Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Tandem Aza-Michael Addition—Vinylogous Aldol Condensation: Synthesis of *N*-Bridged Pyridine Fused Quinolones

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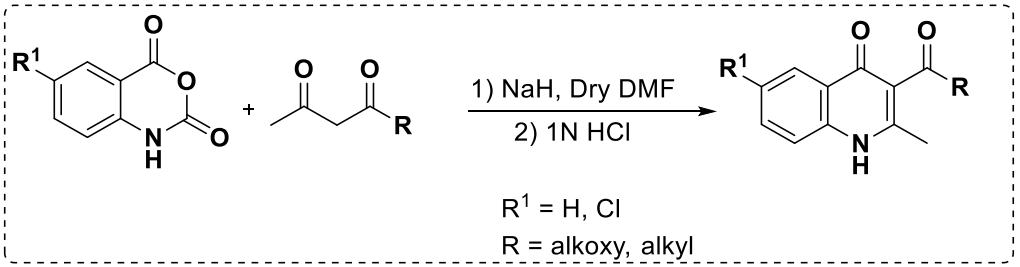
# Equal contribution

Contents:

1. General Information

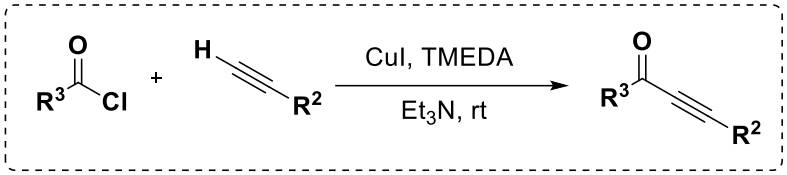
All the reactions were performed using oven-dried standard glassware or screw-caped vials. The reactions were performed by using sealed screw caped vials and heating metal block. The reactions are stirred magnetically and monitored by analytical thin layer chromatography (TLC). TLC was made by silica gel 60 F254, and UV lamp was used as visualizing agent. Iodine, 5% aqueous potassium permanganate solution was used as a developing agents followed by heating. Purification of products was performed using column chromatography on silica gel (60−120 and 100− 120, mesh) where it is required. Hexane/ethyl acetate was used as eluents. The solvents were removed by rotary evaporator at 40−45 °C under reduced pressure. All the reagents and solvents were purchased from commercial suppliers. Melting points reported in this work are uncorrected. 1H NMR spectra were recorded on 300, 400, and 500 MHz instruments. Chemical shifts (δ) are reported in parts per million (ppm) with the reference solvent and the internal standards (TMS = 0; $CDCl_3$ = 7.26) *via* residual solvent as $CDCl_3$. Peaks that appear at 1.26, 0.86 ppm in 1H NMR, and 29.7 ppm in 13C{1H}NMR correspond to the residual grease present in the solvent.[1] The following abbreviations were used to explain the multiplicity of the spectra (s = singlet, d = doublet, dd = doublet of doublet, t = triplet, q = quartet, sep = septet, and m = multiplet). 13C NMR spectra were recorded on 75, 100, and 125 MHz spectrometers. Infrared spectroscopy was performed neat on a BRUKER FT-IR spectrophotometer in chloroform, IR[KBr] spectra were recorded on a Thermo Nicolet-NEXUS 670 FT-IR instrument. Mass spectrometric analyses were performed using ESI techniques, mass spectra obtained on a SHIMADZU LCMS-2020 mass spectrometer. High Resolution Mass Spectra data were obtained on a Thermo scientific Exactive^{TM} Orbitrap mass spectrometer or Q STAR XL Hybrid MS/MS.

2. Synthesis of quinoline-3-carboxylate derivatives



In a dry, clean round bottom flask, suspension of sodium hydride (15 mmol, 1.0 equiv) and β-ketoesters or 1,3-diketones (15 mmol, 1.0 equiv) were taken in a dry DMF (50 mL), followed by the drop wise addition of isatoic anhydride derivative (15 mmol, 1.0 equiv) in dry DMF (30 mL) and stirred overnight. After most of the solvent had been removed under reduced pressure, the residue was treated with 1M HCl to yield the oxoquinolone derivatives as yellow solids. The synthesized oxoquinolones were good agreement with reported data.[2]

3. Synthesis of ynones



An oven-dried Schlenk reaction tube was charged with CuI (0.02 mmol, 3 mg), TMEDA (0.05 mmol, 6 mg), and acid chloride (1.2 mmol), followed by alkyne derivatives (1 mmol) and Et_3N (3.0 mmol, 0.42 mL). The mixture was stirred at room temperature for 1 h under N_2. After completion of the reaction, saturated aqueous $NaHCO_3$ (5 mL) and EtOAc (20 mL) were added. The organic layer was dried over anhydrous Na_2SO_4, filtered, and solvent removed under reduced pressure. The residue was purified by chromatography (silica gel) to give the cross-coupled ynones**.** The synthesized ynones were good agreement with reported data.[3]

4. Optimization survey

An oven-dried reaction vial equipped with a magnetic stirrer bar, was charged with ethyl 1,4-dihydro-2-methyl-4-oxoquinoline-3-carboxylate (0.5 mmol, 115 mg), 1,3-diphenylprop-2-yn-1-one (1 equiv, 0.5 mmol, 103 mg) and base (x equiv) followed by the addition of solvent (2 mL). The reaction vial was closed and placed in a metal heating block, heated to mentioned time and temperature according to optimization table. After the reaction completion, the reaction mixture was cooled to room temperature, extracted with ethyl acetate (2 x 20 mL), washed with brine, dried over anhydrous Na_2SO_4 and filtered. The solvent was removed from organic layer under vacuum to afford a crude residue. The residue was purified by flash column chromatography (hexane/EtOAc, 80:20) on silica gel to afford methyl 6-oxo-1,3-diphenyl-6H-pyrido[1,2-*a*]quinoline-5-carboxylate **3b**.

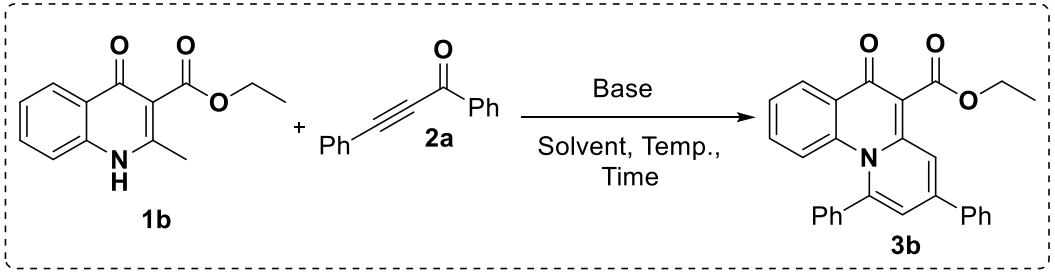
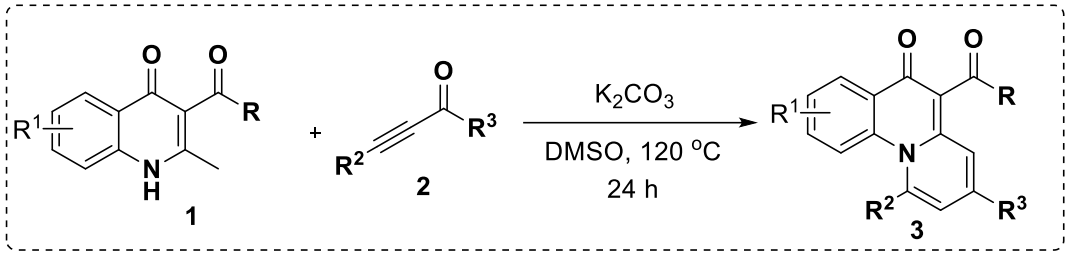


Table S1: Optimization study

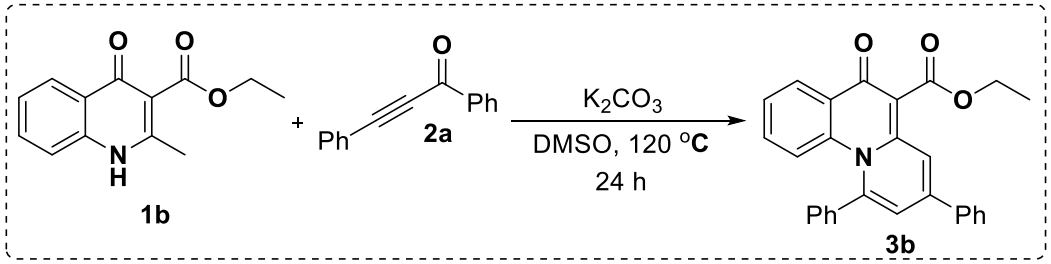
S. No	Base	Equiv (Base)	Solvent	Time	Temp (°C)	Yields of 3a
1	K_2CO_3	1	DMSO	24 h	**RT**	-
2	K_2CO_3	1	DMSO	24 h	**100**	66%
3	K_2CO_3	1	DMSO	24 h	**120**	93%
4	K_2CO_3	1	DMSO	24 h	**140**	87%
5	K_2CO_3	**1.2**	DMSO	24 h	120	90%
6	K_2CO_3	**1.5**	DMSO	24 h	120	88%
7	K_2CO_3	**2**	DMSO	24 h	120	72%
8	K_2CO_3	**2.5**	DMSO	24 h	120	67%
9	K_2CO_3	**3**	DMSO	24 h	120	66%
10	**NaH**	1	DMSO	24 h	120	52%
11	**^{t}BuOK**	1	DMSO	24 h	120	54%
12	**Cs_2CO_3**	1	DMSO	24 h	120	76%
13	**K_3PO_4**	1	DMSO	24 h	120	68%
14	**NaOH**	1	DMSO	24 h	120	58%
15	**DBU**	1	DMSO	24 h	120	35%
16	K_2CO_3	1	**DMF**	24 h	120	86%
17	K_2CO_3	1	**1,4-Dioxane**	24 h	120	80%
18	K_2CO_3	1	**^{t}Butanol**	24 h	120	64%
19	K_2CO_3	1	**DCE**	24 h	120	61%
20	K_2CO_3	1	**Toluene**	24 h	120	49%
21	K_2CO_3	1	**MeOH**	24 h	120	23%
22	K_2CO_3	1	**Water**	24 h	120	-
23	K_2CO_3	1	DMSO	**18 h**	120	85%
24	K_2CO_3	1	DMSO	**12 h**	120	72%
25	-	1	DMSO	**24 h**	120	-

5. Experimental procedure for the synthesis of pyridine fused quinolone derivatives 3a-y



An oven-dried reaction vial equipped with a magnetic stirrer bar charged with quinoline-3-carboxylate derivatives (0.5 mmol), ynone (1 equiv, 0.5 mmol) and K_2CO_3 (1 equiv, 0.5 mmol, 69 mg) followed by the addition of DMSO (2 mL). The reaction vial was closed and placed in a metal heating block and the reaction mixture was stirred at 120 ^oC for 24 h. After reaction completion, the reaction mixture was cooled to room temperature, then extracted with ethyl acetate (2 x 20 mL), washed with brine, dried over anhydrous Na_2SO_4 and filtered. The solvent was removed under vacuum from organic layer to afford a crude residue. The residue was purified by flash column chromatography (hexane/EtOAc 80:20 to 60:40) on silica gel to afford pyridine fused quinolone derivatives **3a-3y**.

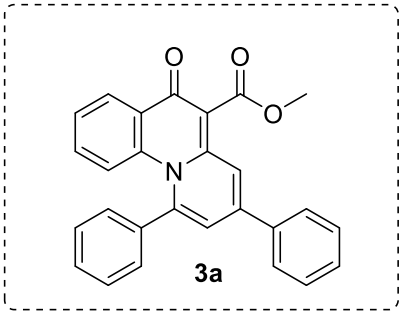
6. Gram scale synthesis of 3b



An oven-dried reaction vial equipped with a magnetic stirrer bar charged with ethyl 1,4-dihydro-2-methyl-4-oxoquinoline-3-carboxylate (10 mmol, 2.31 g), 1,3-diphenylprop-2-yn-1-one (1 equiv, 10 mmol, 2.06 g) and K_2CO_3 (1 equiv, 10 mmol, 1.38 g) followed by the addition of DMSO (40 mL). The reaction vial was closed and placed in a metal heating block and the reaction mixture was stirred at 120 °C for 24 h. After reaction completion, the reaction mixture was cooled to room temperature, then extracted with ethyl acetate (3x100 mL), washed with brine, dried over anhydrous Na_2SO_4 and filtered. The solvent was removed from organic layer under vacuum to afford a crude residue. The residue was purified by flash column chromatography (hexane/EtOAc 80:20) on silica gel to afford methyl 6-oxo-1,3-diphenyl-6H-pyrido[1,2-*a*]quinoline-5-carboxylate **3b** (80% yield, 3.36 g).

7. Spectroscopic data of 3a-y

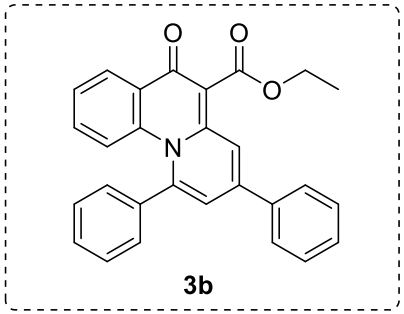
Methyl 6-oxo-1,3-diphenyl-6H-pyrido[1,2-*a*]quinoline-5-carboxylate (3a)



3a

Yellow solid, 182 mg (0.450), 90%, $\mathbf{R_f}$ = 0.6 (EtOAC/Hexane, 60:40); **MP** 160-162 ºC; **IR** ($CHCl_3$) 756, 1215, 1449, 1594, 1696, 1717, 2853, 2923 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.01 (s, 3H), 7.01 (d, *J* = 2.0 Hz, 1H), 7.08–7.16 (m, 2H), 7.28–7.31 (m, 2H), 7.33–7.39 (m, 4H), 7.45–7.53 (m, 3H), 7.73 (dd, *J* = 7.8, 1.5 Hz, 2H), 8.20 (d, *J* = 2.0 Hz, 1H), 8.43 (dd, *J* = 7.9, 0.9 Hz, 1H); **^{13}C{1H}NMR** (101 MHz, $CDCl_3$) δ 52.3, 107.9, 117.4, 117.7, 123.8, 126.4, 126.5, 126.9, 127.2, 128.7, 129.2, 129.3, 129.4, 130.0, 130.4, 136.2, 137.3, 137.9, 144.3, 145.9, 149.6, 168.1, 173.1; **MS** (ESI) m/z 406 $[M+H]^+$**HRMS** (ESI, m/z): calcd for $C_{27}H_{20}NO_3$ $[M+H]^+$406.15823, found 406.15942.

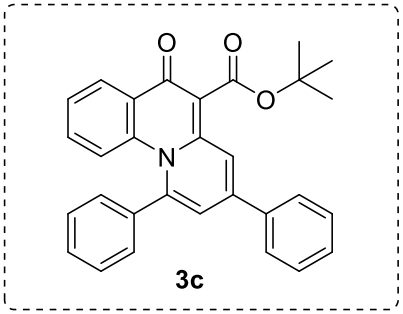
Ethyl 6-oxo-1,3-diphenyl-6H-pyrido[1,2-*a*]quinoline-5-carboxylate (3b)



3b

Yellow solid, 195 mg (0.465 mmol), 93%, **R_f** = 0.4 (EtOAC/Hexane, 60:40); **MP** 160-162 ºC; **IR** ($CHCl_3$) 759, 1217, 1595, 1614, 1718, 2923, 2959 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCL_3$) δ 1.47 (t, *J* = 8.9, 5.3 Hz, 3H), 4.52 (q, *J* = 7.1 Hz, 2H), 7.00 (d, *J* = 2.0 Hz, 1H), 7.07–7.19 (m, 2H), 7.27–7.34 (m, 2H), 7.35–7.42 (m, 4H), 7.47–7.54 (m, 3H), 7.71–7.76 (m, 2H), 8.06 (d, *J* = 2.0 Hz, 1H), 8.46 (dd, *J* = 7.9, 1.2 Hz, 1H); **^{13}C{1H}NMR** (101 MHz, $CDCL_3$) δ 14.5, 61.4, 109.1, 117.4, 117.7, 123.8, 126.5, 126.9, 127.3, 128.7, 129.1, 129.2, 129.3, 129.4, 130.0, 130.4, 136.4, 137.4, 138.1, 144.1, 145.9, 149.1, 167.6, 172.8; **MS** (ESI) m/z 420 $[M+H]^+$ **HRMS** (ESI, m/z): calcd for $C_{28}H_{22}NO_3$ $[M+H]^+$420.15823, found 420.15942.

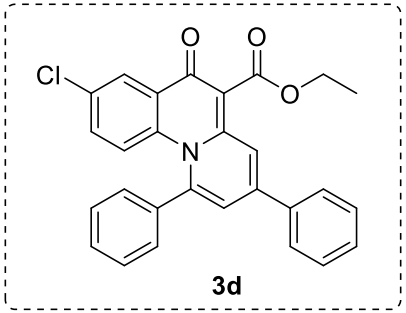
tert-Butyl 6-oxo-1,3-diphenyl-6H-pyrido[1,2-*a*]quinoline-5-carboxylate (3c)



3c

Yellow solid, 206 mg (0.460 mmol), 92 %, **R_f** = 0.5 (EtOAC/Hexane, 60:40); **MP** 165-167 ºC; **IR** (KBr) cm^{-1} 766, 1149, 1459, 1530, 1601, 1724, 2922, 2973; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 1.70 (s, 9H), 6.94 (d, *J* = 2.0 Hz, 1H), 7.07–7.18 (m, 2H), 7.29–7.32 (m, 2H), 7.35–7.40 (m, 4H), 7.48–7.54 (m, 3H), 7.68–7.73 (m, 2H), 7.78 (d, *J* = 2.0 Hz, 1H), 8.46 (dd, *J* = 8.0, 1.3 Hz, 1H); **^{13}C{1H}NMR** (101 MHz, $CDCl_3$) δ 28.5, 82.1, 111.9, 117.2, 1173, 123.7, 126.3, 126.4, 126.7, 127.2, 128.6, 129.3, 129.4, 129.7, 129.9, 130.3, 136.5, 137.4, 138.2, 143.4, 145.6, 147.7, 166.6, 172.3; **MS** (ESI) m/z 448 $[M+H]^+$ **HRMS** (ESI, m/z): calcd for $C_{30}H_{26}NO_3$ $[M+H]^+$ 448.19072, found 448.18958.

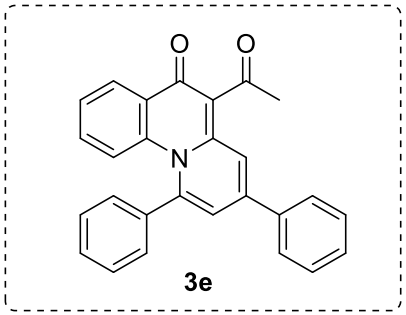
Ethyl 8-chloro-6-oxo-1,3-diphenyl-6H-pyrido[1,2-a]quinoline-5-carboxylate (3d)



3d

Yellow solid, 137 mg (0.300 mmol) 60%, $\mathbf{R_f}$ = 0.6 (EtOAC/Hexane, 60:40); **MP** 163-165 ^{o}C; **IR** ($CHCl_3$) 719, 1158, 1461, 1589, 1615, 1725, 2919, 2957 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.45 (t, *J* = 7.1 Hz, 3H), 4.50 (q, *J* = 7.1 Hz, 2H), 7.02 (d, *J* = 2.0 Hz, 1H), 7.06 (dd, *J* = 9.1, 2.5 Hz, 1H), 7.11 (d, *J* = 9.1 Hz, 1H), 7.28–7.32 (m, 2H), 7.37–7.42 (m, 3H), 7.49–7.53 (m, 3H), 7.72 (dt, *J* = 4.4, 2.4 Hz, 2H), 8.04 (t, *J* = 2.8 Hz, 1H), 8.43 (d, *J* = 2.5 Hz, 1H); **^{13}C{1H}NMR** (101 MHz) δ 14.4, 61.5, 109.3, 117.6, 117.7, 125.2, 125.9, 126.8, 127.2, 128.4, 128.9, 129.3, 129.7, 130.2, 131.5, 132.9, 135.7, 136.1, 137.7, 144.4, 145.7, 149.0, 167.2, 171.5; **MS** (ESI) m/z 453 $[M+H]^+$**HRMS** (ESI, m/z): calcd for $C_{28}H_{21}NO_3Cl$ $[M]^+$454.12045, found 454.11996.

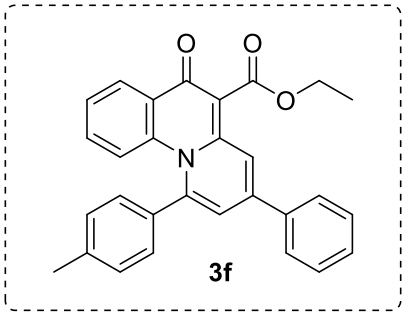
5-Acetyl-1,3-diphenyl-6H-pyrido[1,2-*a*]quinolin-6-one (3e)



3e

Yellow solid, 161 mg (0.415 mmol), 83%, **R_f** = 0.6 (EtOAC/Hexane, 60:40); **MP** 156-158 ^oC; **IR** ($CHCl_3$) 769, 1462, 1530, 1643, 1728, 2922, 2957 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.83 (s, 3H), 7.10–7.18 (m, 3H), 7.32 (dd, *J* = 6.4, 2.9 Hz, 2H), 7.36–7.42 (m, 4H), 7.51 (q, *J* = 5.7 Hz, 3H), 7.76–7.83 (m, 2H), 8.42 (d, *J* = 7.8 Hz, 1H), 8.92 (d, *J* = 1.7 Hz, 1H); **^{13}C{1H}NMR** (101 MHz, $CDCl_3$) δ 29.5, 114.5, 118.1, 118.5, 124.1, 126.3, 126.9, 127.1, 127.4, 128.9, 129.2, 129.4, 129.5, 130.2, 131.1, 136.3, 137.4, 138.1, 145.4, 146.2, 150.5, 175.2, 201.1; **MS** (ESI) m/z 390 $[M+H]^+$**HRMS** (ESI, m/z): calcd for $C_{27}H_{20}NO_2$ $[M+H]^+$390.14886, found 390.15080.

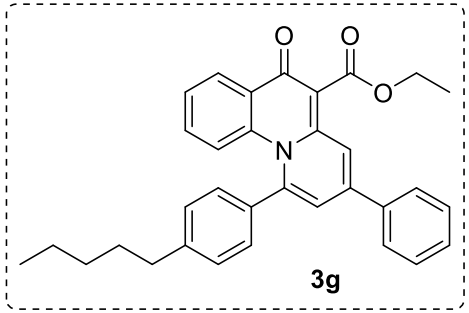
Ethyl 6-oxo-3-phenyl-1-p-tolyl-6H-pyrido[1,2-*a*]quinoline-5-carboxylate (3f)



3f

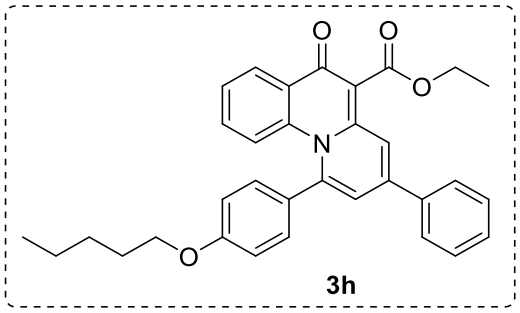
Yellow solid, 191 mg (0.441 mmol), 88%, **R_f** = 0.5 (EtOAC/Hexane, 60:40); **MP** 166-168 ^oC; **IR** (KBr) cm^{-1} 772, 1227, 1495, 1690, 1735, 2677, 2842; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 1.47 (t, *J* = 7.1 Hz, 3H), 2.38 (s, 3H), 4.52 (q, *J* = 7.1 Hz, 2H), 6.97 (d, *J* = 1.7 Hz, 1H), 7.10–7.22 (m, 6H), 7.39 (t, *J* = 7.1 Hz, 1H), 7.51 (d, *J* = 6.2 Hz, 3H), 7.69–7.75 (m, 2H), 8.04 (d, *J* = 1.7 Hz, 1H), 8.46 (d, *J* = 7.8 Hz, 1H); **^{13}C{1H}NMR** (101 MHz, $CDCl_3$) δ 14.5, 21.4, 61.3, 108.9, 117.1, 117.5, 123.8, 126.4, 126.6, 126.9, 127.2, 128.7, 129.3, 130.0, 130.1, 130.4, 135.3, 136.5, 137.6, 139.7, 144.1, 146.1, 149.2, 167.7, 172.9; **MS** (ESI) m/z 434, $[M+H]^+$**HRMS** (ESI, m/z): calcd for $C_{29}H_{24}NO_3$ $[M+H]^+$ 434.17507, found 434.17411.

Ethyl 6-oxo-1-(4-pentylphenyl)-3-phenyl-6H-pyrido[1,2-*a*]quinoline-5-carboxylate (3g)



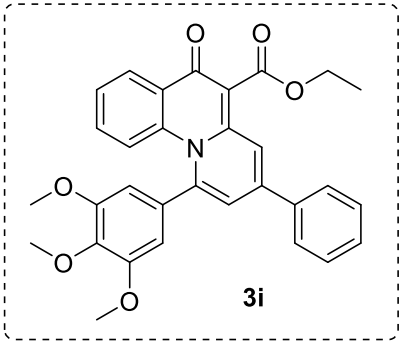
Yellow solid, 232 mg (0.475 mmol), 95%, $\mathbf{R_f}$= 0.6 (EtOAC/Hexane, 60:40); **MP** 168-170 ^{o}C; **IR** ($CHCl_3$) 2956, 2922, 1722, 1615, 1596, 1457, 1217, 765 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 0.90 (t, *J* = 7.0 Hz, 3H), 1.29–1.36 (m, 4H), 1.47 (t, *J* = 7.1 Hz, 3H), 1.61 (dt, *J* = 14.8, 7.5 Hz, 2H), 2.59–2.66 (m, 2H), 4.56 (q, *J* = 5.0 Hz, 2H), 6.98 (d, *J* = 2.0 Hz, 1H), 7.08–7.13 (m, 1H), 7.18 (q, *J* = 8.1 Hz, 5H), 7.38 (t, *J* = 7.5 Hz, 1H), 7.46–7.53 (m, 3H), 7.74 (dd, *J* = 10.7, 9.3 Hz, 2H), 8.04 (d, *J* = 1.9 Hz, 1H), 8.45 (d, *J* = 7.9 Hz, 1H); **^{13}C{1H}NMR** (101 MHz, $CDCl_3$) δ 14.0, 14.5, 22.5, 30.9, 31.3, 35.6, 61.4, 108.9, 117.0, 117.6, 123.7, 126.4, 126.5, 126.9, 127.1, 128.5, 129.2, 129.4, 129.9, 130.4, 135.4, 136.4, 137.5, 144.1, 144.7, 146.1, 149.1, 167.4, 172.8; **MS** (ESI) m/z 490 $[M+H]^+$**HRMS** (ESI, m/z): calcd for $C_{33}H_{32}NO_3$ $[M+H]^+$490.15823, found 490.15942.

Ethyl 6-oxo-1-(4-(pentyloxy)phenyl)-3-phenyl-6H-pyrido[1,2-*a*]quinoline-5-carboxylate (3h)



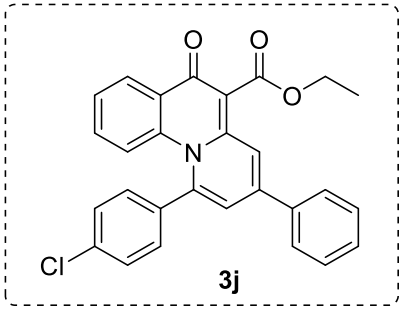
Yellow solid, 230 mg (0.450), 91%, **R_f** = 0.6 (EtOAC/Hexane, 60:40); **MP** 168-170 ºC; **IR** ($CHCl_3$) 767, 1259, 1461, 1599, 1731, 2920, 2957 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 0.94 (t, *J* = 7.1 Hz, 3H), 1.36–1.44 (m, 4H), 1.47 (dd, *J* = 8.2, 5.2 Hz, 3H), 1.79 (dd, *J* = 14.5, 6.7 Hz, 2H), 3.96 (t, *J* = 6.6 Hz, 2H), 4.51 (q, *J* = 7.1 Hz, 2H), 6.86 (d, *J* = 8.8 Hz, 2H), 6.94 (d, *J* = 2.0 Hz, 1H), 7.11-7.18 (m, 1H), 7.18–7.24 (m, 3H), 7.35–7.40 (m, 1H), 7.47–7.53 (m, 3H), 7.72 (dd, *J* = 7.9, 1.6 Hz, 2H), 8.03 (d, *J* = 2.0 Hz, 1H), 8.45 (dd, *J* = 8.0, 1.4 Hz, 1H); **^{13}C{1H}NMR** (101 MHz, $CDCl_3$) δ 13.9, 14.5, 22.4, 28.1, 28.8, 61.1, 68.7, 108.7, 115.3, 116.6, 117.1, 123.7, 126.4, 126.5, 126.9, 127.6, 128.6, 128.7 ,129.2, 129.9, 130.2, 130.4, 136.5, 144.2, 146.2, 149.3, 159.9, 167.6, 172.8; **MS** (ESI) m/z 506 $[M+H]^+$**HRMS** (ESI, m/z): calcd for $C_{33}H_{32}NO_4$ $[M+H]^+$506.15823, found 506.15942.

Ethyl 6-oxo-3-phenyl-1-(3,4,5-trimethoxyphenyl)-6H-pyrido[1,2-*a*]quinoline-5-carboxylate (3i)



Yellow solid, 209 mg (0.410), 82%, **R_f** = 0.6 (EtOAC/Hexane, 60:40); **MP** 169-171 ºC; **IR** ($CHCl_3$) 762, 1126, 1216, 1454, 1594, 1717, 2922, 2958 cm^{-1}; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 1.47 (t, *J* = 7.1 Hz, 3H), 3.69 (s, 6H), 3.88 (s, 3H), 4.52 (q, *J* = 7.1 Hz, 2H), 6.48 (s, 2H), 7.01 (d, *J* = 1.9 Hz, 1H), 7.15–7.25 (m, 2H), 7.40 (d, *J* = 6.6 Hz, 1H), 7.49–7.56 (m, 3H), 7.73 (dd, *J* = 7.6, 1.8 Hz, 2H), 8.00 (d, *J* = 1.9 Hz, 1H), 8.46 (d, *J* = 7.7 Hz, 1H); **^{13}C{1H}NMR** (101 MHz) δ 14.5, 56.3, 61.1, 61.4, 104.6, 109.3, 116.7, 117.7, 121.6, 123.3, 126.5, 126.9, 128.9, 129.3, 129.8, 130.0, 130.1, 133.2, 136.4, 137.9, 139.1, 145.8, 148.9, 153.9, 167.0, 172.6; **MS** (ESI) m/z 510 $[M+H]^+$**HRMS** (ESI, m/z): calcd for $C_{31}H_{28}NO_6$ $[M+H]^+$510.15823, found 510.15942.

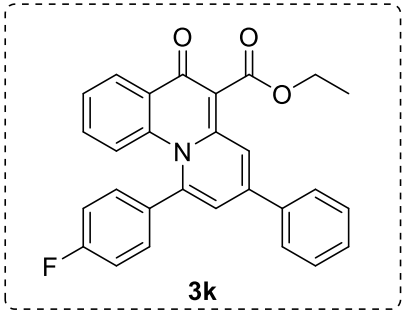
Ethyl 1-(4-chlorophenyl)-6-oxo-3-phenyl-6H-pyrido[1,2-*a*]quinoline-5-carboxylate (3j)



3j

Yellow solid, 143 mg (0.315 mmol), 63%, $\mathbf{R_f}$ = 0.6 (EtOAC/Hexane, 60:40); **MP** 163-165 ^{o}C; **IR** ($CHCl_3$) 769, 1093, 1460, 1597, 1715, 2921, 2957 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 1.47 (t, *J* = 7.1 Hz, 3H), 4.51 (q, *J* = 7.1 Hz, 2H), 6.96 (d, *J* = 2.0 Hz, 1H), 7.12 (d, *J* = 8.4 Hz, 1H), 7.16–7.21 (m, 1H), 7.23–7.25 (m, 1H), 7.34–7.37 (m, 2H), 7.41 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.44–7.55 (m, 4H), 7.70–7.73 (m, 2H), 8.07 (d, *J* = 2.0 Hz, 1H), 8.47 (dd, *J* = 8.0, 1.4 Hz, 1H); **^{13}C{1H}NMR** (75 MHz, $CDCl_3$) δ 14.5, 61.4, 117.5, 118.1, 123.6, 124.4, 126.6, 126.7, 126.8, 128.5, 128.7, 129.0, 129.3, 129.8, 130.1, 135.5, 136.2, 136.5, 137.2, 143.7,144.9, 149.0, 158.5, 172.8; **MS** (ESI) m/z 454 $[M+H]^+$**HRMS** (ESI, m/z): calcd for $C_{28}H_{21}ClNO_3$ $[M+H]^+$454.15823, found 454.15942.

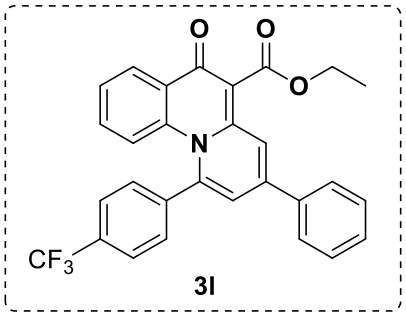
Ethyl 1-(4-fluorophenyl)-6-oxo-3-phenyl-6H-pyrido[1,2-*a*]quinoline-5-carboxylate (3k)



3k

Yellow solid, 155 mg (0.355 mmol), 71%, **R_f**= 0.6 (EtOAC/Hexane, 60:40); **MP** 151-153 ^oC; **IR** ($CHCl_3$) 765, 1156, 1220, 1458, 1596, 1719, 2921, 2957 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.47 (t, *J* = 7.1 Hz, 3H), 4.51 (q, *J* = 7.1 Hz, 2H), 6.96 (d, *J* = 1.9 Hz, 1H), 7.08 (t, *J* = 8.5 Hz, 2H), 7.11–7.16 (m, 2H), 7.28–7.32 (m, 2H), 7.40 (t, *J* = 7.3 Hz, 1H), 7.48–7.54 (m, 3H), 7.72 (dd, *J* = 8.0, 1.5 Hz, 2H), 8.06 (d, *J* = 1.9 Hz, 1H), 8.47 (d, *J* = 7.9 Hz, 1H); **^{13}C{1H}NMR** (101 MHz) δ 14.5, 61.4, 108.9, 116.6, 116.8, 117.3, 117.9, 123.7, 126.6, 126.8, 126.9, 128.4, 128.9, 129.2, 129.3, 130.1, 134.6, 136.3, 137.9, 144.0, 145.0, 149.0, 159.7, 168.0; **MS** (ESI) m/z 438 $[M+H]^+$**HRMS** (ESI, m/z): calcd for $C_{28}H_{21}FNO_3$ $[M+H]^+$438.15823, found 438.15942.

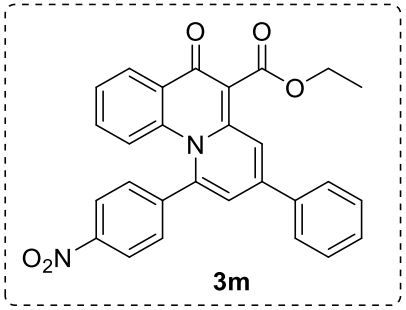
Ethyl 6-oxo-3-phenyl-1-(4-(trifluoromethoxy)phenyl)-6H-pyrido[1,2-*a*]quinoline-5-carboxylate (3l)



3l

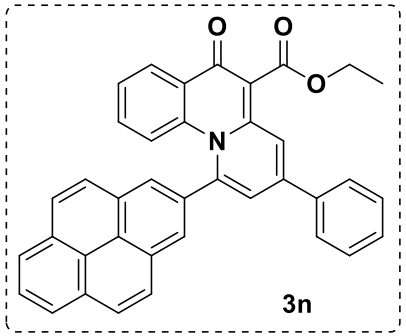
Yellow solid, 97 mg (0.200 mmol), 40%, **R_f** = 0.6 (EtOAC/Hexane, 60:40); **MP** 153-155 ^oC; **IR** ($CHCl_3$) 767, 1131, 1311, 1514, 1597, 1677, 1723, 2853, 2922, 2956 cm^{-1}; **^{1}H NMR** (400 MHz) δ 1.47 (t, *J* = 7.1 Hz, 3H), 4.53 (q, *J* = 7.1 Hz, 2H), 7.01 (d, *J* = 2.0 Hz, 1H), 7.08 (d, *J* = 7.8 Hz, 1H), 7.14 (dd, *J* = 4.6, 1.2 Hz, 2H), 7.37–7.41 (m, 1H), 7.46–7.52 (m, 4H), 7.69–7.73 (m, 2H), 7.82 (dd, *J* = 5.3, 3.2 Hz, 1H), 7.88 (d, *J* = 7.4 Hz, 1H), 8.11 (d, *J* = 2.0 Hz, 1H), 8.48 (d, *J* = 7.8 Hz, 1H); **^{13}C{1H}NMR** (101 MHz, $CDCl_3$) δ 31.9, 61.6, 118.4, 118.5, 122.2, 126.8, 126.9, 127.1, 127.4, 128.5, 128.7, 129.3, 129.4, 129.6, 130.2, 130.8, 132.3, 132.6, 133.6, 135.9, 137.0, 142.1, 148.4, 167.8, 171.5; **MS** (ESI) m/z 487 $[M+H]^+$**HRMS** (ESI, m/z): calcd for $C_{29}H_{21}F_3NO_3$ $[M+H]^+$488.14680, found 488.14556.

Ethyl 1-(4-nitrophenyl)-6-oxo-3-phenyl-6H-pyrido[1,2-*a*]quinoline-5-carboxylate (3m)



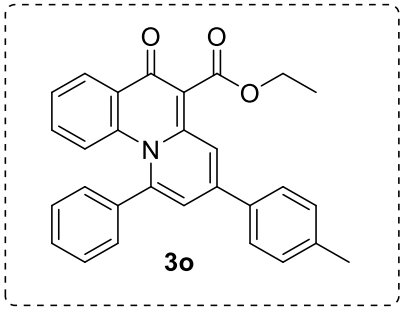
Yellow solid, 125 mg (0.270 mmol), 54%, $\mathbf{R_f}$ = 0.6 (EtOAC/Hexane, 60:40); **MP** 165-167 ºC; **IR** ($CHCl_3$) 700, 1291, 1346, 1463, 1598, 1643, 1726, 2200, 2920, 2957 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.47 (t, *J* = 7.1 Hz, 3H), 4.51 (q, *J* = 8.5 Hz, 2H), 7.00 (d, *J* = 8.5 Hz, 1H), 7.05 (d, *J* = 1.9 Hz, 1H), 7.17–7.21 (m, 1H), 7.42–7.46 (m, 1H), 7.48–7.54 (m, 5H), 7.69–7.75 (m, 2H), 8.10–8.12 (m, 1H), 8.24 (d, *J* = 8.9 Hz, 2H), 8.48 (dd, *J* = 8.0, 1.4 Hz, 1H); **^{13}C{1H}NMR** (126 MHz, $CDCl_3$) δ 14.5, 61.5, 109.9, 118.7, 119.1, 123.4, 124.8, 126.7, 126.8, 126.9, 127.0, 128.0, 128.4, 128.6, 129.4, 130.1, 130.3, 133.5, 135.9, 143.1, 143.5, 147.8, 148.5, 167.0; **MS** (ESI) m/z 465 $[M+H]^+$**HRMS** (ESI, m/z): calcd for $C_{28}H_{21}N_2O_5$ $[M+H]^+$465.18563, found 465.18573.

Ethyl 6-oxo-3-phenyl-1-(pyren-2-yl)-6H-pyrido[1,2-*a*]quinoline-5-carboxylate (3n)



Yellow solid, 85 mg (0.149 mmol), 31%, **R_f** = 0.4 (EtOAC/Hexane, 60:40); **MP** 166-168 ^oC; **IR** ($CHCl_3$) 763, 1062, 1218, 1458, 1596, 1614, 1722, 2922, 2956 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.52 (t, *J* = 7.1 Hz, 3H), 4.58 (q, *J* = 7.1 Hz, 2H), 6.64–6.70 (m, 1H), 7.10 (d, *J* = 8.7 Hz, 1H), 7.13–7.18 (m, 1H), 7.20–7.24 (m, 1H), 7.45–7.56 (m, 3H), 7.74–7.81(m, 2H), 7.87 (d, *J* = 8.0 Hz, 1H), 8.03–8.11 (m, 4H), 8.16 (dd, *J* = 10.4, 8.5 Hz, 2H), 8.19–8.24 (m, 2H), 8.27 (d, *J* = 7.6 Hz, 1H), 8.41 (dd, *J* = 8.0, 1.5 Hz, 1H); **^{13}C{1H}NMR** (101 MHz, $CDCl_3$) δ 14.5, 61.4, 109.5, 117.8, 119.5, 122.2, 122.8, 124.5, 125.3, 126.0, 126.3, 126.5, 126.7, 126.9, 127.2, 128.9, 129.3, 129.8, 130.2, 130.7, 131.3, 131.9, 132.4, 136.3, 137.3, 143.8, 144.9, 148.9, 167.7, 172.7; **MS** (ESI) m/z 544 $[M+H]^+$**HRMS** (ESI, m/z): calcd for $C_{38}H_{26}NO_3$ $[M+H]^+$544.19072, found 544.19226.

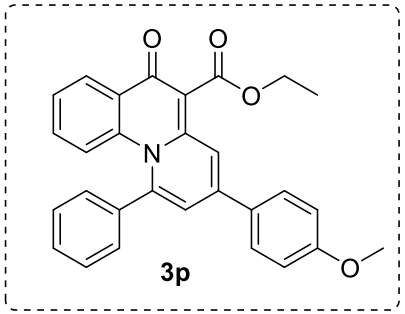
Ethyl 6-oxo-1-phenyl-3-p-tolyl-6H-pyrido[1,2-a]quinoline-5-carboxylate (3o)



3o

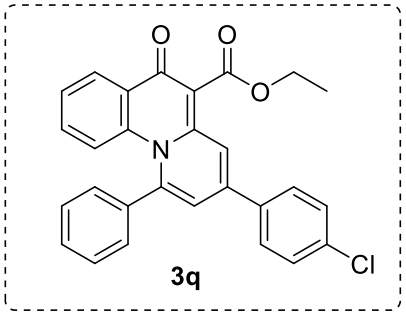
Orange solid, 180 mg (0.415 mmol), 83%, **R_f** = 0.3 (EtOAC/Hexane, 60:40); **MP** 169-171 ^oC; **IR** (KBr) cm^{-1} 767, 1224, 1460, 1526, 1611, 1687, 1727, 2922, 2972; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 1.47 (t, *J* = 7.1 Hz, 3H), 2.43 (s, 3H), 4.52 (q, *J* = 7.1 Hz, 2H), 6.99 (d, *J* = 2.0 Hz, 1H), 7.08–7.16 (m, 2H), 7.29–7.33 (m, 4H), 7.35–7.40 (m, 4H), 7.63 (d, *J* = 8.2 Hz, 2H), 8.04 (d, *J* = 2.0 Hz, 1H), 8.46 (dd, *J* = 7.9, 1.4 Hz, 1H); **^{13}C{1H}NMR** (101 MHz, $CDCl_3$) δ 14.5, 21.4, 61.4, 108.9, 117.0, 117.4, 123.8, 126.4, 126.5, 126.8, 127.3, 128.7, 129.3, 129.5, 130.0, 130.4, 133.4, 137.4, 138.2, 140.5, 143.9, 145.8, 149.2, 167.5, 172.9; **MS** (ESI) m/z 434 $[M+H]^+$**HRMS** (ESI, m/z): calcd for $C_{29}H_{24}NO_3$ $[M+H]^+$ 434.17507, found 434.17329.

Ethyl 3-(4-methoxyphenyl)-6-oxo-1-phenyl-6H-pyrido[1,2-a]quinoline-5-carboxylate (3p)



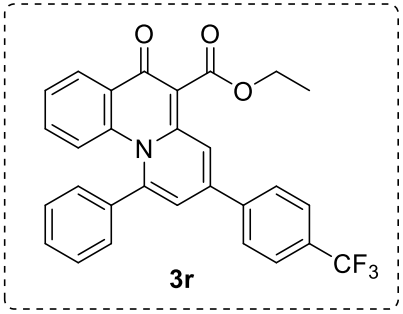
Yellow solid, 196 mg (0.450), 87%, $\mathbf{R_f}$ = 0.3 (EtOAC/Hexane, 60:40); **MP** 152-154 ºC; **IR** ($CHCl_3$) 720, 1286, 1462, 1516, 1600, 1727, 2923, 2957 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.48 (t, *J* = 7.1 Hz, 3H), 3.88 (s, 3H), 4.52 (q, *J* = 7.1 Hz, 2H), 6.99 (d, *J* = 2.1 Hz, 1H), 7.01–7.06 (m, 2H), 7.07–7.18 (m, 2H), 7.29–7.32 (m, 2H), 7.34–7.40 (m, 4H), 7.67–7.73 (m, 2H), 8.02 (d, *J* = 2.0 Hz, 1H), 8.43–8.48 (m, 1H); **^{13}C{1H}NMR** (101 MHz) δ 14.5, 55.5, 61.3, 108.5, 113.5, 114.7, 116.2, 117.2, 123.7, 126.4, 126.5, 127.3, 128.3, 128.6, 129.3, 129.4, 130.3, 137.4, 138.2, 143.5, 145.8, 149.3, 161.3, 167.7, 172.9; **MS** (ESI) m/z 450 $[M+H]^+$ **HRMS** (ESI, m/z): calcd for $C_{29}H_{24}NO_4$ $[M+H]^+$450.16998, found 450.16938.

Ethyl 3-(4-chlorophenyl)-6-oxo-1-phenyl-6H-pyrido[1,2-*a*]quinoline-5-carboxylate (3q)



Yellow solid, 190 mg (0.420 mmol), 84 %, **R_f** = 0.4 (EtOAC/Hexane, 60:40); **MP** 158-160 ^oC; **IR** (KBr) cm^{-1} 768, 1225, 1459, 1529, 1601, 1689, 1732, 2851, 2930; ^1H NMR (400 MHz, $CDCl_3$) δ 1.47 (t, *J* = 7.1 Hz, 3H), 4.52 (q, *J* = 7.1 Hz, 2H), 6.93 (d, *J* = 2.1 Hz, 1H), 7.10–7.15 (m, 2H), 7.28–7.32 (m, 2H), 7.35–7.43 (m, 4H), 7.45–7.52 (m, 2H), 7.61–7.72 (m, 2H), 8.07 (d, *J* = 2.1 Hz, 1H), 8.42–8.50 (m, 1H); **^{13}C{1H}NMR** (101 MHz, CDCl3) δ 14.5, 61.4, 109.1, 116.9, 117.7, 123.8, 126.5, 126.6, 127.3, 128.2, 128.4, 128.6, 128.8, 129.5, 130.4, 134.8, 136.3, 137.4, 137.9, 142.7, 146.1, 149.0, 167.6, 172.9; **MS** (ESI) m/z 454, $[M+H]^+$**HRMS** (ESI, m/z): calcd for $C_{28}H_{21}ClNO_3$ $[M+H]^+$ 454.12045, found 454.12051

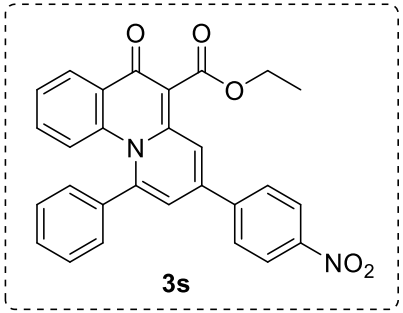
Ethyl 3-(4-(trifluoromethyl)phenyl)-6-oxo-1-phenyl-6H-pyrido[1,2-*a*]quinoline-5-carboxylate (3r)



3r

Yellow solid, 204 mg (0.420 mmol), 84%, **R_f** = 0.5 (EtOAC/Hexane, 60:40); **MP** 163-165 ^oC; **IR** (KBr) cm^{-1}764, 1135, 1329, 1535, 1686, 1734, 2937, 2972; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.47 (t, *J* = 7.1 Hz, 3H), 4.52 (q, *J* = 7.1 Hz, 2H), 6.95 (d, *J* = 2.0 Hz, 1H), 7.11–7.18 (m, 2H), 7.28–7.33 (m, 2H), 7.36–7.43 (m, 4H), 7.77 (d, *J* = 8.3 Hz, 2H), 7.83 (d, *J* = 8.2 Hz, 2H), 8.10 (d, *J* = 2.0 Hz, 1H), 8.46 (dd, *J* = 7.9, 1.1 Hz, 1H); **^{13}C{1H}NMR** (101 MHz, $CDCl_3$) δ 14.5, 61.5, 109.5, 116.8, 118.8, 122.5, 123.8, 126.3 (*J* = 4 Hz), 126.6, 126.7, 127.3 (*J* = 12 Hz), 128.9, 129.5, 129.6, 130.5, 131.9, 137.4, 137.9, 140.0, 142.5, 146.3, 147.1, 148.9, 167.5, 173.0; **MS** (ESI) m/z 488 $[M+H]^+$**HRMS** (ESI, m/z): calcd for $C_{29}H_{21}F_3NO_3$ $[M+H]^+$ 488.14680, found 488.14368.

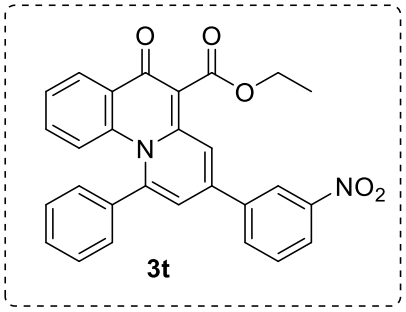
Ethyl 3-(4-nitrophenyl)-6-oxo-1-phenyl-6H-pyrido[1,2-*a*]quinoline-5-carboxylate (3s)



3s

Yellow solid, 179 mg (0.385 mmol), 77 %, $\mathbf{R_f}$ = 0.5 (EtOAC/Hexane, 60:40); **MP** 168-170 ^{o}C; **IR** (KBr) cm^{-1} 766, 1344, 1458, 1597, 1689, 1731, 2849, 2931; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.47 (t, *J* = 2.1 Hz, 3H), 4.5 (q, *J* = 2.1 Hz, 2H), 6.93 (d, *J* = 2.1 Hz, 1H), 7.12–7.18 (m, 2H), 7.30–7.32 (m, 2H), 7.36–7.43 (m, 4H), 7.87–7.91 (m, 2H), 8.17 (d, *J* = 2.0 Hz, 1H), 8.35–8.39 (m, 2H), 8.46 (dd, *J* = 8.0, 0.9 Hz, 1H); **^{13}C{1H}NMR** (101 MHz, $CDCl_3$) δ 14.5, 61.5, 109.6, 116.3, 118.9, 121.7, 123.8, 124.5, 126.6, 126.9, 127.3, 129.0, 129.6, 129.7, 130.5, 132.7, 137.4, 137.7, 138.3, 141.4, 146.6, 148.9, 167.4, 173.1; **MS** (ESI) m/z 465 $[M+H]^+$**HRMS** (ESI, m/z): calcd for $C_{28}H_{21}N_2O_5$ $[M+H]^+$465.14450, found 465.14292.

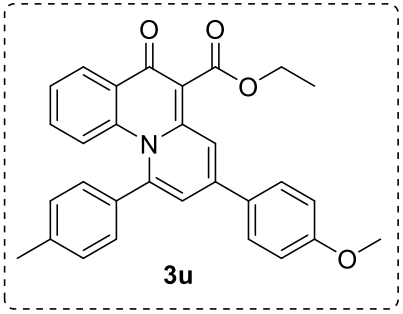
Ethyl 3-(3-nitrophenyl)-6-oxo-1-phenyl-6H-pyrido[1,2-*a*]quinoline-5-carboxylate (3t)



3t

Yellow solid, 167 mg (0.360 mmol), 72%, **R_f** = 0.4 (EtOAC/Hexane, 60:40); **MP** 174-176 ^oC; **IR** (KBr) cm^{-1} 770, 1350, 1532, 1685, 1727, 2976; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 1.48 (t, *J* = 7.1 Hz, 3H), 4.53 (q, *J* = 7.1 Hz, 2H), 6.97 (d, *J* = 2.1 Hz, 1H), 7.13–7.20 (m, 2H), 7.32–7.35 (m, 2H), 7.37–7.45 (m, 4H), 7.73 (t, *J* = 8.0 Hz, 1H), 8.05–8.10 (m, 1H), 8.15 (d, *J* = 2.0 Hz, 1H), 8.32–8.37 (m, 1H), 8.46 (dd, *J* = 7.9, 1.1 Hz, 1H), 8.56 (t, *J* = 1.9 Hz, 1H); **^{13}C{1H}NMR** (101 MHz, $CDCl_3$) δ 14.5, 61.5, 109.6, 116.3, 118.8, 121.7, 123.8, 124.5, 126.8, 126.9, 127.0, 127.3, 129.0, 129.6, 129.7, 130.5, 132.7, 137.4, 137.7, 138.3, 141.4, 146.6, 148.7, 148.9, 167.3, 173.1; **MS** (ESI) m/z 465 $[M+H]^+$**HRMS** (ESI, m/z): calcd for $C_{28}H_{21}N_2O_5$ $[M+H]^+$ 465.14450, found 465.14214.

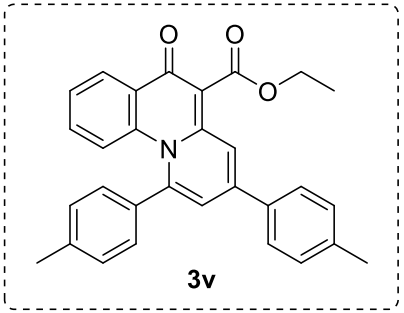
Ethyl 3-(4-methoxyphenyl)-6-oxo-1-(*p*-tolyl)-6H-pyrido[1,2-*a*]quinoline-5-carboxylate (3u)



3u

Yellow solid, 211 mg (0.450 mmol), 91%, **R_f** = 0.6 (EtOAC/Hexane, 60:40); **MP** 164-166 ^oC; **IR** ($CHCl_3$) 763, 1181, 1253, 1456, 1515, 1596, 1718, 2921, 2957 cm^{-1}; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 1.46 (t, *J* = 7.1 Hz, 3H), 2.38 (s, 3H), 3.87 (d, *J* = 8.1 Hz, 3H), 4.5 (q, *J* = 6.0 Hz,, 2H), 6.93–6.98 (m, 1H), 7.02 (d, *J* = 8.8 Hz, 2H), 7.09–7.22 (m, 6H), 7.37 (t, *J* = 6.8 Hz, 1H), 7.69 (d, *J* = 8.8 Hz, 2H), 8.01 (d, *J* = 2.0 Hz, 1H), 8.45 (d, *J* = 7.8 Hz, 1H); **^{13}C{1H}NMR** (101 MHz, $CDCl_3$) δ 14.5, 21.3, 55.5, 61.2, 108.4, 113.8, 114.7, 115.9, 116.9, 123.7, 126.3, 126.40, 127.1, 128.3, 128.6, 130.0, 130.3, 135.3, 137.5, 139.6, 143.7, 146.0, 149.3, 161.3, 167.7, 172.7; **MS** (ESI) m/z 464 $[M+H]^+$**HRMS** (ESI, m/z): calcd for $C_{30}H_{26}NO_4$ $[M+H]^+$464.18563, found 464.18573.

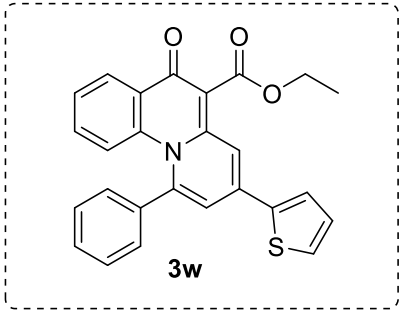
Ethyl 6-oxo-1,3-dip-tolyl-6H-pyrido[1,2-*a*]quinoline-5-carboxylate (3v)



3v

Yellow solid, 199 mg (0.445 mmol), 89 %, $\mathbf{R_f}$ = 0.6 (EtOAC/Hexane, 60:40); **MP** 170-172 ^{o}C; **IR** (KBr) cm^{-1} 765, 1171, 1285, 1460, 1599, 1731, 2929; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 1.47 (t, *J* = 7.1 Hz, 3H), 2.38 (s, 3H), 2.43 (s, 3H), 4.52 (q, *J* = 7.1 Hz, 2H), 6.96 (d, *J* = 1.8 Hz, 1H), 7.08–7.19 (m, 5H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.38 (t, *J* = 7.4 Hz, 2H), 7.63 (d, *J* = 8.1 Hz, 2H), 8.03 (d, *J* = 1.7 Hz, 1H), 8.46 (d, *J* = 7.8 Hz, 1H); **^{13}C{1H}NMR** (101 MHz, $CDCl_3$) δ 29.7, 61.3, 79.3, 105.2, 115.4, 115.9, 115.7, 118.2, 119.7, 121.8, 125.1, 125.3, 127.2, 127.4, 127.5, 128.5, 129.8, 130.9, 131.2, 131.3, 131.6, 138.5, 150.0, 152.9, 161.4, 163.8; **MS** (ESI) m/z 448 $[M+H]^+$**HRMS** (ESI, m/z): calcd for $C_{30}H_{26}NO_3$ $[M+H]^+$ 448.19072, found 448.18844.

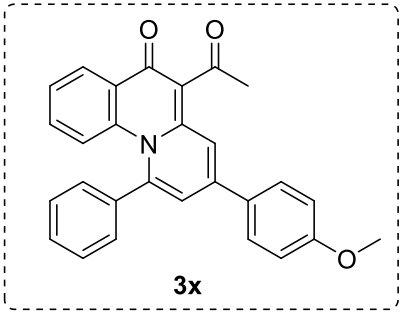
Ethyl 6-oxo-1-phenyl-3-(thiophen-2-yl)-6H-pyrido[1,2-*a*]quinoline-5-carboxylate (3w)



3w

Yellow solid, 0.196 mg (0.460 mmol), 92%, **R_f** = 0.4 (EtOAC/Hexane, 60:40); **MP** 160-162 ^oC; **IR** (KBr) cm^{-1} 762, 1226, 1459, 1529, 1604, 1692, 1727, 2855, 2946; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 1.49 (t, *J* = 7.1 Hz, 3H), 4.53 (q, *J* = 7.1 Hz, 2H), 6.94 (d, *J* = 1.9 Hz, 1H), 7.10 (d, *J* = 3.8 Hz, 2H), 7.15–7.20 (m, 1H), 7.28–7.33 (m, 2H), 7.34–7.42 (m, 4H), 7.50 (d, *J* = 5.1 Hz, 1H), 7.58 (d, *J* = 3.7 Hz, 1H), 8.02 (s, 1H), 8.44 (d, *J* = 7.9 Hz, 1H); **^{13}C{1H}NMR** (101 MHz, $CDCl_3$) δ 14.6, 61.4, 108.9, 115.4, 116.0, 123.6, 126.2, 126.4, 126.6, 127.0, 127.3, 127.8, 128.8, 129.5, 130.4, 137.3, 137.4, 137.9, 139.9, 145.8, 148.8, 148.9, 167.4, 172.9; **MS** (ESI) m/z 426 $[M+H]^+$**HRMS** (ESI, m/z): calcd for $C_{26}H_{20}NO_3S$ $[M+H]^+$ 426.11584, found 426.11603

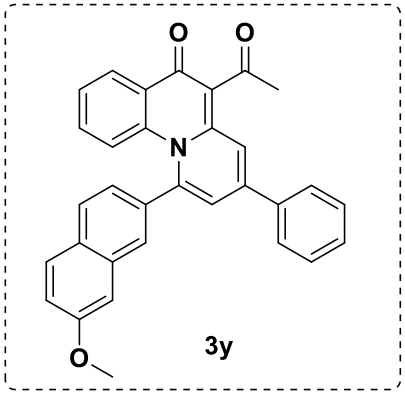
5-Acetyl-3-(4-methoxyphenyl)-1-phenyl-6H-pyrido[1,2-*a*]quinolin-6-one (3x)



3x

Yellow solid, 191 mg (0.450 mmol), 91%, **R_f** = 0.4(EtOAC/Hexane, 60:40); **MP** 162-164 ^oC; **IR** ($CHCl_3$) 766, 1255, 1383, 1440, 1599, 1726, 2919, 2957 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 2.83 (s, 3H), 3.89 (s, 3H), 6.91 (t, *J* = 9.2 Hz, 1H), 7.02 (d, *J* = 8.8 Hz, 2H), 7.09–7.13 (m, 3H), 7.30–7.32 (m, 2H), 7.36–7.41 (m, 3H), 7.77 (d, *J* = 8.8 Hz, 2H), 8.41 (d, *J* = 7.6 Hz, 1H), 8.94 (t, *J* = 6.4 Hz, 1H); **^{13}C{1H}NMR** (126 MHz, $CDCl_3$) δ 33.4, 55.8, 113.6, 113.9, 114.7, 116.9, 117.8, 124.1, 126.3, 126.7, 127.5, 128.2, 128.6, 128.8, 129.5, 131.1, 137.2, 138.5, 144.9, 146.1, 150.7, 161.5, 175.1, 201.1; **MS** (ESI) m/z 420 $[M+H]^+$**HRMS** (ESI, m/z): calcd for $C_{28}H_{22}NO_3$ $[M+H]^+$420.15942, found 420.15816.

5-Acetyl-1-(6-methoxynaphthalen-2-yl)-3-phenyl-6H-pyrido[1,2-*a*]quinolin-6-one (3y)



Yellow solid, 145 mg (0.310 mmol), 62%, $\mathbf{R_f}$ = 0.6 (EtOAC/Hexane, 60:40); **MP** 148-150 ^{o}C; **IR** ($CHCl_3$) 763, 1204, 1392, 1451, 1598, 1725, 2919, 2958 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.85 (s, 3H), 3.94 (s, 3H), 7.02–7.12 (m, 3H), 7.18–7.25 (m, 2H), 7.38 (dd, *J* = 13.4, 6.1 Hz, 2H), 7.51 (t, *J* = 7.2 Hz, 3H), 7.62 (d, *J* = 8.6 Hz, 1H), 7.75 (d, *J* = 9.0 Hz, 1H), 7.82 (d, *J* = 6.6 Hz, 2H), 7.95 (s, 1H), 8.43 (d, *J* = 7.0 Hz, 1H), 8.95 (d, *J* = 1.9 Hz, 1H); **^{13}C{1H}NMR** (101 MHz, $CDCl_3$) δ 33.3, 55.4, 106.8, 114.4, 118.1, 118.2, 120.1, 123.9, 125.1, 126.2, 126.4, 126.8, 127.1, 127.8, 128.8, 129.2, 129.8, 130.1, 131.1, 132.2, 133.3, 134.7, 136.4, 137.9, 145.5, 146.4, 150.6, 158.9, 175.2, 201.02; **MS** (ESI) m/z 470 $[M+H]^+$**HRMS** (ESI, m/z): calcd for $C_{32}H_{24}NO_3$ $[M+H]^+$470.15823, found 470.15942.

8. Crystallographic data and ORTEP Diagram of 3o

Method of Crystallization: The crystals of compound **3o** were obtained using slow evaporation method in acetonitrile/ethanol (1:1) at room temperature. A single crystal was subjected to X-ray crystallographic data collection, analysis and the structure was determined as follows:

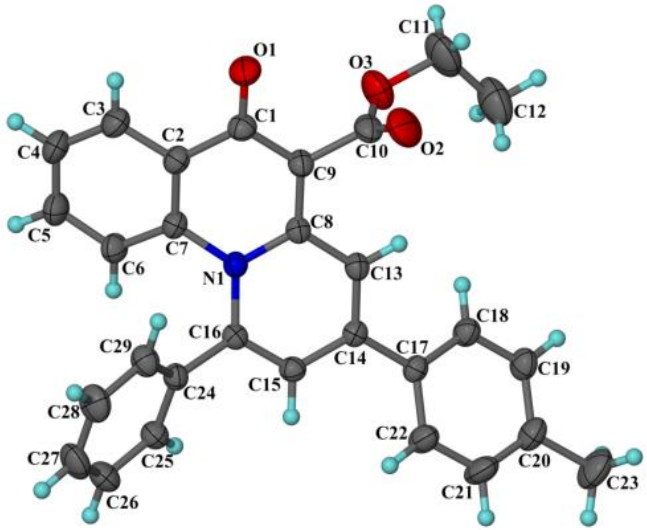


Figure caption: ORTEP diagram of 3o compound with the atom-numbering. Displacement ellipsoids are drawn at the 35% probability level and H atoms are shown as small spheres of arbitrary radius. Only the major component of the disordered ethyl ester atoms is shown for clarity purpose. **CCDC** deposition number 2128795 contains the supplementary crystallographic data for this paper which can be obtained free of charge at https://www.ccdc.cam.ac.uk/structures/

Crystal data for 3o: $C_{29}H_{23}NO_3$, M = 433.48, Monoclinic, Space group $P2_1/n$ (No.14), a = 11.493(4)Å, b = 14.034(6)Å, c = 14.667(6)Å, α = 90°, β = 102.249(10)°, γ = 90°, V = 2311.8(16)Å^3, Z = 4, D_c = 1.245 g/cm^3, F_{000} = 912, Bruker D8 QUEST PHOTON III C7, Mo-Kα radiation, λ = 0.71073 Å, T = 293(2)K, $2\theta_{max}$ = 56.6º, μ = 0.080 mm^{-1}, 22049 reflections collected,

5694 unique (R_{int} = 0.0563), 329 parameters, *R1* = 0.0541, *wR2* =0.1282, *R* indices based on 3145 reflections with I > 2σ(I) (refinement on F^2), Final *GooF* = 1.020, largest difference hole and peak = -0.167 and 0.188 e.$Å^{-3}$.

Data collection and Structure solution details: Single crystal X-ray data were collected at room temperature on a Bruker D8 QUEST equipped with a four-circle kappa diffractometer and Photon III C7 detector. An Iμs microfocus Mo source (λ=0.71073Å) supplied the multi-mirror monochromated incident beam. A combination of Phi and Omega scans were used to collect the necessary data. Integration and scaling of intensity data were accomplished using SAINT program.[4] The structures were solved by Direct Methods using SHELXS97[5-6] and refinement was carried out by full-matrix least-squares technique using SHELXL-2014/7.[5-6] Anisotropic displacement parameters were included for all non-hydrogen atoms. All H atoms were positioned geometrically and treated as riding on their parent C atoms, with C-H distances of 0.93--0.97 Å, and with Uiso(H) = 1.2Ueq (C) or 1.5Ueq for methyl atoms. Ethyl ester was disordered over two sites with site occupancy factors of 0.632(13) for major component (O3/C11/C12) and 0.368(13) for minor component (O3D/C11D/C12D) of the disordered atoms. Structural disorder was modelled using PART, FVAR, DFIX, DELU and SIMU instructions in the refinement which can be found in the supplementary CIF file. CCDC deposition number 2128795 contains the supplementary crystallographic data for this paper which can be obtained free of charge at https://www.ccdc.cam.ac.uk/structures/

9. References

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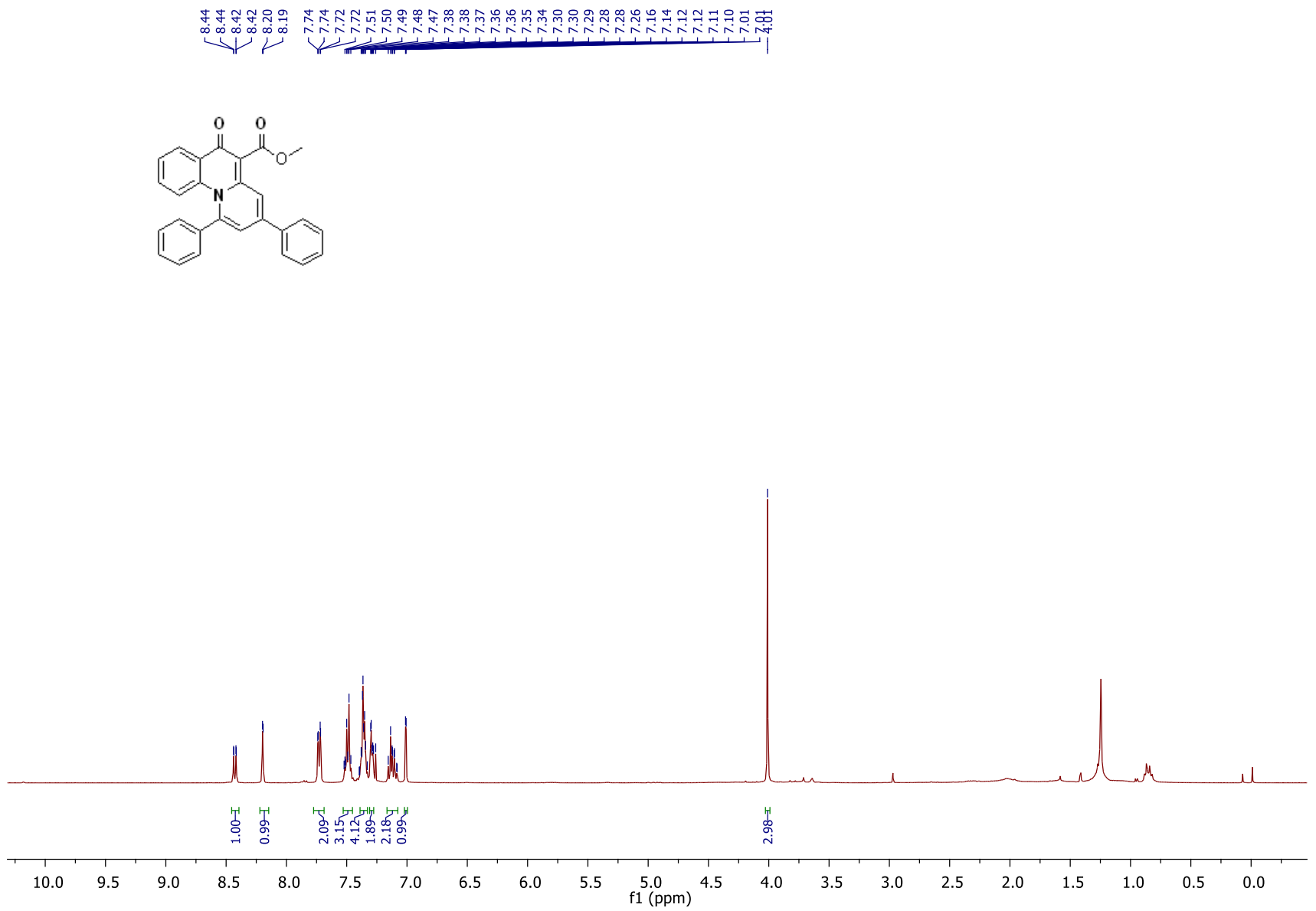
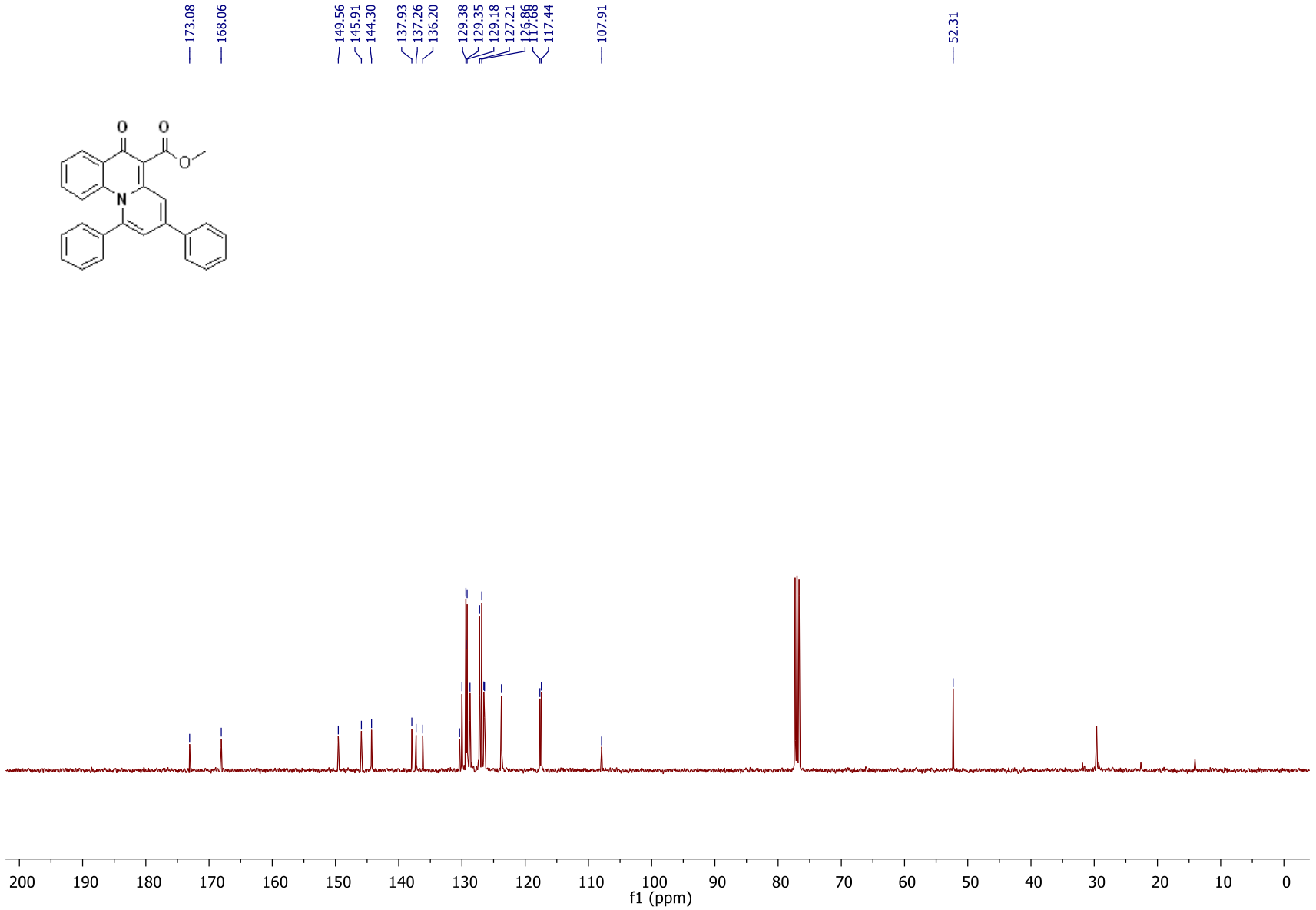
Copies of ^{1}H and ^{13}C NMR spectra of 3a-y

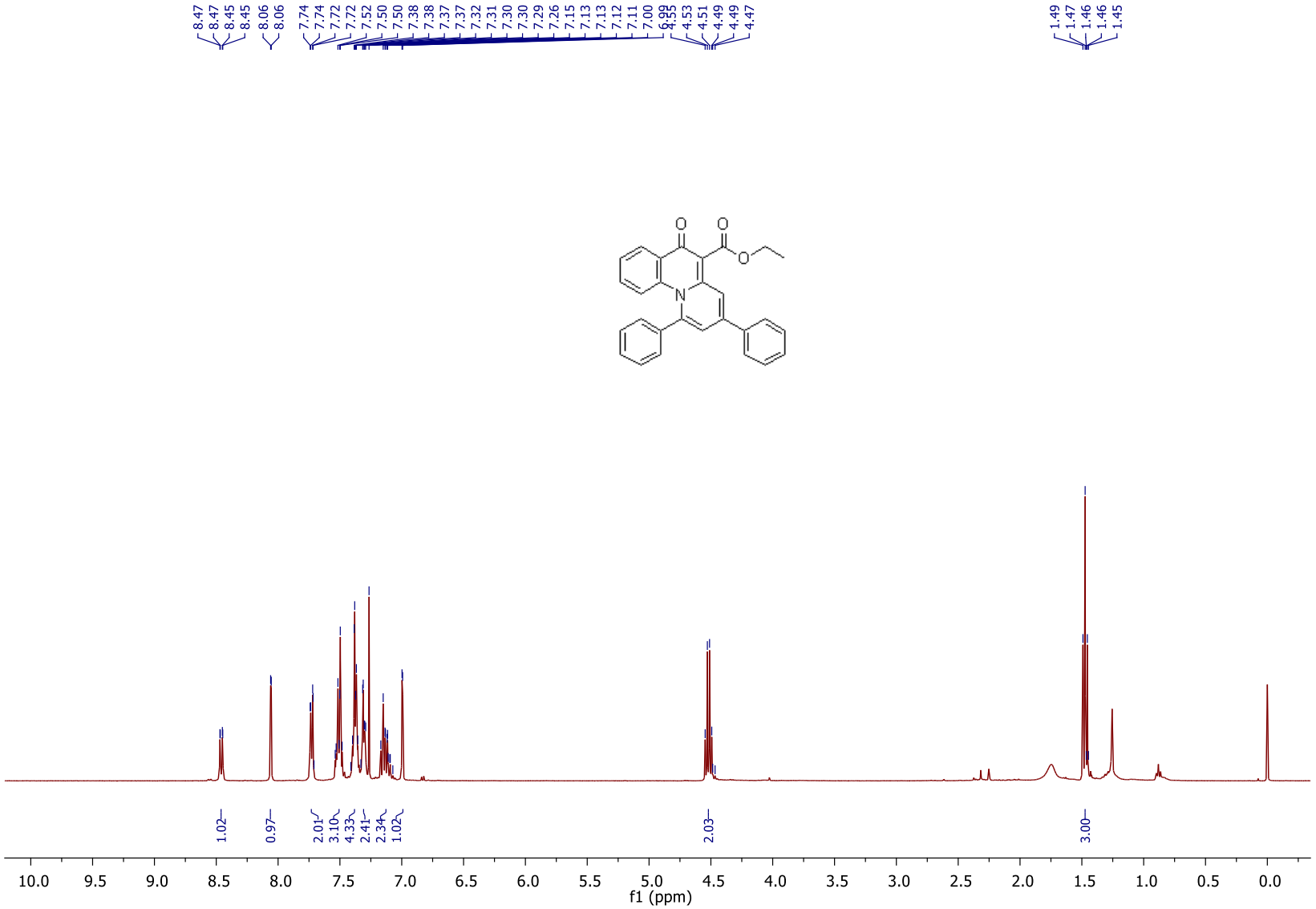
^{1}H NMR of **3a** (400 MHz, $CDCl_3$)



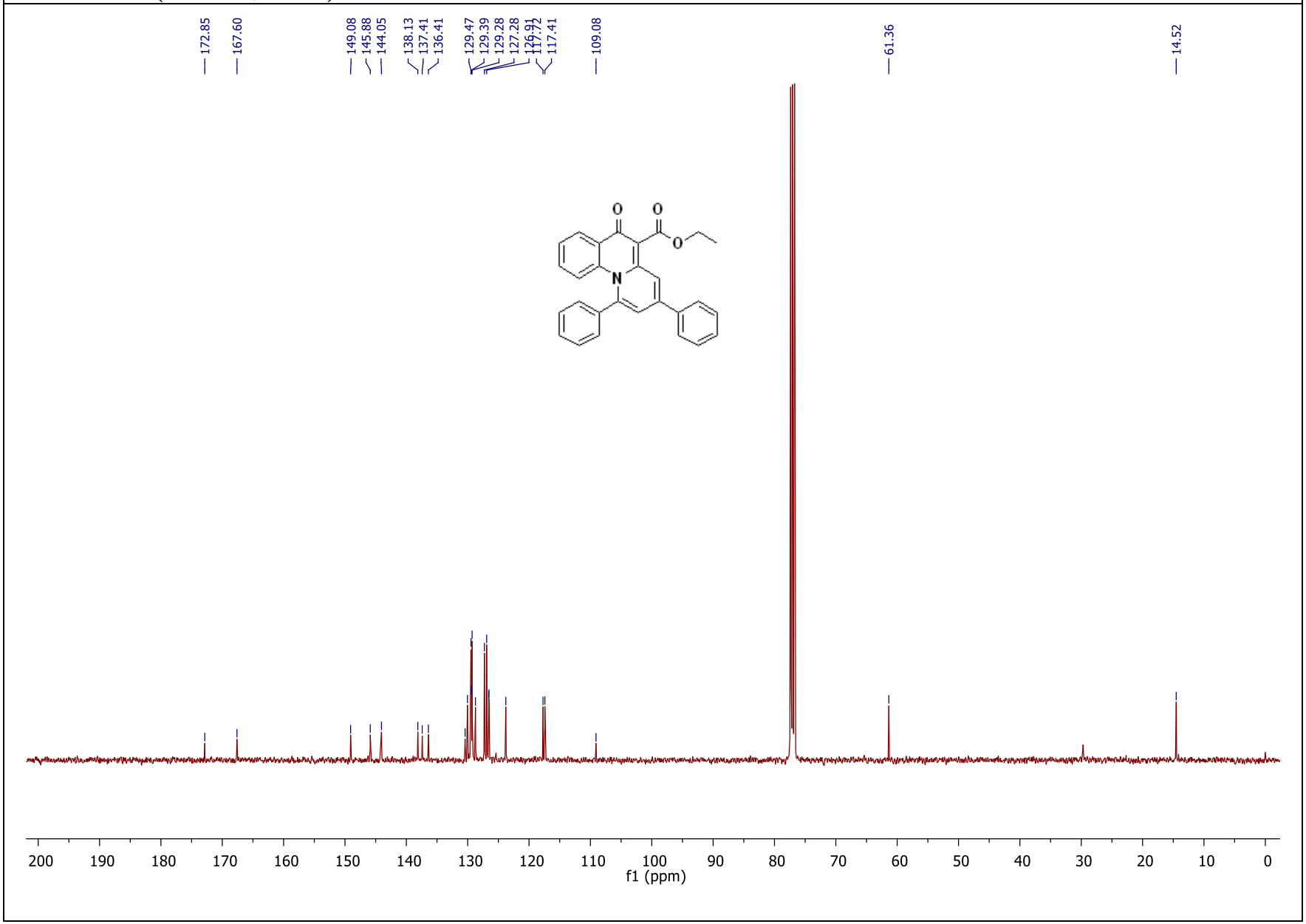
^{13}C NMR of **3a** (101 MHz, $CDCl_3$)



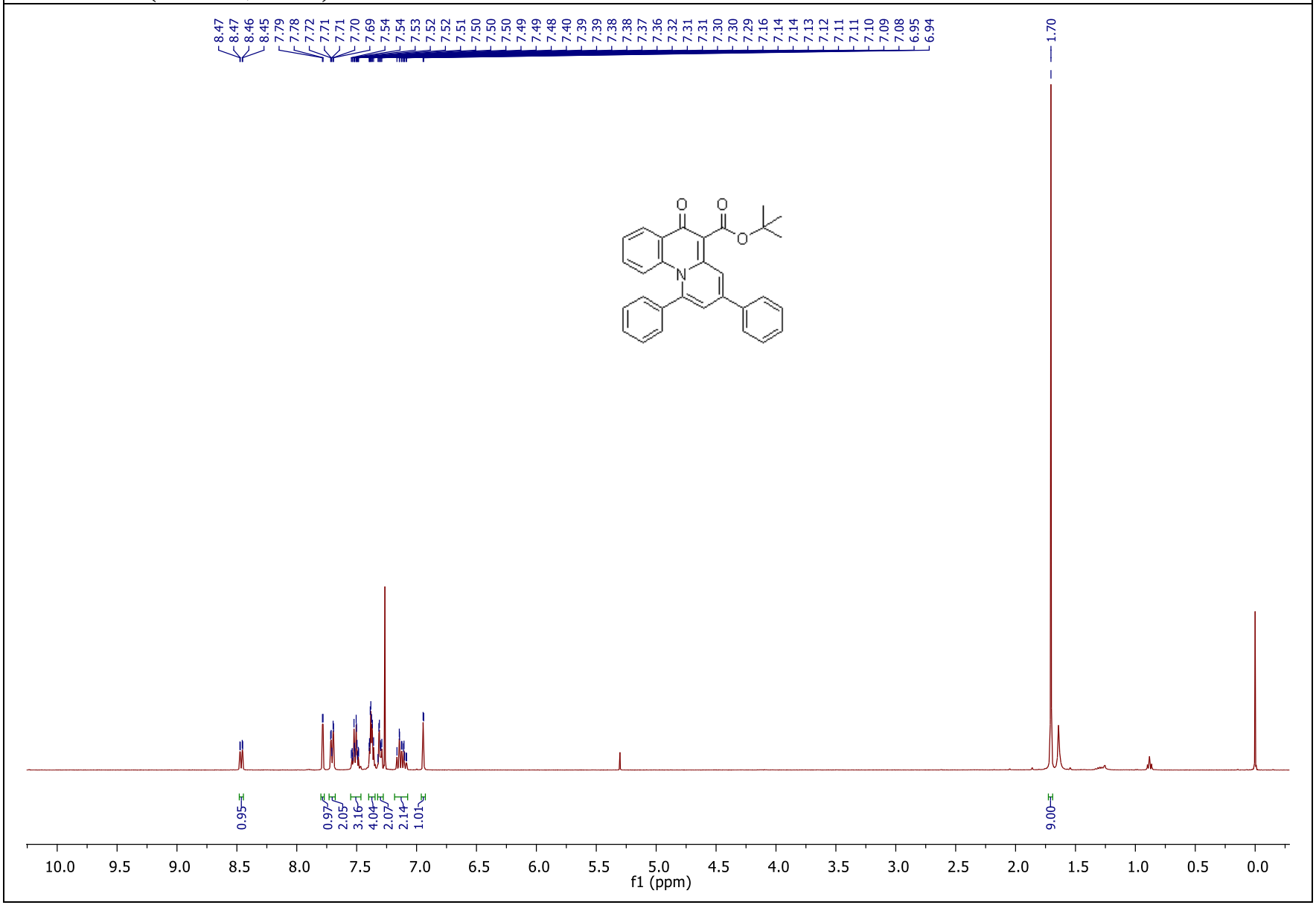
^{1}H NMR of **3b** (400 MHz, $CDCl_3$)



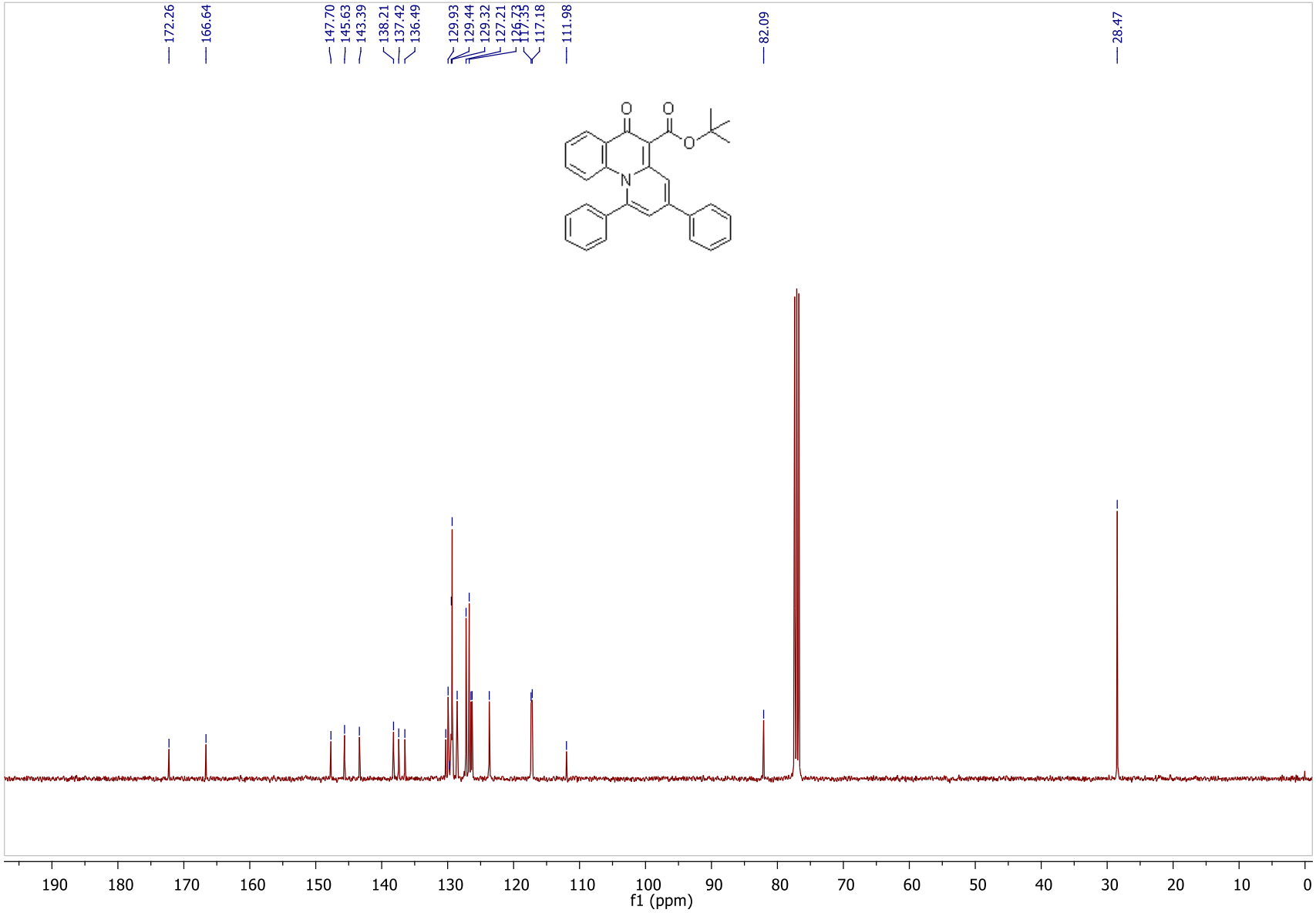
^{13}C NMR of **3b** (101 MHz, $CDCl_3$)



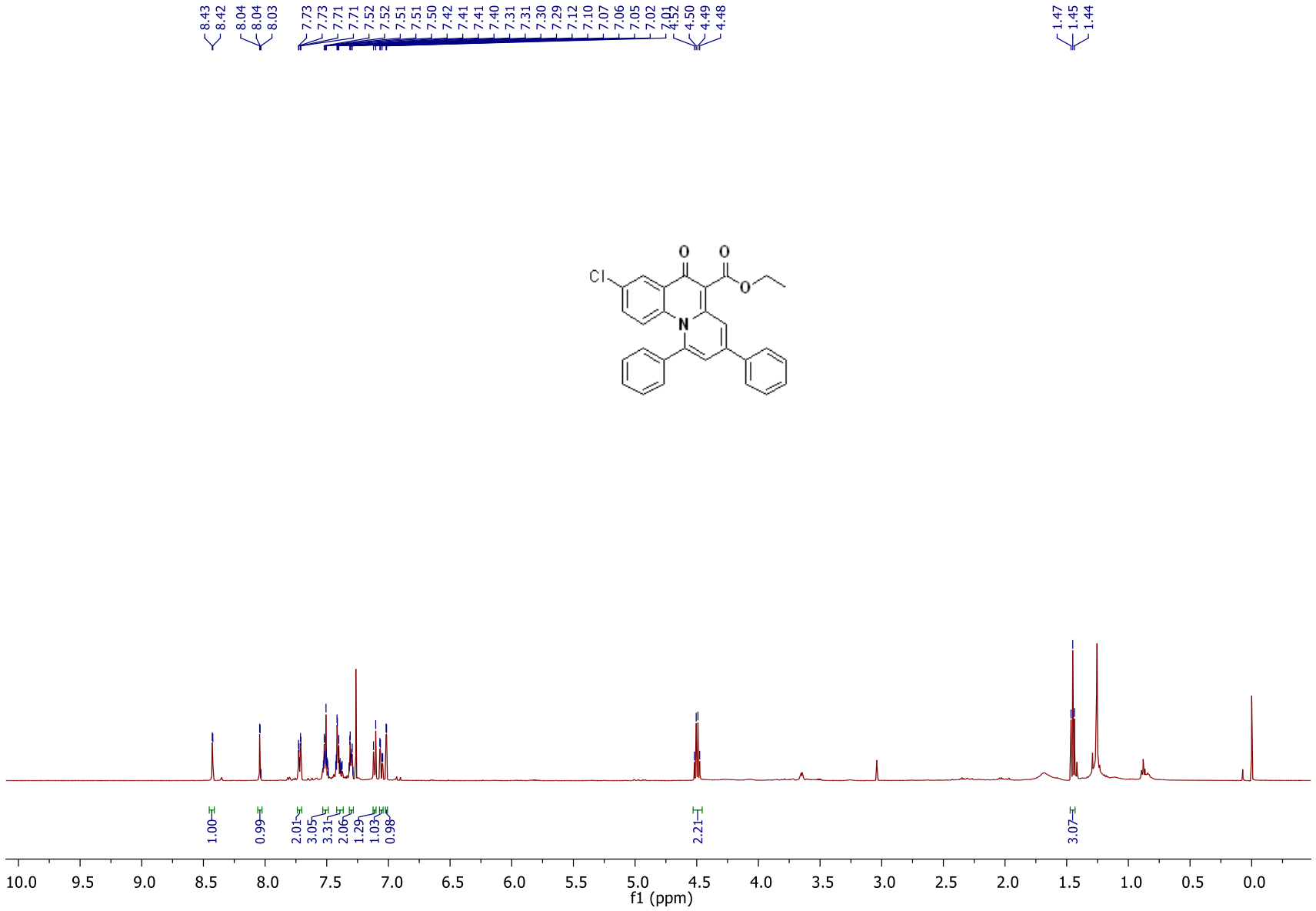
^{1}H NMR of **3c** (400 MHz, $CDCl_3$)



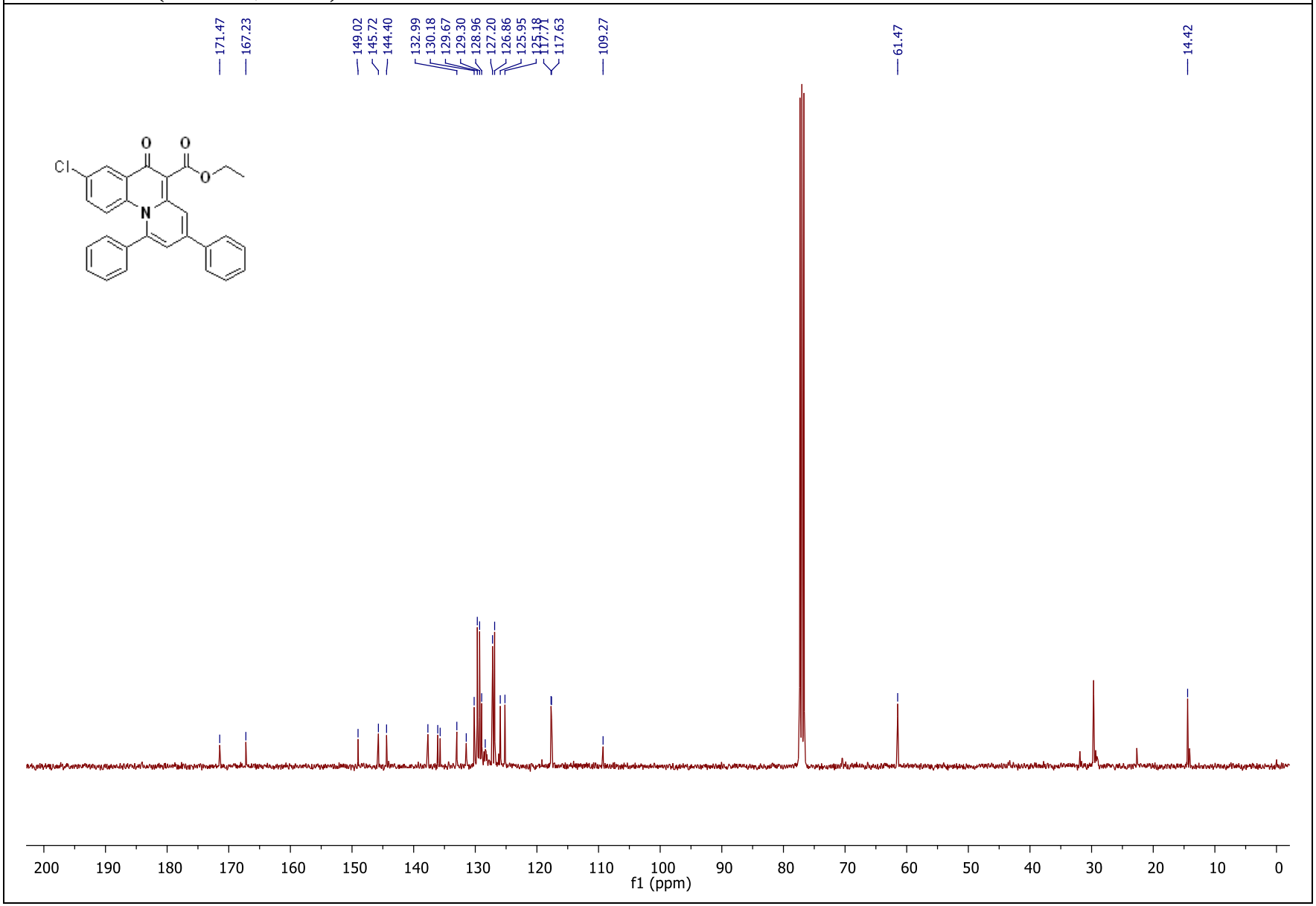
^{13}C NMR of **3c** (101 MHz, $CDCl_3$)



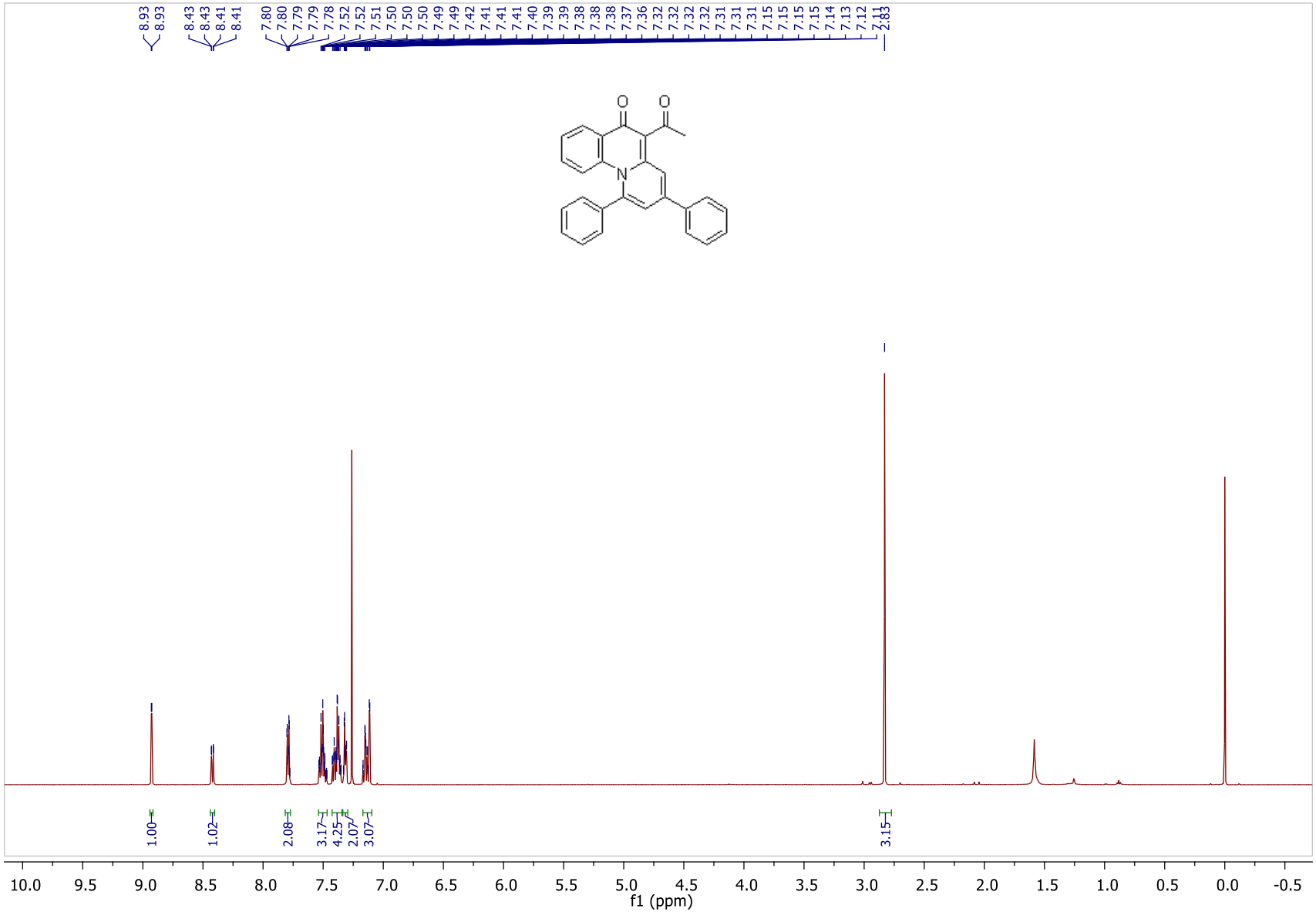
^{1}H NMR of **3d** (500 MHz, $CDCl_3$)



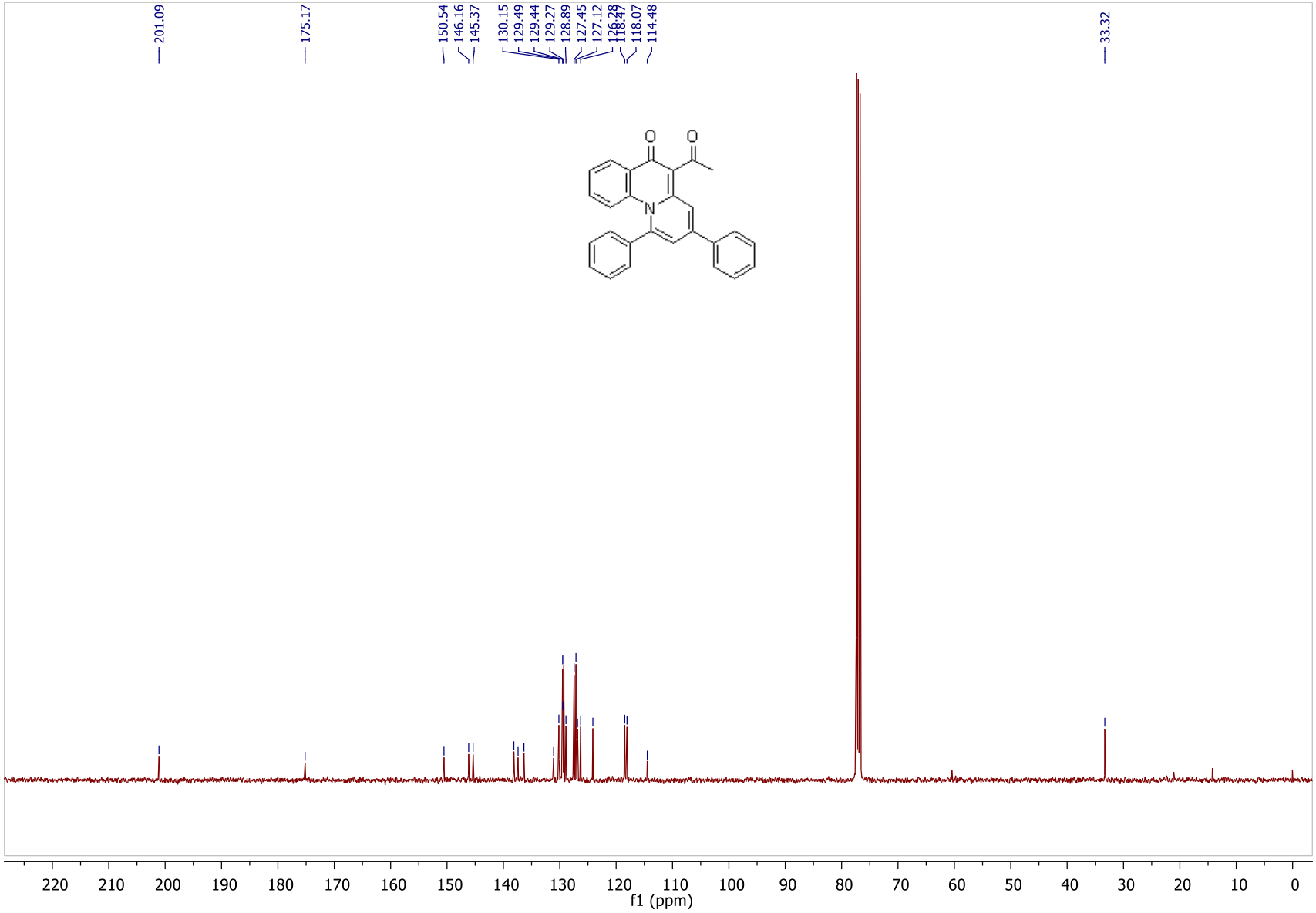
^{13}C NMR of **3d** (101 MHz, $CDCl_3$)



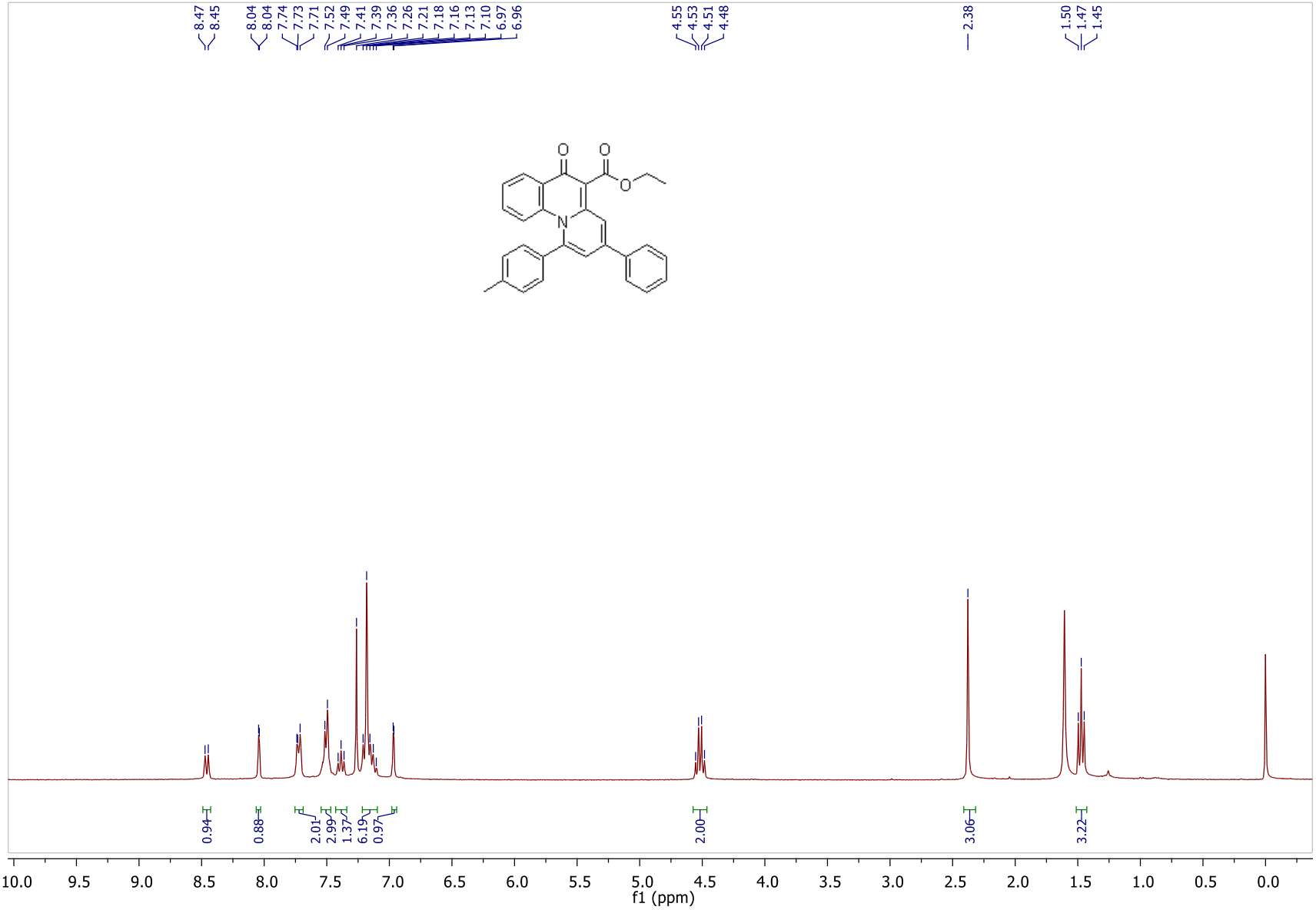
^{1}H NMR of **3e** (400 MHz, $CDCl_3$)



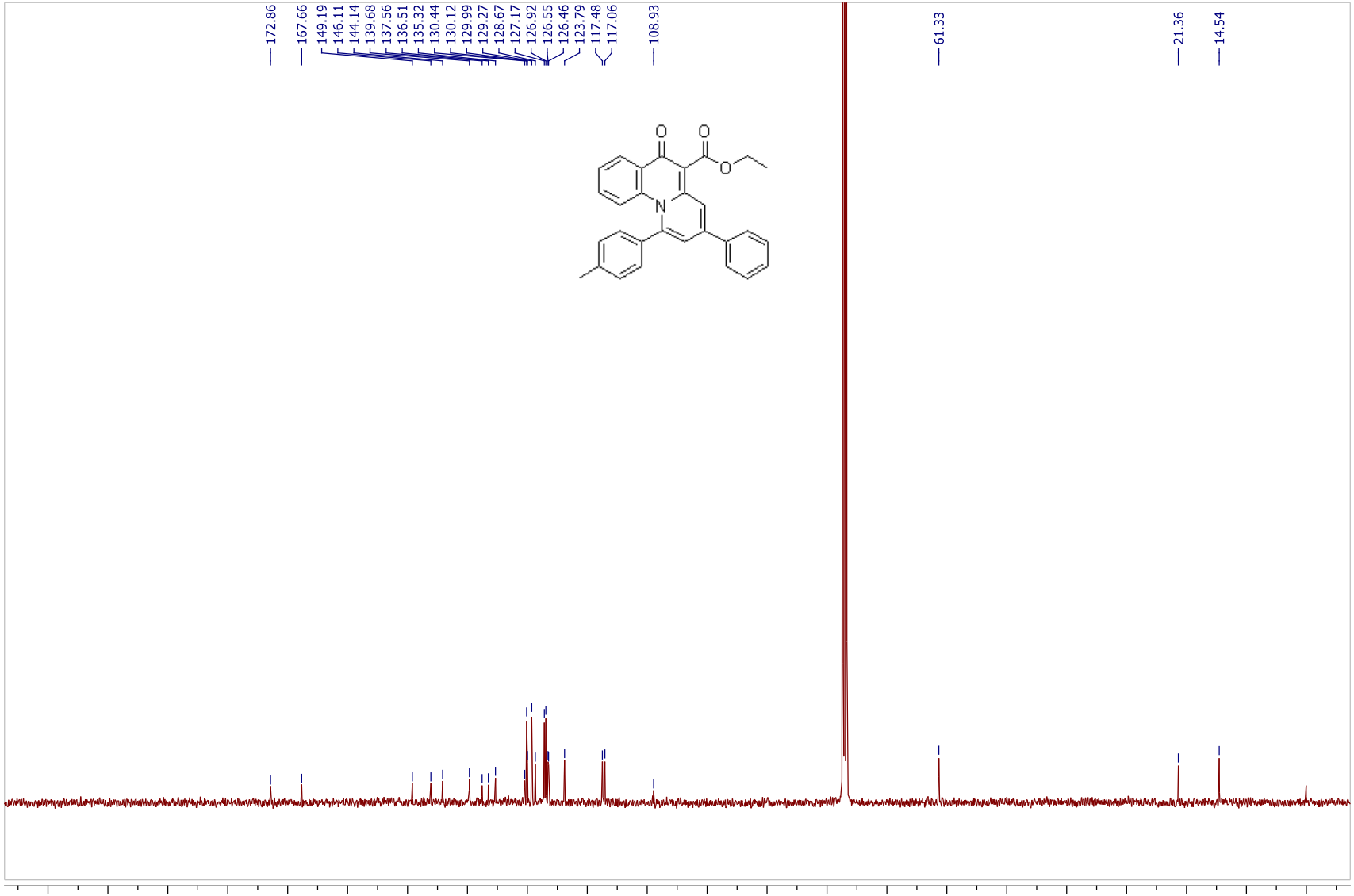
^{13}C NMR of **3e** (101 MHz, $CDCl_3$)



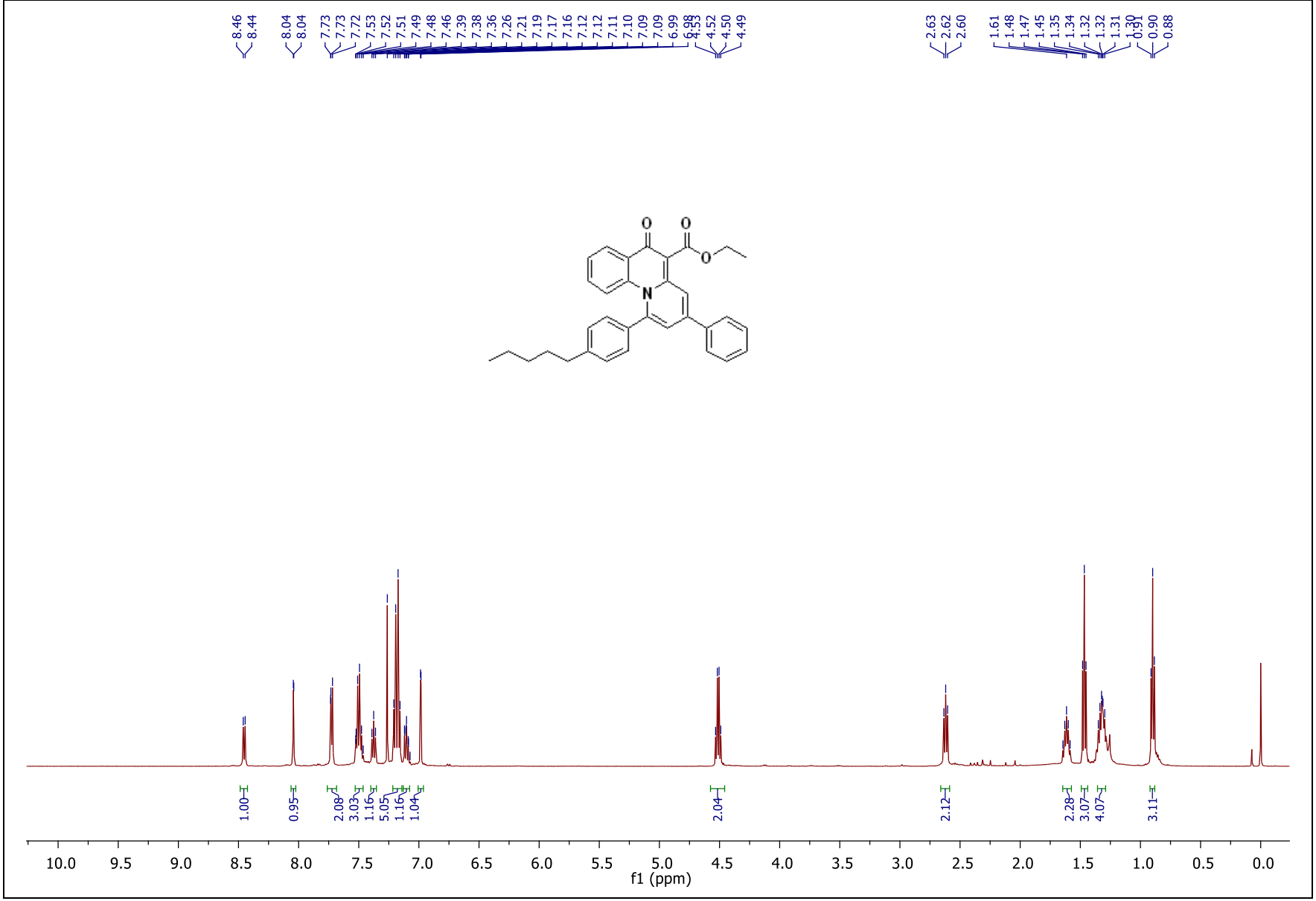
^{1}H NMR of **3f** (300 MHz, $CDCl_3$)



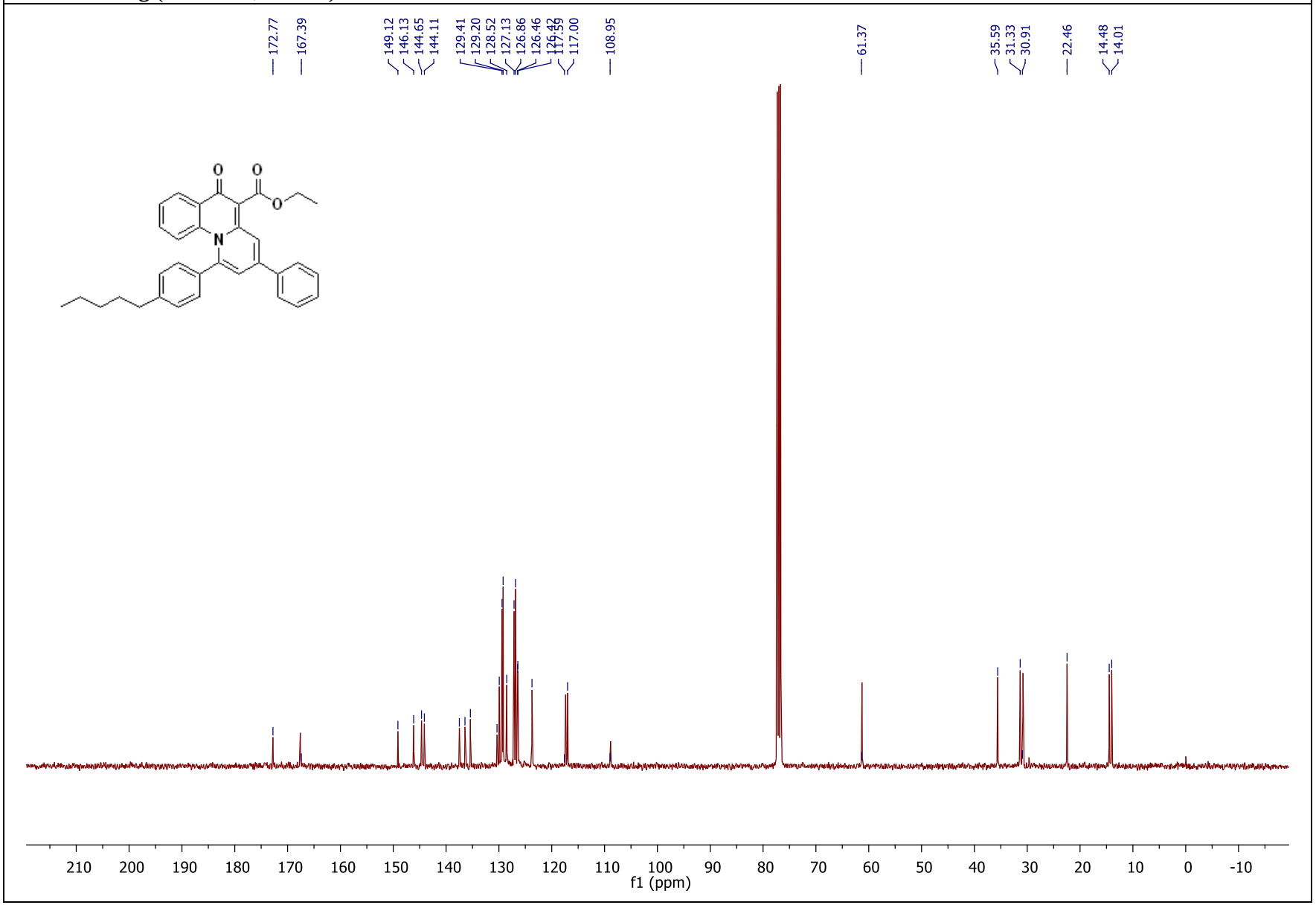
^{13}C NMR of **3f** (101 MHz, $CDCl_3$)



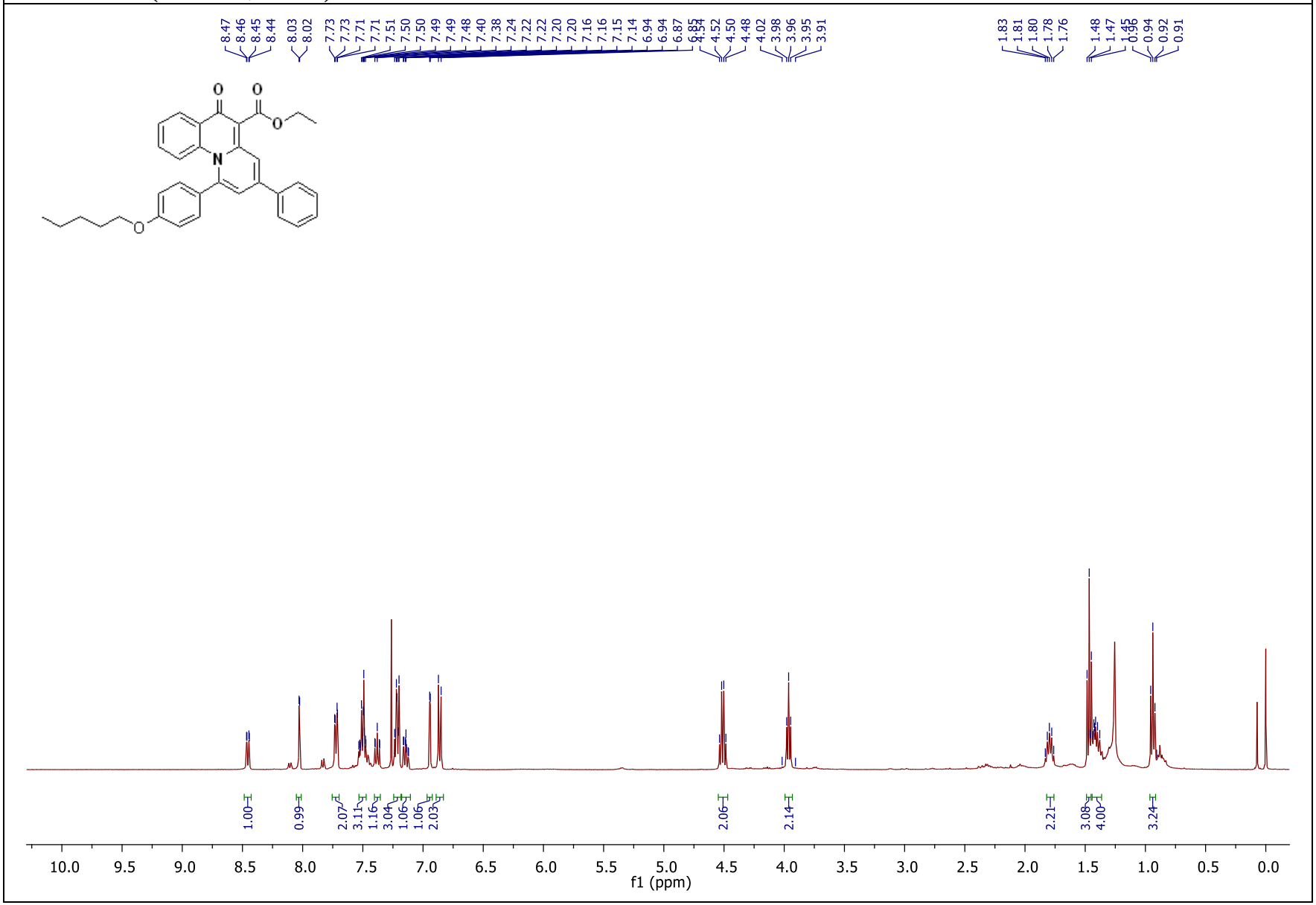
^{1}H NMR of **3g** (500 MHz, $CDCl_3$)



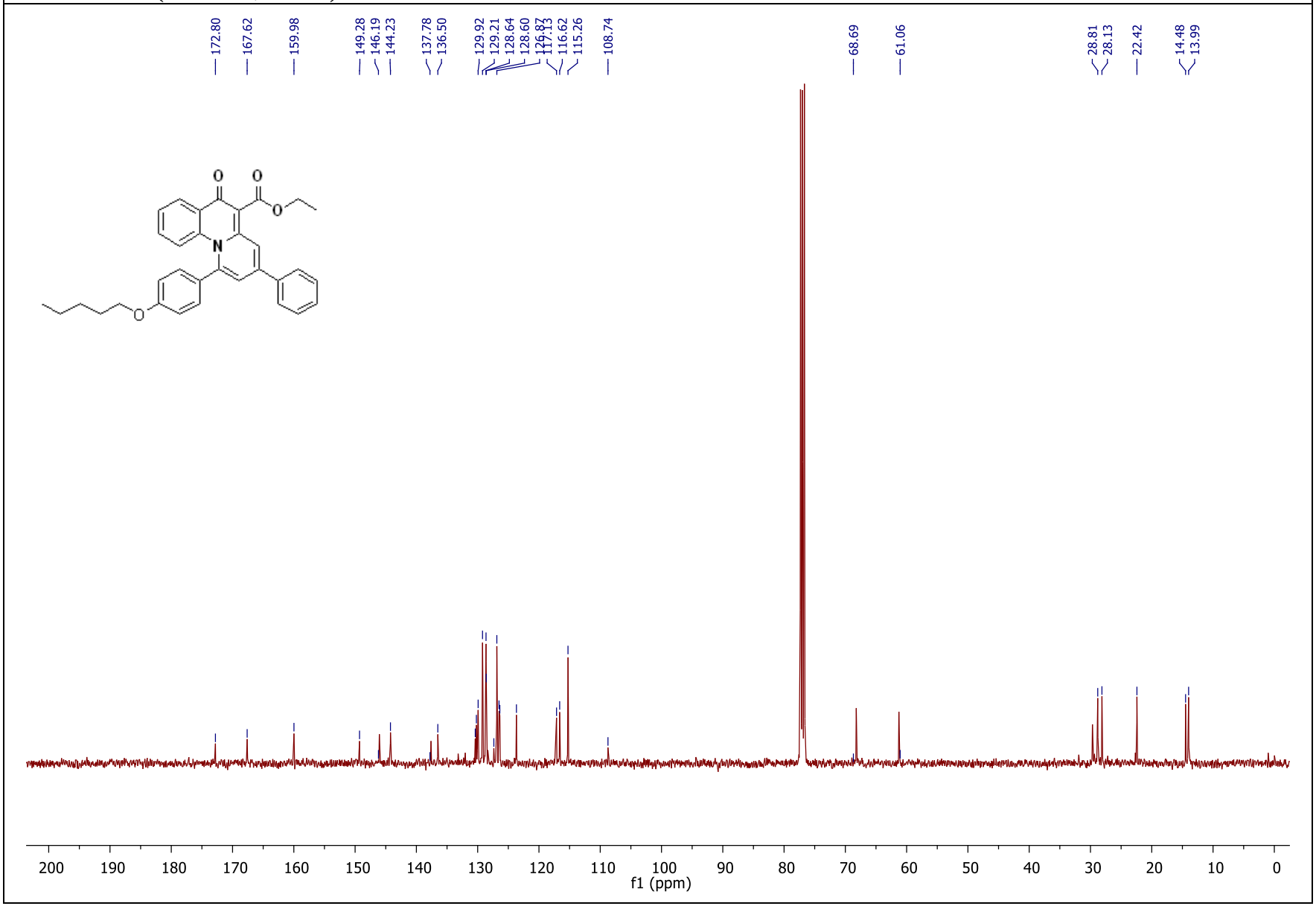
^{13}C NMR of **3g** (101 MHz, $CDCl_3$)



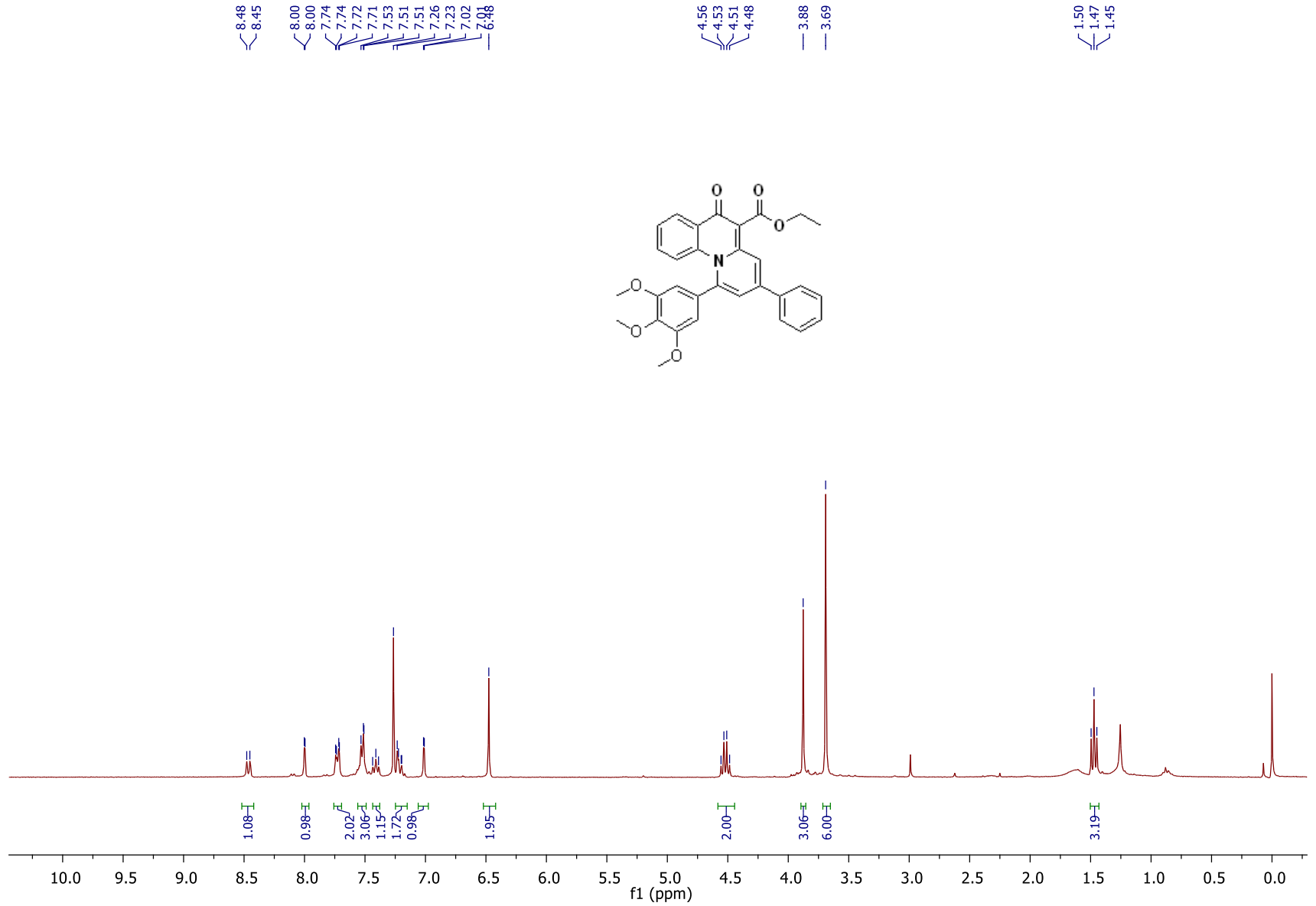
^{1}H NMR of **3h** (400 MHz, $CDCl_3$)



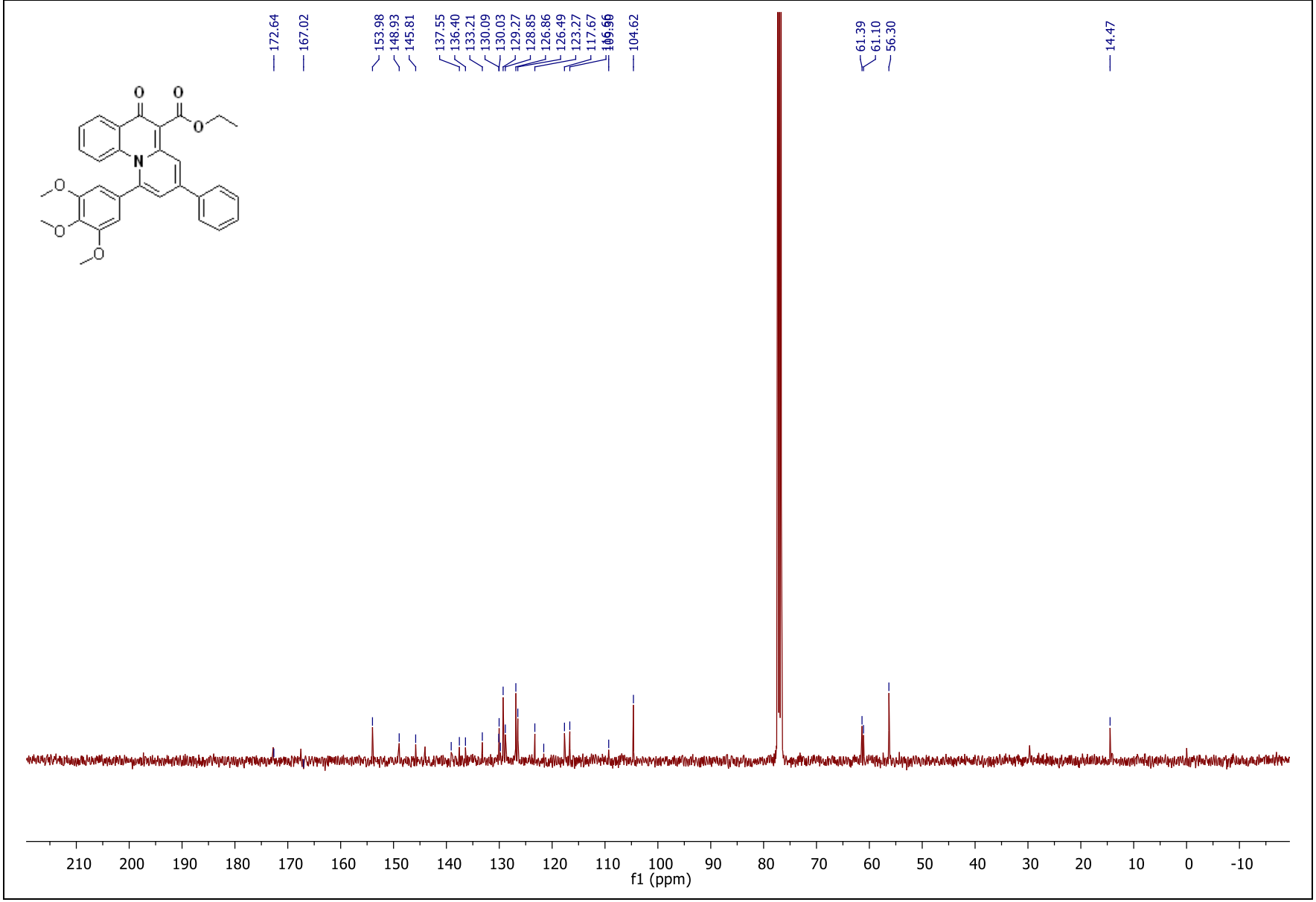
^{13}C NMR of **3h** (101 MHz, $CDCl_3$)



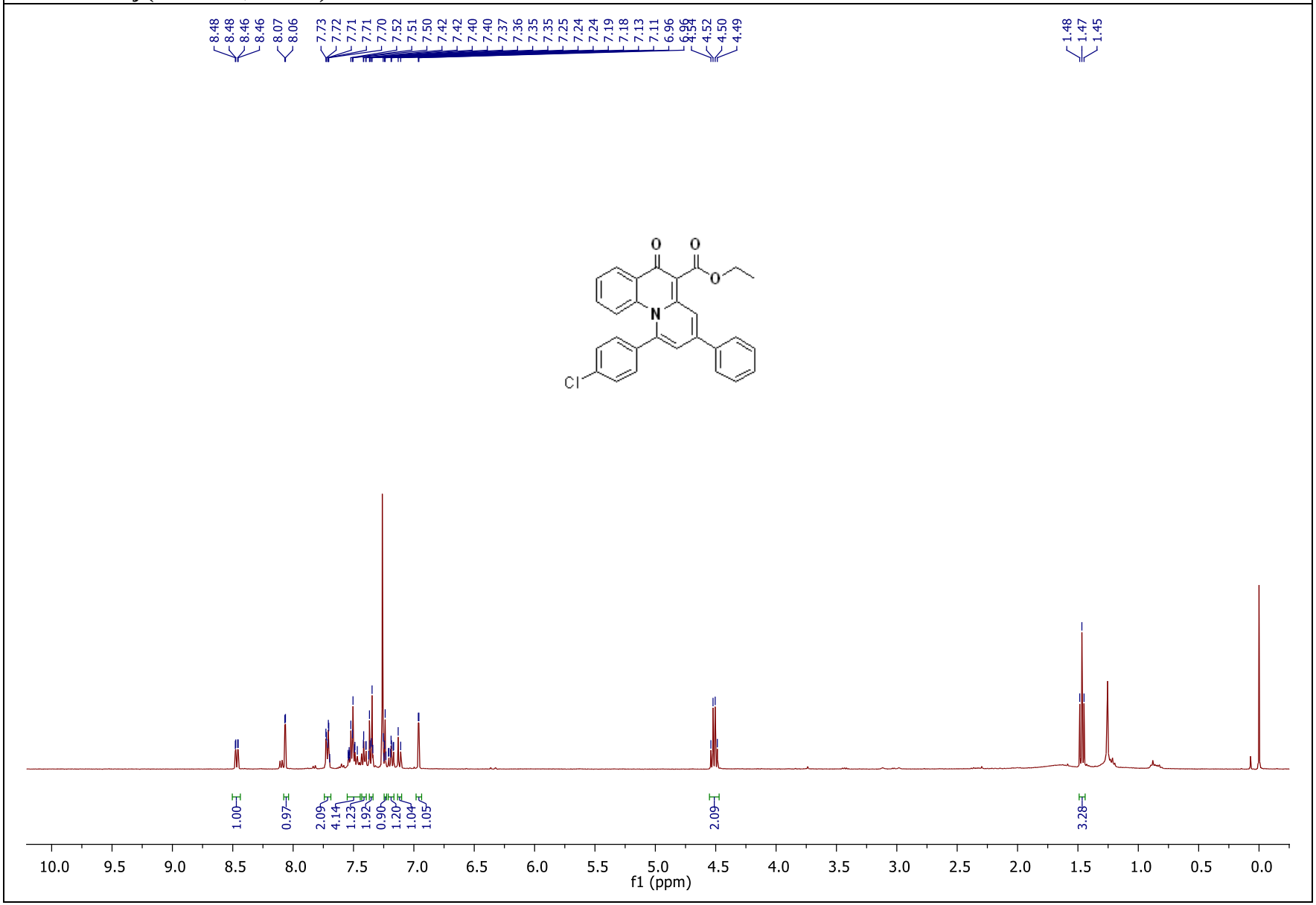
^{1}H NMR of **3i** (300 MHz, $CDCl_3$)



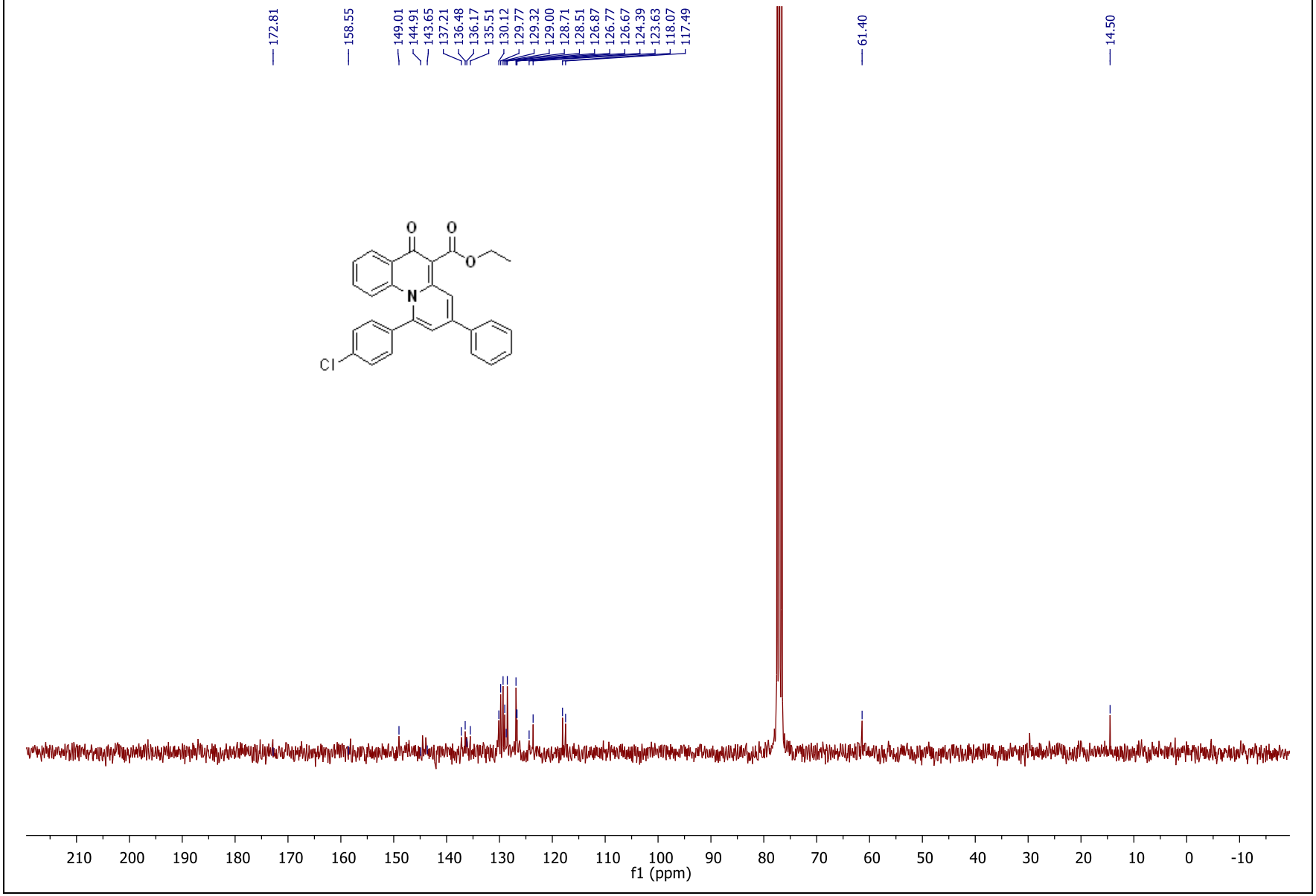
^{13}C NMR of **3i** (101 MHz, $CDCl_3$)



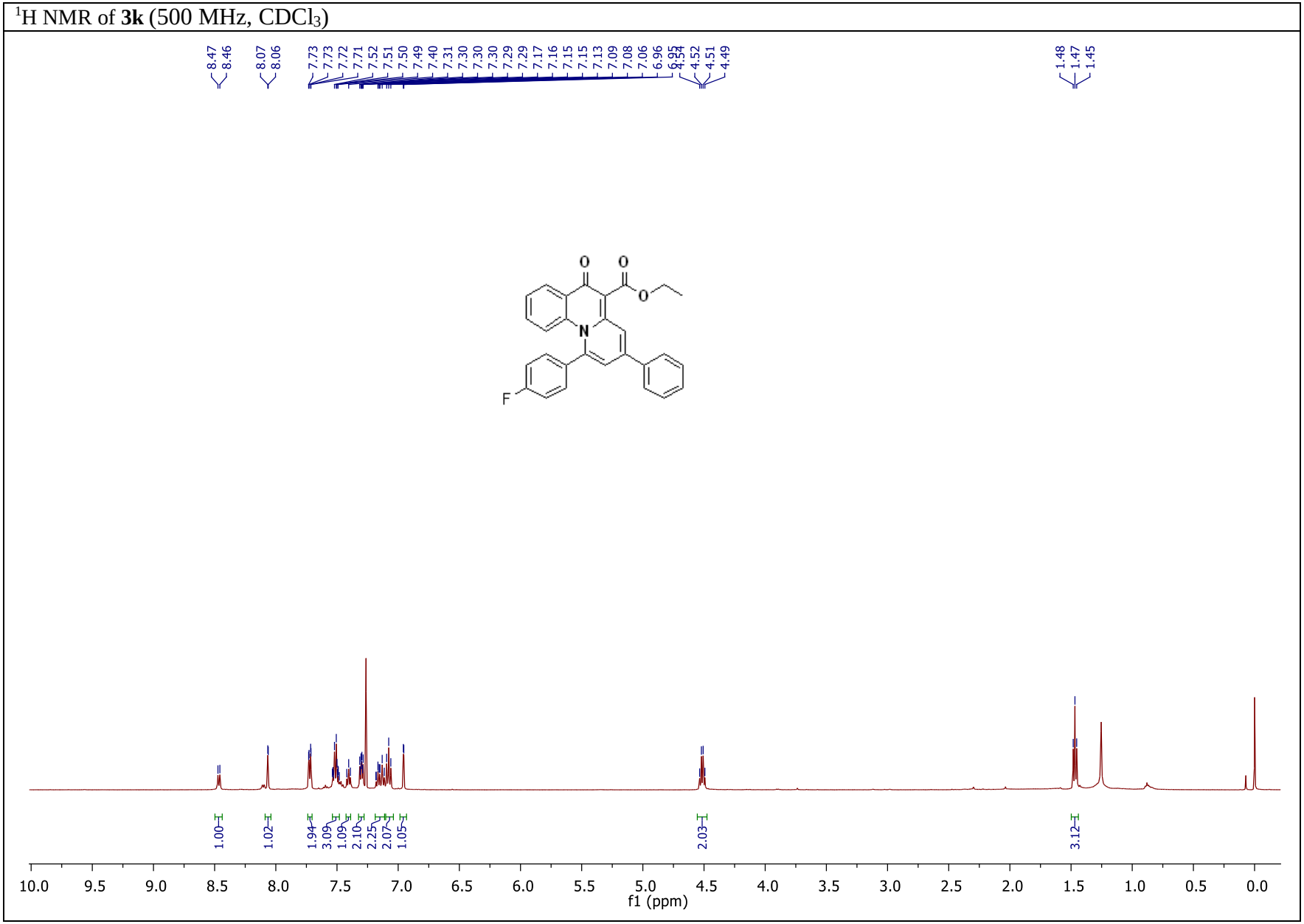
^{1}H NMR of **3j** (400 MHz, $CDCl_3$)



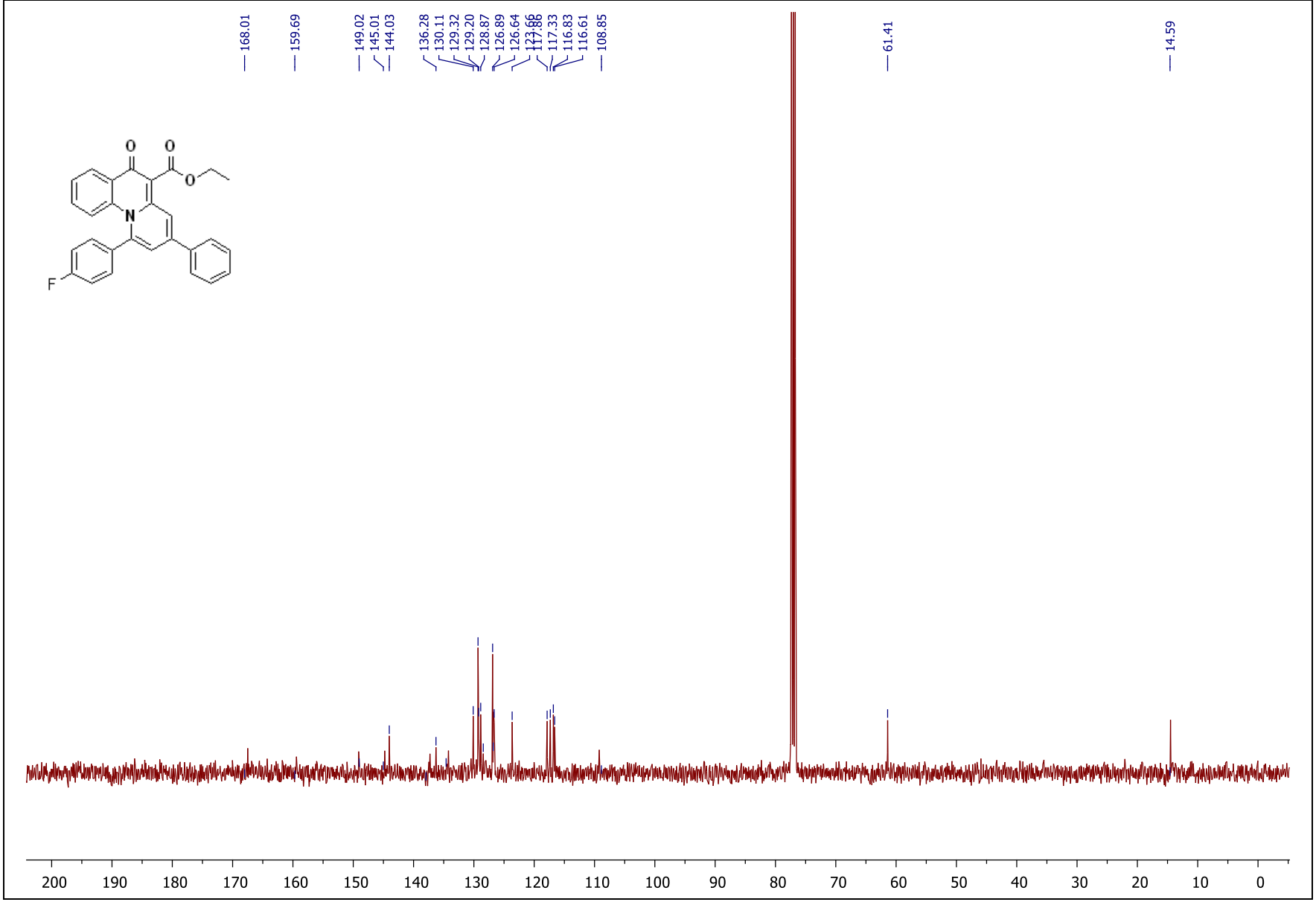
^{13}C NMR of **3j** (101 MHz, $CDCl_3$)



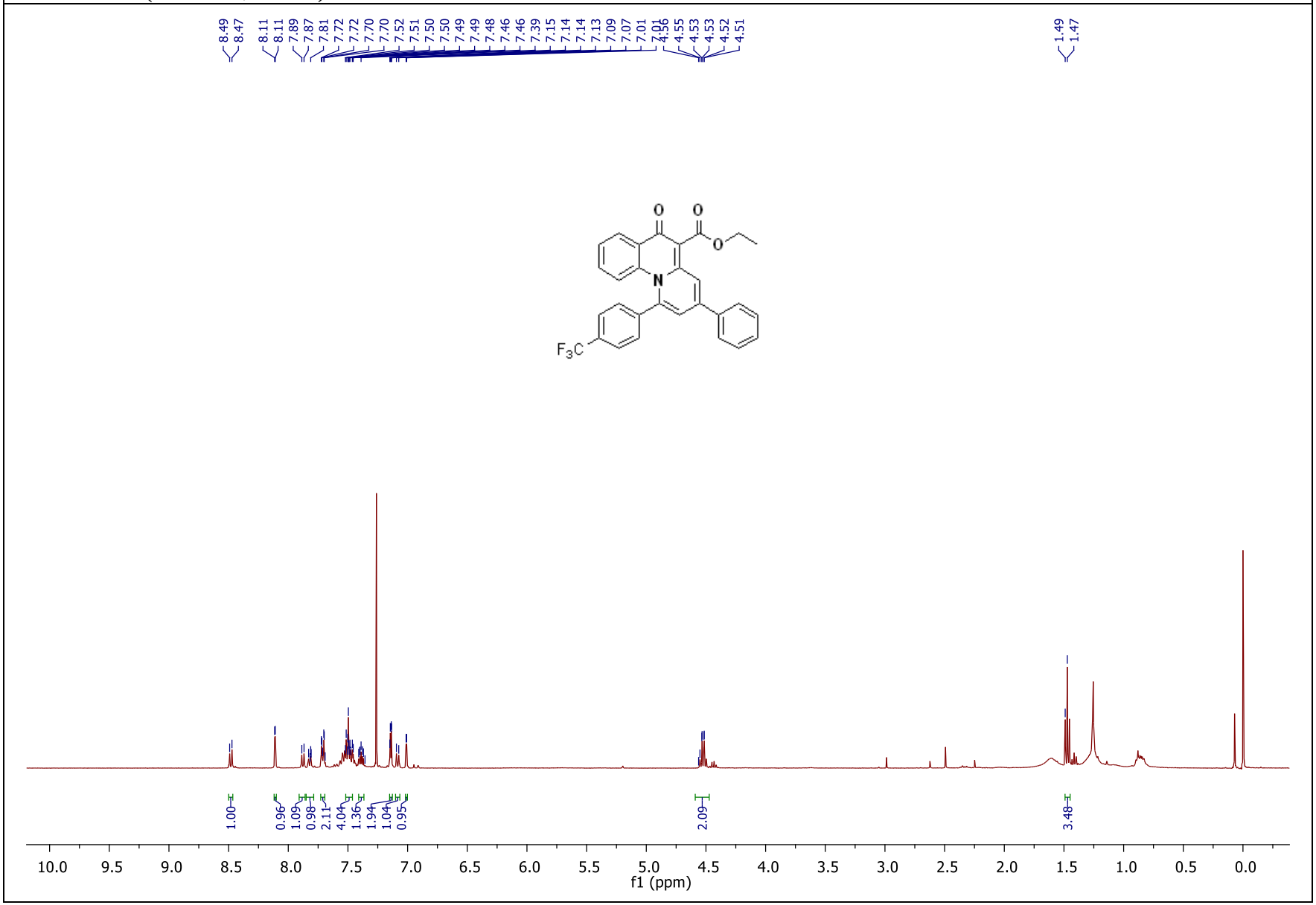
^{1}H NMR of **3k** (500 MHz, $CDCl_3$)



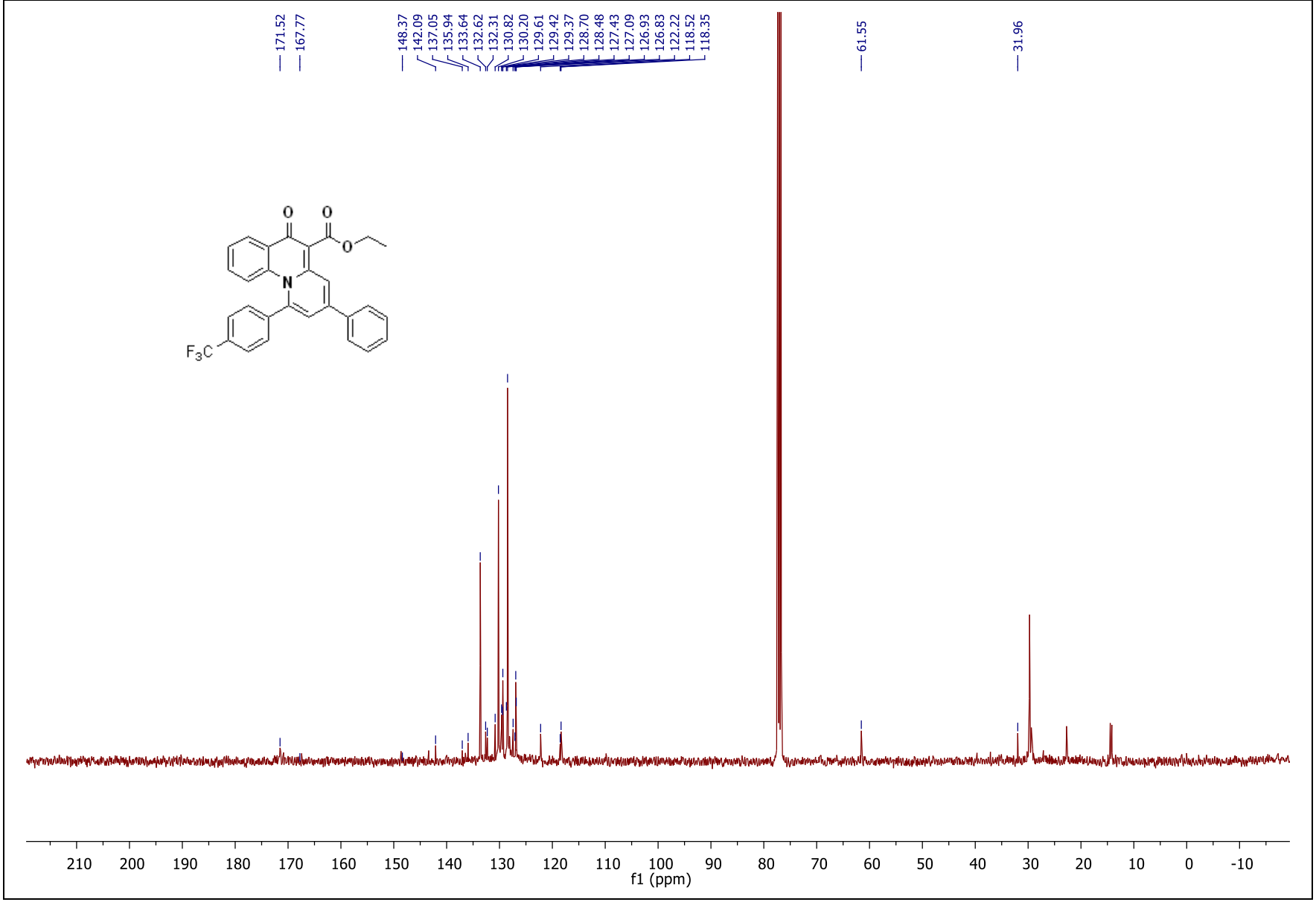
^{13}C NMR of **3k** (101 MHz, $CDCl_3$)



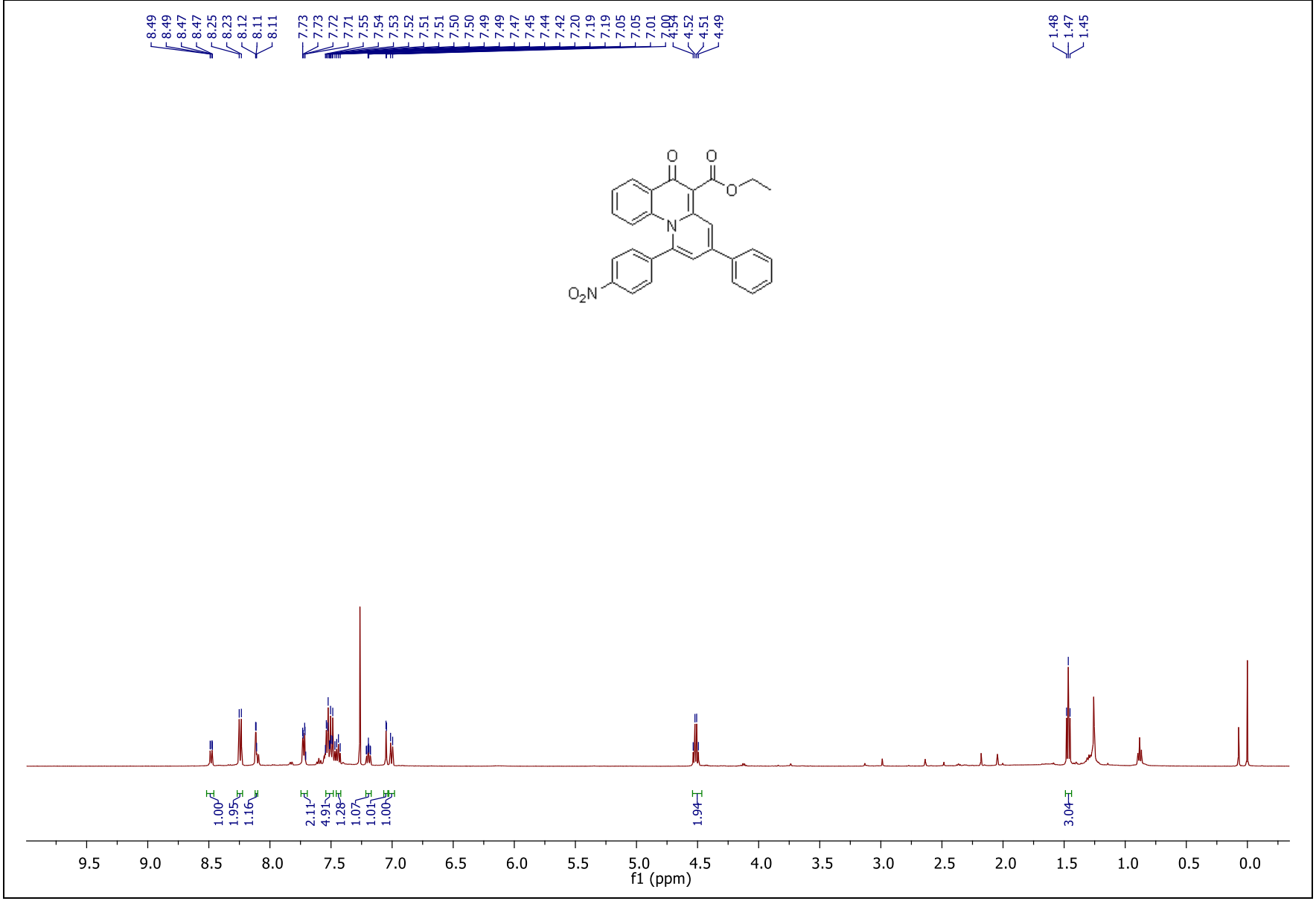
^{1}H NMR of **3l** (400 MHz, $CDCl_3$)



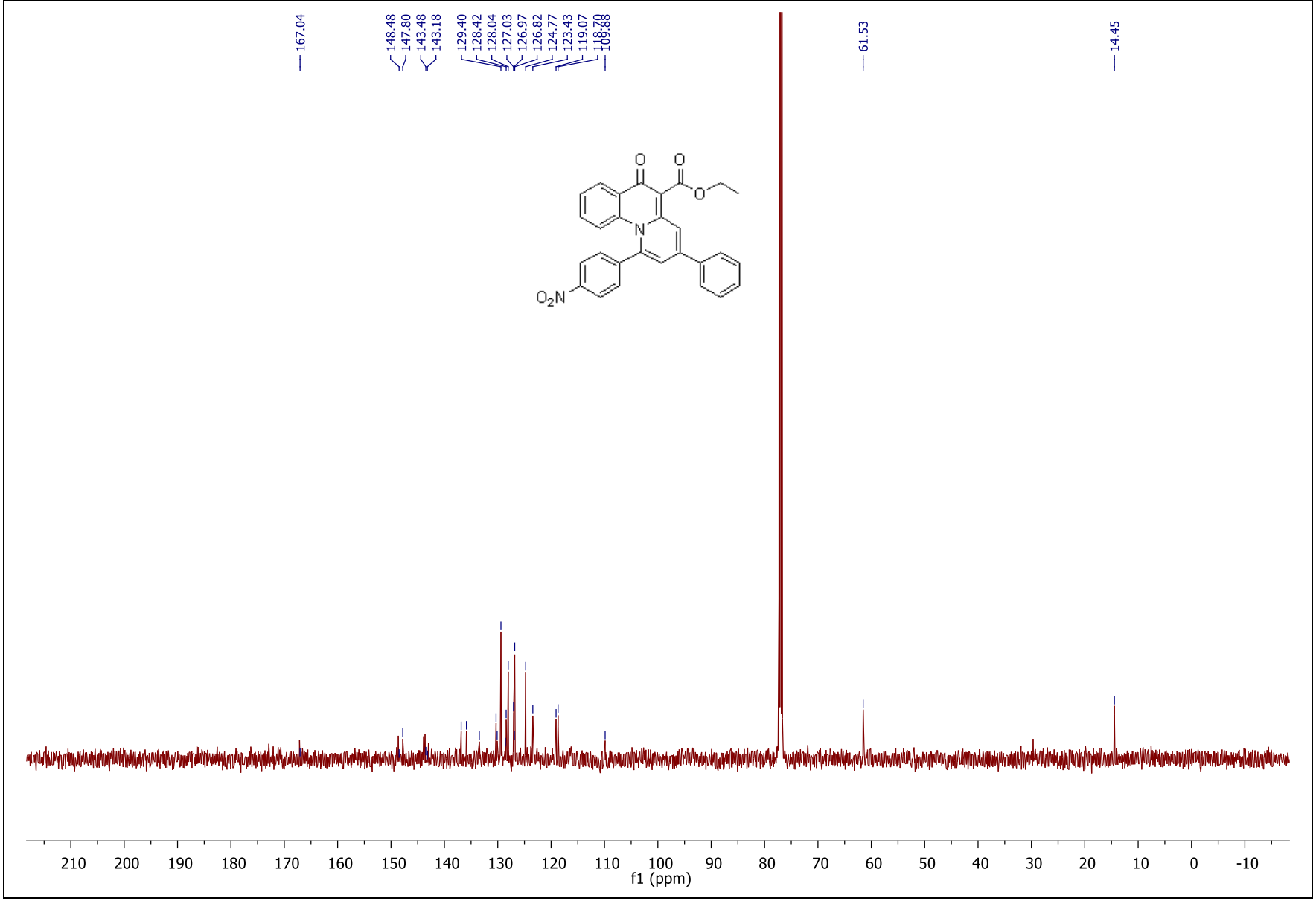
^{13}C NMR of **3l** (101 MHz, $CDCl_3$)



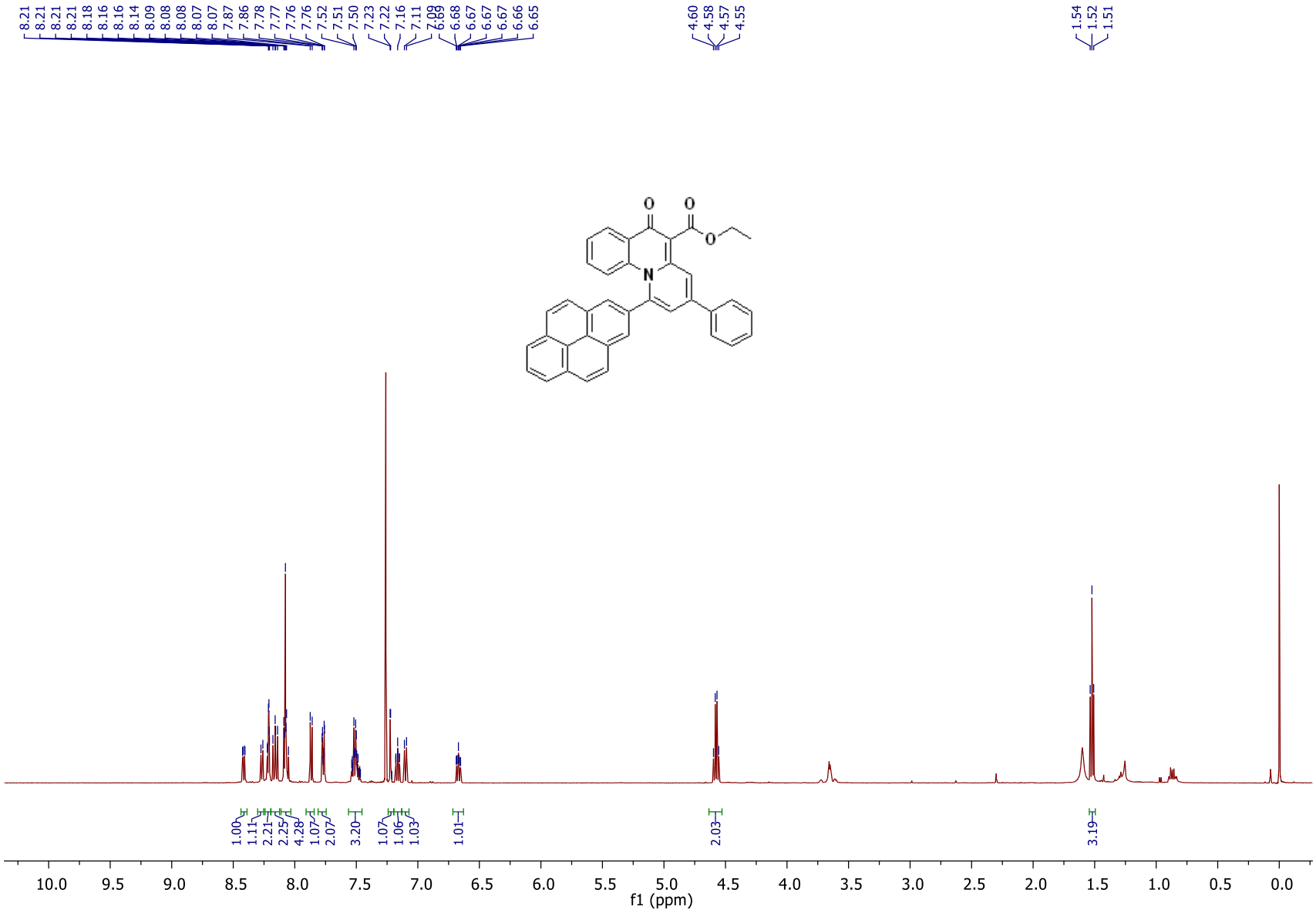
^{1}H NMR of **3m** (500 MHz, $CDCl_3$)



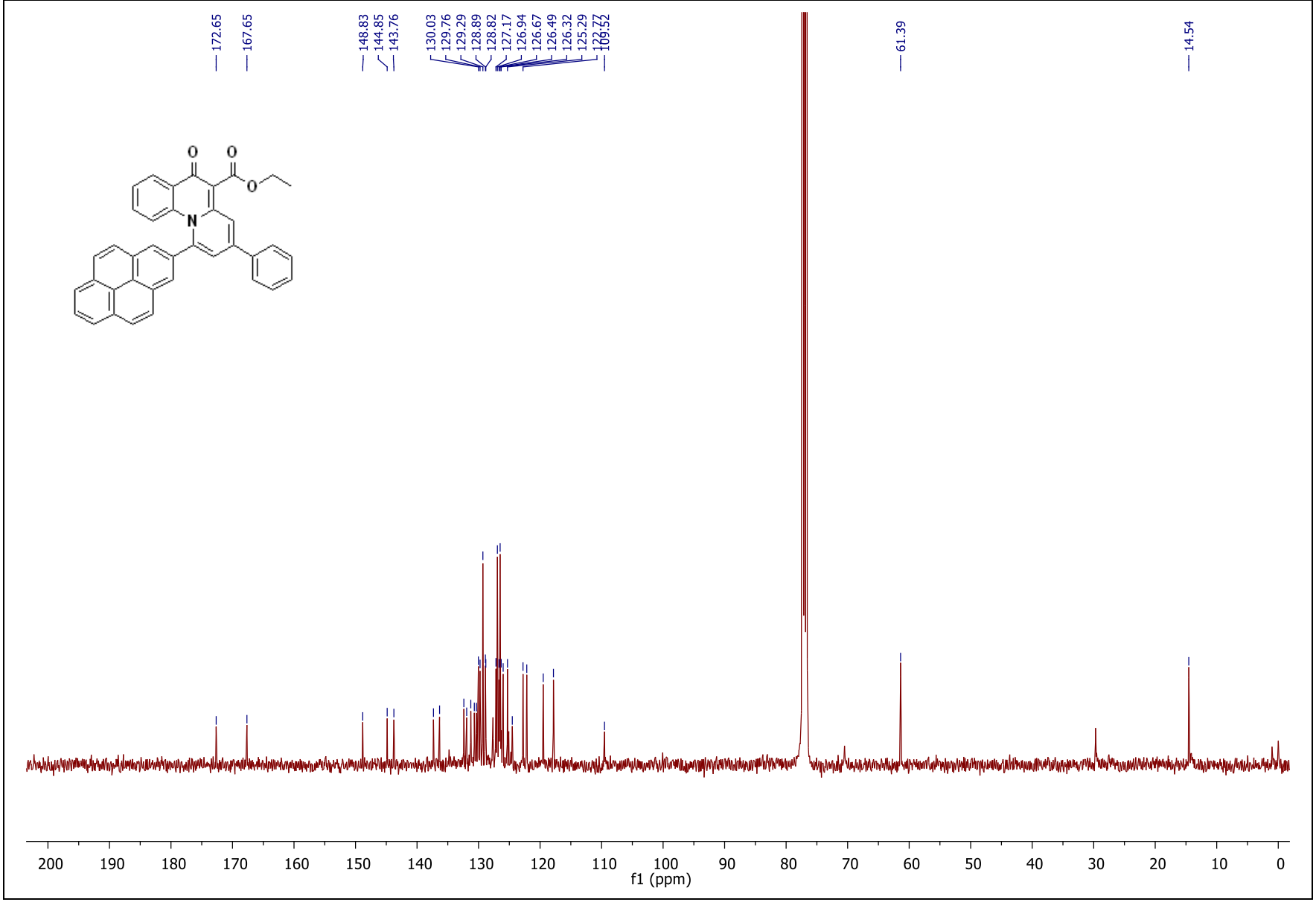
^{13}C NMR of **3m** (126 MHz, $CDCl_3$)



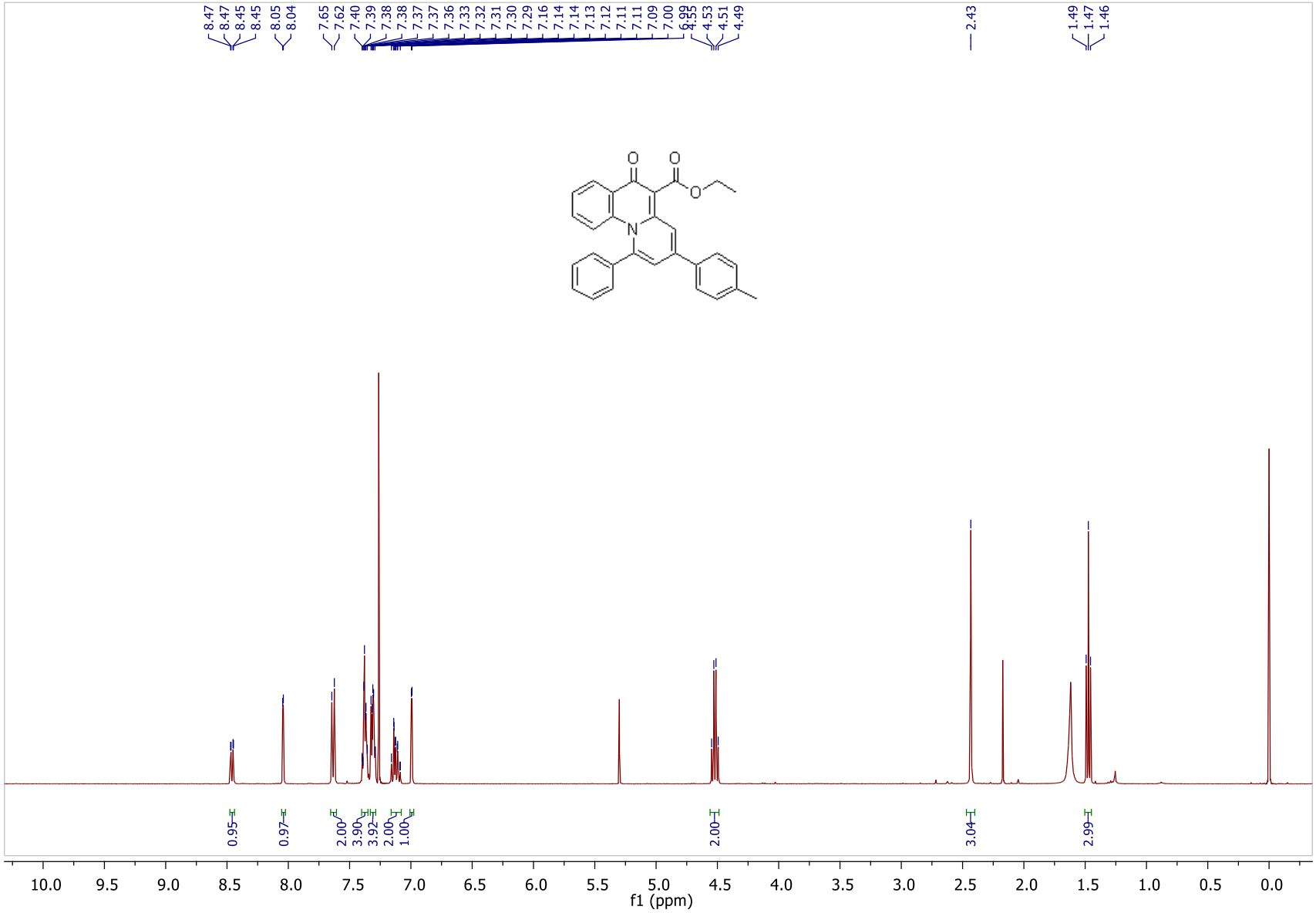
^{1}H NMR of **3n** (500 MHz, $CDCl_3$)



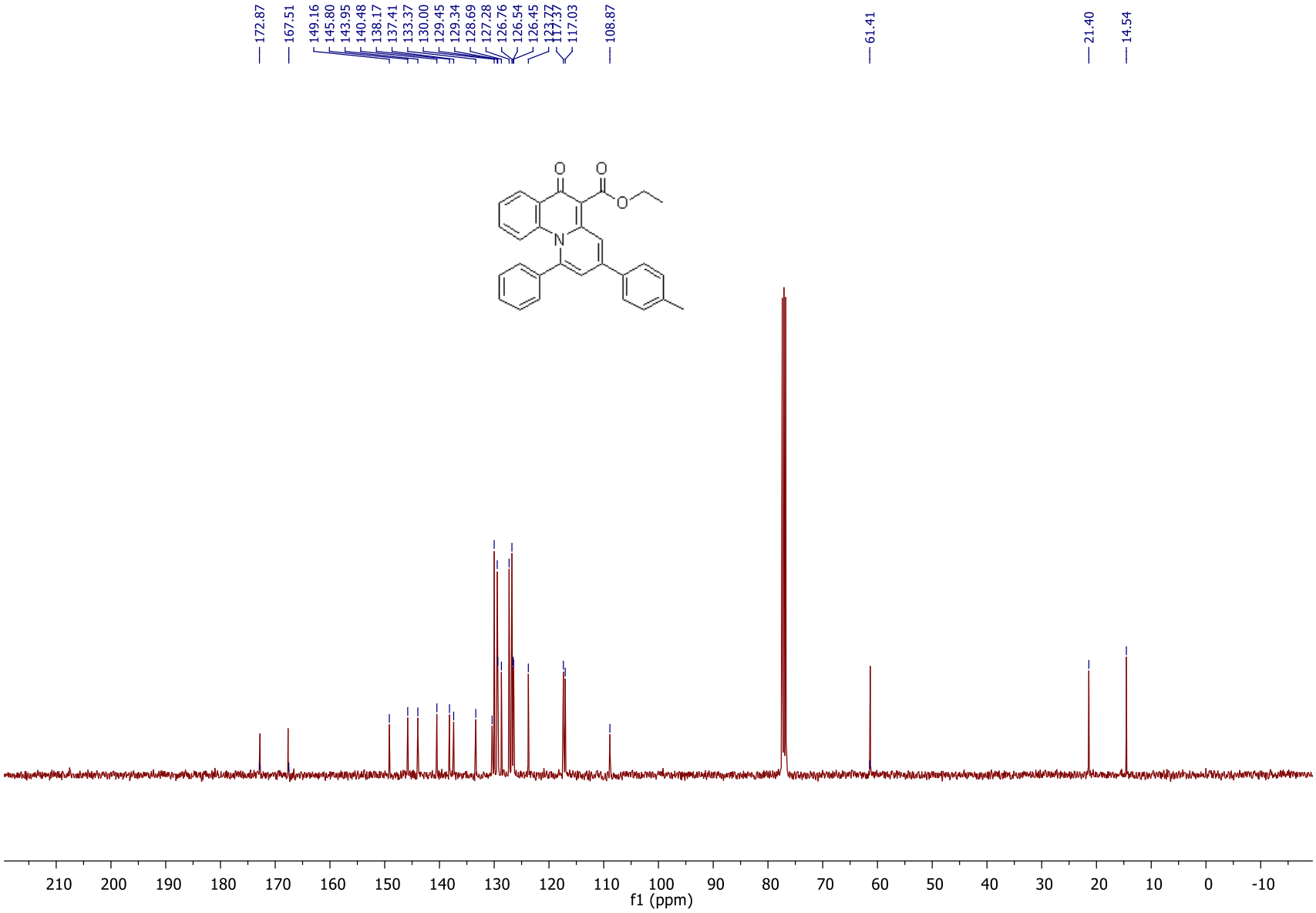
^{13}C NMR of **3n** (101 MHz, $CDCl_3$)



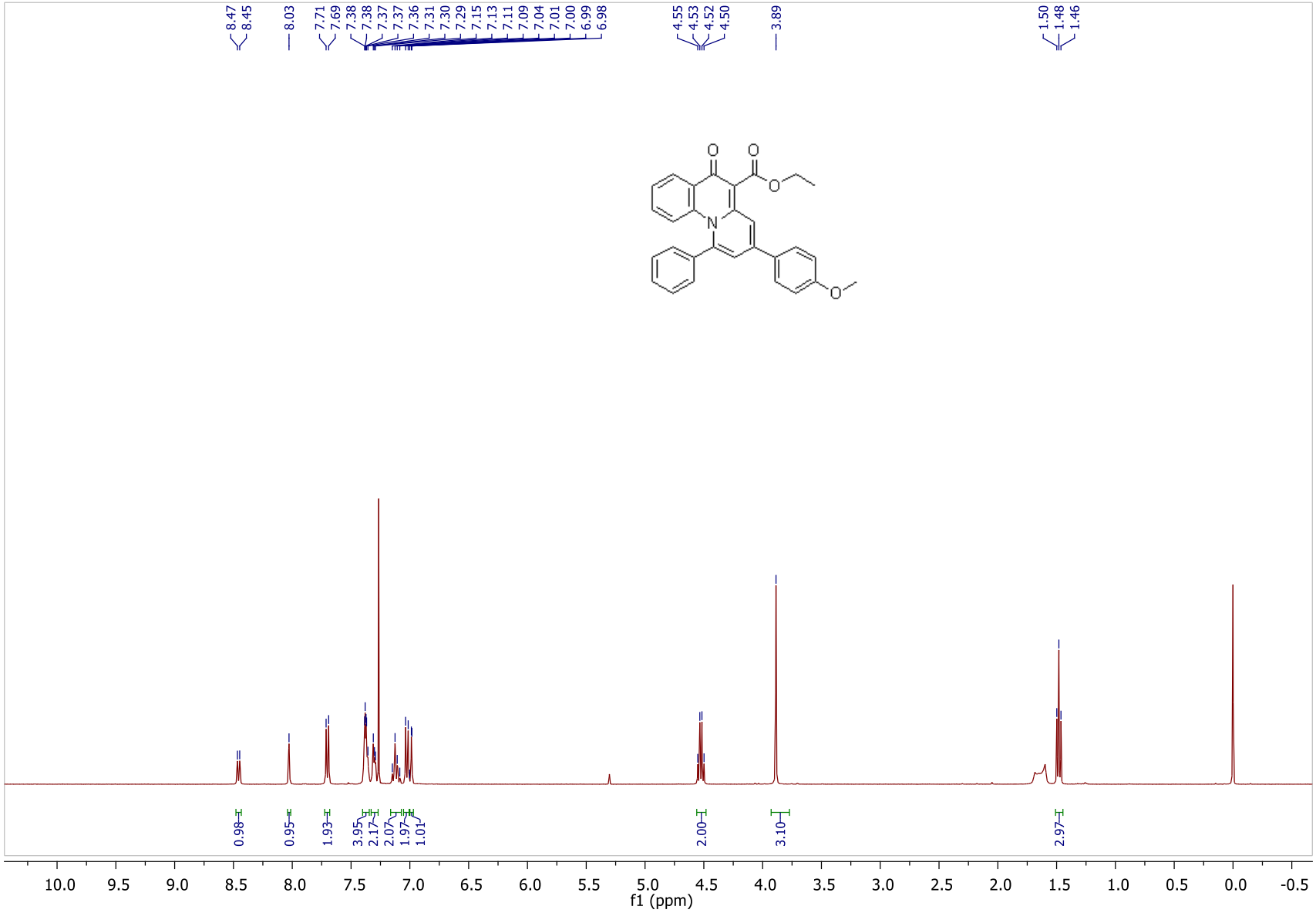
^{1}H NMR of **3o** (400 MHz, $CDCl_3$)



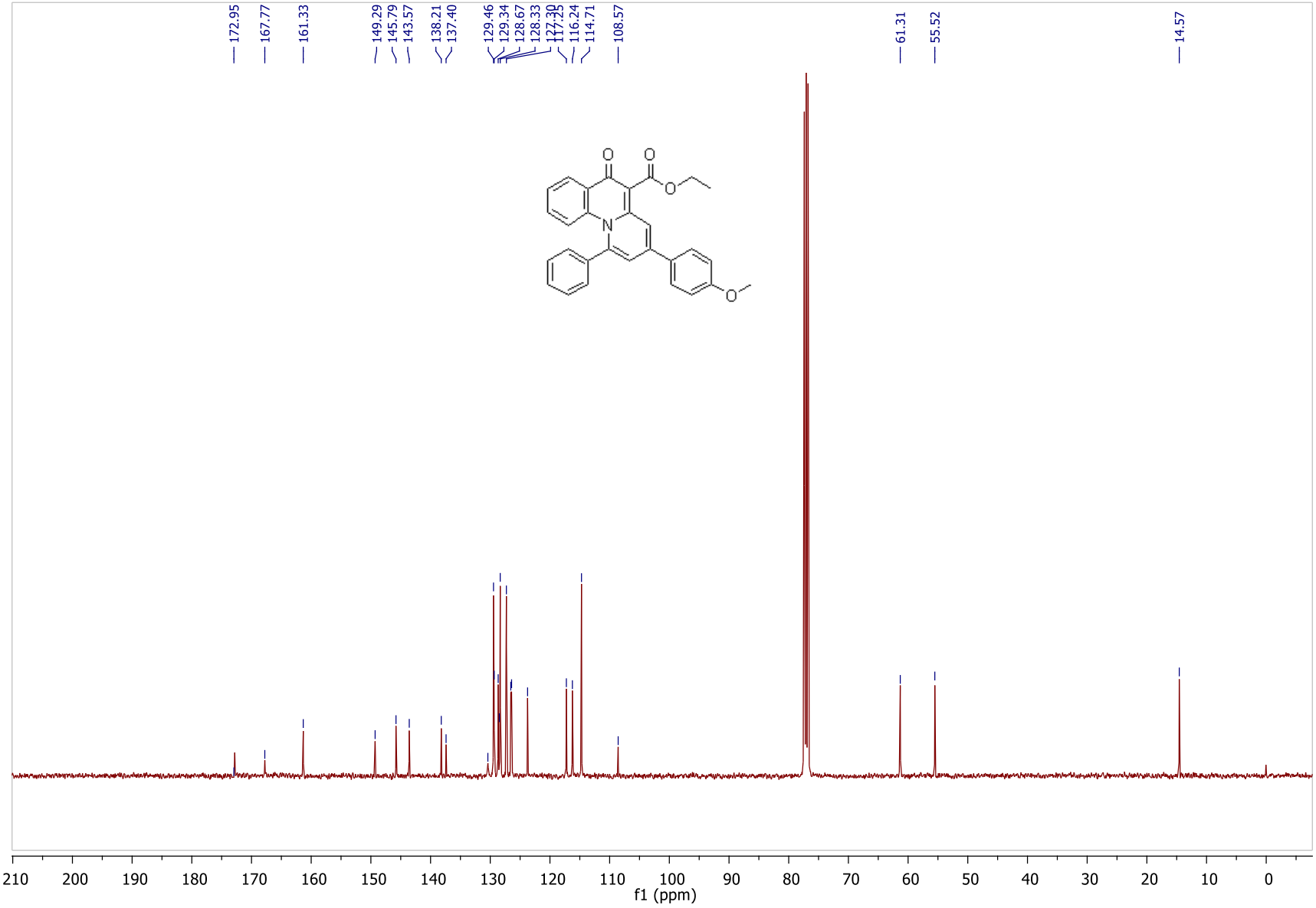
^{13}C NMR of **3o** (101 MHz, $CDCl_3$)



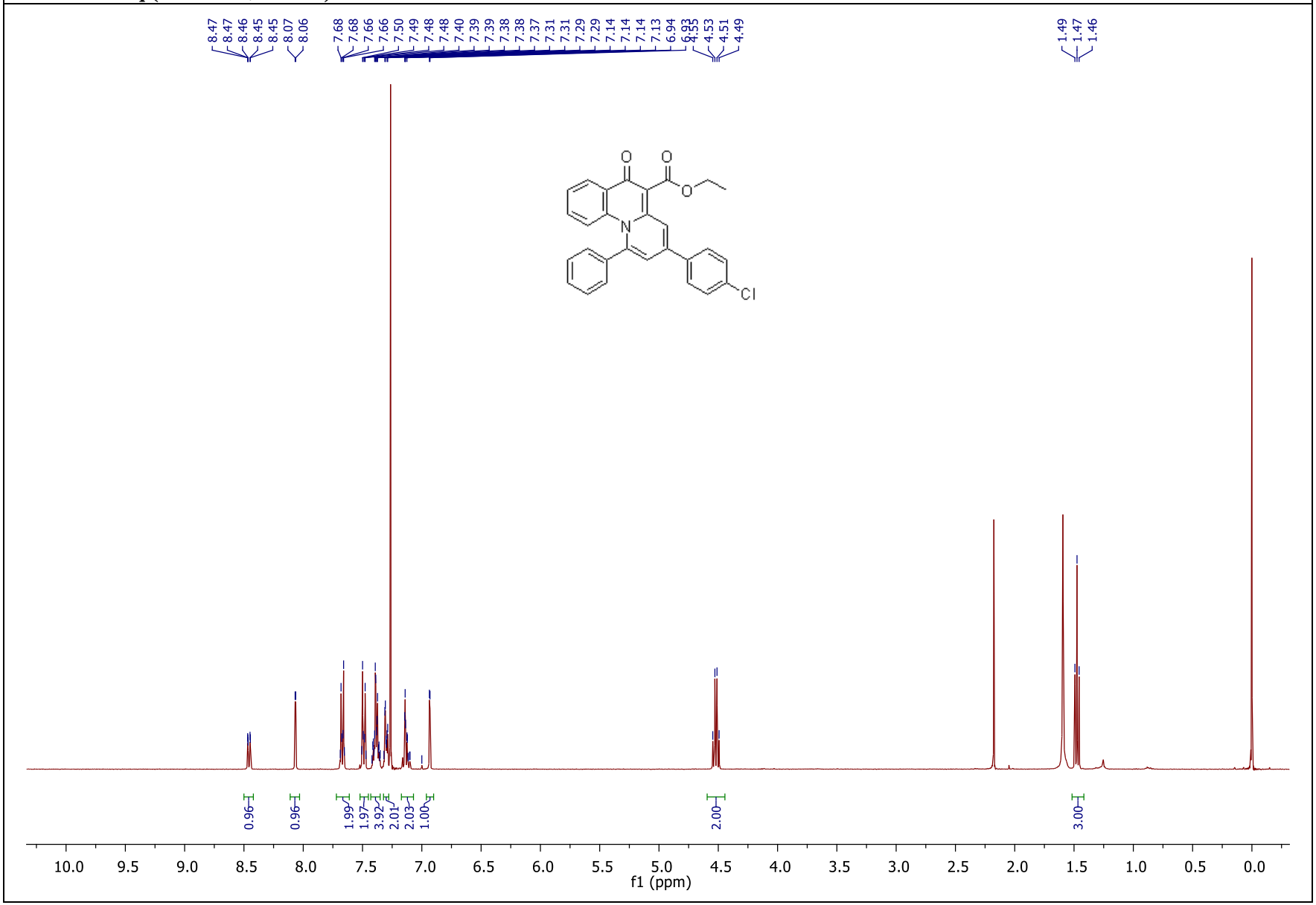
^{1}H NMR of **3p** (500 MHz, $CDCl_3$)



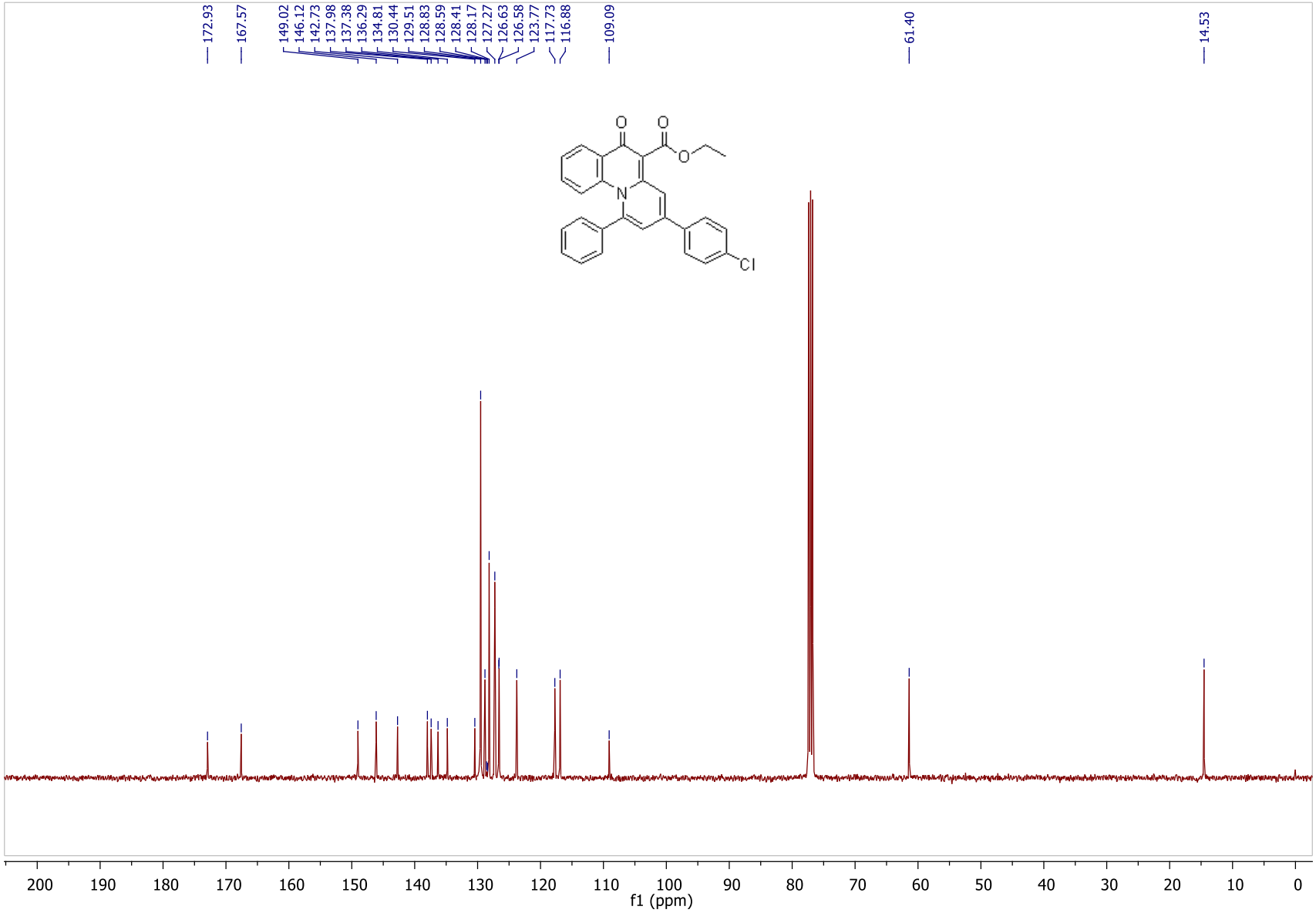
^{13}C NMR of **3p** (101 MHz, $CDCl_3$)



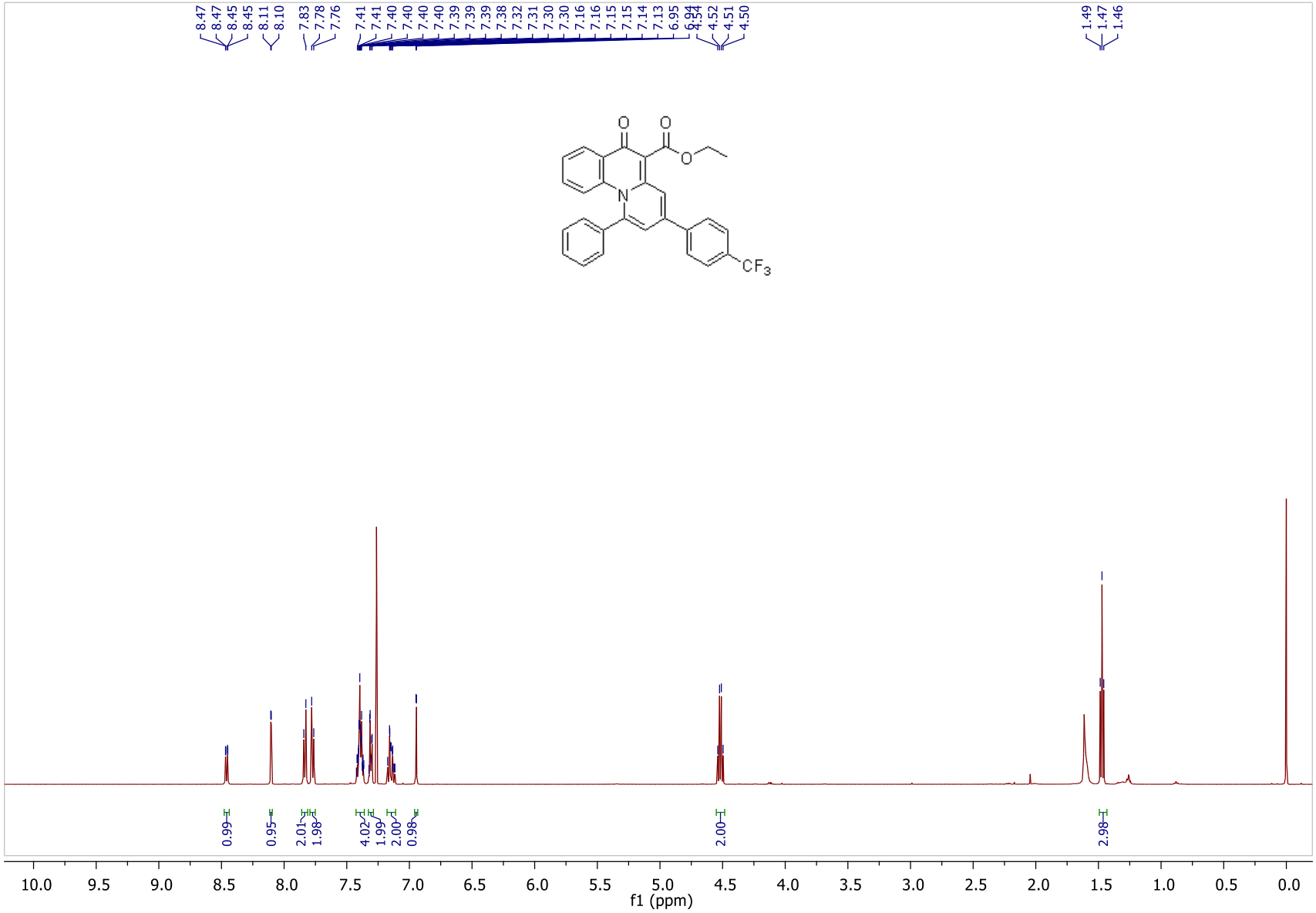
^{1}H NMR of **3q** (400 MHz, $CDCl_3$)



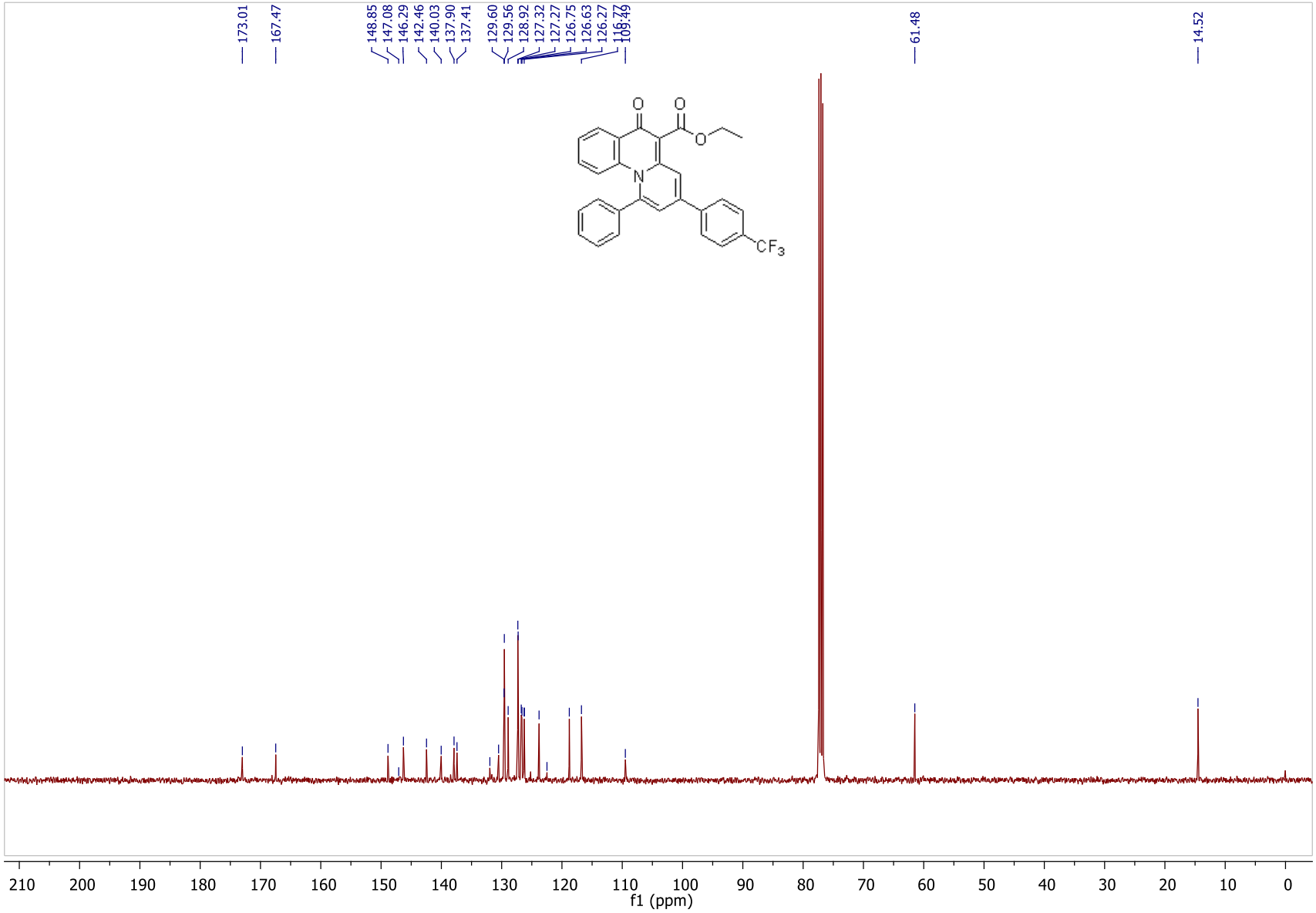
^{13}C NMR of **3q** (101 MHz, $CDCl_3$)



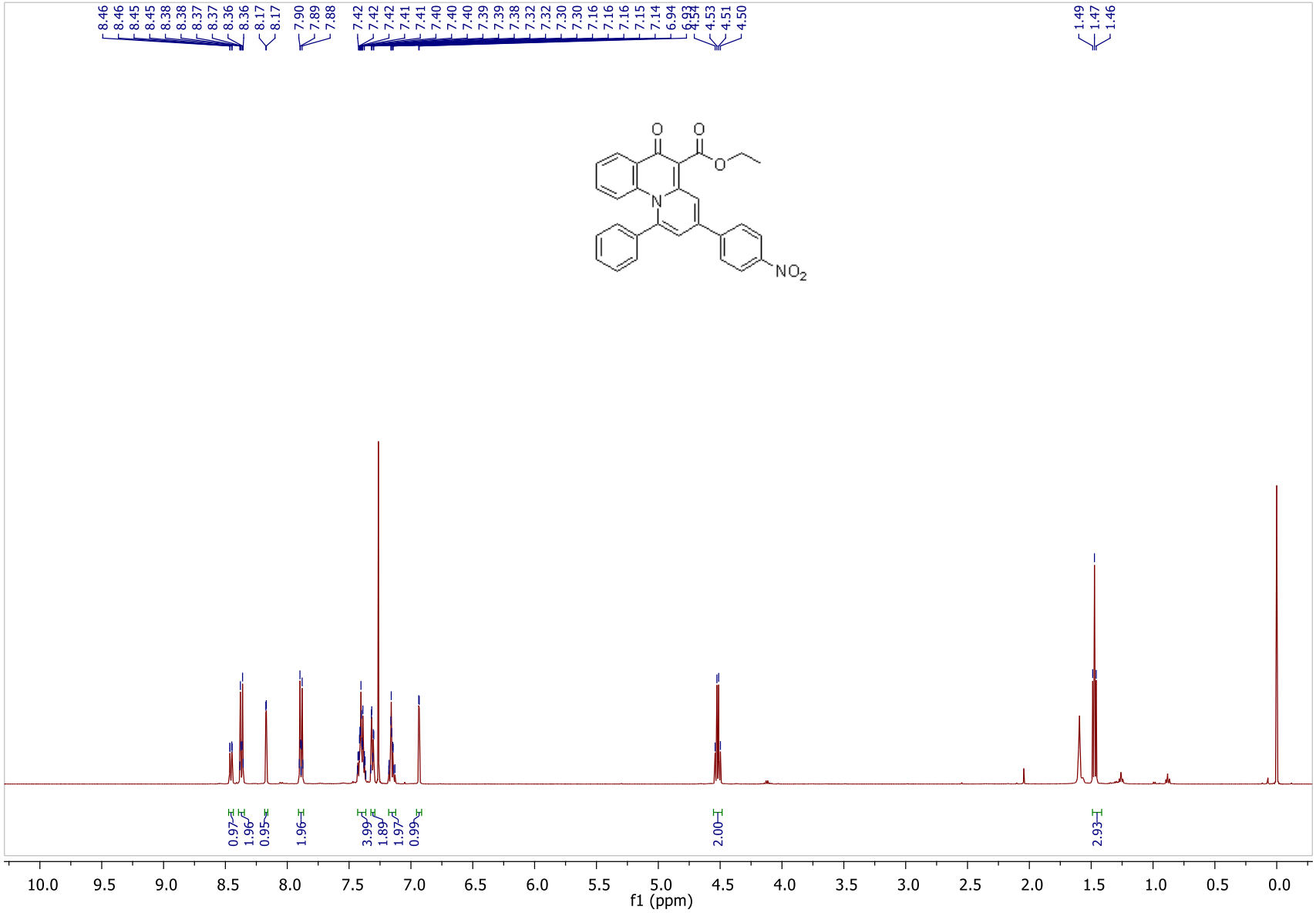
^{1}H NMR of **3r** (500 MHz, $CDCl_3$)



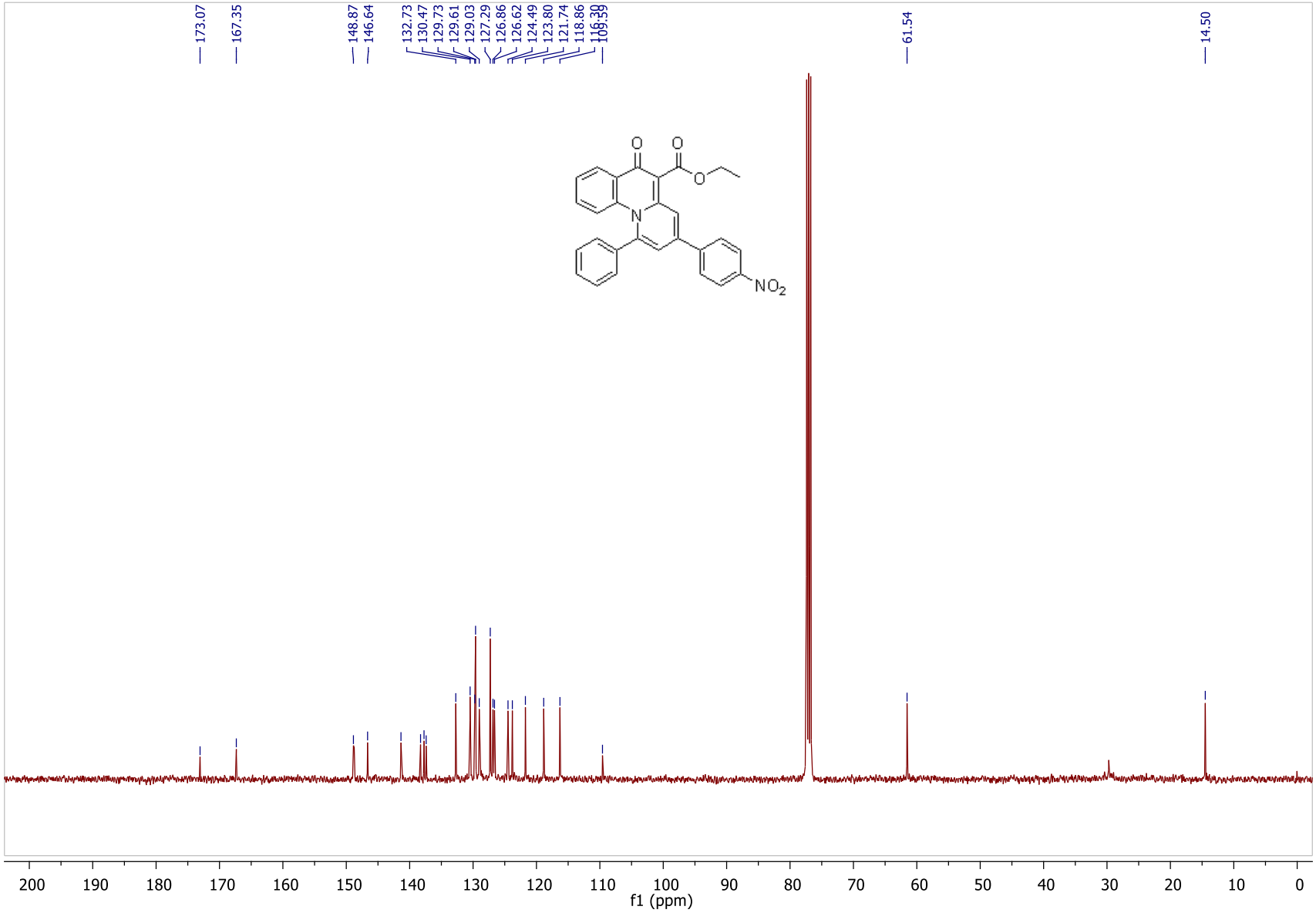
^{13}C NMR of **3r** (101 MHz, $CDCl_3$)



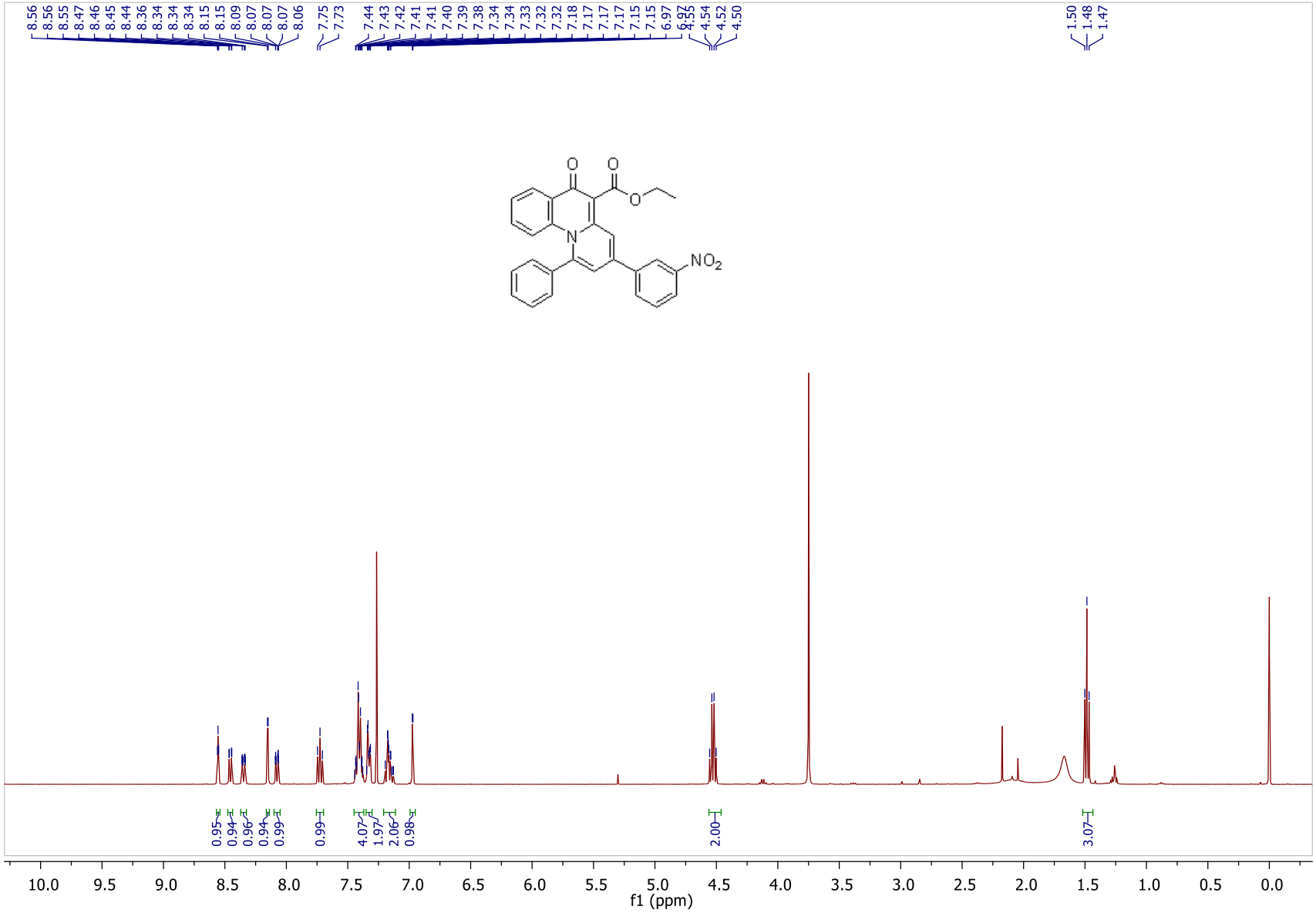
^{1}H NMR of **3s** (500 MHz, $CDCl_3$)



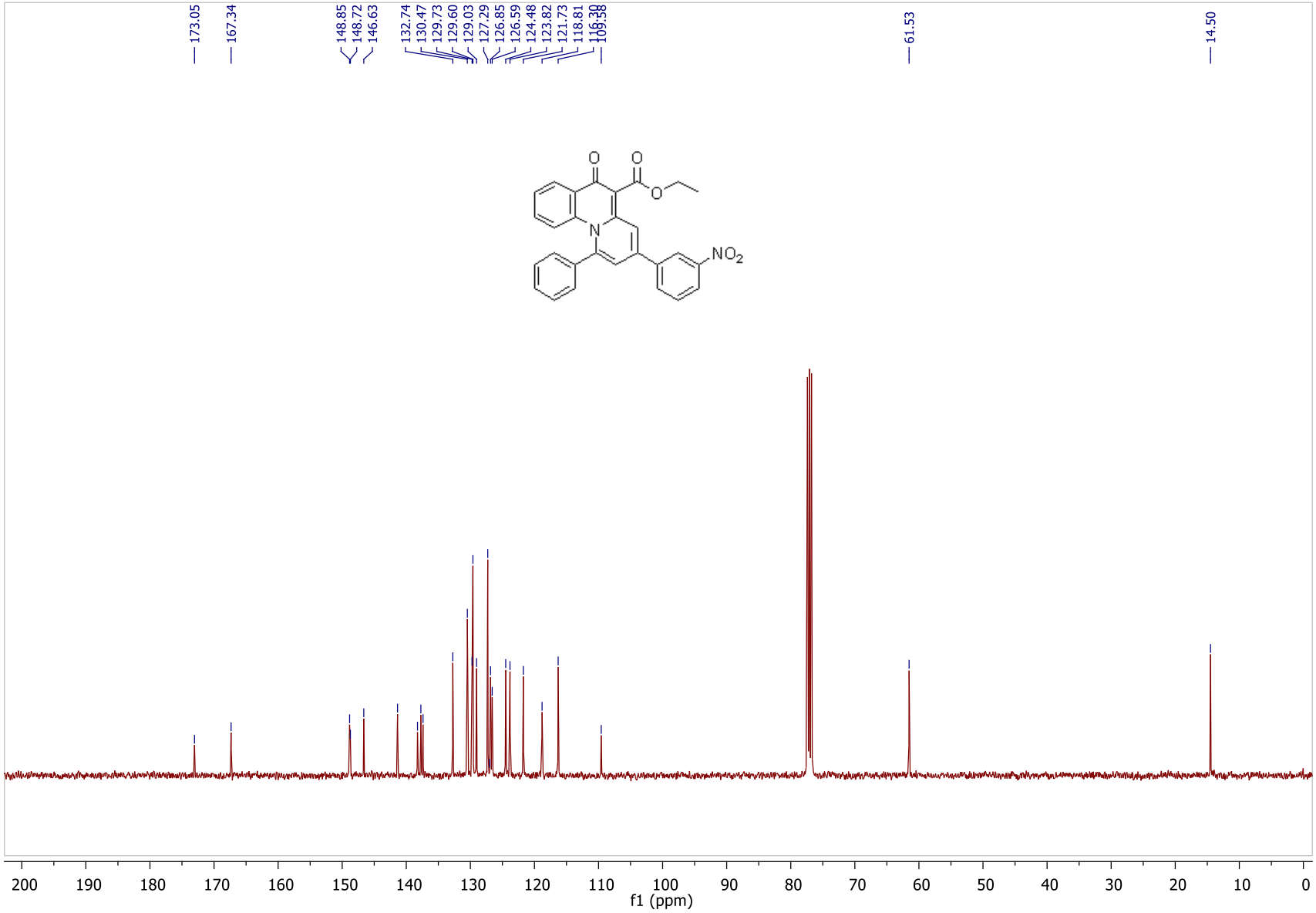
^{13}C NMR of **3s** (101 MHz, $CDCl_3$)



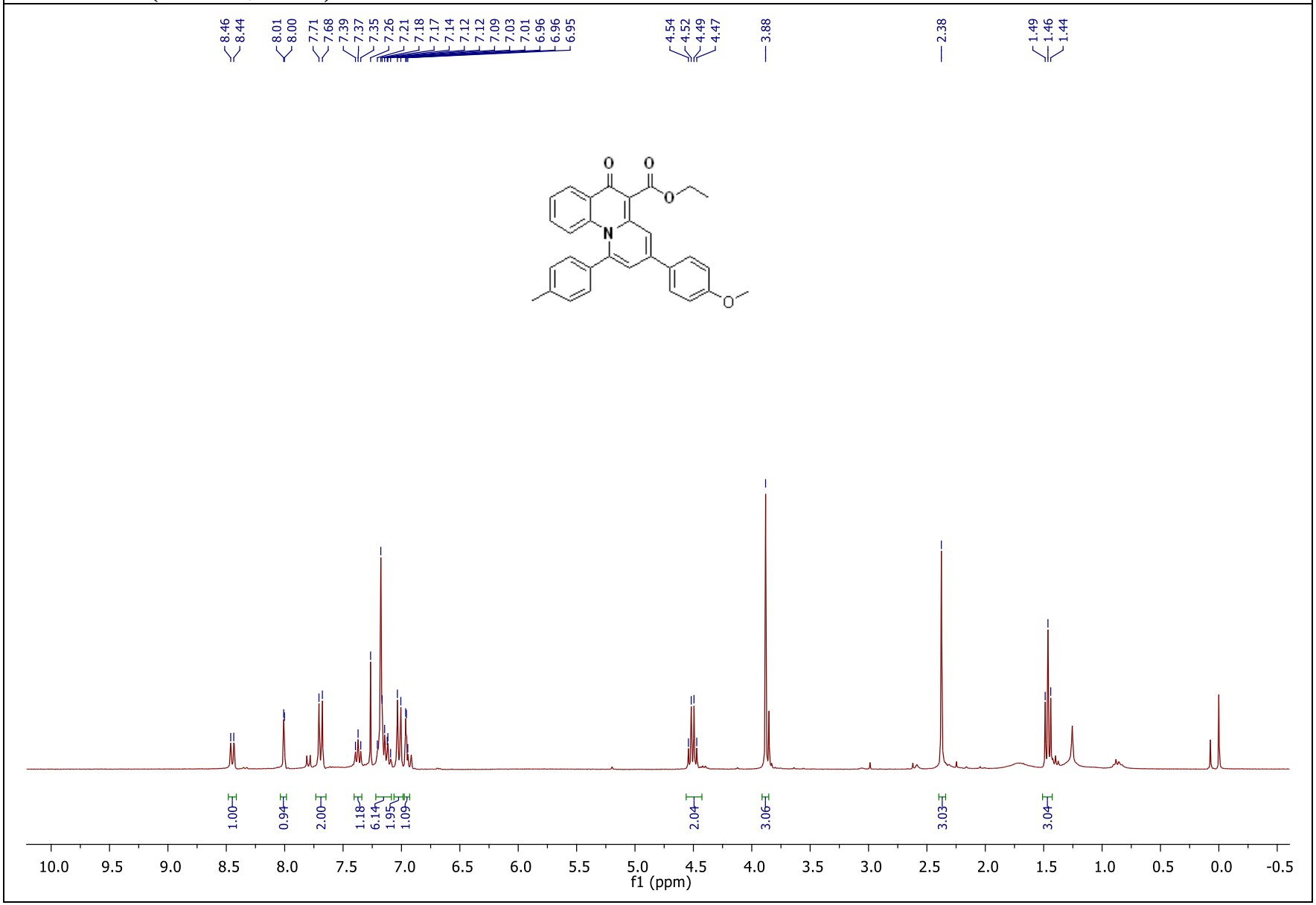
^{1}H NMR of **3t** (400 MHz, $CDCl_3$)



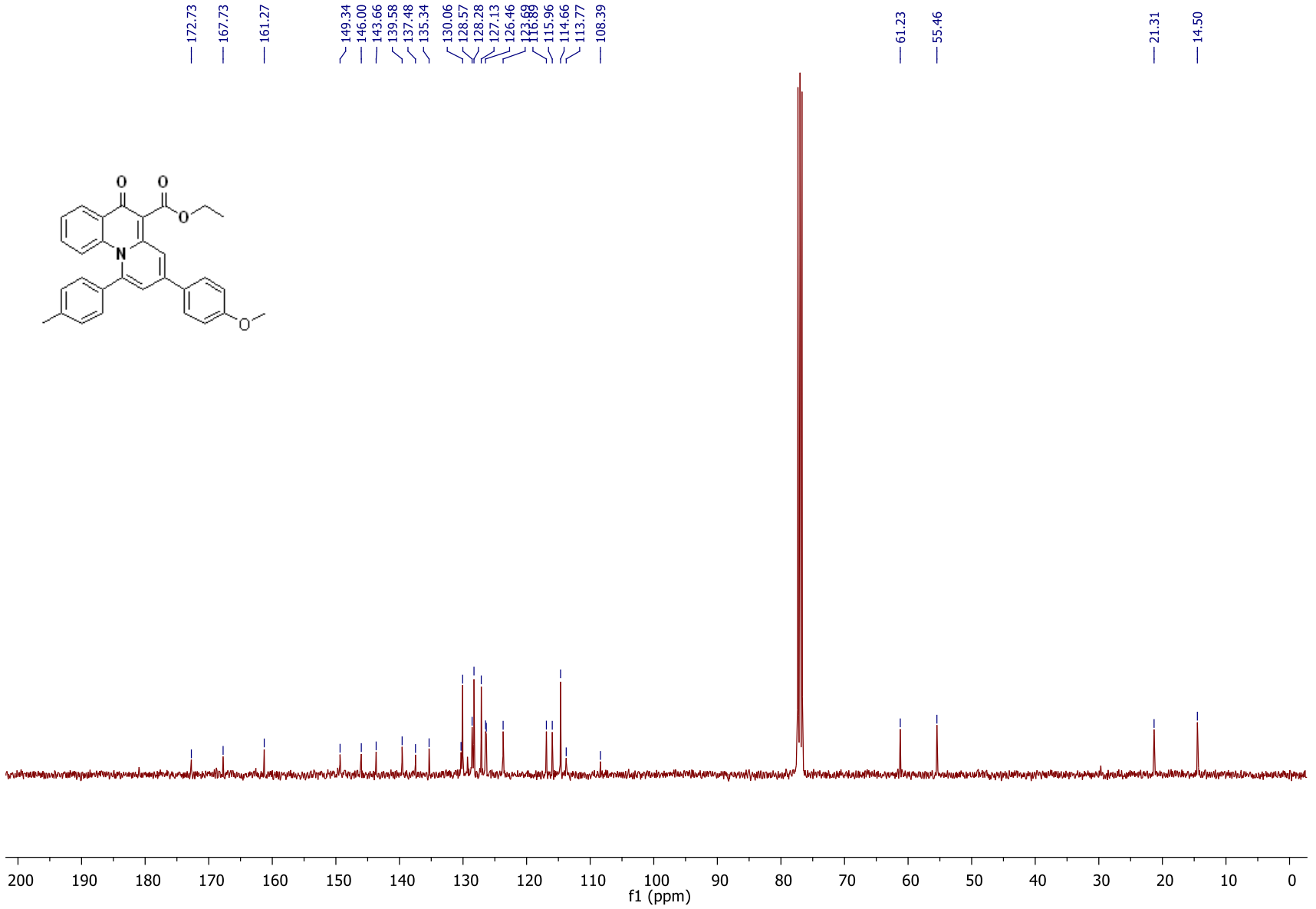
^{13}C NMR of **3t** (101 MHz, $CDCl_3$)



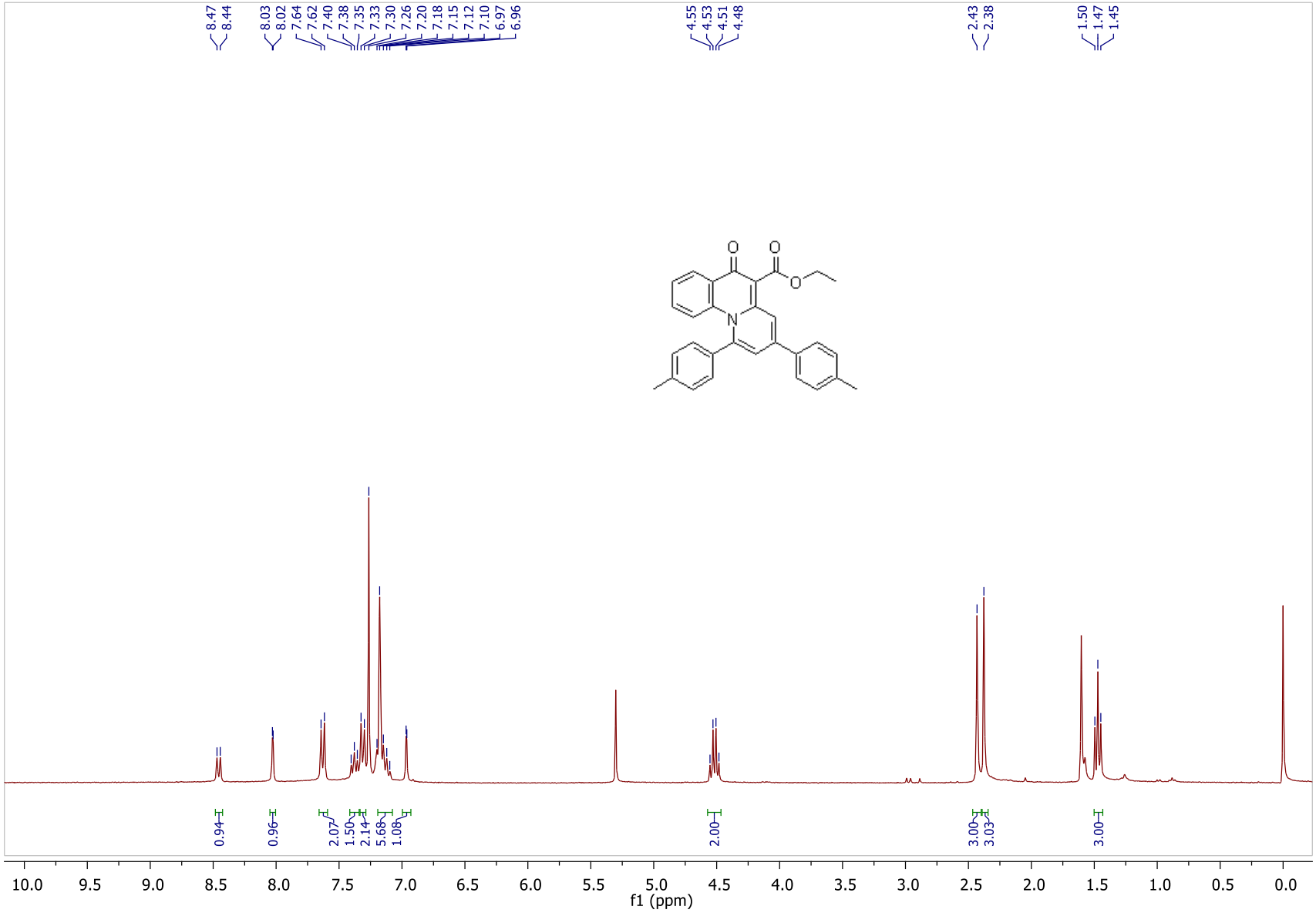
^{1}H NMR of **3u** (300 MHz, $CDCl_3$)



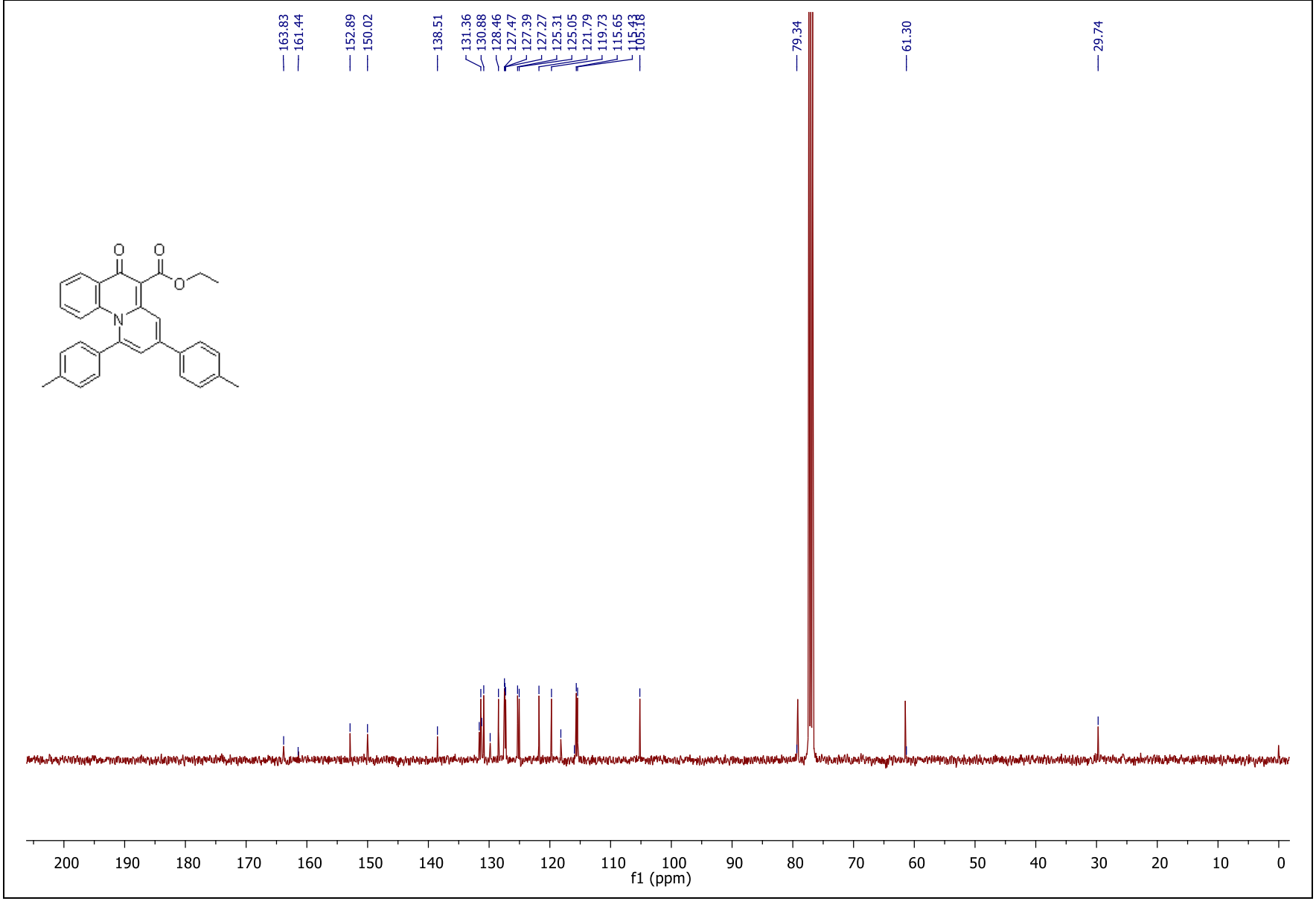
^{13}C NMR of **3u** (101 MHz, $CDCl_3$)



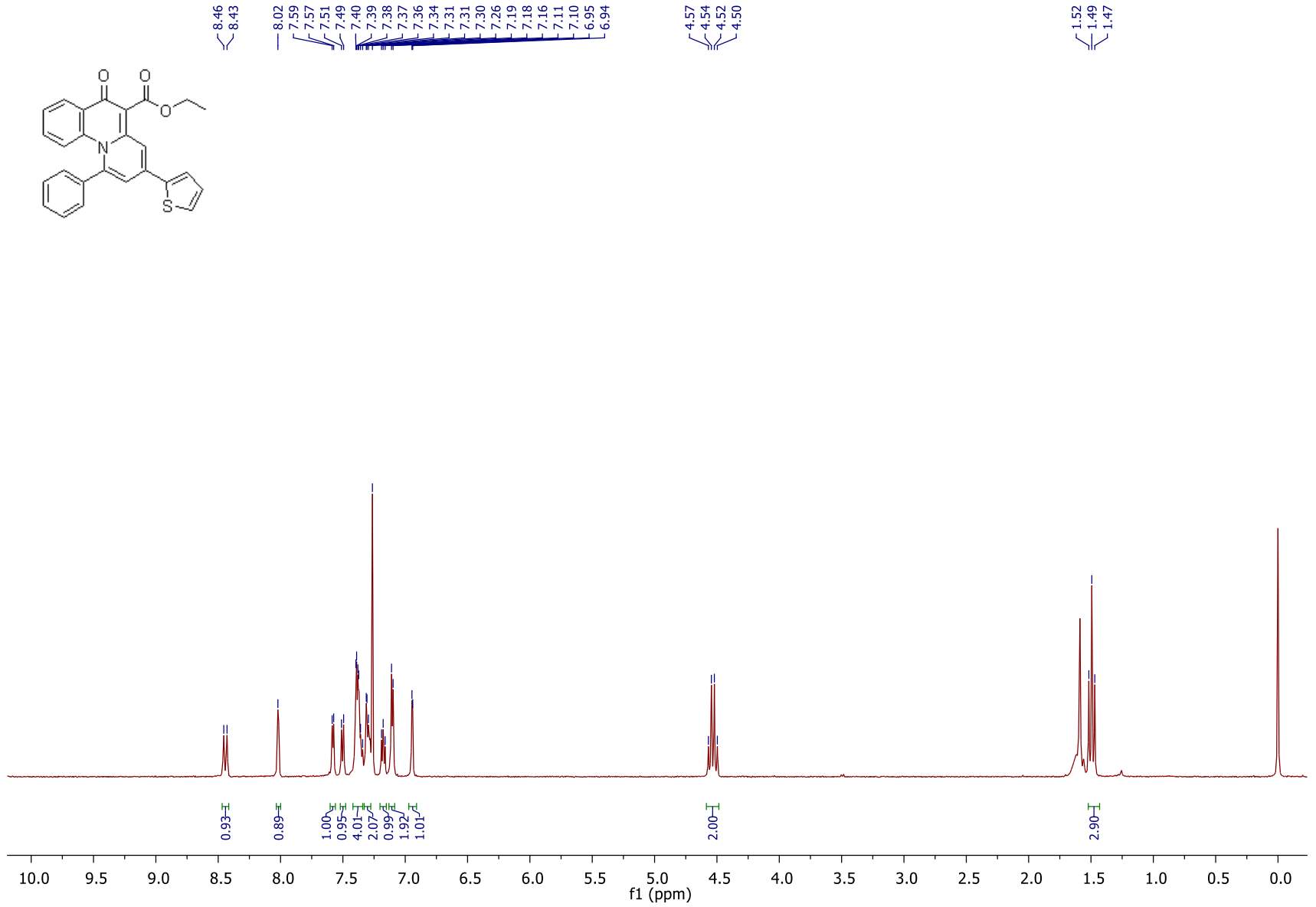
^{1}H NMR of **3v** (300 MHz, $CDCl_3$)



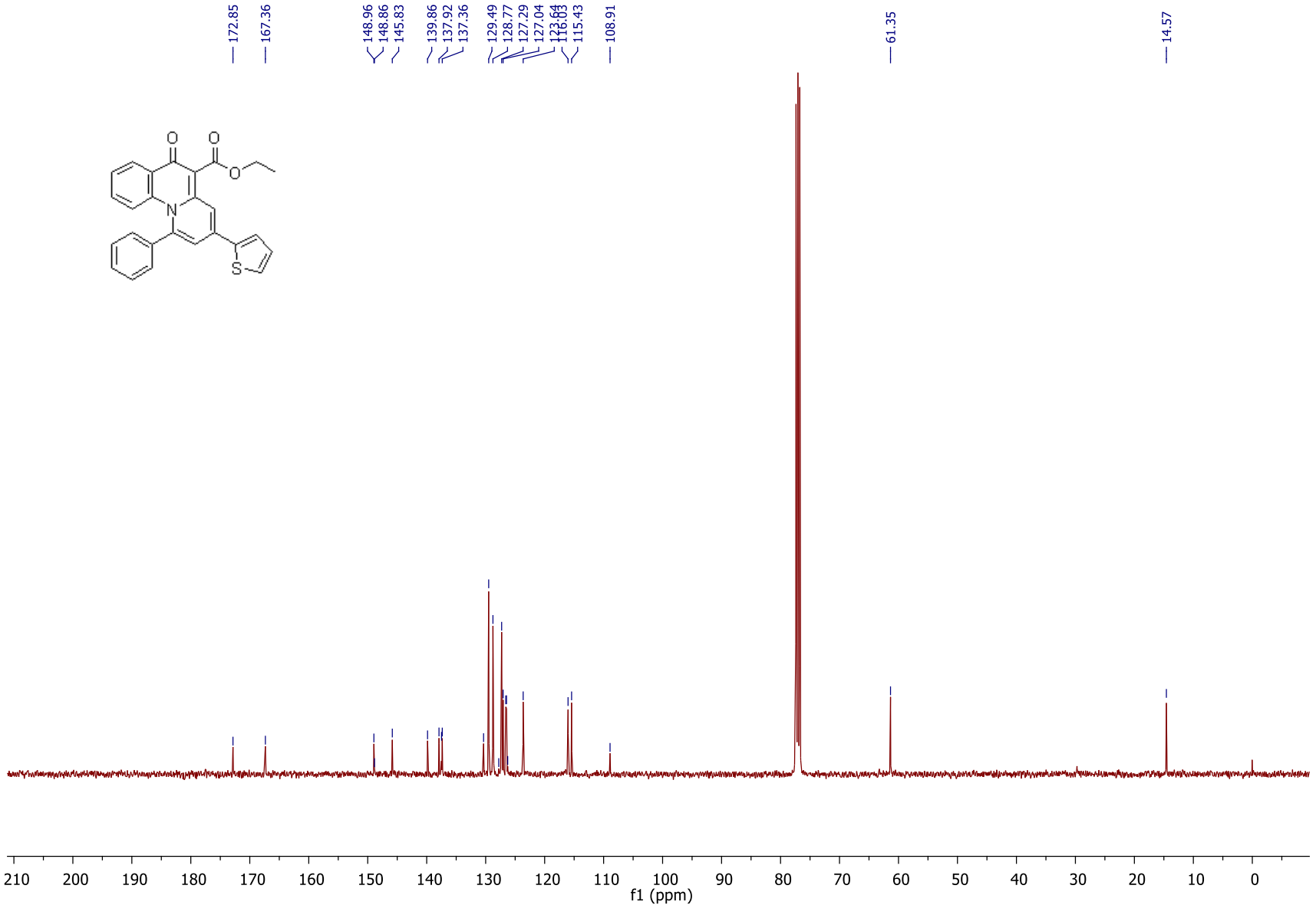
^{13}C NMR of **3v** (101 MHz, $CDCl_3$)



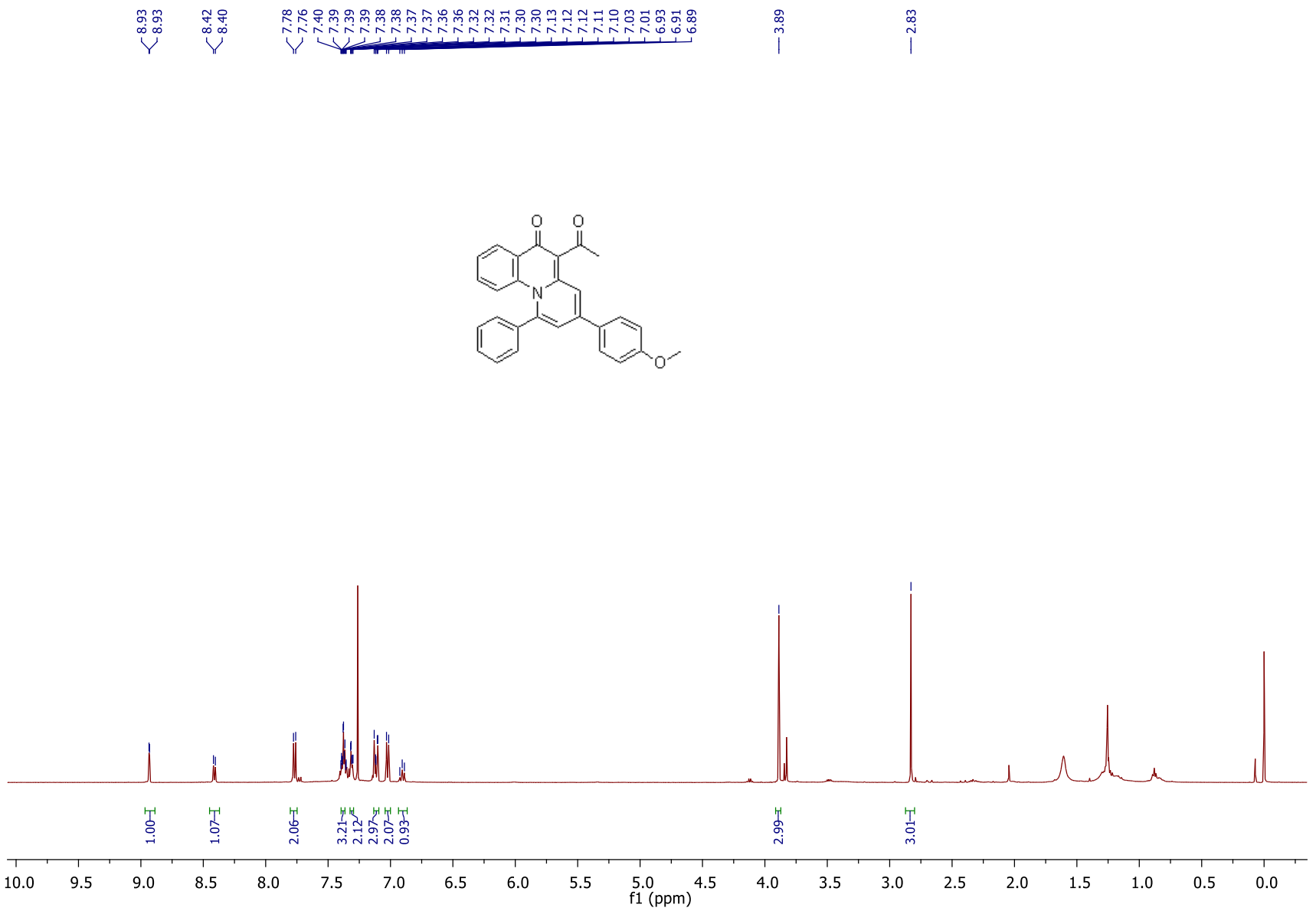
^{1}H NMR of **3w** (101 MHz, $CDCl_3$)



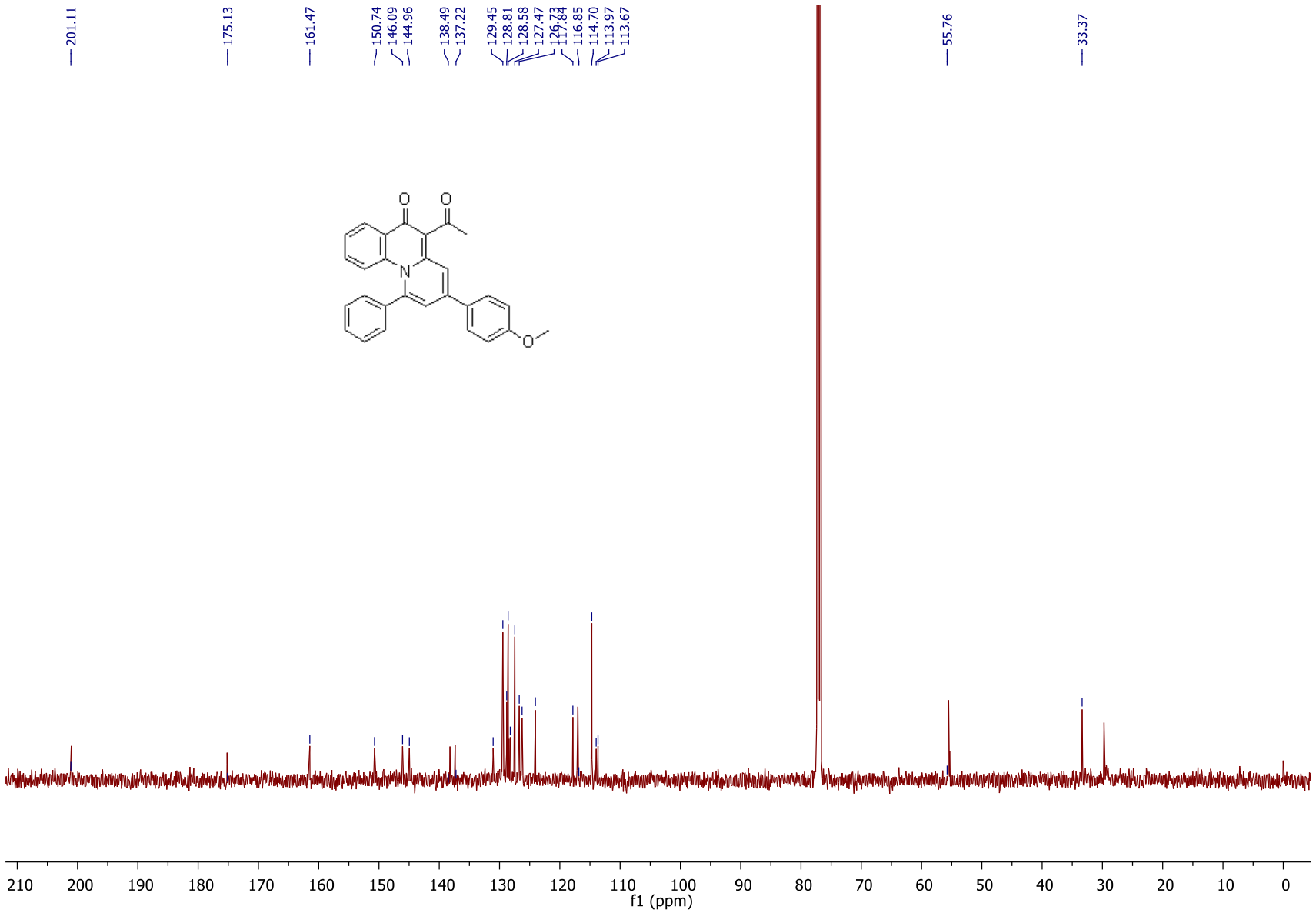
^{13}C NMR of **3w** (101 MHz, $CDCl_3$)



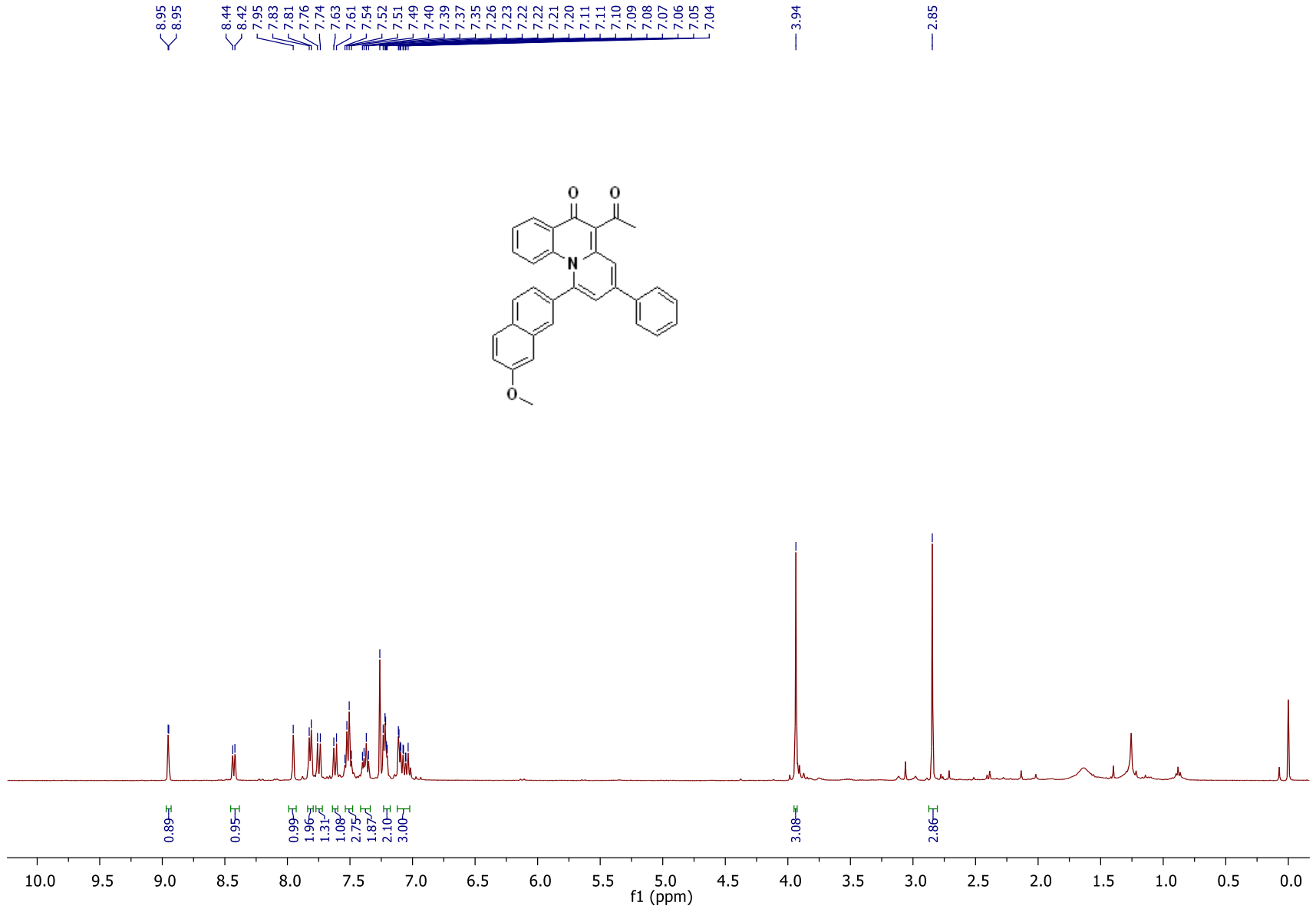
^{1}H NMR of **3x** (500 MHz, $CDCl_3$)



^{13}C NMR of **3x** (101 MHz, $CDCl_3$)



^{1}H NMR of **3y** (400 MHz, $CDCl_3$)



^{13}C NMR of **3y** (101 MHz, $CDCl_3$)