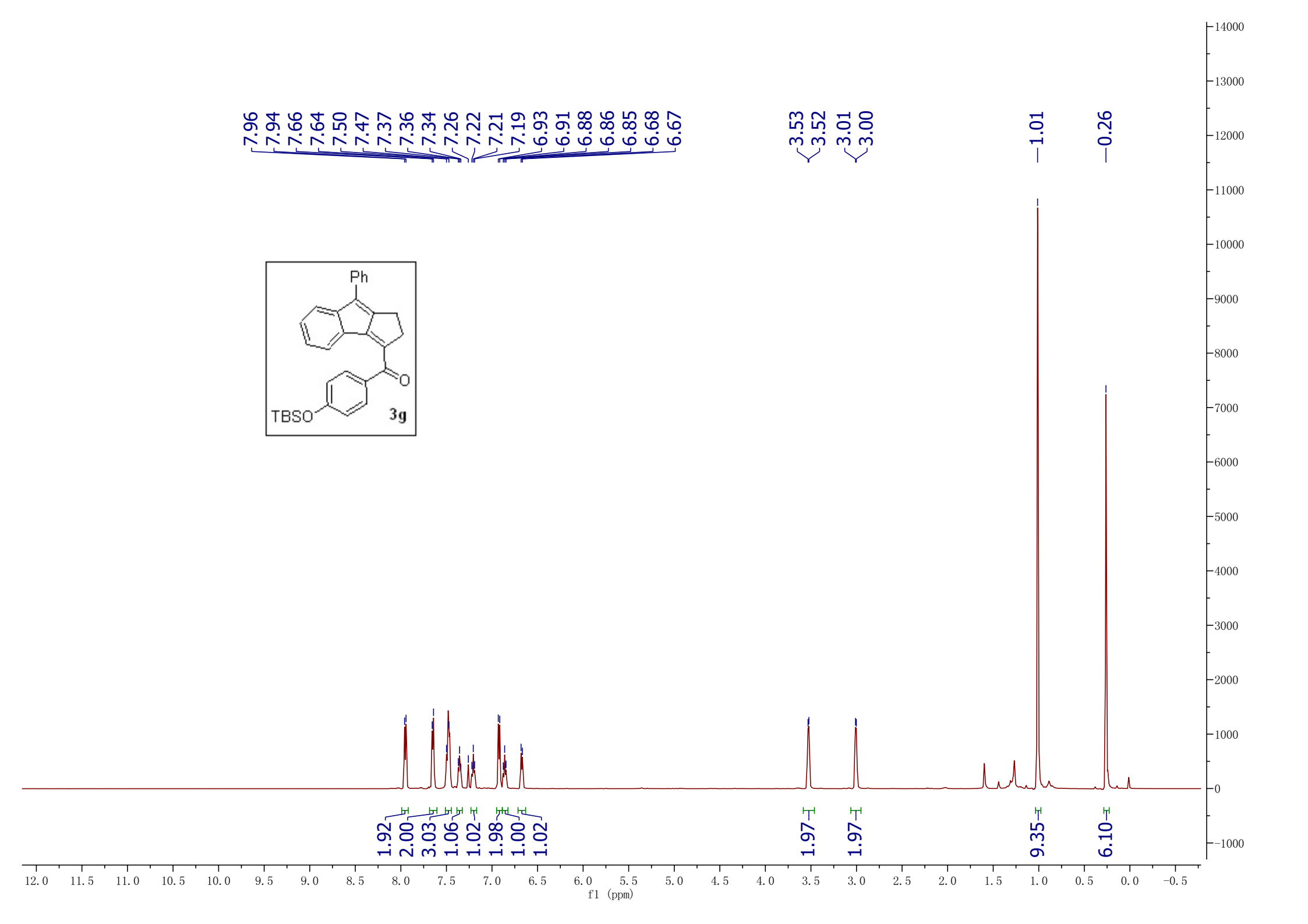
f1 (ppm)

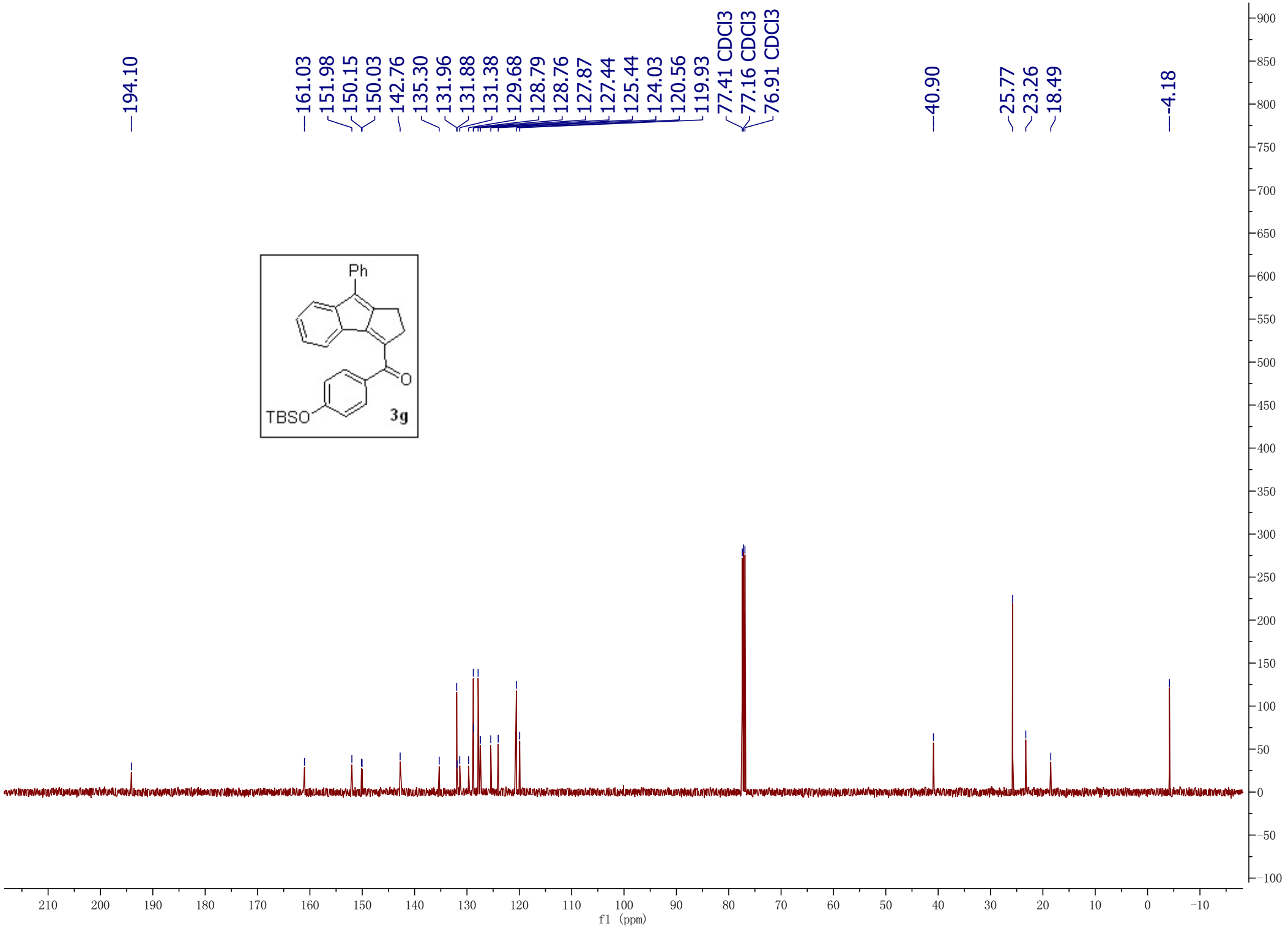
JKG-20180913-240-P2/12
C13CPD CDCl3 {D:\2018-3} ZHL 41

195.15
160.20
151.76
151.27
150.16
141.98
139.46
135.20
132.49
130.02
129.69
129.01
128.80
127.88
127.54
125.59
124.28
122.60
120.28
120.00
113.00
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
55.68
40.79
23.22

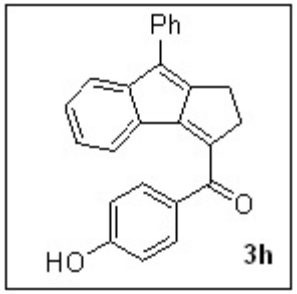


f1 (ppm)


7.96
7.94
7.66
7.64
7.50
7.47
7.37
7.36
7.34
7.26
7.22
7.21
7.19
6.93
6.91
6.88
6.86
6.85
6.68
6.67
3.53
3.52
3.01
3.00
1.01
0.26
Ph
O
TBSO
3g
1.92
2.00
3.03
1.06
1.02
1.98
1.00
1.02
1.97
1.97
9.35
6.10
f1 (ppm)

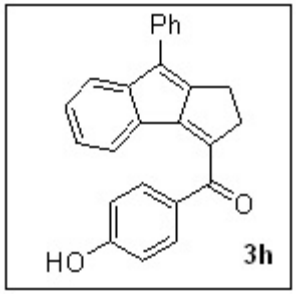

194.10
161.03
151.98
150.15
150.03
142.76
135.30
131.96
131.88
131.38
129.68
128.79
128.76
127.87
127.44
125.44
124.03
120.56
119.93
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
40.90
25.77
23.26
18.49
-4.18
Ph
O
TBSO
3g
f1 (ppm)

JKG-20181102-249-P7/10
PROTON Acetone {D:\2018-3} ZHL 3



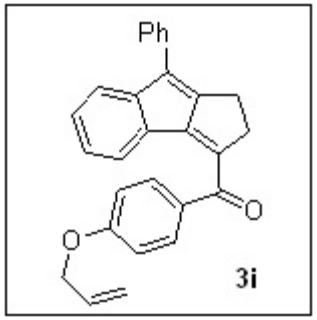
JKG-20181102-249-P7/11
C13CPD Acetone {D:\2018-3} ZHL 3

206.21
206.17
193.75
163.49
152.87
150.66
149.36
144.88
136.03
132.79
131.66
130.45
130.39
129.57
129.39
128.49
128.12
125.54
124.68
120.52
116.51
41.62
30.30 Acetone
30.15 Acetone
29.99 Acetone
29.84 Acetone
29.69 Acetone
29.53 Acetone
29.38 Acetone
23.83



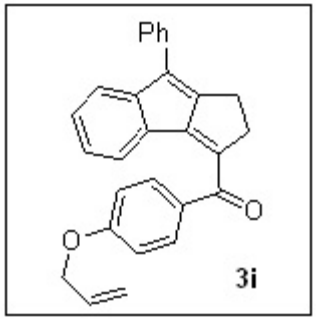
f1 (ppm)

JKG-20180913-241-P1A/10
PROTON CDCl3 {D:\2018-3} ZHL 42

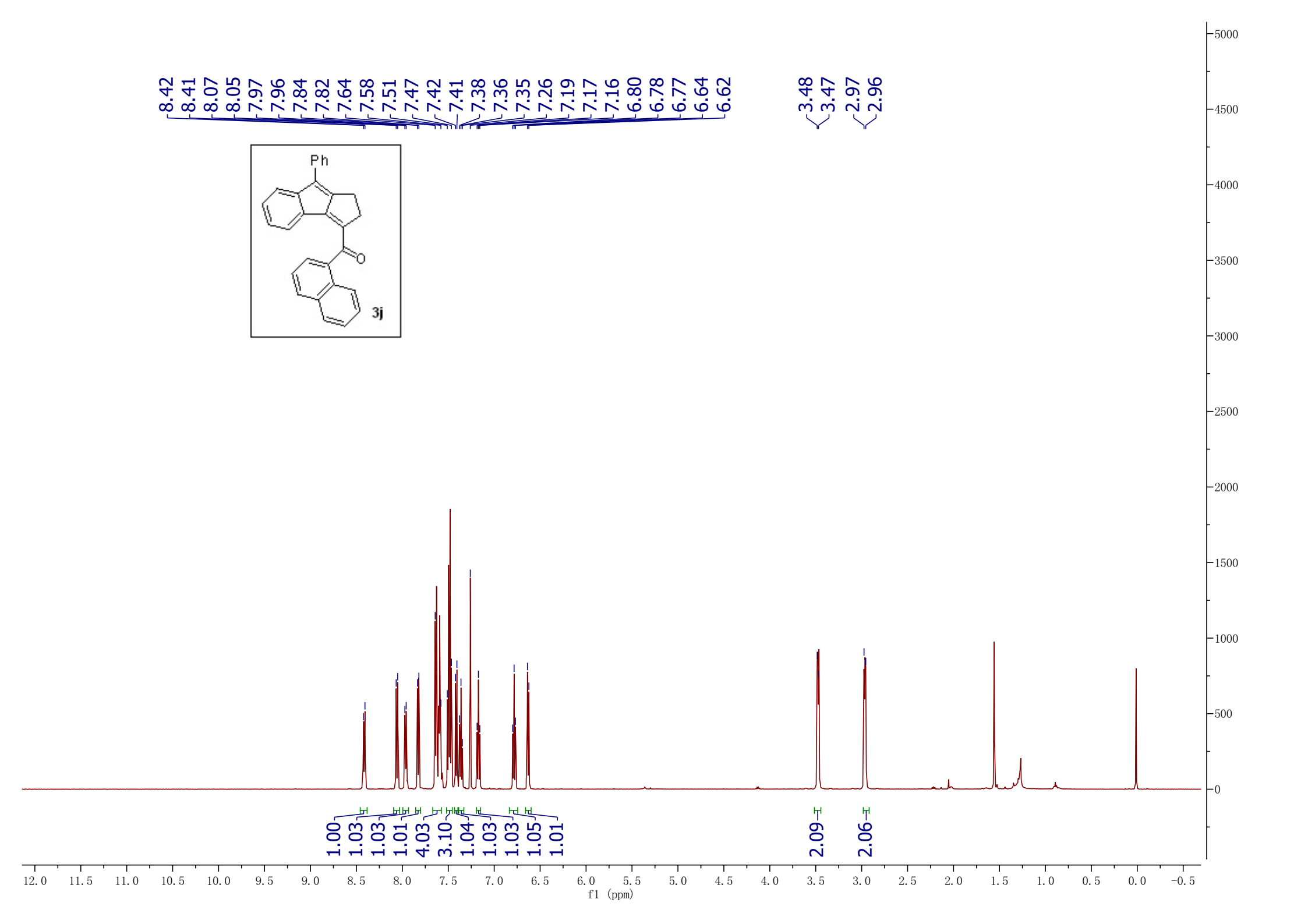


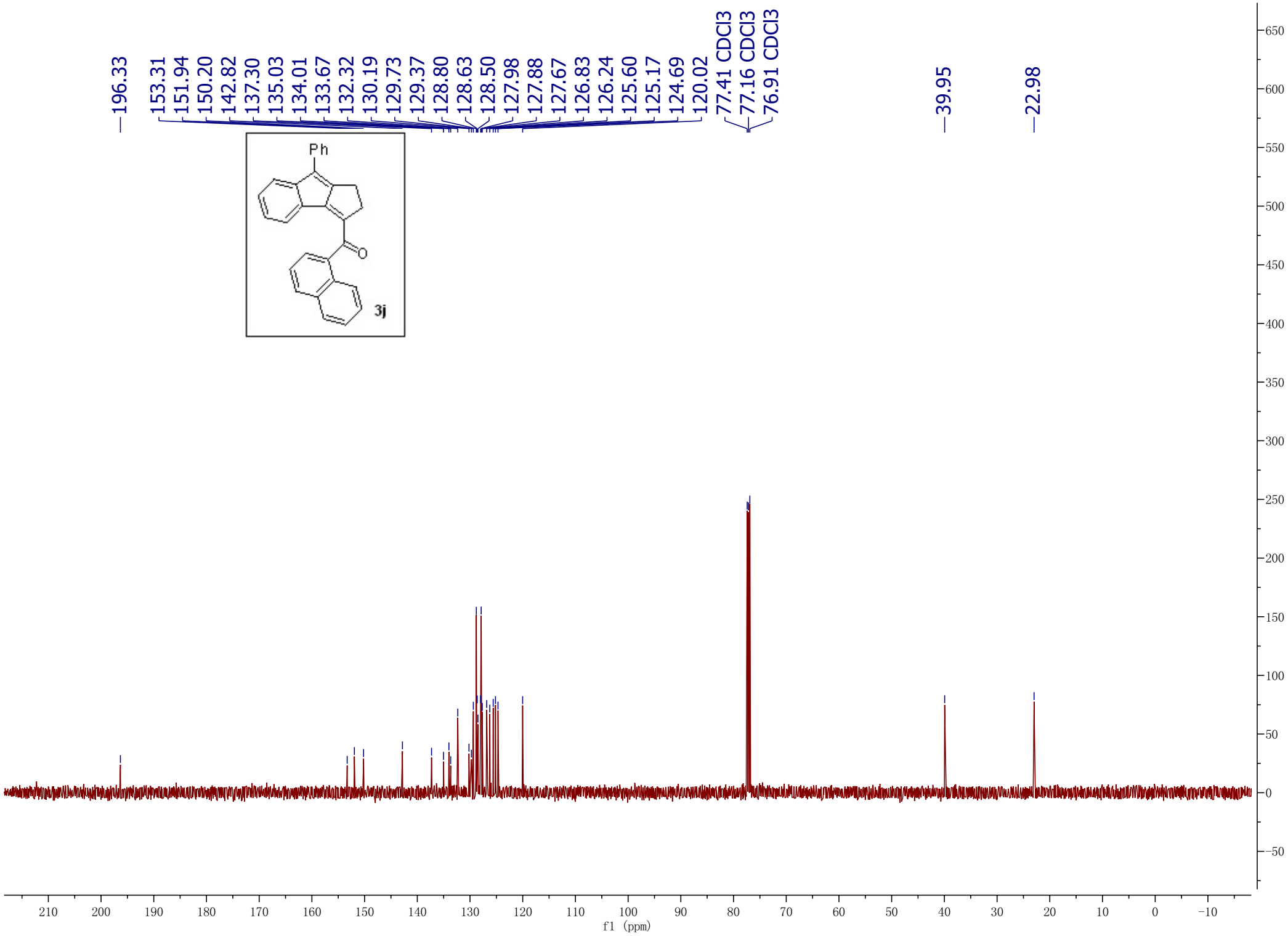
JKG-20180913-241-P1A/11
C13CPD CDCl3 {D:\2018-3} ZHL 42

193.92
163.19
151.91
150.11
149.83
142.77
135.32
132.52
132.05
131.80
130.73
129.67
128.78
128.73
127.86
127.42
125.32
124.10
119.94
118.39
114.96
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
69.10
41.02
23.31

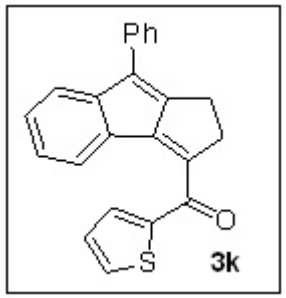


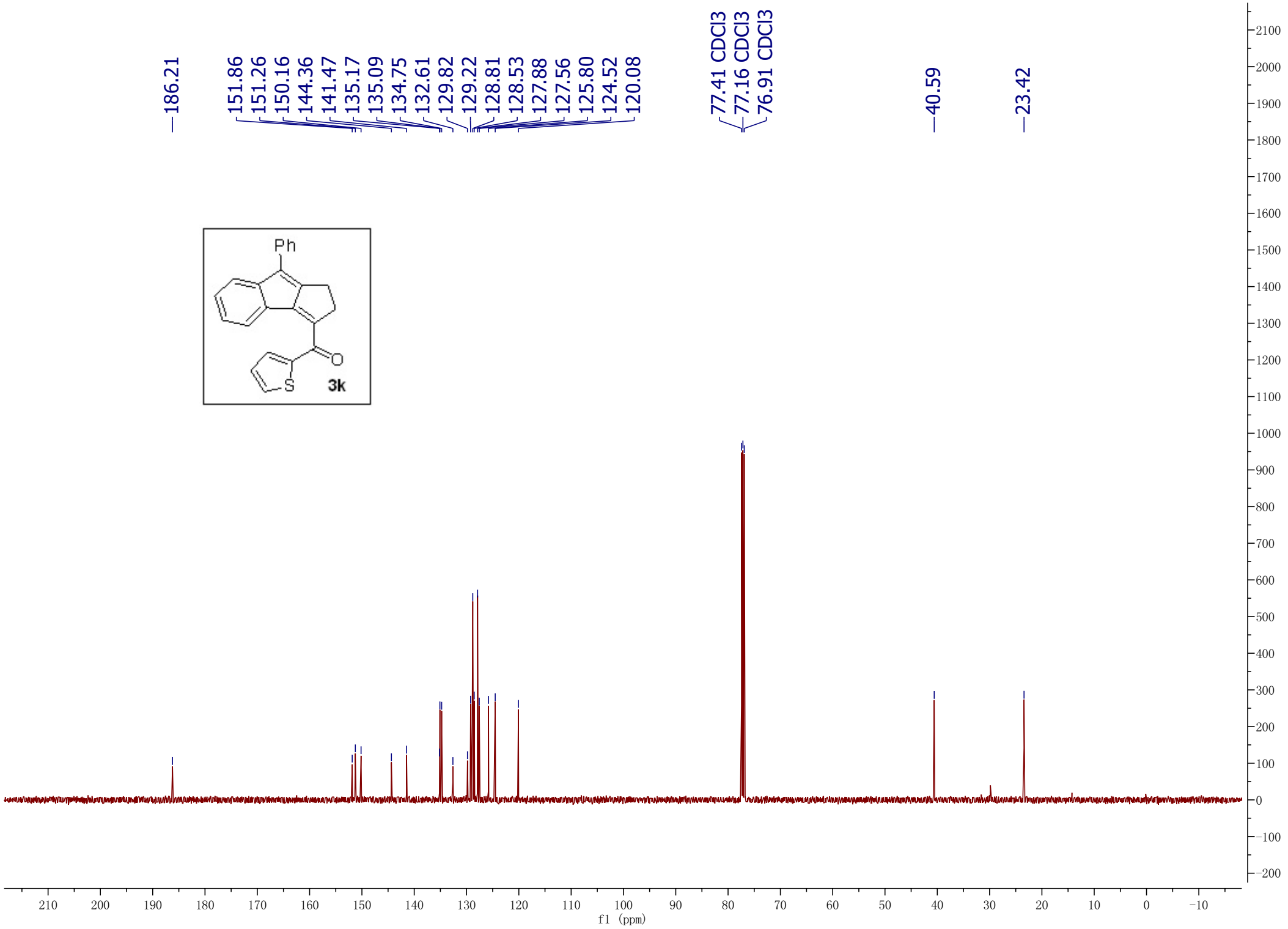
f1 (ppm)

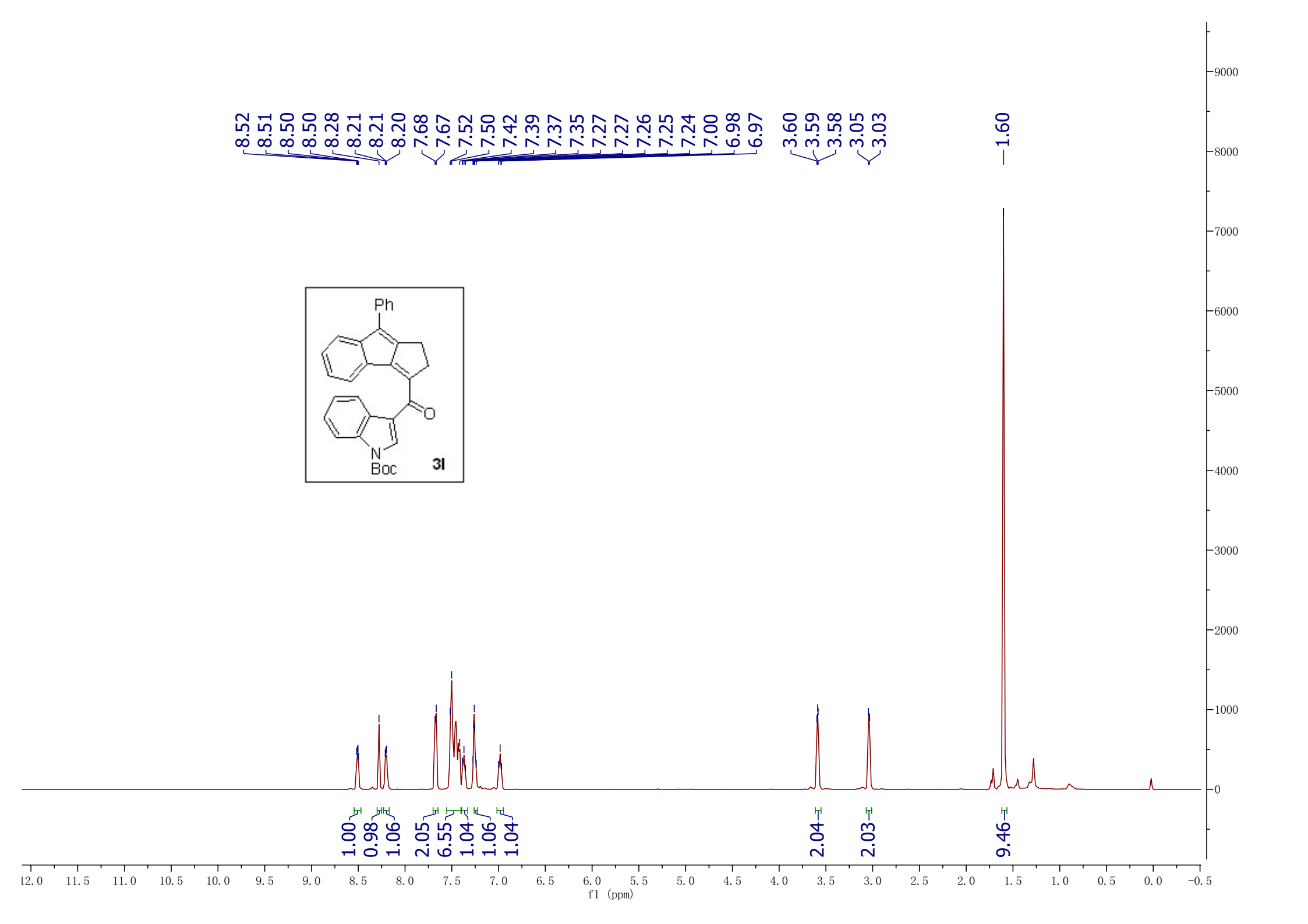

8.42
8.41
8.07
8.05
7.97
7.96
7.84
7.82
7.64
7.58
7.51
7.47
7.42
7.41
7.38
7.36
7.35
7.26
7.19
7.17
7.16
6.80
6.78
6.77
6.64
6.62
3.48
3.47
2.97
2.96
Ph
O
3j
1.00
1.03
1.03
1.01
4.03
3.10
1.04
1.03
1.03
1.05
1.01
2.09
2.06
f1 (ppm)

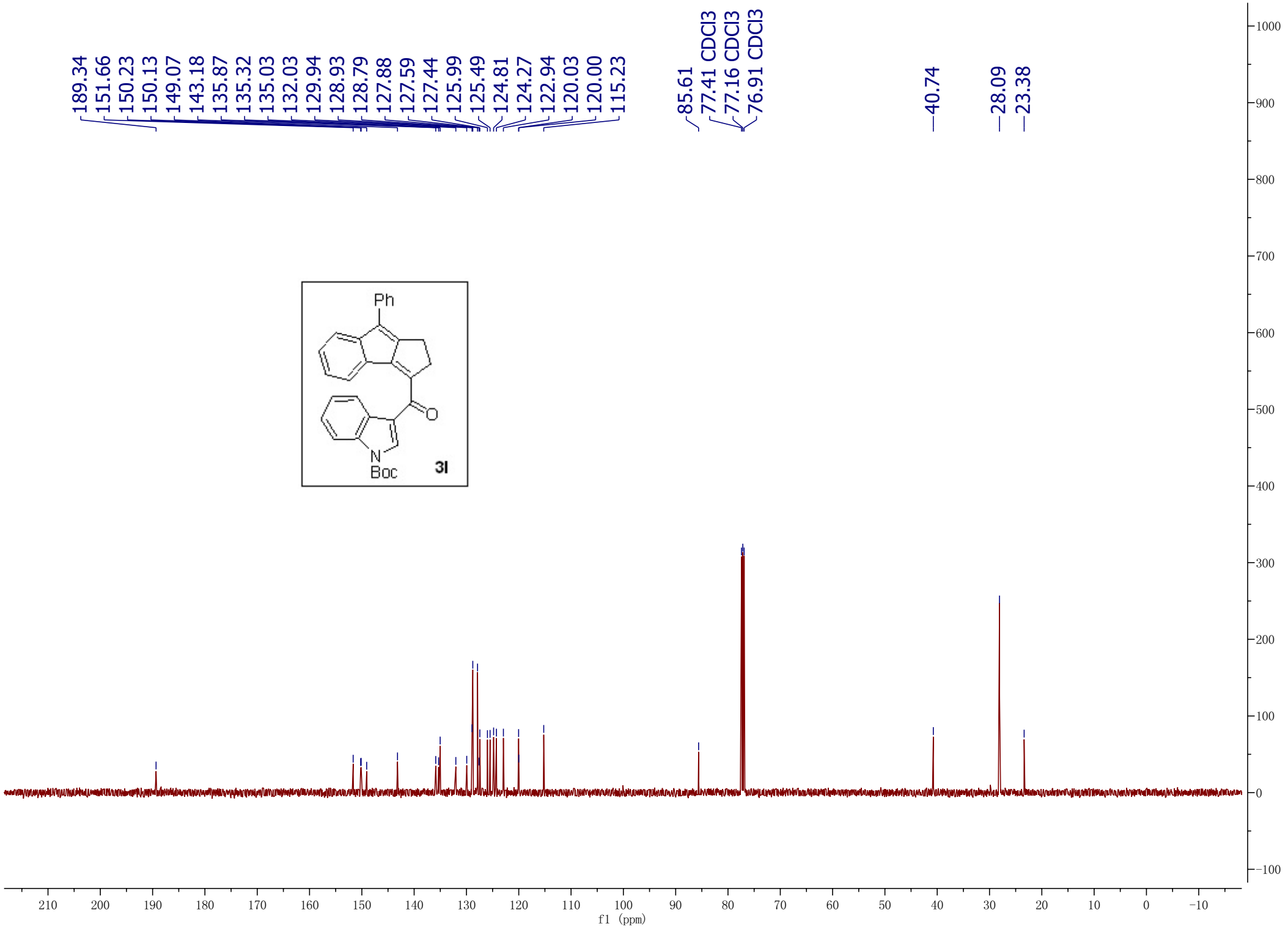

196.33
153.31
151.94
150.20
142.82
137.30
135.03
134.01
133.67
132.32
130.19
129.73
129.37
128.80
128.63
128.50
127.98
127.88
127.67
126.83
126.24
125.60
125.17
124.69
120.02
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
39.95
22.98
Ph
O
3j
650
600
550
500
450
400
350
300
250
200
150
100
50
0
−50
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

237-P8A/10
PROTON CDCl3 {D:\2018-3} ZHL 40

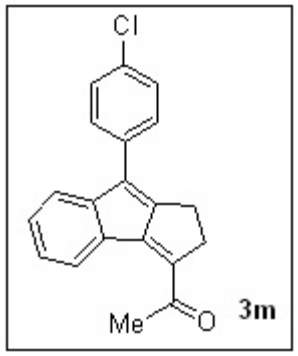



186.21
151.86
151.26
150.16
144.36
141.47
135.17
135.09
134.75
132.61
129.82
129.22
128.81
128.53
127.88
127.56
125.80
124.52
120.08
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
40.59
23.42
Ph
O
S
3k
f1 (ppm)


8.52
8.51
8.50
8.50
8.28
8.21
8.21
8.20
7.68
7.67
7.52
7.50
7.42
7.39
7.37
7.35
7.27
7.27
7.26
7.25
7.24
7.00
6.98
6.97
3.60
3.59
3.58
3.05
3.03
1.60
Ph
O
N
Boc
3l
1.00
0.98
1.06
2.05
6.55
1.04
1.06
1.04
2.04
2.03
9.46
f1 (ppm)


189.34
151.66
150.23
150.13
149.07
143.18
135.87
135.32
135.03
132.03
129.94
128.93
128.79
127.88
127.59
127.44
125.99
125.49
124.81
124.27
122.94
120.03
120.00
115.23
85.61
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
40.74
28.09
23.38
Ph
O
N
Boc
3l
f1 (ppm)

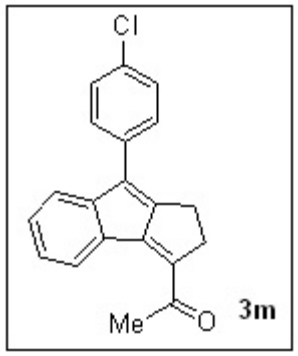
JKG-20180919-242-P3A/10
PROTON CDCl3 {D:\2018-3} ZHL 12



f1 (ppm)

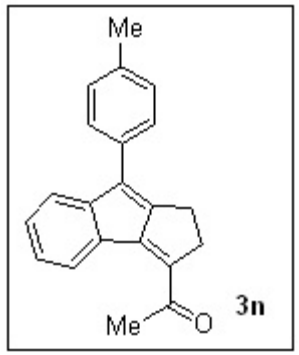
JKG-20180919-242-P3A/11
C13CPD CDCl3 {D:\2018-3} ZHL 12

197.47
153.63
151.38
149.78
140.60
133.53
133.27
132.93
130.06
129.86
129.12
129.01
127.16
125.64
119.87
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
39.30
30.31
23.08



f1 (ppm)

JKG-20180919-241-P3A/10
PROTON CDCl3 {D:\2018-3} ZHL 11



8.45 8.43 7.51 7.50 7.46 7.44 7.32 7.26 7.22 7.20 7.19

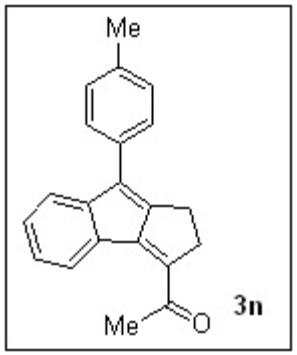
3.33 3.31 2.88 2.87 2.45 2.42

0.98 2.03 1.00 3.00 1.06 2.08 2.08 3.00 3.01

f1 (ppm)

JKG-20180919-241-P3A/11
C13CPD CDCl3 {D:\2018-3} ZHL 11

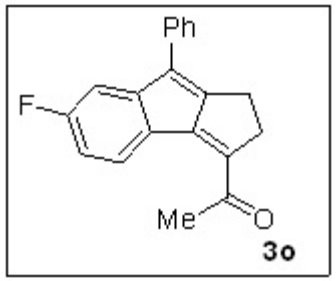
197.50
153.97
150.38
150.26
139.87
137.48
134.06
132.14
130.04
129.92
129.45
127.76
126.98
125.39
120.11
77.41 CDCl3
77.16 CDCl3
76.90 CDCl3
39.22
30.27
23.08
21.50



3n

f1 (ppm)

JKG-20181025-245-P4A/10
PROTON CDCl3 {D:\2018-3} ZHL 11

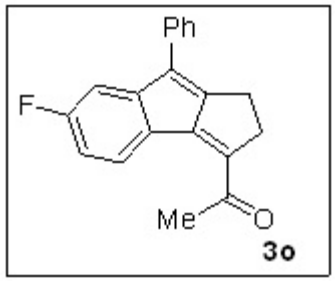


8.44 8.41 7.57 7.56 7.49 7.47 7.46 7.37 7.36 7.35 7.26 7.14 7.14 7.12 7.12 6.88 6.87 6.86 6.86 6.84 6.84 3.37 3.35 2.94 2.92 2.46

0.93 2.06 2.02 1.02 0.99 0.98 2.00 1.99 3.01

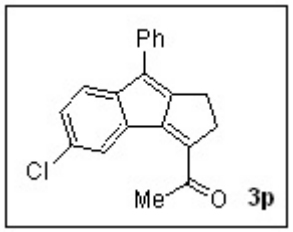
f1 (ppm)

JKG-20181025-245-P4A/11
C13CPD CDCl3 {D:\2018-3} ZHL 11



f1 (ppm)

JKG-20181025-248-P2A/10
PROTON CDCl3 {D:\2018-3} ZHL 12



8.45 8.43 7.57 7.57 7.56 7.48 7.47 7.41 7.37 7.34 7.33 7.31 7.26 7.24 7.22 7.21

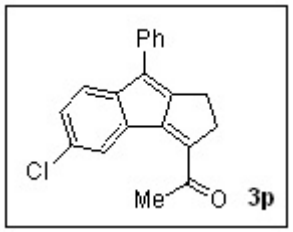
3.38 3.36 2.91 2.89 2.48

0.99 0.98 1.02 2.21 2.00 1.01 2.00 2.00 3.09

f1 (ppm)

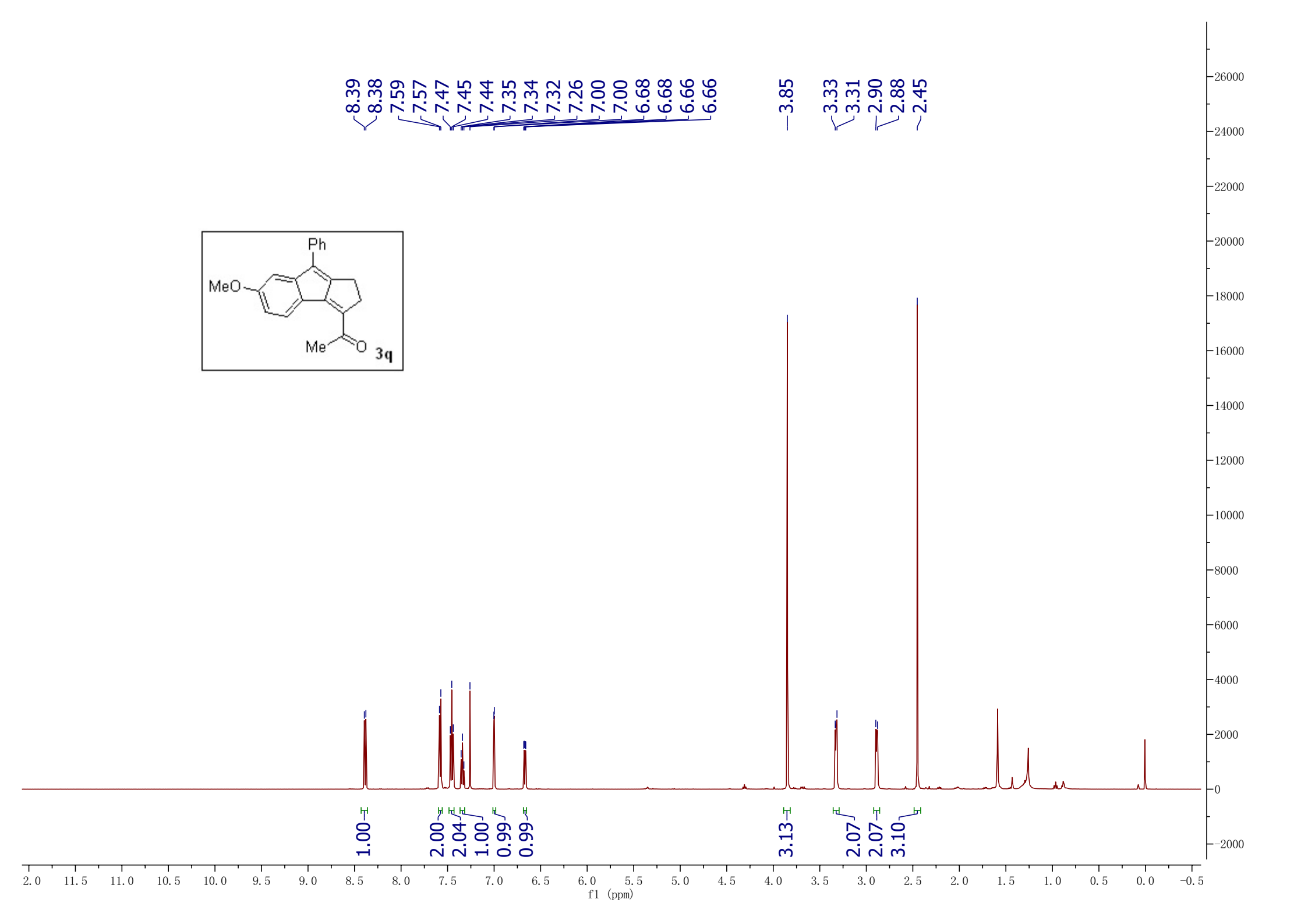
JKG-20181025-248-P2A/11
C13CPD CDCl3 {D:\2018-3} ZHL 12

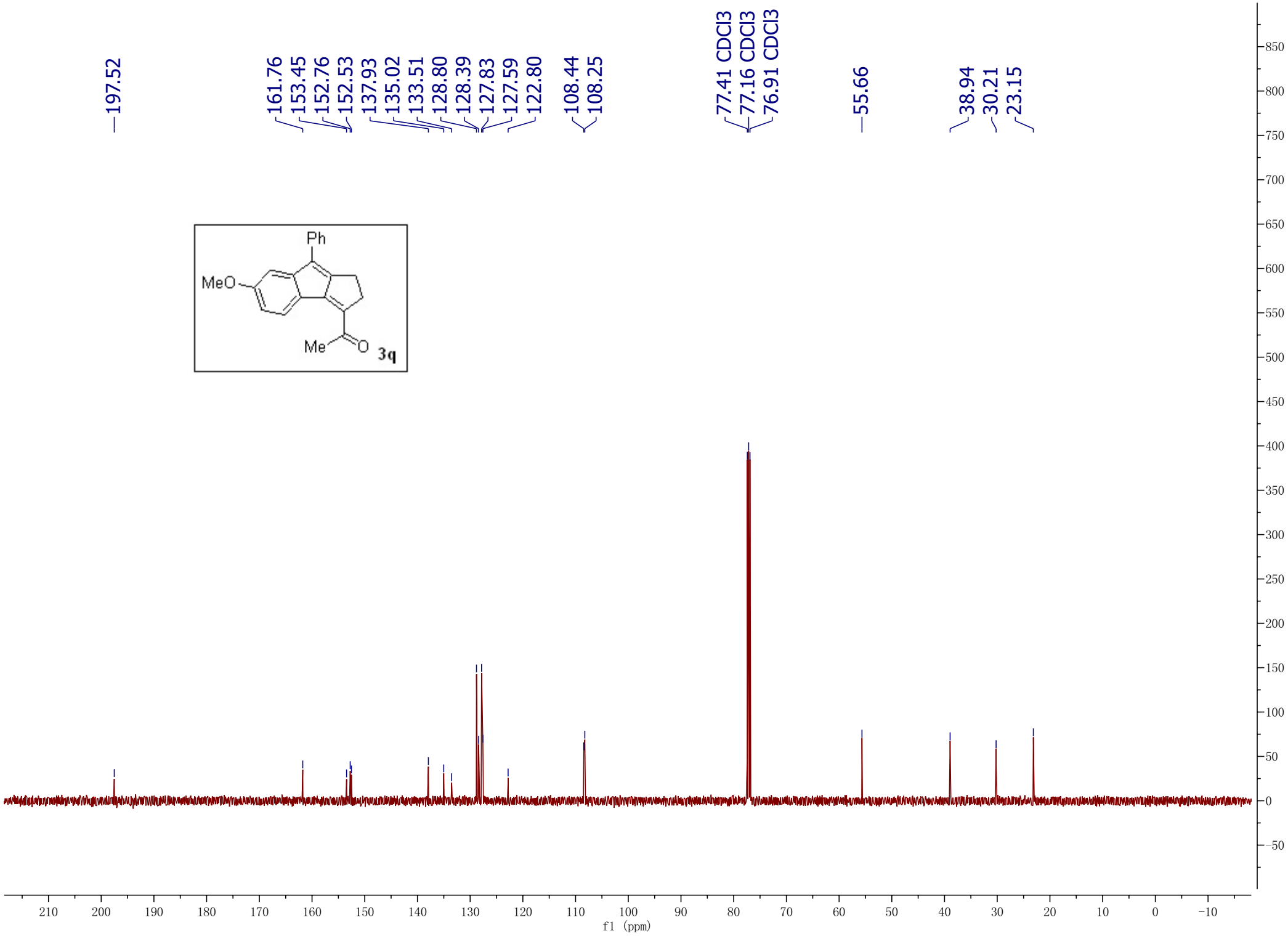
197.50
153.53
151.93
149.64
140.90
136.92
134.74
132.69
130.11
130.05
129.76
127.80
127.63
127.18
125.97
125.68
119.90
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
39.32
30.34
23.09



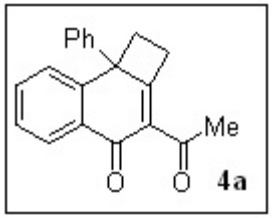
3p

f1 (ppm)


8.39
8.38
7.59
7.57
7.47
7.45
7.44
7.35
7.34
7.32
7.26
7.00
7.00
6.68
6.68
6.66
6.66
3.85
3.33
3.31
2.90
2.88
2.45
Ph
MeO
Me
O
3q
1.00
2.00
2.04
1.00
0.99
0.99
3.13
2.07
2.07
3.10
f1 (ppm)


197.52
161.76
153.45
152.76
152.53
137.93
135.02
133.51
128.80
128.39
127.83
127.59
122.80
108.44
108.25
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
55.66
38.94
30.21
23.15
Ph
MeO
Me
O
3q
f1 (ppm)

JKG-20181010-218-P5A/10
PROTON CDCl3 {D:\2018-3} ZHL 24



8.08 8.06 7.44 7.43 7.42 7.41 7.41 7.38 7.35 7.34 7.28 7.23 7.21 7.20

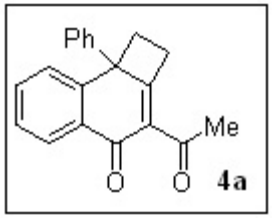
3.42 3.35 3.33 3.33 3.28 3.22 3.18 2.58 2.55 2.50

0.92 1.02 6.00 1.00 1.00 1.03 1.01 3.01 0.96

f1 (ppm)

JKG-20180118-218-P4/10C
C13CPD CDCl3 {D:\2018-1} ZHL 40

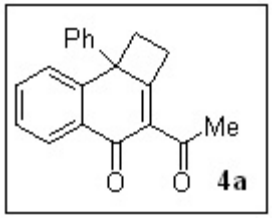
197.38
184.72
176.03
147.17
142.04
133.01
132.48
130.93
129.30
127.69
127.56
127.34
126.22
125.14
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
57.88
34.81
31.27
29.46



4a

f1 (ppm)

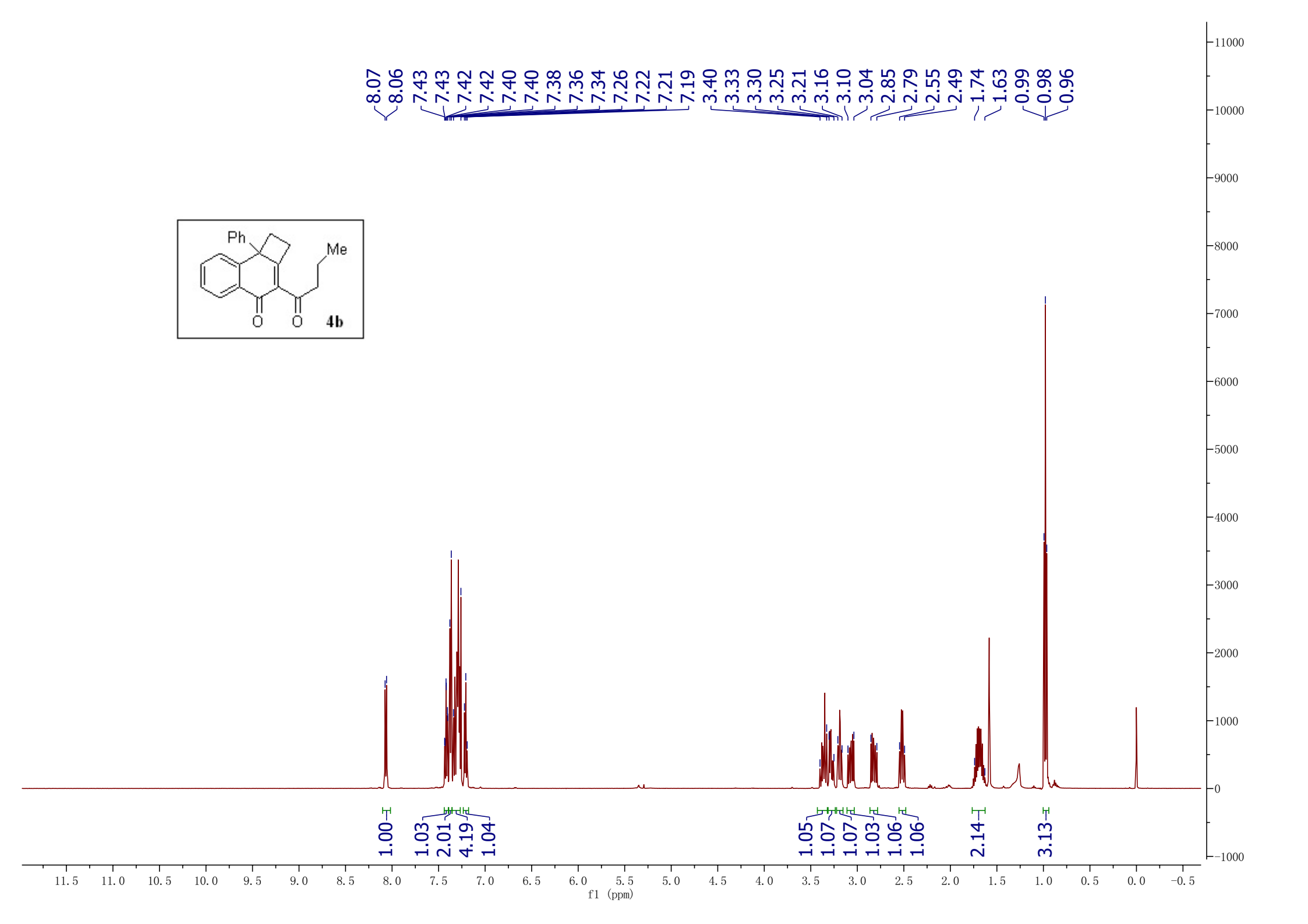
218-P4/DEPT135
C13DEPT135 CDC13 {D:\2018-1} ZHL 24

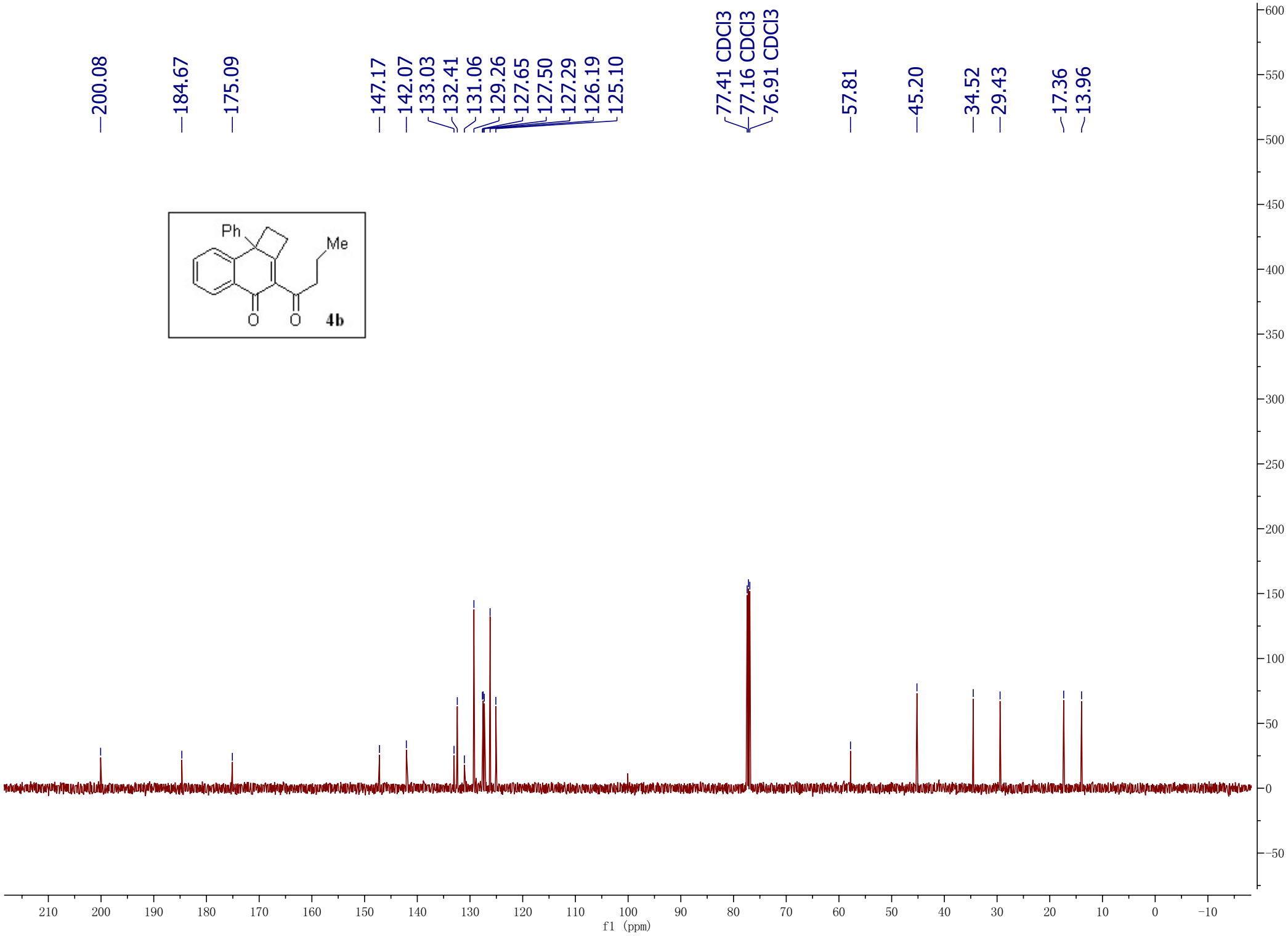


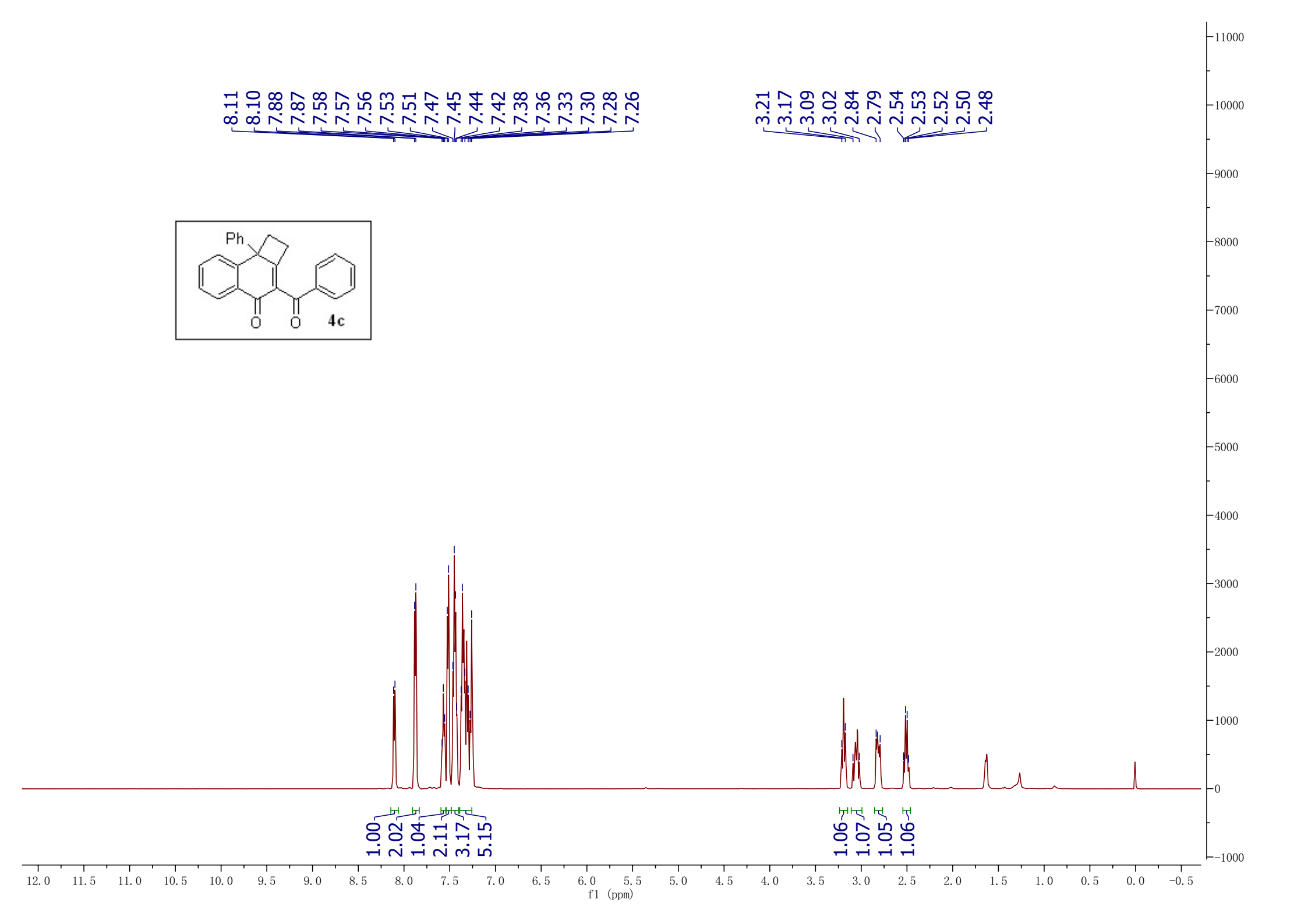
700
600
500
400
300
200
100
0
-100
-200
-300
-400
-500

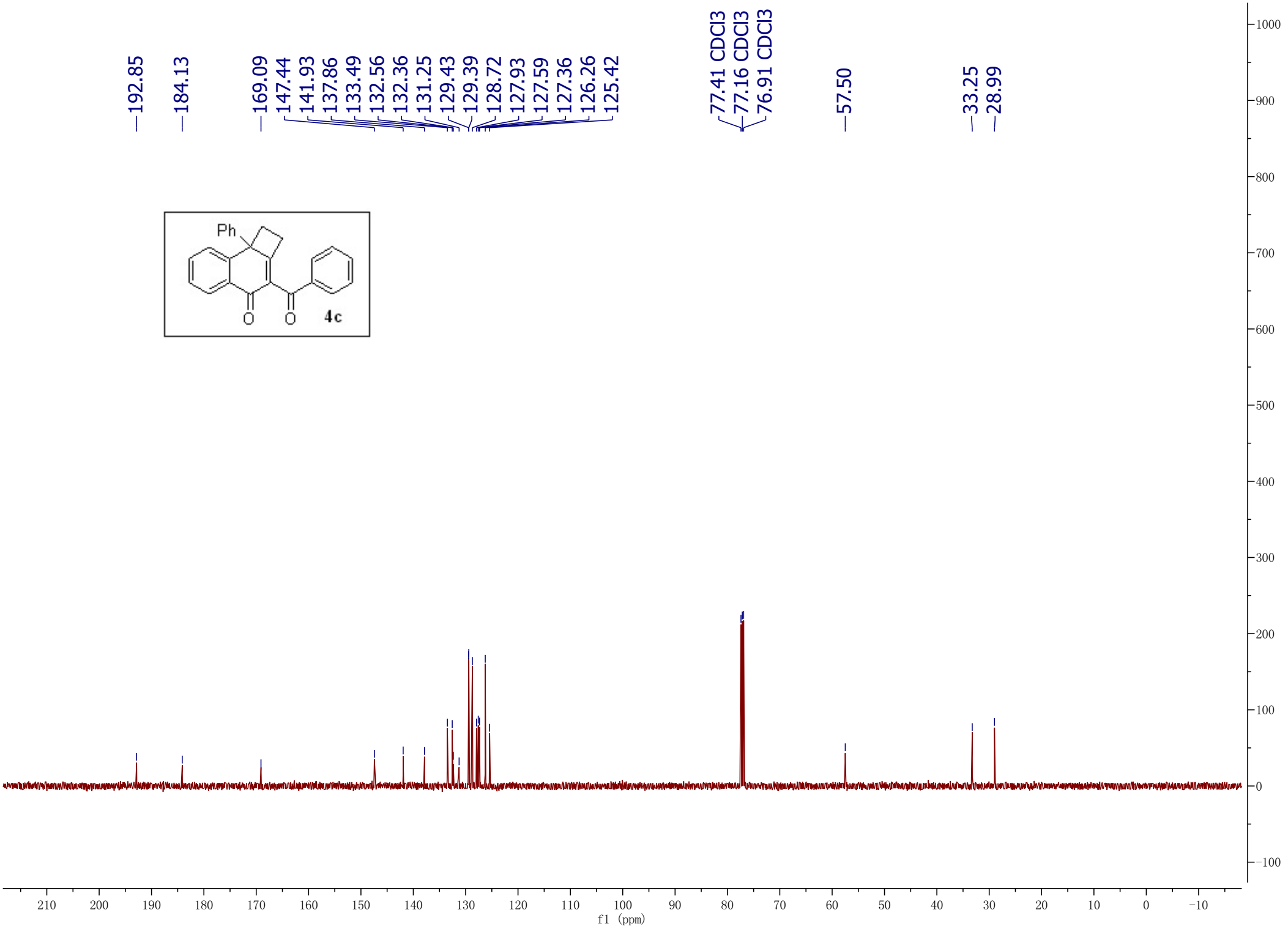
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

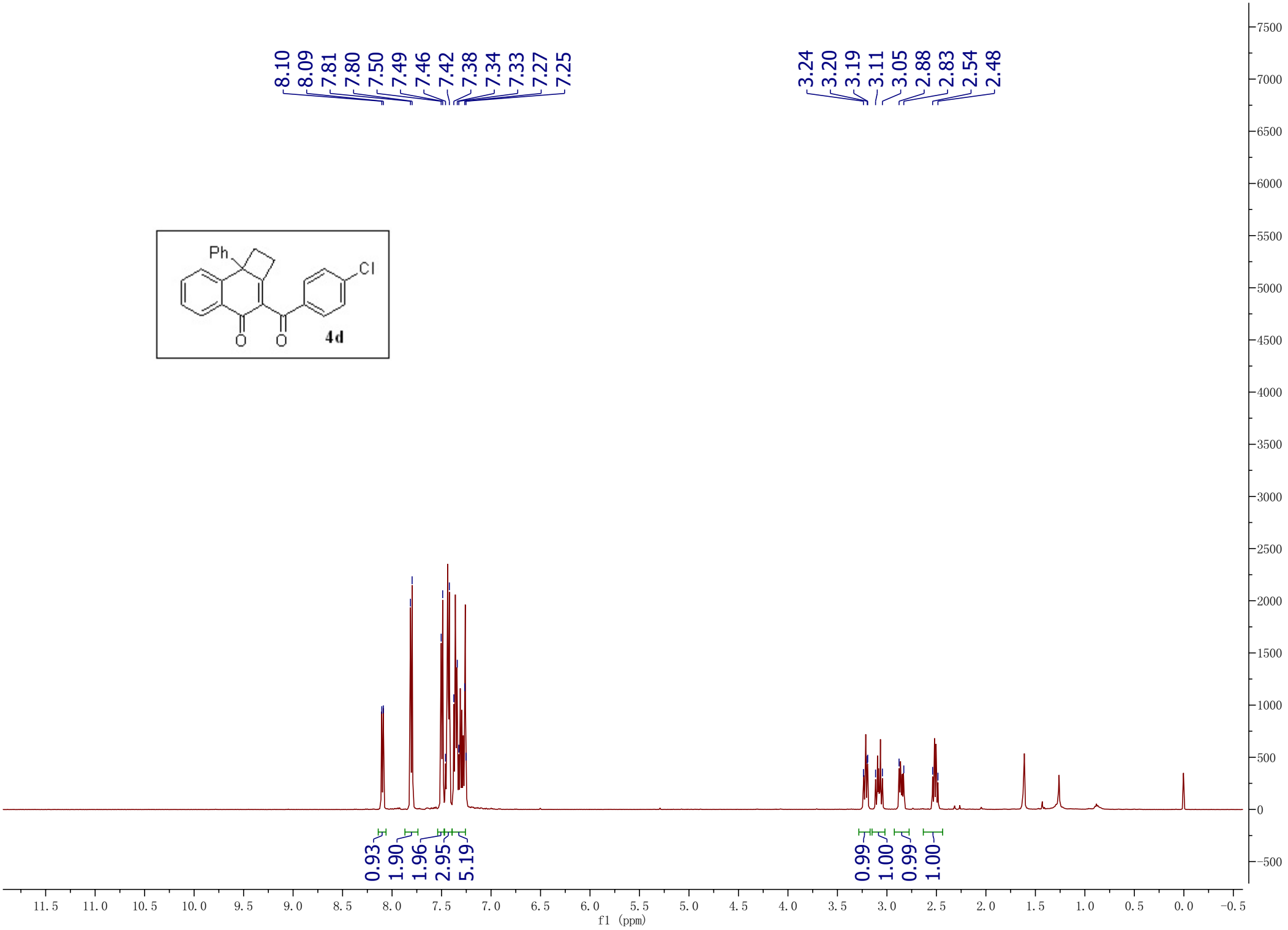
f1 (ppm)

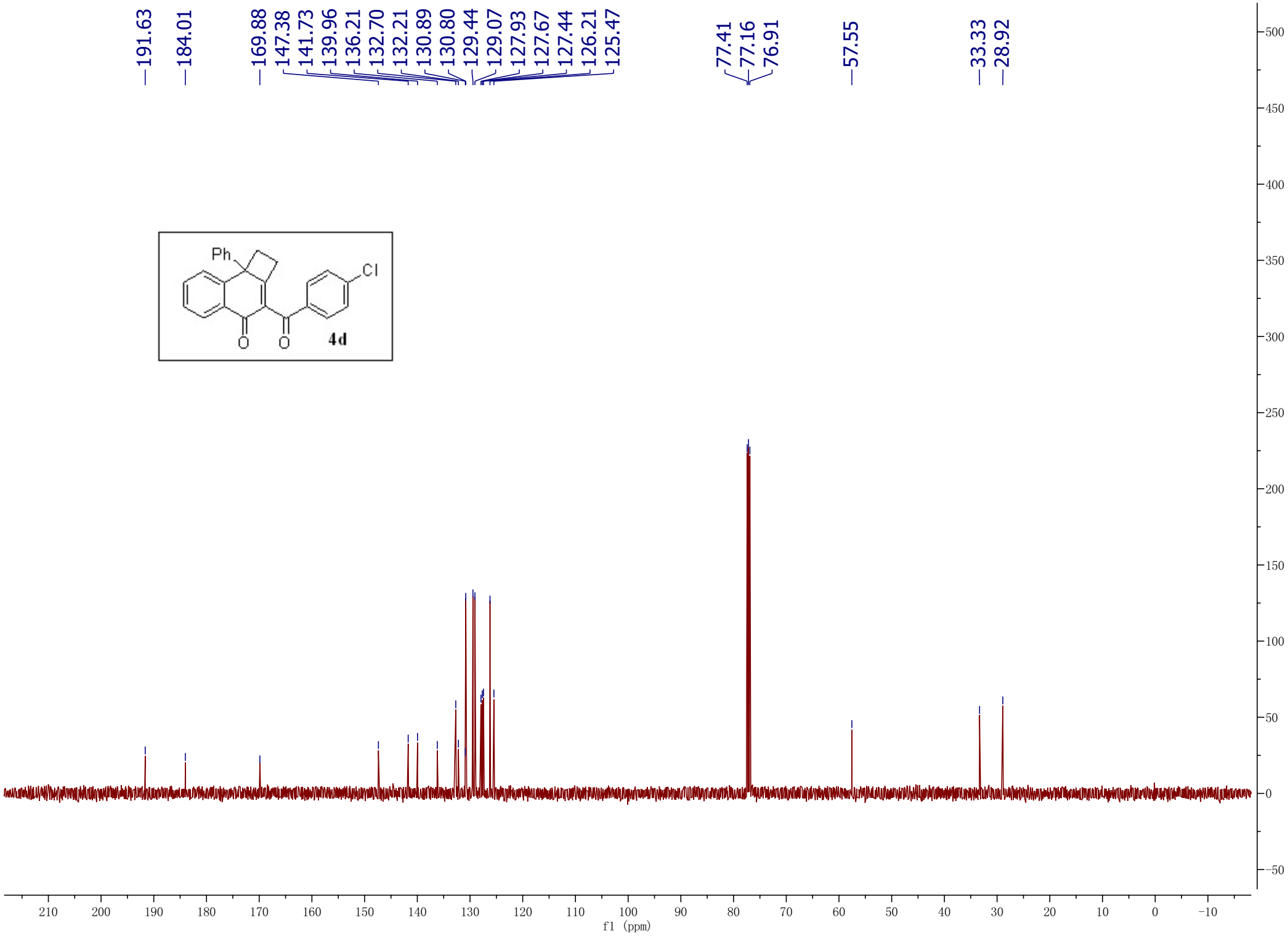

8.07
8.06
7.43
7.43
7.42
7.42
7.40
7.40
7.38
7.36
7.34
7.26
7.22
7.21
7.19
3.40
3.33
3.30
3.25
3.21
3.16
3.10
3.04
2.85
2.79
2.55
2.49
1.74
1.63
0.99
0.98
0.96
Ph
Me
O
O
4b
1.00
1.03
2.01
4.19
1.04
1.05
1.07
1.07
1.03
1.06
1.06
2.14
3.13
f1 (ppm)

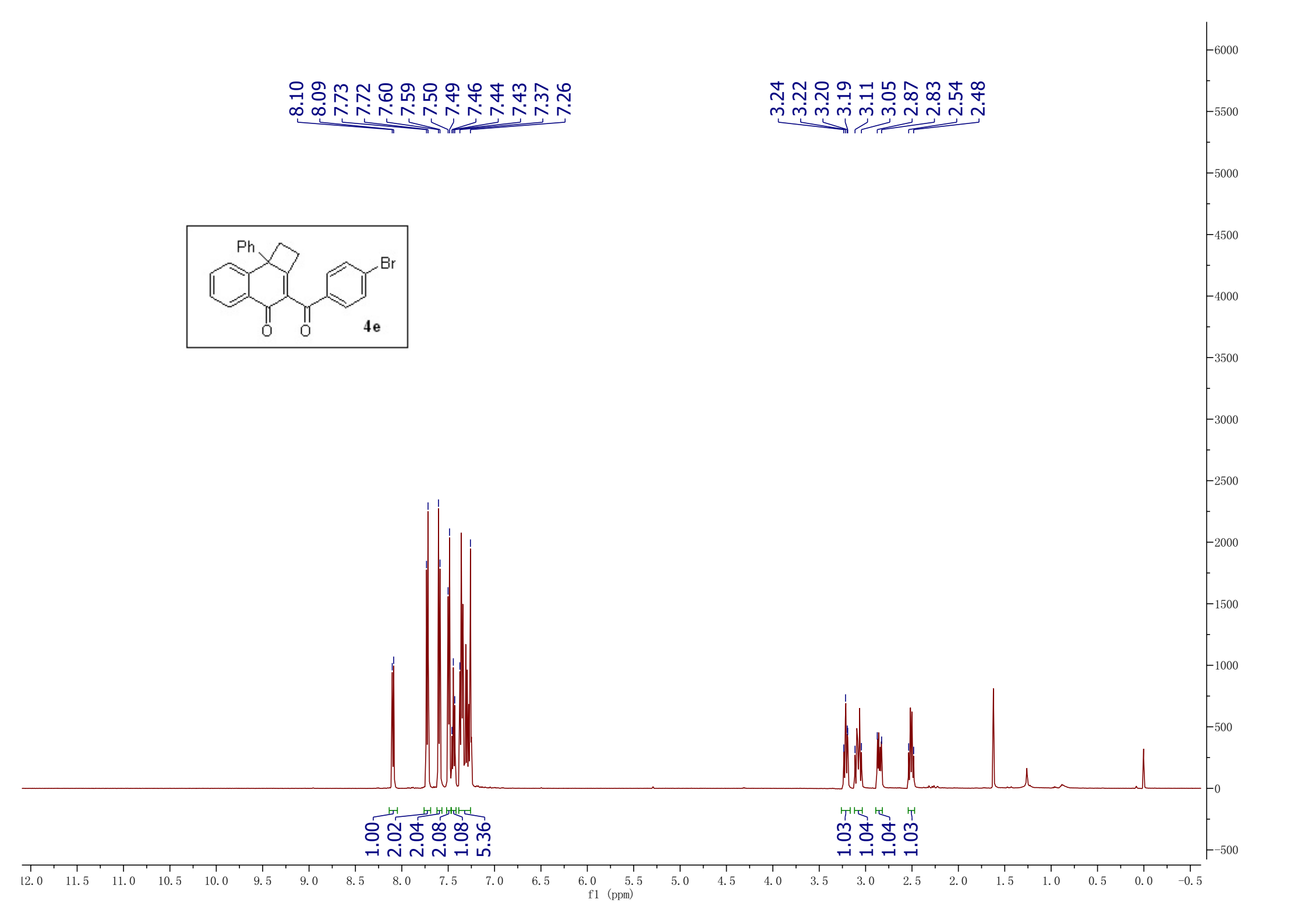

200.08
184.67
175.09
147.17
142.07
133.03
132.41
131.06
129.26
127.65
127.50
127.29
126.19
125.10
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
57.81
45.20
34.52
29.43
17.36
13.96
Ph
Me
O
O
4b
f1 (ppm)

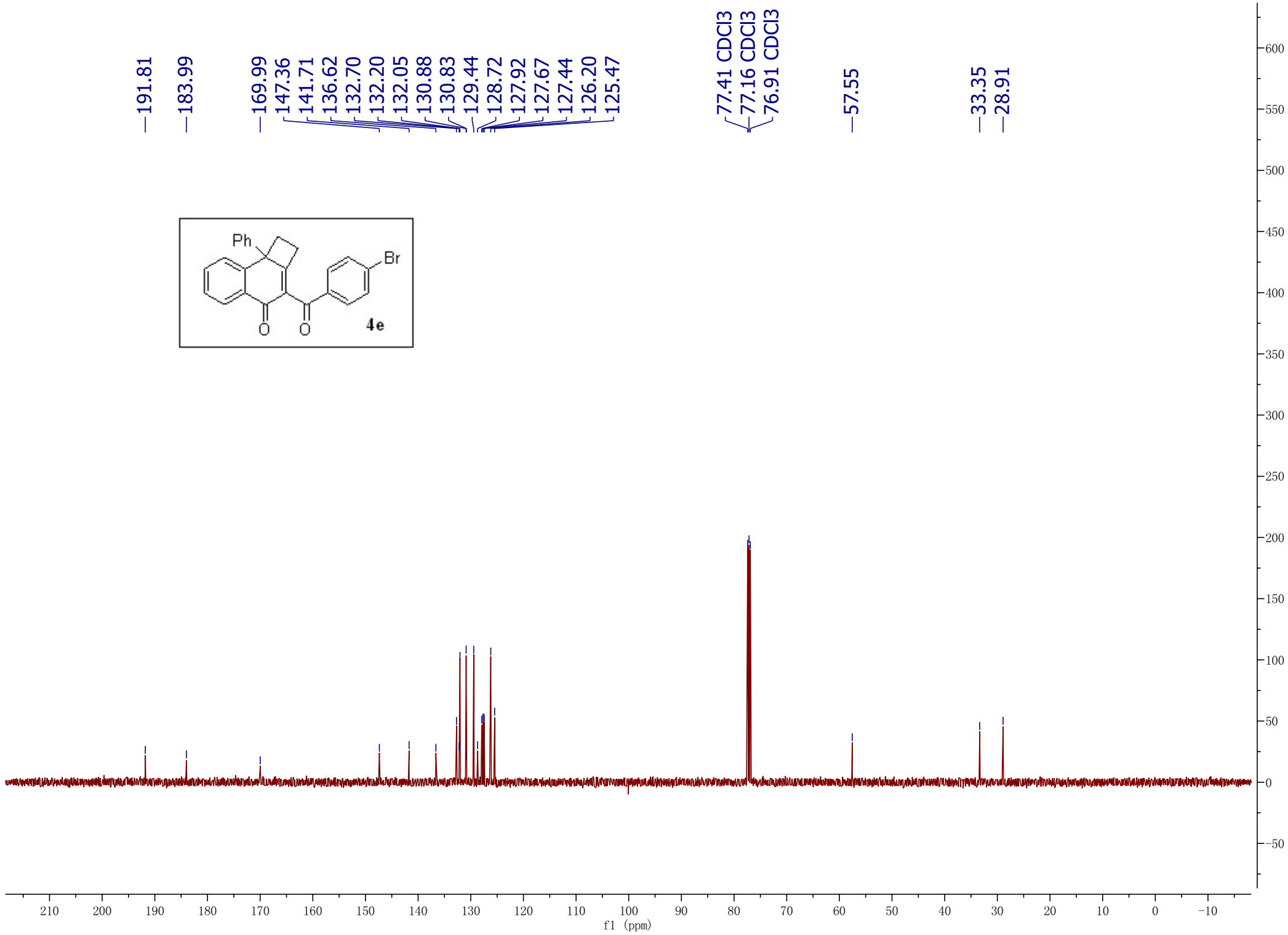

8.11
8.10
7.88
7.87
7.58
7.57
7.56
7.53
7.51
7.47
7.45
7.44
7.42
7.38
7.36
7.33
7.30
7.28
7.26
3.21
3.17
3.09
3.02
2.84
2.79
2.54
2.53
2.52
2.50
2.48
Ph
O
O
4c
1.00
2.02
1.04
2.11
3.17
5.15
1.06
1.07
1.05
1.06
f1 (ppm)

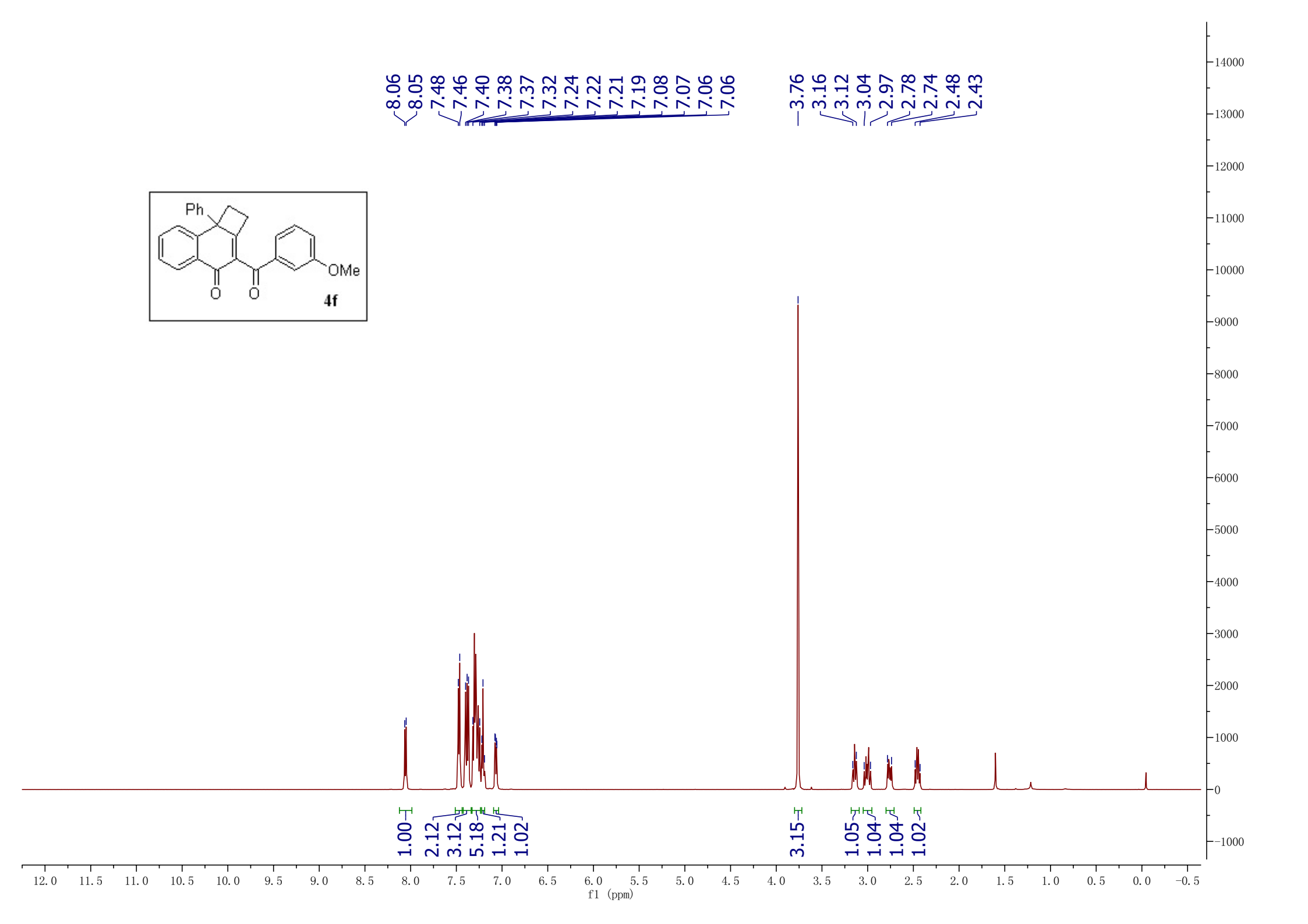

192.85
184.13
169.09
147.44
141.93
137.86
133.49
132.56
132.36
131.25
129.43
129.39
128.72
127.93
127.59
127.36
126.26
125.42
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
57.50
33.25
28.99
Ph
O
O
4c
f1 (ppm)

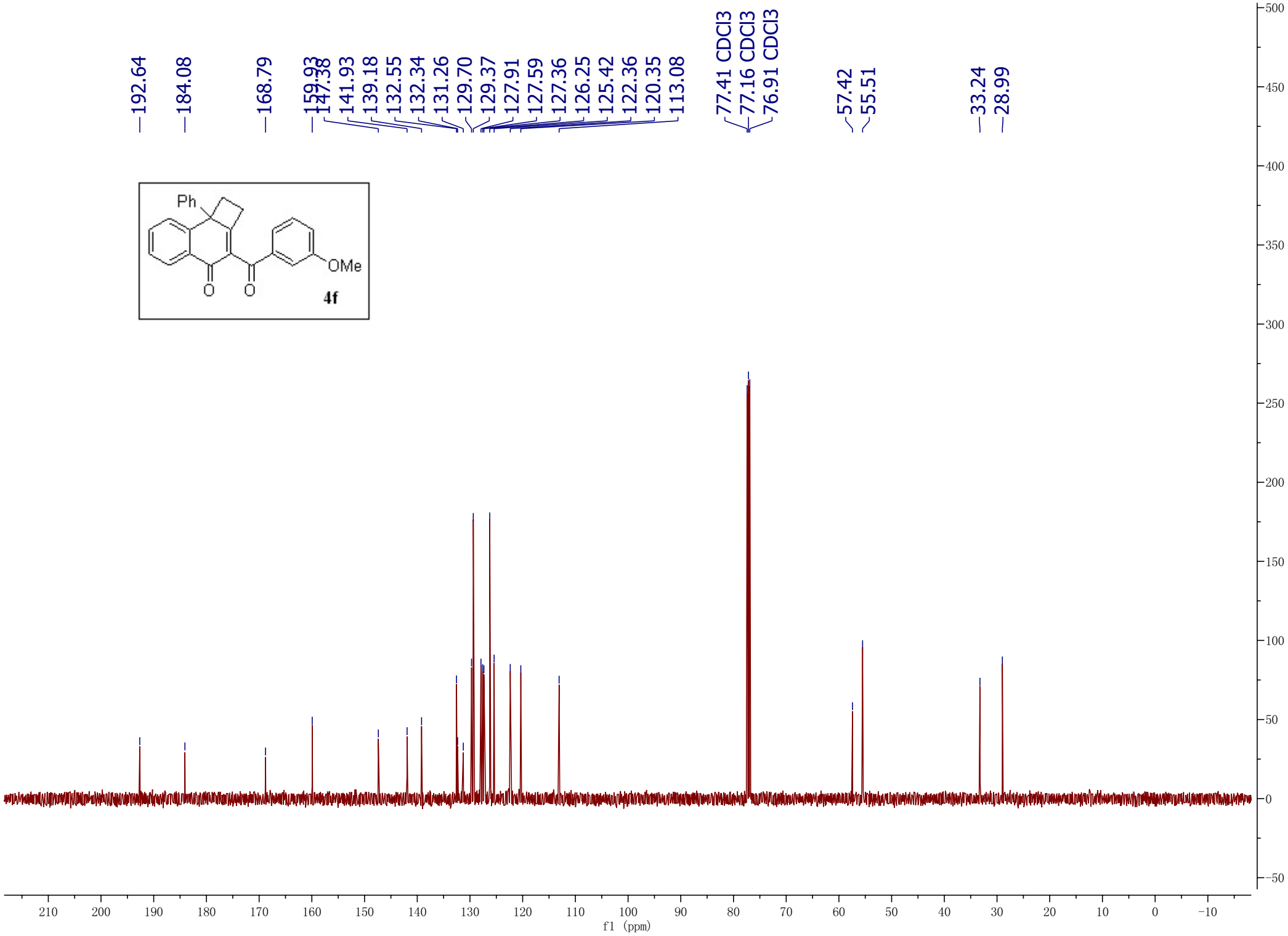

8.10
8.09
7.81
7.80
7.50
7.49
7.46
7.42
7.38
7.34
7.33
7.27
7.25
3.24
3.20
3.19
3.11
3.05
2.88
2.83
2.54
2.48
Ph
Cl
O
O
4d
0.93
1.90
1.96
2.95
5.19
0.99
1.00
0.99
1.00
f1 (ppm)

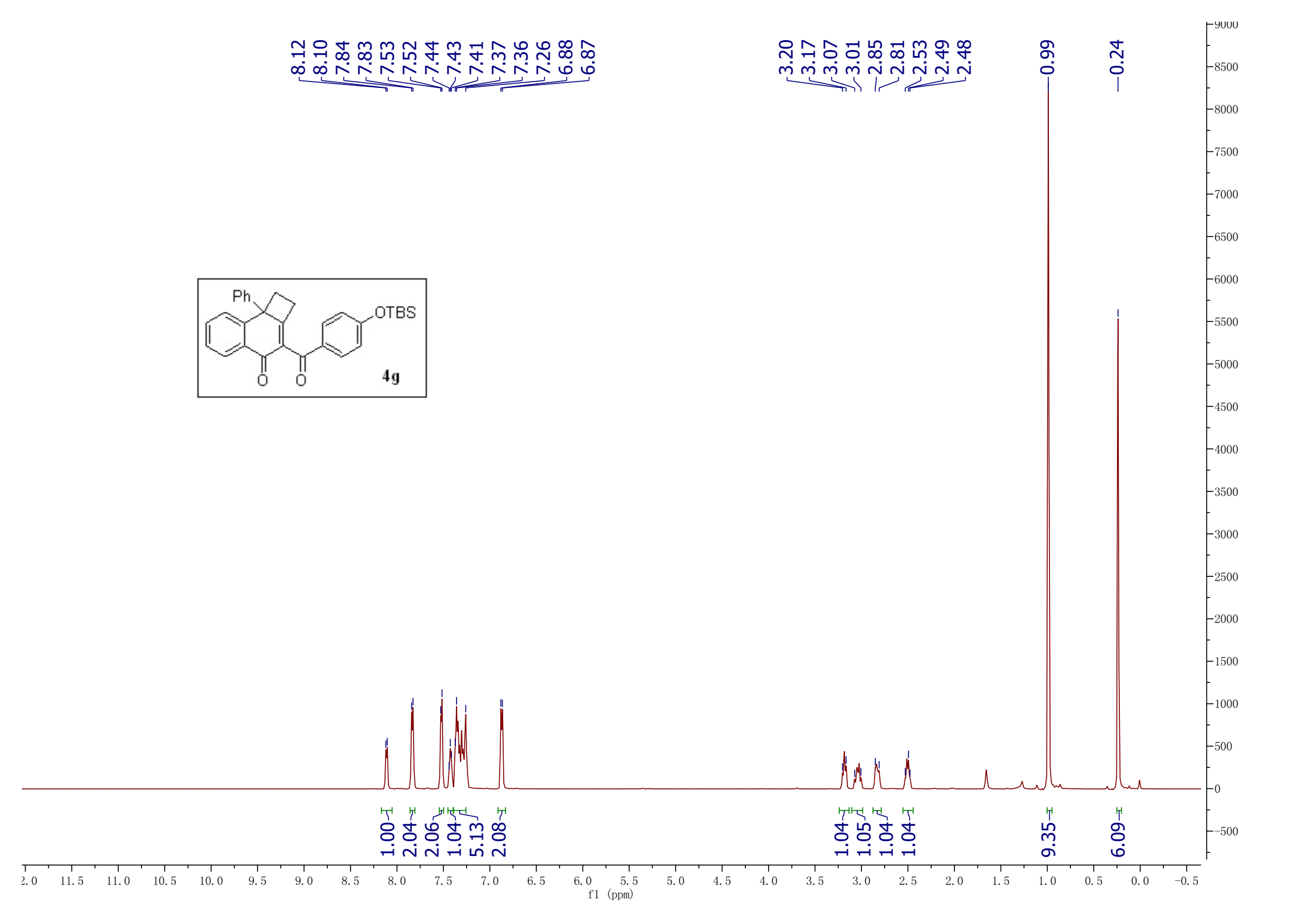

191.63
184.01
169.88
147.38
141.73
139.96
136.21
132.70
132.21
130.89
130.80
129.44
129.07
127.93
127.67
127.44
126.21
125.47
77.41
77.16
76.91
57.55
33.33
28.92
Ph
Cl
O
O
4d
f1 (ppm)

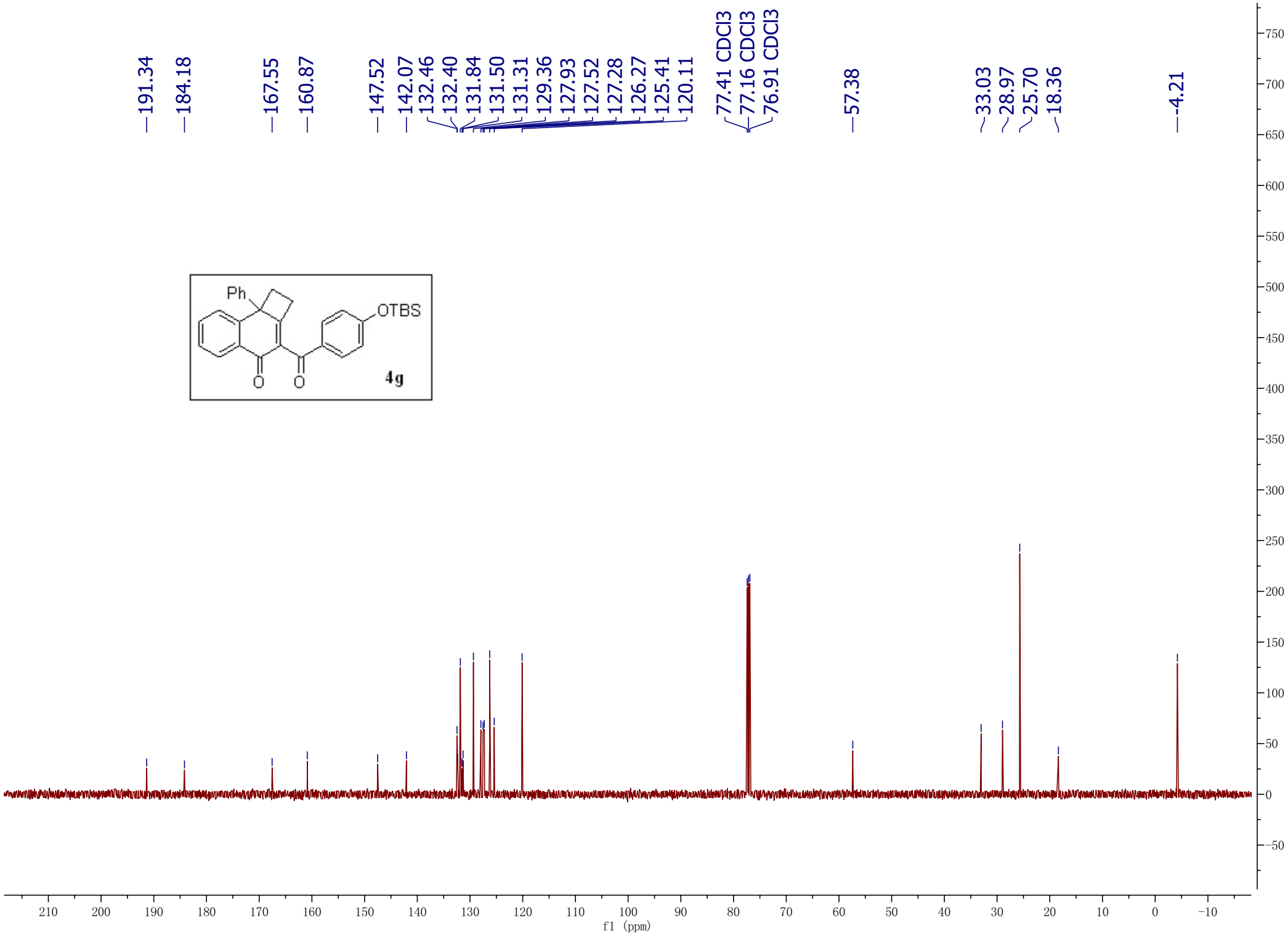

8.10
8.09
7.73
7.72
7.60
7.59
7.50
7.49
7.46
7.44
7.43
7.37
7.26
3.24
3.22
3.20
3.19
3.11
3.05
2.87
2.83
2.54
2.48
Ph
Br
O
O
4e
1.00
2.02
2.04
2.08
1.08
5.36
1.03
1.04
1.04
1.03
f1 (ppm)


191.81
183.99
169.99
147.36
141.71
136.62
132.70
132.20
132.05
130.88
130.83
129.44
128.72
127.92
127.67
127.44
126.20
125.47
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
57.55
33.35
28.91
Ph
Br
O
O
4e
600
550
500
450
400
350
300
250
200
150
100
50
0
−50
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

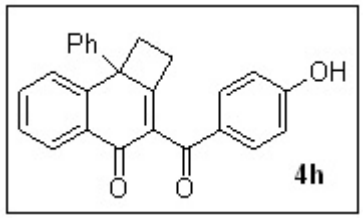

8.06
8.05
7.48
7.46
7.40
7.38
7.37
7.32
7.24
7.22
7.21
7.19
7.08
7.07
7.06
7.06
3.76
3.16
3.12
3.04
2.97
2.78
2.74
2.48
2.43
Ph
OMe
O
O
4f
1.00
2.12
3.12
5.18
1.21
1.02
3.15
1.05
1.04
1.04
1.02
f1 (ppm)


192.64
184.08
168.79
159.93
147.38
141.93
139.18
132.55
132.34
131.26
129.70
129.37
127.91
127.59
127.36
126.25
125.42
122.36
120.35
113.08
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
57.42
55.51
33.24
28.99
Ph
OMe
O
O
4f
f1 (ppm)


8.12
8.10
7.84
7.83
7.53
7.52
7.44
7.43
7.41
7.37
7.36
7.26
6.88
6.87
3.20
3.17
3.07
3.01
2.85
2.81
2.53
2.49
2.48
0.99
0.24
Ph
OTBS
O
O
4g
1.00
2.04
2.06
1.04
5.13
2.08
1.04
1.05
1.04
1.04
9.35
6.09
f1 (ppm)

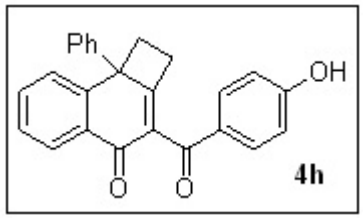

191.34
184.18
167.55
160.87
147.52
142.07
132.46
132.40
131.84
131.50
131.31
129.36
127.93
127.52
127.28
126.27
125.41
120.11
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
57.38
33.03
28.97
25.70
18.36
-4.21
Ph
OTBS
O
O
4g
f1 (ppm)

JKG-20181102-249-P8/10
PROTON DMSO {D:\2018-3} ZHL 4

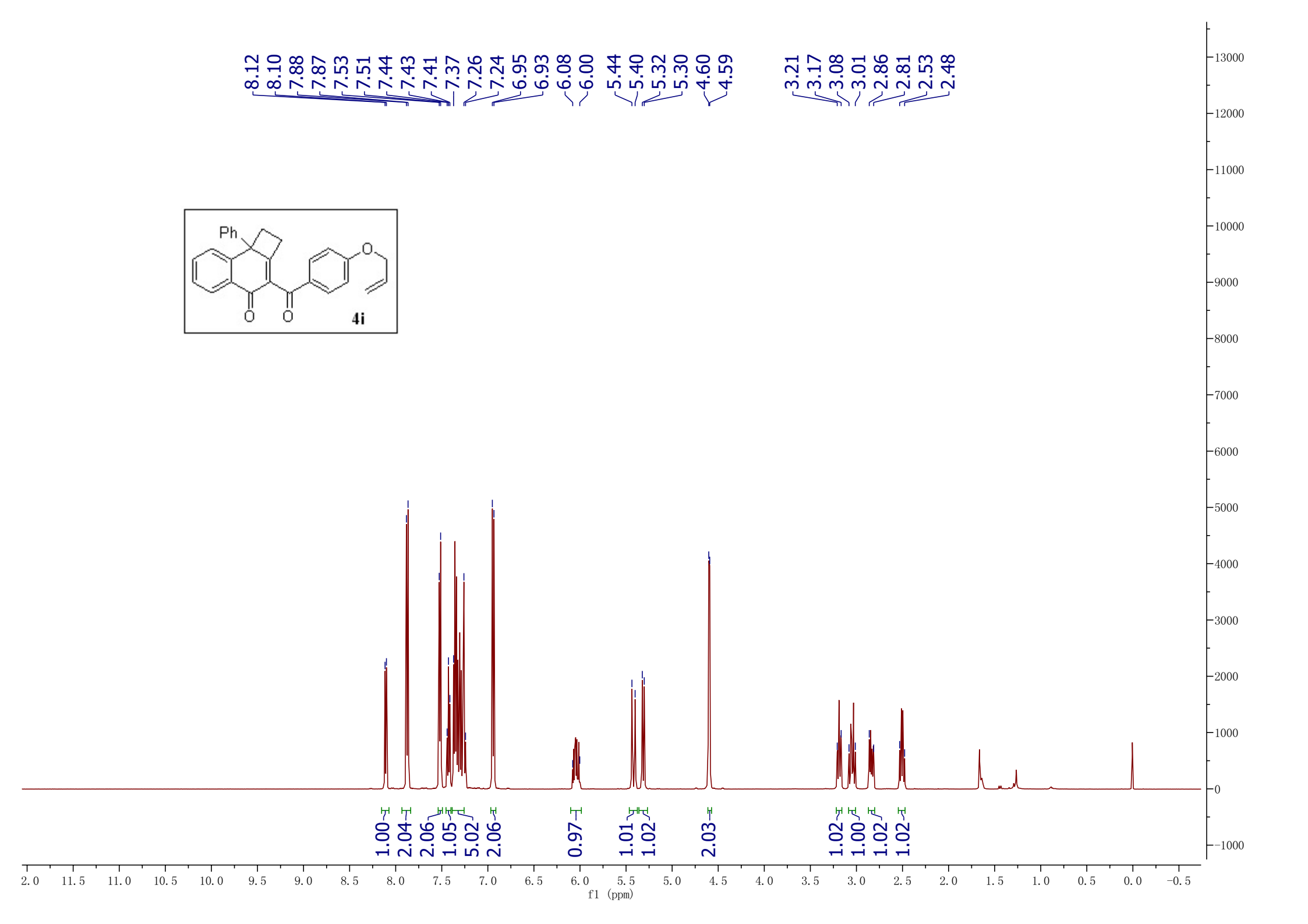


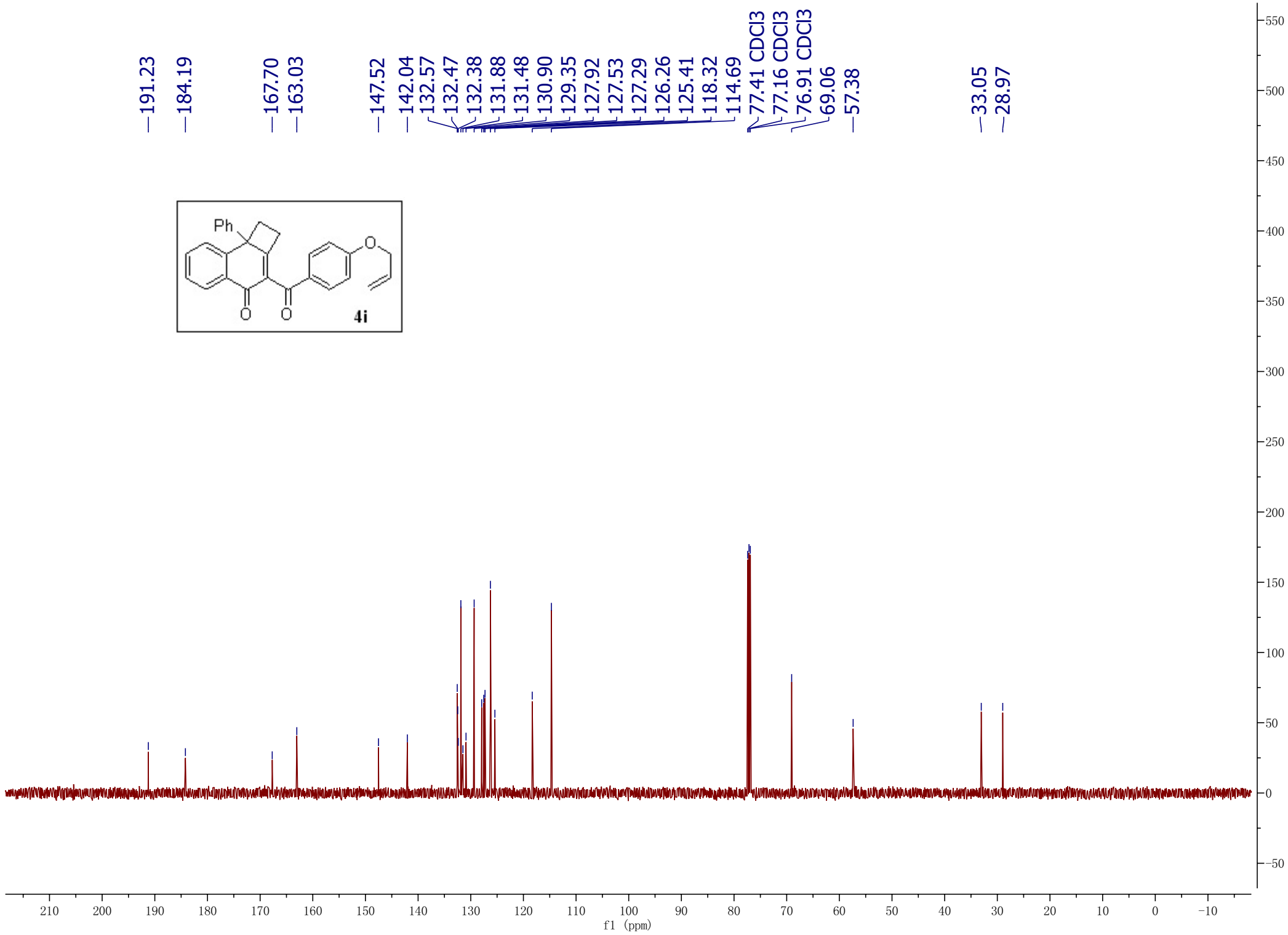
f1 (ppm)

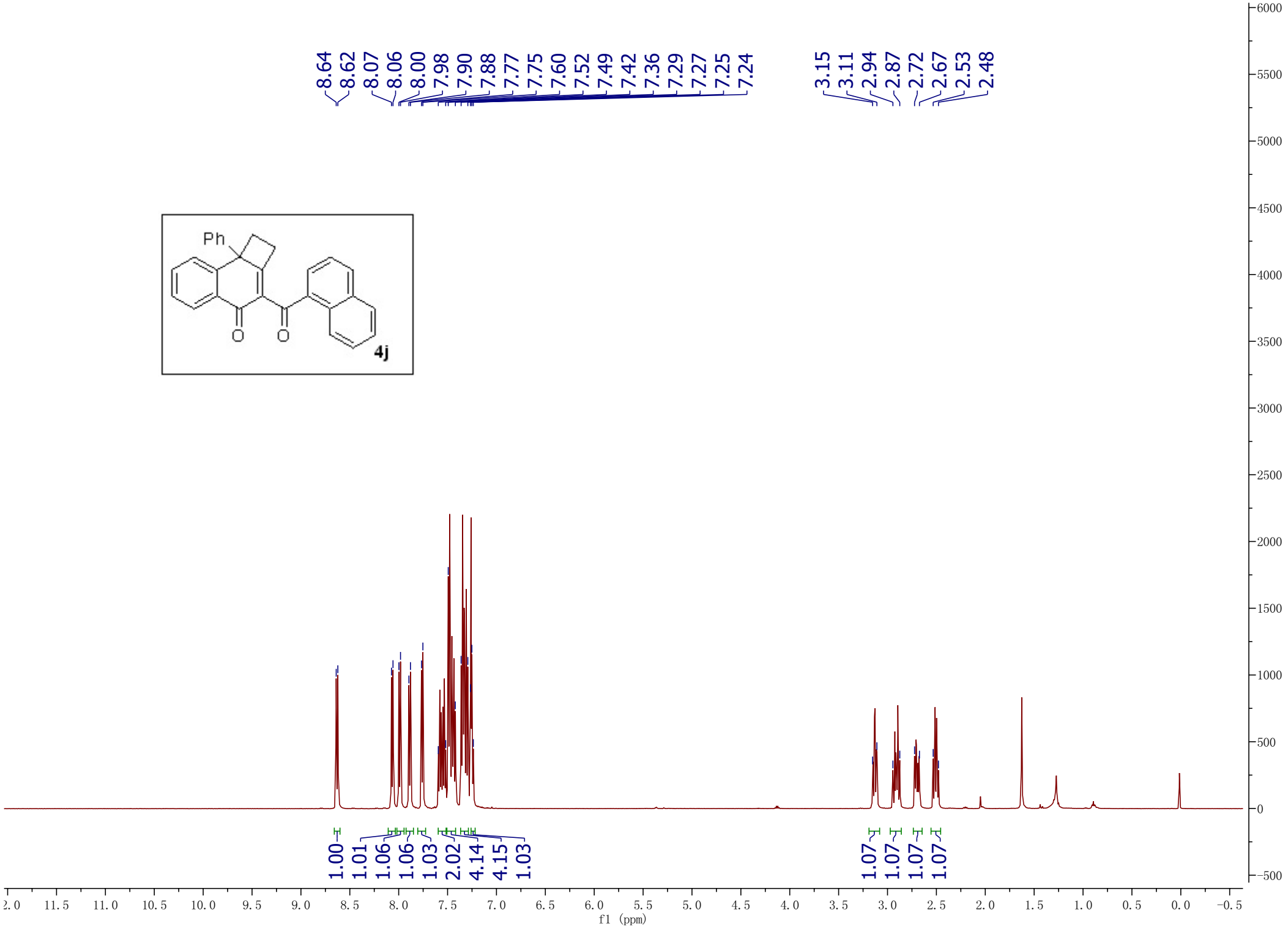
JKG-20181102-249-P8/11
C13CPD DMSO {D:\2018-3} ZHL 4

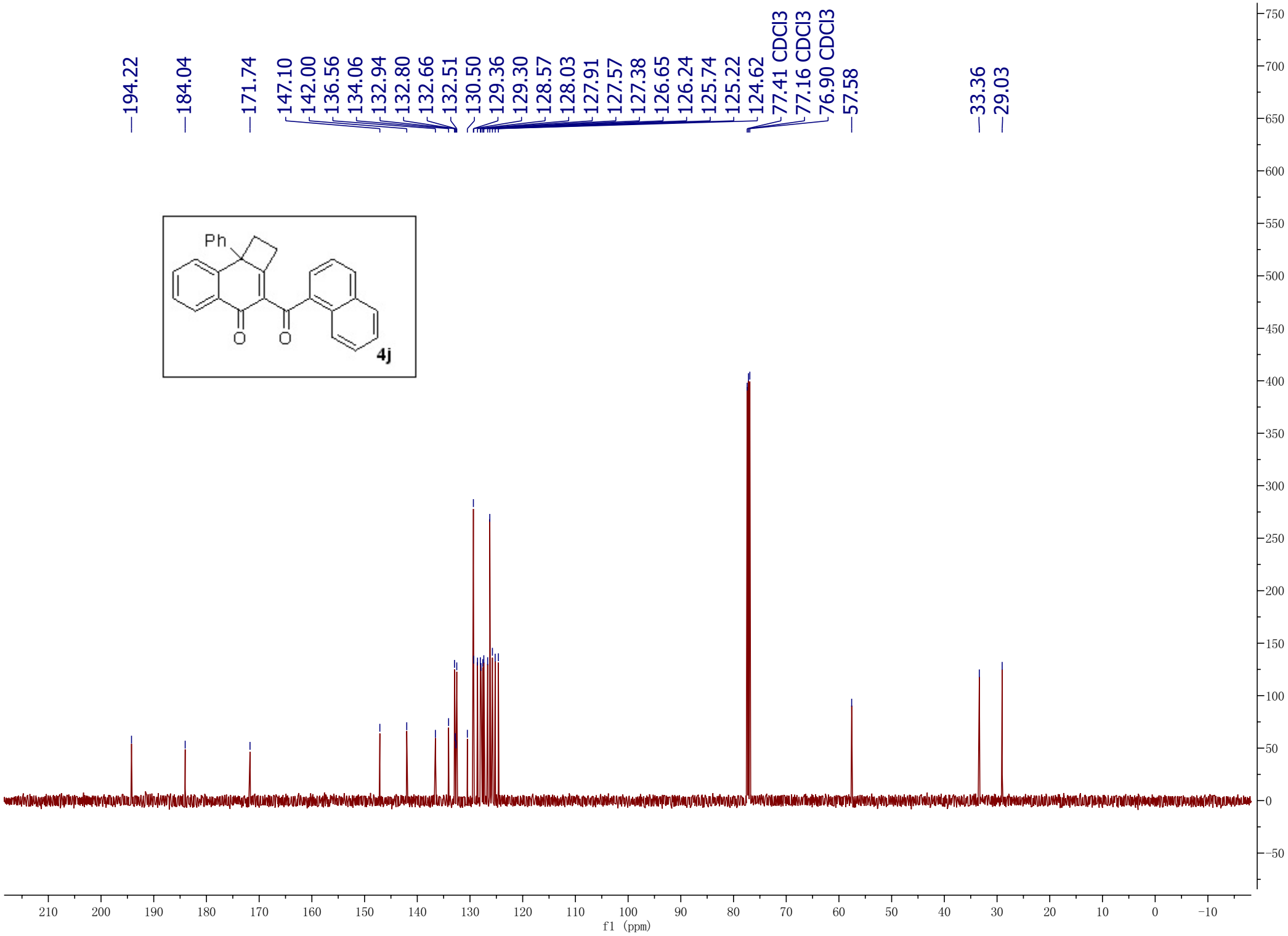


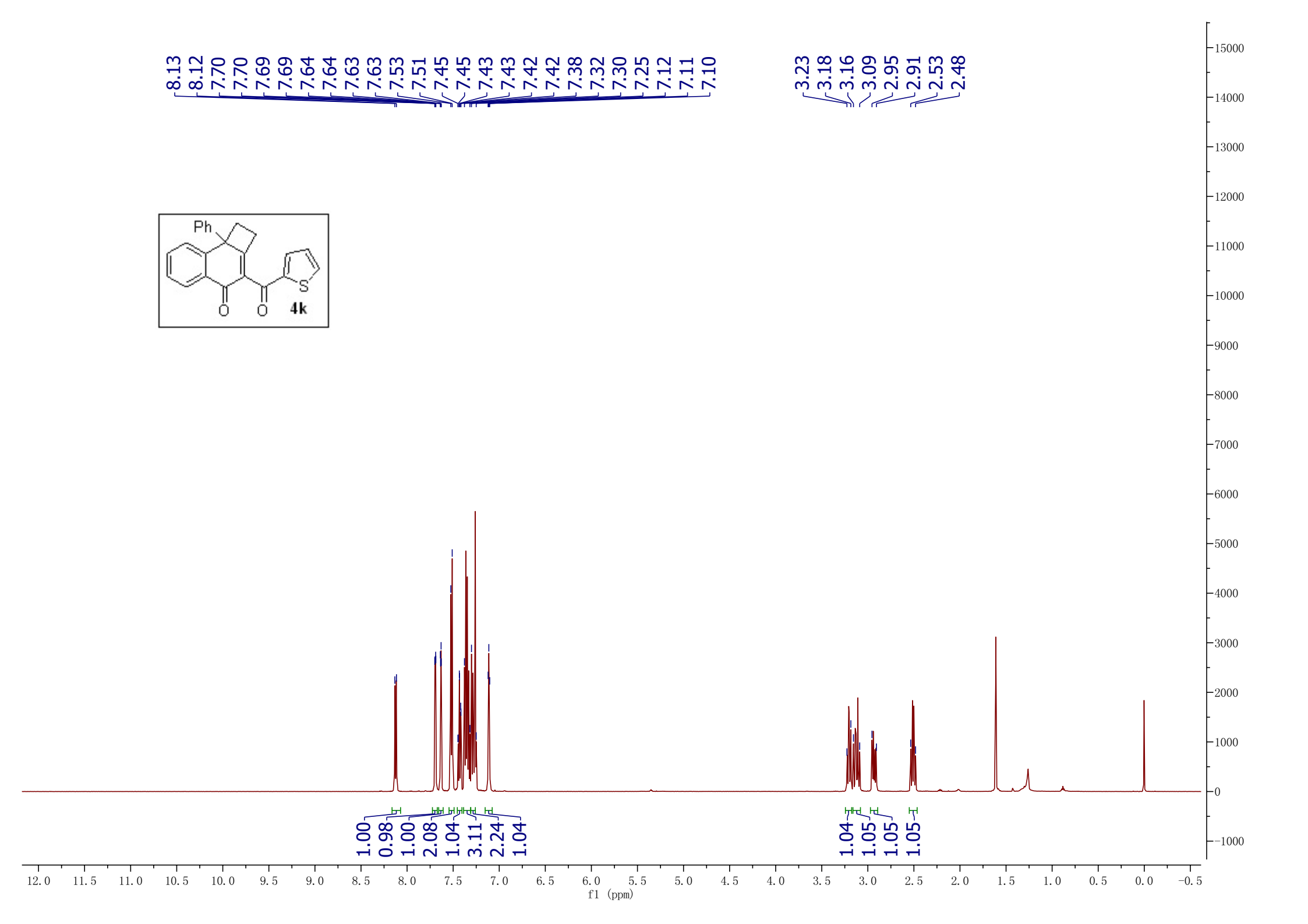
f1 (ppm)

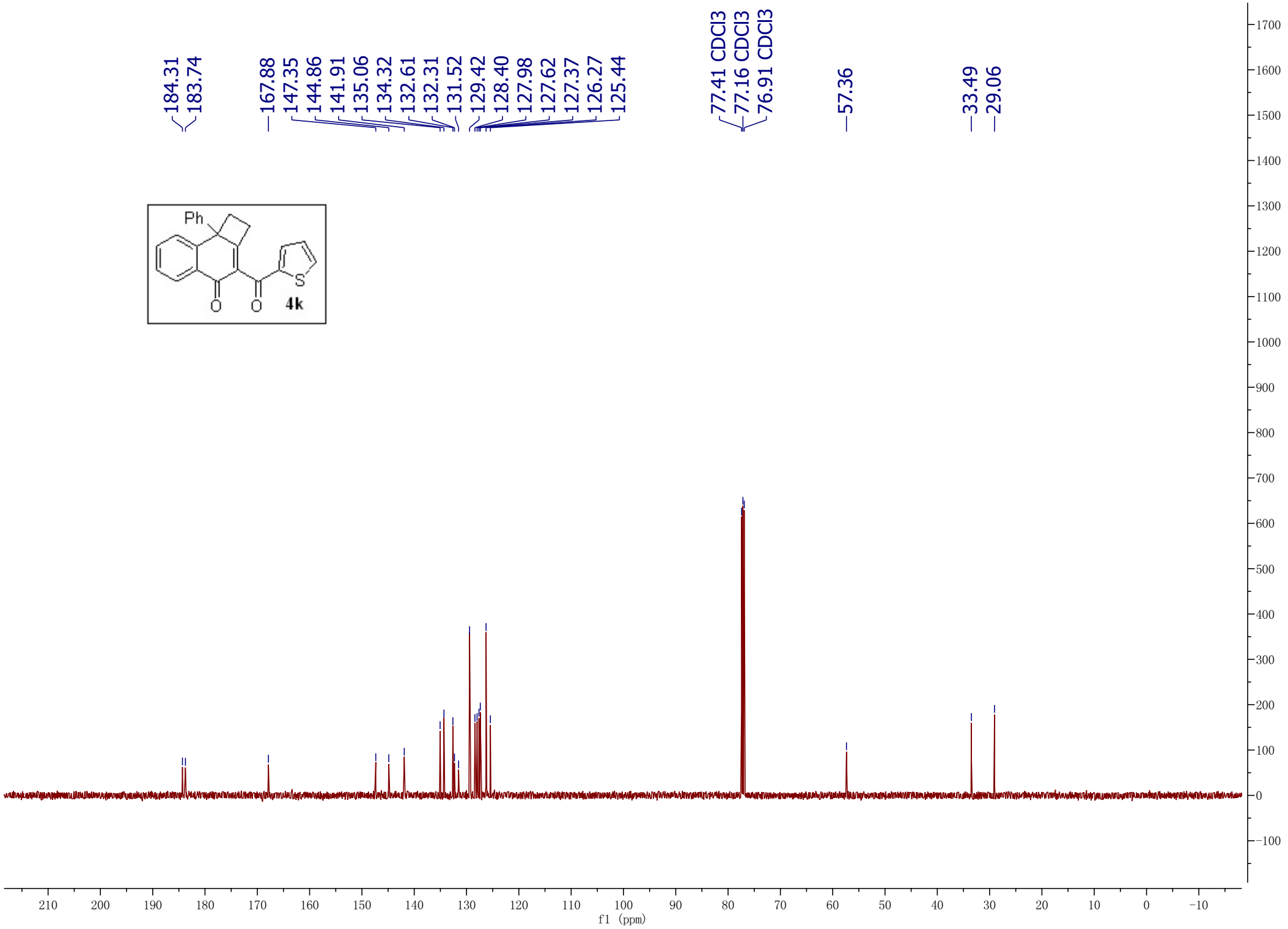

8.12
8.10
7.88
7.87
7.53
7.51
7.44
7.43
7.41
7.37
7.26
7.24
6.95
6.93
6.08
6.00
5.44
5.40
5.32
5.30
4.60
4.59
3.21
3.17
3.08
3.01
2.86
2.81
2.53
2.48
Ph
O
O
O
4i
1.00
2.04
2.06
1.05
5.02
2.06
0.97
1.01
1.02
2.03
1.02
1.00
1.02
1.02
f1 (ppm)

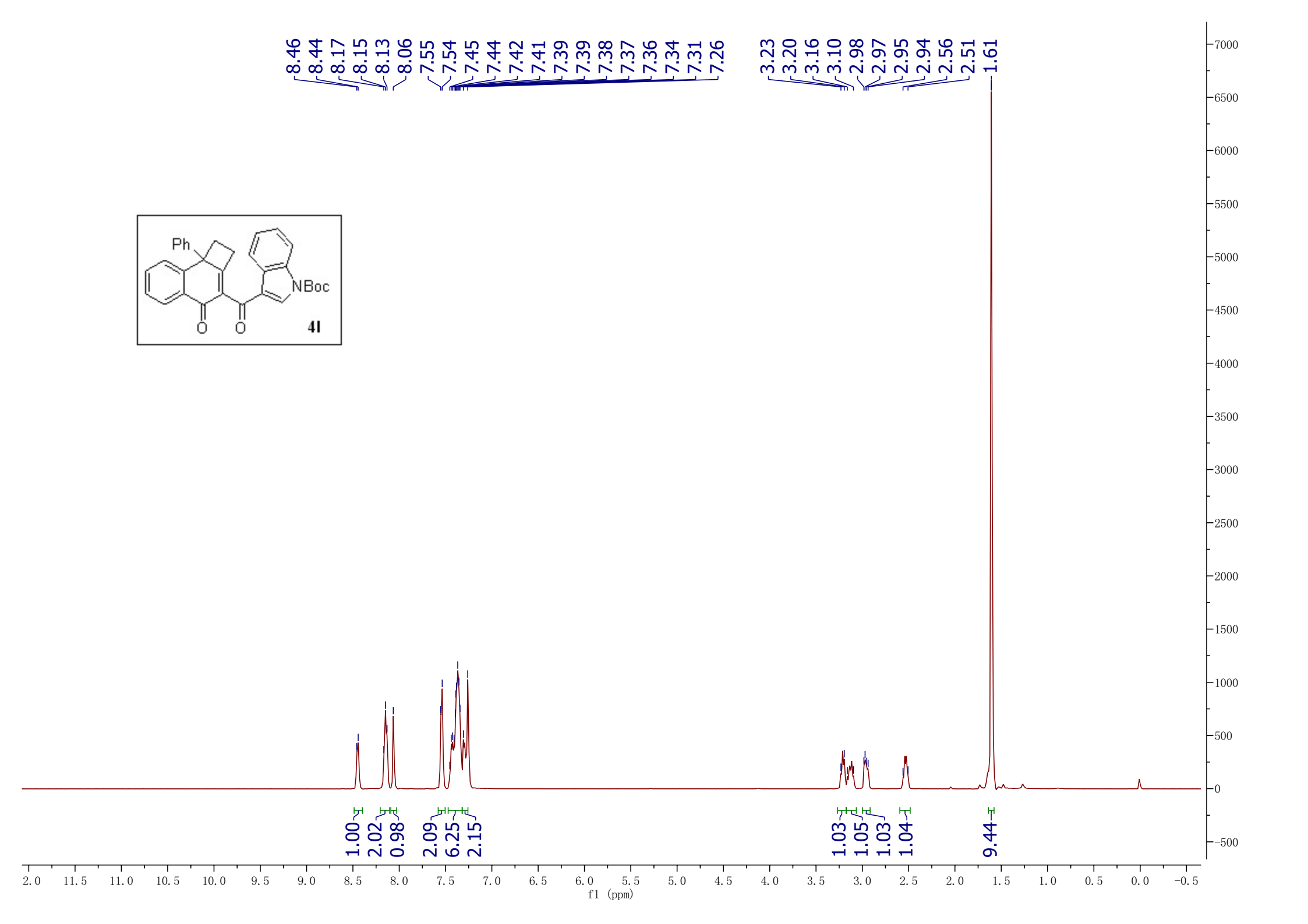

191.23
184.19
167.70
163.03
147.52
142.04
132.57
132.47
132.38
131.88
131.48
130.90
129.35
127.92
127.53
127.29
126.26
125.41
118.32
114.69
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
69.06
57.38
33.05
28.97
Ph
O
O
O
4i
f1 (ppm)

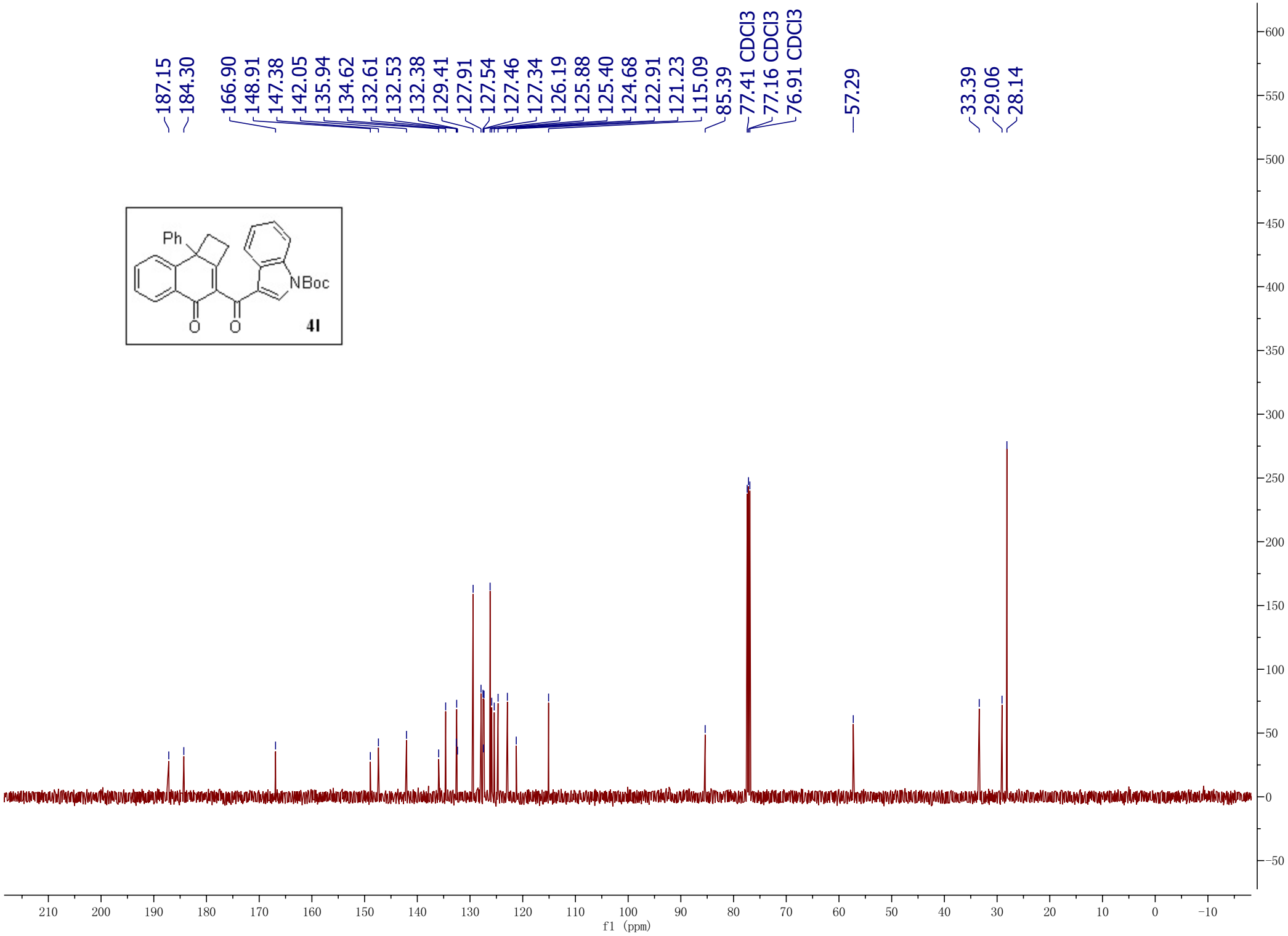

8.64
8.62
8.07
8.06
8.00
7.98
7.90
7.88
7.77
7.75
7.60
7.52
7.49
7.42
7.36
7.29
7.27
7.25
7.24
3.15
3.11
2.94
2.87
2.72
2.67
2.53
2.48
Ph
O
O
4j
1.00
1.01
1.06
1.06
1.03
2.02
4.14
4.15
1.03
1.07
1.07
1.07
1.07
f1 (ppm)


194.22
184.04
171.74
147.10
142.00
136.56
134.06
132.94
132.80
132.66
132.51
130.50
129.36
129.30
128.57
128.03
127.91
127.57
127.38
126.65
126.24
125.74
125.22
124.62
77.41 CDCl3
77.16 CDCl3
76.90 CDCl3
57.58
33.36
29.03
Ph
O
O
4j
f1 (ppm)

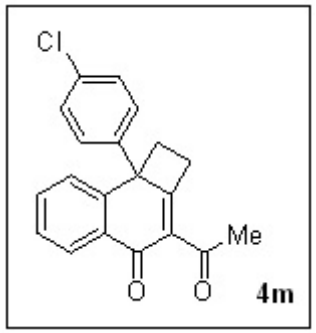

8.13
8.12
7.70
7.70
7.69
7.69
7.64
7.64
7.63
7.63
7.53
7.51
7.45
7.45
7.43
7.43
7.42
7.42
7.38
7.32
7.30
7.25
7.12
7.11
7.10
3.23
3.18
3.16
3.09
2.95
2.91
2.53
2.48
Ph
S
O
O
4k
1.00
0.98
1.00
2.08
1.04
3.11
2.24
1.04
1.04
1.05
1.05
1.05
f1 (ppm)


184.31
183.74
167.88
147.35
144.86
141.91
135.06
134.32
132.61
132.31
131.52
129.42
128.40
127.98
127.62
127.37
126.27
125.44
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
57.36
33.49
29.06
Ph
S
O
O
4k
f1 (ppm)


8.46
8.44
8.17
8.15
8.13
8.06
7.55
7.54
7.45
7.44
7.42
7.41
7.39
7.39
7.38
7.37
7.36
7.34
7.31
7.26
3.23
3.20
3.16
3.10
2.98
2.97
2.95
2.94
2.56
2.51
1.61
Ph
NBoc
O
O
4l
1.00
2.02
0.98
2.09
6.25
2.15
1.03
1.05
1.03
1.04
9.44
f1 (ppm)


187.15
184.30
166.90
148.91
147.38
142.05
135.94
134.62
132.61
132.53
132.38
129.41
127.91
127.54
127.46
127.34
126.19
125.88
125.40
124.68
122.91
121.23
115.09
85.39
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
57.29
33.39
29.06
28.14
Ph
NBoc
O
O
4l
f1 (ppm)

JKG-20180926-242-P4A/10
PROTON CDCl3 {D:\2018-3} ZHL 21



8.02 8.00 7.36 7.28 7.26 7.25 7.23 3.41 3.28 3.21 3.17 2.58 2.55 2.50

0.97 5.16 1.98 2.04 1.00 3.01 0.99

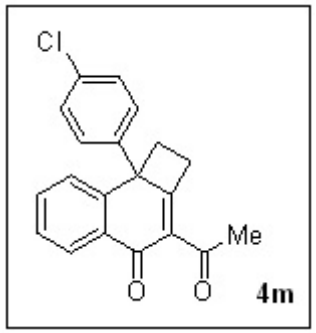
30000 25000 20000 15000 10000 5000 0

11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

f1 (ppm)

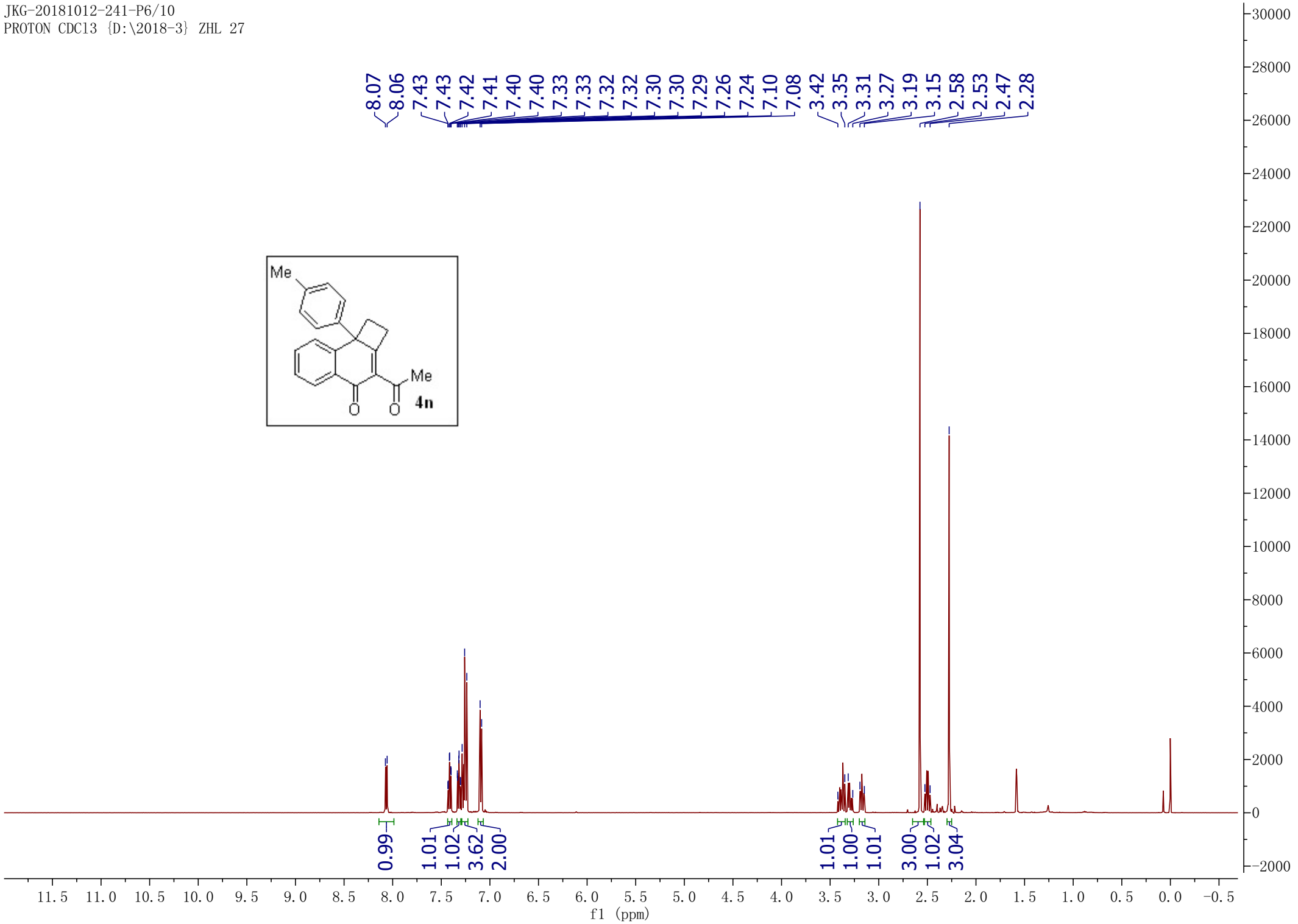
JKG-20180926-242-P4A.11.fid
C13CPD CDCl3 {D:\2018-3} ZHL 21

197.08
183.68
175.75
148.63
141.28
138.97
131.40
130.75
129.49
129.47
127.89
127.87
126.18
125.30
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
57.47
34.87
31.30
29.40

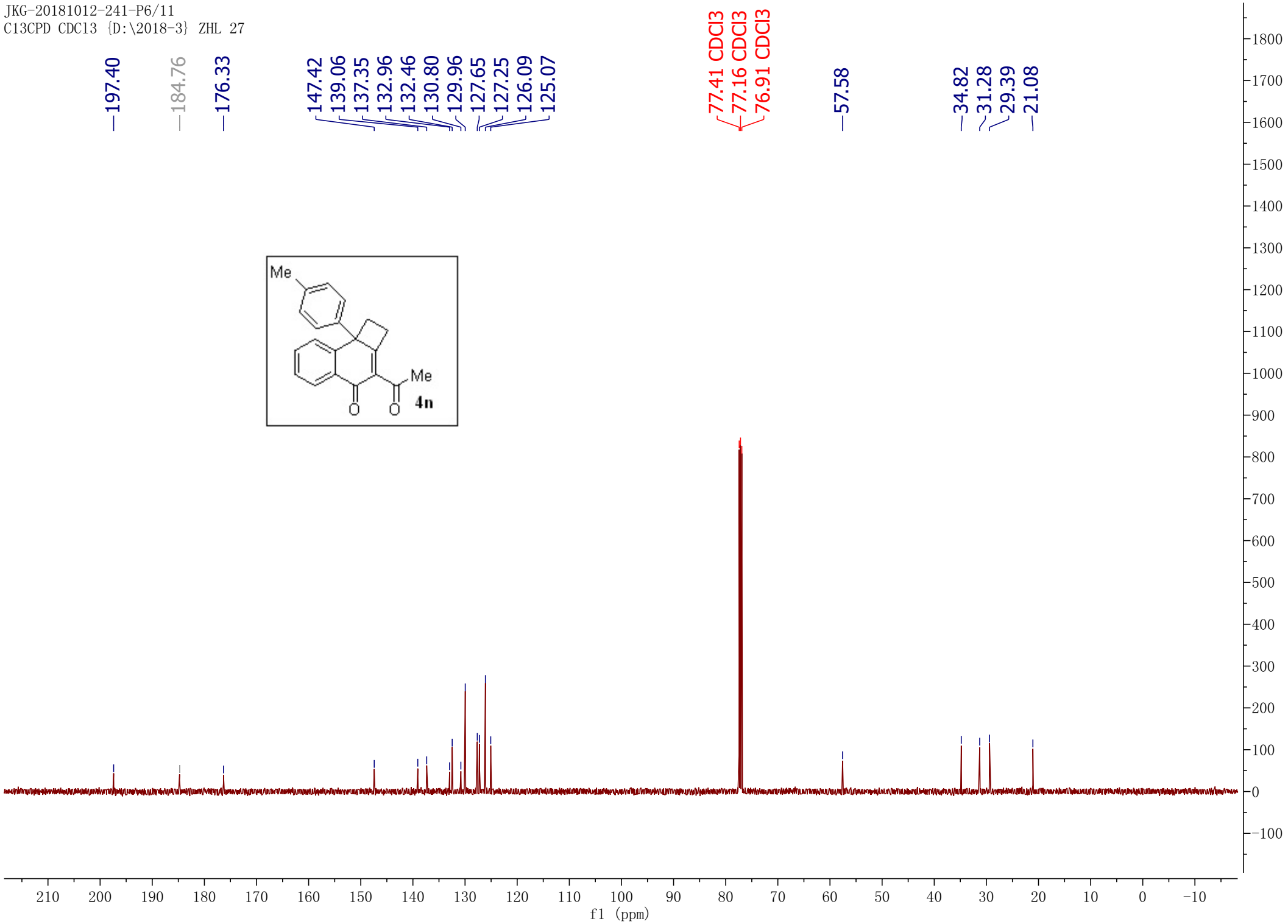


f1 (ppm)

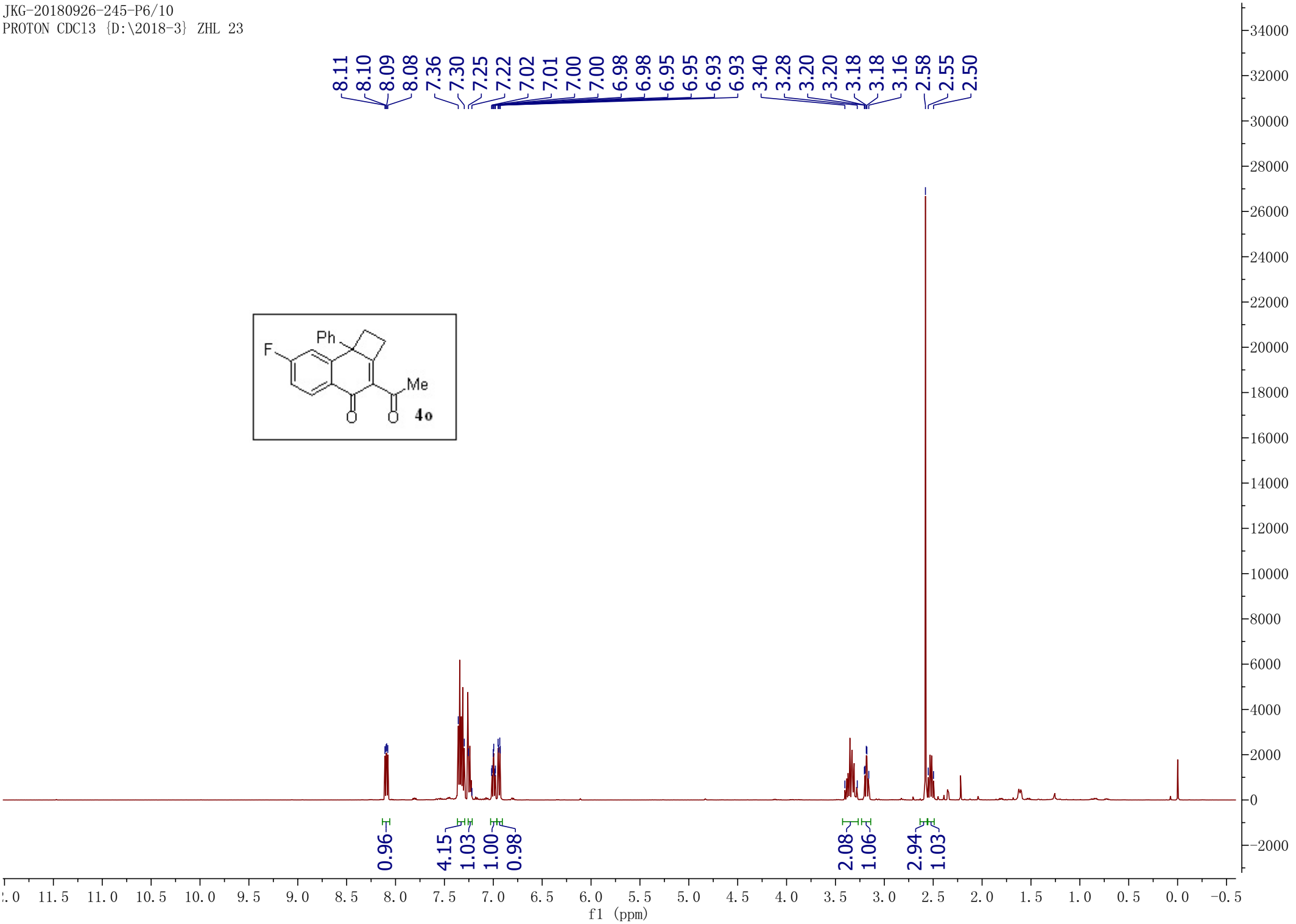
JKG-20181012-241-P6/10
PROTON CDCl3 {D:\2018-3} ZHL 27



JKG-20181012-241-P6/11
C13CPD CDCl3 {D:\2018-3} ZHL 27

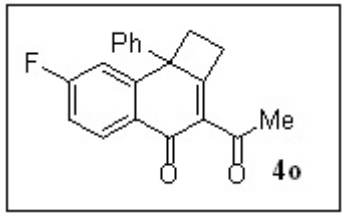


JKG-20180926-245-P6/10
PROTON CDCl3 {D:\2018-3} ZHL 23



JKG-20180926-245-P6.11.fid
C13CPD CDCl3 {D:\2018-3} ZHL 23

197.22
183.47
175.63
166.11
164.08
150.01
149.94
141.41
130.87
130.79
130.75
129.45
127.85
126.16
115.13
114.96
112.02
111.84
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
57.64
57.62
34.80
31.31
29.39

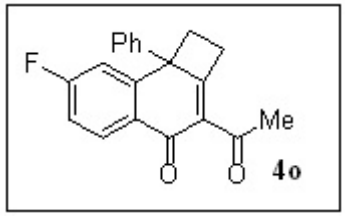


4o

f1 (ppm)

JKG-20180929-245-P6/10

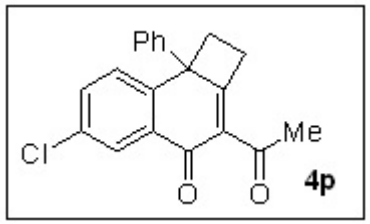
-105.16



4o

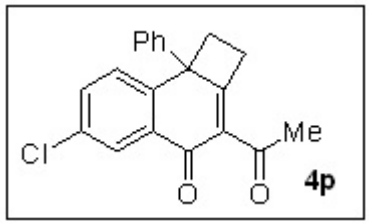
f1 (ppm)

JKG-20180921-248-P1/10
PROTON CDCl3 {D:\2018-3} ZHL 41

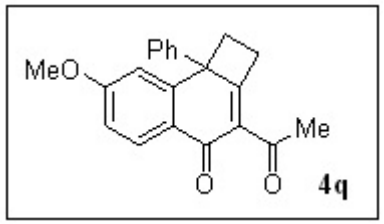


JKG-20180921-248-P1/11
C13CPD CDCl3 {D:\2018-3} ZHL 41

197.25
184.43
174.84
146.34
144.12
135.15
132.95
132.65
131.11
130.52
127.91
127.87
127.65
126.46
125.10
124.54
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
57.54
34.80
31.27
29.63



JKG-20180929-244-P8A/10

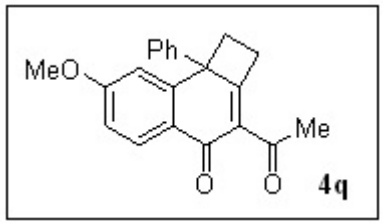


4q

f1 (ppm)

JKG-20180926-244-P8.11.fid
C13CPD CDCl3 {D:\2018-3} ZHL 22

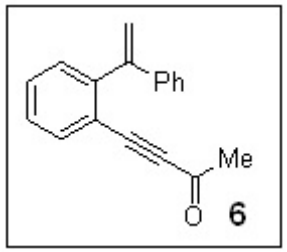
197.71
183.89
175.13
162.82
149.60
141.99
130.89
130.13
129.27
127.55
126.42
126.20
113.12
110.05
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
57.76
55.60
34.76
31.34
29.38



4q

f1 (ppm)

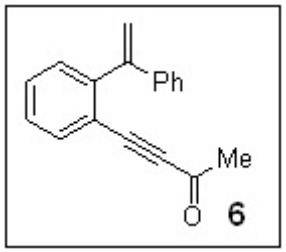
JKG-20190412-256-P6/10
H



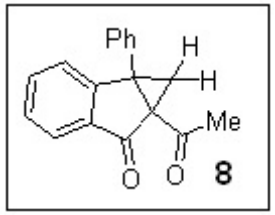
f1 (ppm)

JKG-20190412-256-P6/11
C

184.64
148.22
146.02
140.56
134.26
130.80
130.39
128.43
127.94
127.79
127.12
119.35
116.97
91.83
89.85
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
32.51



JKG-20190522-257-P1/10
PROTON CDCl3 {D:\2019-1} ZHL 8



7.78 7.77 7.50 7.49 7.47 7.41 7.39 7.30 7.26 7.14 7.12

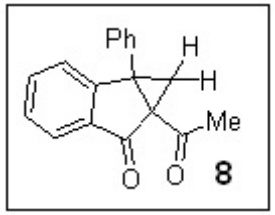
3.09 3.08 2.34 2.12 2.12

0.96 1.04 5.97 1.00 1.04 3.03 1.04

f1 (ppm)

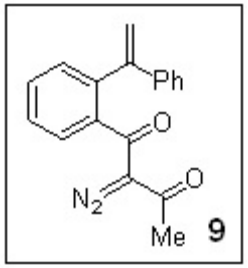
JKG-20190522-257-P1/11
C13CPD CDCl3 {D:\2019-1} ZHL 8

198.83
198.72
155.36
134.67
133.46
132.85
129.87
128.80
128.53
128.23
124.97
124.76
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
54.11
51.08
42.22
30.31



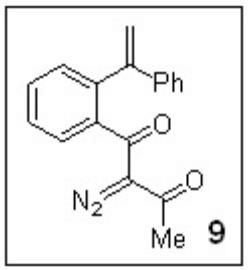
f1 (ppm)

JKG-20190522-257-P2/10
PROTON CDCl3 {D:\2019-1} ZHL 10

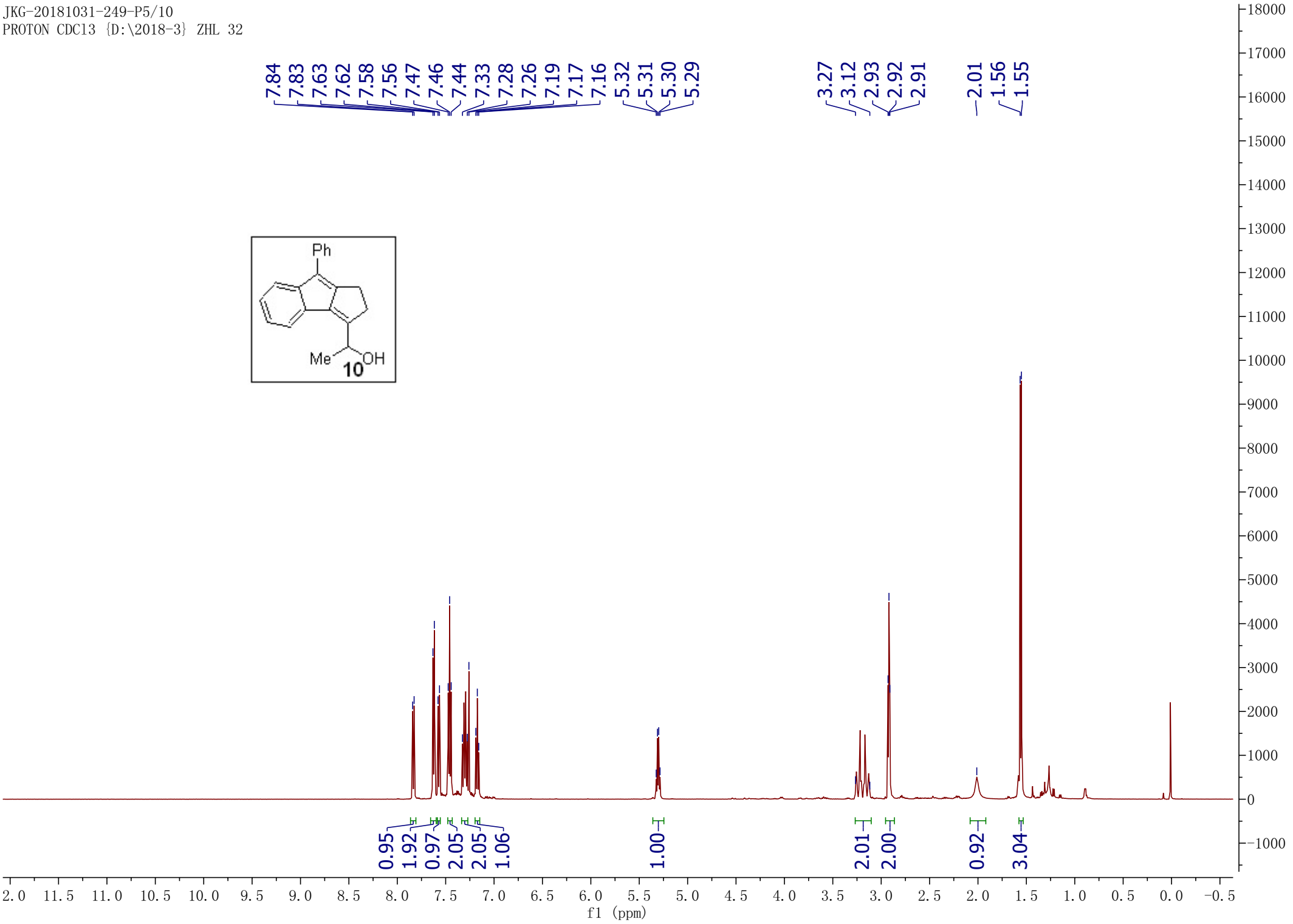


f1 (ppm)

JKG-20190522-257-P2/11
C13CPD CDCl3 {D:\2019-1} ZHL 10

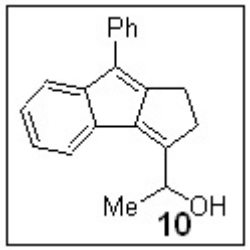


JKG-20181031-249-P5/10
PROTON CDCl3 {D:\2018-3} ZHL 32



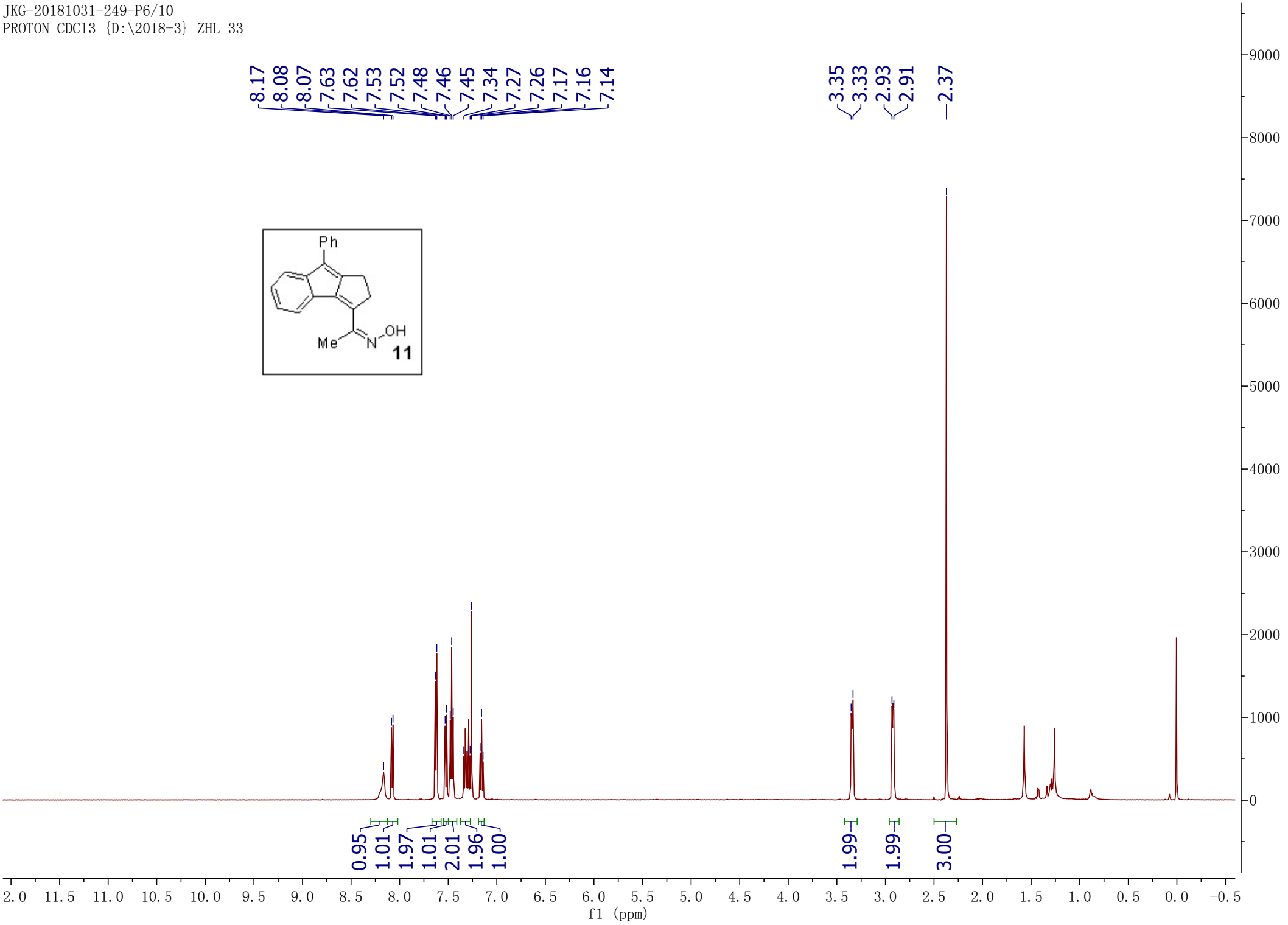
JKG-20181031-249-P5/11
C13CPD CDCl3 {D:\2018-3} ZHL 32

154.62
152.25
149.36
142.88
136.06
129.90
128.68
128.19
127.81
127.52
126.72
124.01
123.45
119.67
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
66.81
37.87
23.37
22.33



f1 (ppm)

JKG-20181031-249-P6/10
PROTON CDCl3 {D:\2018-3} ZHL 33

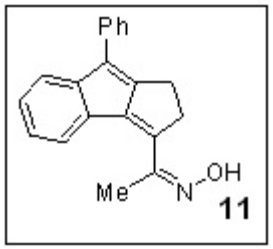


JKG-20181031-249-P6/11
C13CPD CDCl3 {D:\2018-3} ZHL 33

155.31
152.32
149.78
146.49
142.35
135.74
130.11
129.71
128.71
128.36
127.93
127.00
125.04
123.99
119.79

77.41 CDCl3
77.16 CDCl3
76.91 CDCl3

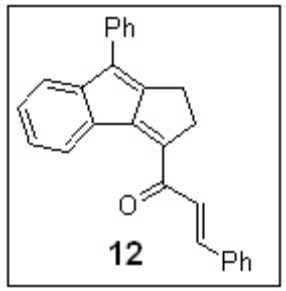
40.06
22.87
14.08



11

f1 (ppm)

JKG-20190104-250-P7/10
PROTON CDCl3 {D:\2019-1} ZHL 31

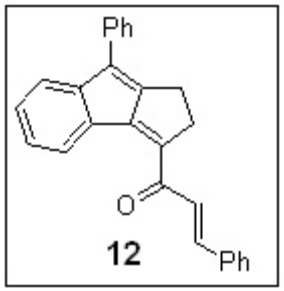


12

f1 (ppm)

JKG-20190104-250-P7/11
C13CPD CDCl3 {D:\2019-1} ZHL 31

189.39
153.80
151.46
150.18
144.62
142.07
135.15
134.90
133.54
130.89
130.13
129.72
129.17
128.79
127.90
127.60
126.87
125.21
124.55
120.21
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
39.10
23.13



12

f1 (ppm)