Metal-free $POCl_3$ Promoted Stereoselective Hydrochlorination of ethynylated azaheterocycles

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Supporting Information

Contents

General Methods

Unless otherwise stated, all reactions were performed under nitrogen atmosphere and air successively. Solvents were purified following standard literature procedures. Melting points were measured in an open capillary tube and are uncorrected. ^{1}H (300, 400 and 600 MHz) and ^{13}C (75, 100 and 150 MHz) NMR spectra were recorded 300 MHz, 400 MHz and 600 MHz spectrometer. Multiplicities are given as: s (singlet), brs (broad singlet), d (doublet), t (triplet), dd (doublet of doublets) or m (multiplet). The chemical shifts (δ ppm) and coupling constants (*J* Hz) are reported in the standard fashion with reference to either internal tetramethylsilane (for ^{1}H) or the central line (77.0 ppm) of $CDCl_3$ (for ^{13}C). Moisture and residual peak of $CDCl_3$ appear at δ 1.5 and 7.2 respectively in ^{1}H NMR. High resolution mass spectra (HRMS) were obtained on TOF/6500 SRIES QTOF B.05.00 (B5042.0) and Thermo Scientific Exactive mass spectrometer. Thin-layer chromatographies (TLC) were performed on glass plates (7.5 x 2.5 and 7.5 x 5.0 cm) coated with silica gel GF 254 and various combinations of ethyl acetate and hexane were used as eluent. Visualisation of spots was accomplished by exposure to UV light. Silica gel (60-120 mesh) was used for column chromatography (approximately 15-20 g per 1g of the crude product).

Procedure for the synthesis of starting material (1, 3, 5 and 7).[1, 2]

The starting materials for final products were synthesized by the known literature procedures which was cited in reference. Individually, 2-arylethynylquinoline-3-carbonitrile/carbaldehyde (**1/3**) was prepared accordingly know literature **1**. Compound 2-phenylethynylquinoline-3-carboxylic acid methyl ester[2a] (**7**) was also prepared via reported literature **23a** which is cited in reference. Further also, the starting compounds (**5**)[2b-e] were prepared by the different known literature procedure which is also cited in reference number 2.

References:

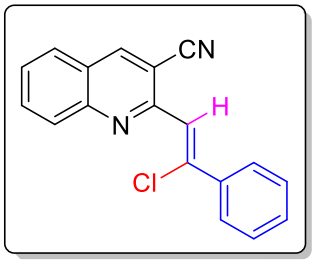
(1) (a) A. Chandra, B. Singh, S. Upadhyay and R. M. Singh, *Tetrahedron*, 2008, **64**, 11680−11685; (b) K. Mishra, J. B. Singh, T. Gupta, R. M. Singh, *Org. Chem. Front*. 2017, **4**, 1926-1930; (c) A. K. Verma, T. Aggarwal, V. Rustagi, R. C. Larock, *Chem Comm*. 2010, **46**, 4064-4066.

(2)(a) N. Sharma, M. Asthana, D. Nandini, R. P. Singh, R. M. Singh, *Tetrahedron*, 2013, **69**, 1822−1829; (b) S. Shi, Y. Zhang, *Synlett*, 2007, 1843–1850; (c) U. S. Sørensen, E. Pombo-Villar, *Tetrahedron*, 2005, **61**, 2607−2703; (d) M. Gazvoda, M. Virant, A. Pevec, D. Urankar, A. Bolje, M. Kočevar, J. Košmrlj, *Chem. Commun.* 2016, **52**, 1571−1574. (e) M. Armengol, J. A. Joule, *J. Chem. Soc., Perkin Trans. 1*, 2001, 154–158.

General procedure for synthesis of 2-(2-chloro-2-phenylvinyl)quinoline-3-carbonitrile/ carbaldehyde (2/4).

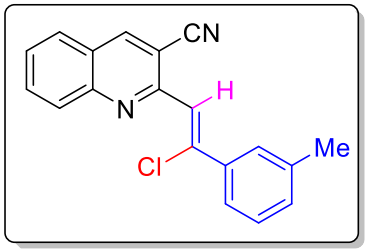
To a solution of compound 2-phenylethynylquinoline-3-carbonitrile/carbaldehyde (**1a/3a**) (0.5 mmol) in 3 equiv $POCl_3$ and stirred at 80 °C under aerobic condition. After completion of the reaction, chilled water was poured into the reaction mixture and extracted with ethyl acetate. The organic layer was washed with water, brine and dried over anhydrous sodium sulphate (Na_2SO_4). The solvent was evaporated under vacuum to give product. The product was further recrystallized from ethanol.

2-(2-Chloro-2-phenylvinyl)quinoline-3-carbonitrile (2a).



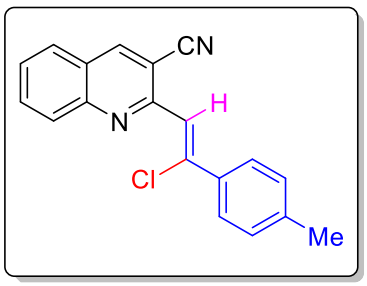
light brown solid; yield 139.2 mg, 96%; mp 129–130 °C; R_f = 0.35 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45 (t, J = 2.1 Hz, 3H), 7.53 (s, 1H), 7.69 (d, J = 7.8 Hz, 1H), 7.82–7.92 (m, 4H), 8.20 (d, J = 8.4 Hz, 1H), 8.58 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 107.4, 116.7, 121.5, 124.9, 127.2, 127.8, 128.3, 128.5, 129.8, 130.0, 132.9, 137.8, 140.6, 142.5, 148.3, 153.6 ppm; IR (KBr, cm−1) 1597, 2203, 2926; HRMS (ESI) m/z calcd for $C_{18}H_{12}ClN_2$ $[M+H]^+$ 291.0684, found 291.0694.

2-(2-Chloro-2-m-tolylvinyl)quinoline-3-carbonitrile (2b).



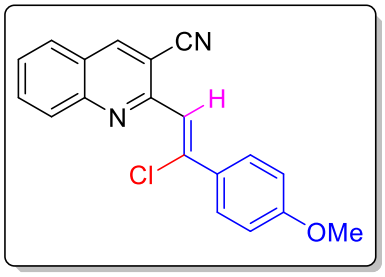
green solid; yield 133.8 mg, 88%; mp 142–143 °C; R_f = 0.30 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.43 (s, 3H), 7.31 (s, 1H), 7.32 (s, 1H), 7.51 (s, 1H), 7.61–7.70 (m, 3H), 7.89 (t, J = 7.5 Hz, 2H), 8.20 (d, J = 9.0 Hz, 1H), 8.58 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 21.3, 107.4, 116.7, 121.3, 124.4, 124.8, 127.8, 128.4, 129.7, 130.8, 132.9, 137.7, 138.2, 140.8, 142.5, 148.3, 153.6 ppm IR (KBr, cm−1) 1607, 2213, 2903; HRMS (ESI) m/z calcd for $C_{19}H_{14}ClN_2$ $[M+H]^+$ 305.0840, found 305.0844.

2-(2-chloro-2-(p-tolyl)vinyl)quinoline-3-carbonitrile (2c).



light yellow solid; yield 136.8 mg, 90%; mp 132–133 °C; R_f = 0.30 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.44 (s, 3H), 7.28–7.38 (m, 1H), 7.53 (s, 1H), 7.63–7.71 (m, 4H), 7.90 (t, J = 7.5 Hz, 2H), 8.22 (d, J = 9.0 Hz, 1H), 8.59 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 21.3, 107.4, 116.8, 121.3, 124.5, 124.9, 127.9, 128.5, 129.8, 130.9, 133.0, 137.8, 138.3, 140.9, 142.7, 148.4, 153.7 ppm; IR (KBr, cm−1) 1613, 2221, 2908; HRMS (ESI) m/z calcd for $C_{19}H_{14}ClN_2$ $[M+H]^+$ 305.0840, found 305.0847.

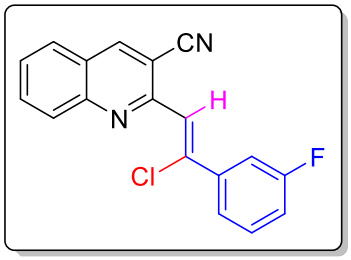
2-[2-Chloro-2-(4-methoxyphenyl)vinyl]quinoline-3-carbonitrile (2d).



white solid; yield 144 mg, 90%; mp 152–153 °C; R_f = 0.25 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.87 (s, 3H), 6.96 (d, J = 8.7 Hz, 2H), 7.45 (s, 1H), 7.66 (t, J = 7.2 Hz, 1H), 7.78 (d, J = 8.7 Hz, 2H), 7.88 (t, J = 7.8 Hz, 2H), 8.19 (d, J = 8.4 Hz, 1H), 8.56 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.8,

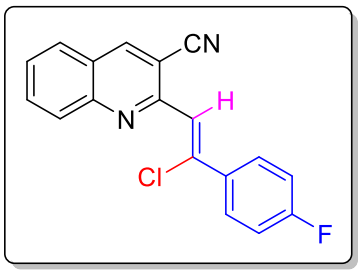
104.7, 117.1, 120.3, 121.7, 121.9, 127.2, 128.5, 128.9, 130.0, 137.9, 140.3, 141.7, 150.5, 154.2, 163.5 ppm; IR (KBr, cm−1) 1590, 2222, 2916; HRMS (ESI) m/z calcd for $C_{19}H_{14}ClN_2O$ $[M+H]^+$ 321.0789, found 321.0788.

2-(2-chloro-2-(3-fluorophenyl)vinyl)quinoline-3-carbonitrile (2e).



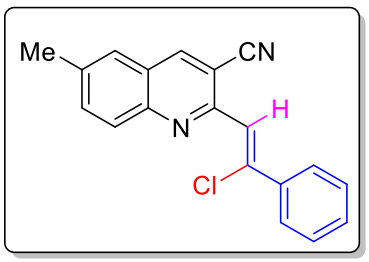
white solid; yield 143.2 mg, 93%; mp 141−143 °C; R_f = 0.30 (05:95 EtOAc/hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13 (t, *J* = 8.8 Hz, 2H), 7.47 (s, 1H), 7.67 (t, *J* = 7.2 Hz, 1H), 7.78−7.82 (m, 2H), 7.89 (t, *J* = 7.6 Hz, 2H) 8.19 (d, *J* = 8.4 Hz, 1H), 8.57 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 107.3, 115.5 (d, *J* = 21.9 Hz), 116.7, 121.4 (d, *J* = 1.3 Hz), 124.9, 127.8, 128.4, 129.1 (d, *J* = 8.6 Hz), 129.8, 131.3 (d, *J* = 8.5 Hz), 132.9, 133.9 (d, *J* = 3.2 Hz), 139.4, 142.5, 148.3, 153.4, 162.4, 164.9 ppm; IR (KBr, cm−1) 1611, 2218, 2925; HRMS (ESI) m/z calcd for $C_{18}H_{11}ClFN_2$ $[M+H]^+$ 309.0589, found 309.0599.

2-[2-Chloro-2-(4-fluoro-phenyl)vinyl]quinoline-3-carbonitrile (2f).



white solid; yield 138.6 mg, 90%; mp 111−112 °C; R_f = 0.30 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.14 (t, *J* = 8.4 Hz, 2H), 7.47 (s, 1H), 7.68 (t, *J* = 7.5 Hz, 1H), 7.79−7.90 (m, 4H), 8.19 (d, *J* = 8.7 Hz, 1H), 8.58 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 107.3, 115.6 (d, *J* = 29.3 Hz), 116.8, 121.4, 124.9, 127.9, 128.4, 129.2 (d, *J* = 11.2 Hz), 129.8, 133.0, 134.0, 139.5, 142.6, 148.4, 153.5, 162.1, 165.4 ppm; IR (KBr, cm−1) 1621, 2214, 2902; HRMS (ESI) m/z calcd for $C_{18}H_{11}ClFN_2$ $[M+H]^+$ 309.0589, found 309.0593.

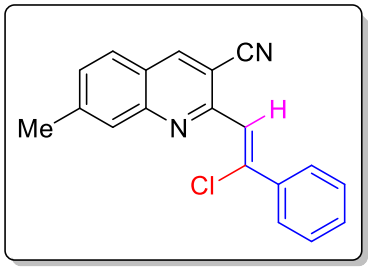
2-(2-Chloro-2-phenylvinyl)6-methyl-quinoline-3-carbonitrile (2h).



brown solid; yield 136.8 mg, 90%; mp 137−138 °C; R_f = 0.30 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.59 (s, 3H), 7.42−7.46 (m, 3H), 7.51 (s, 1H), 7.64 (s, 1H), 7.72 (d, *J* = 9.3 Hz, 1H), 7.80−7.84 (m, 2H), 8.09 (d, *J* = 8.7 Hz, 1H), 8.48 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 22.3, 106.2, 115.9, 121.8, 124.0, 127.3, 127.4, 128.5, 128.6, 129.9, 130.7, 137.9, 140.7, 142.5, 144.0, 148.6, 154.6 ppm;

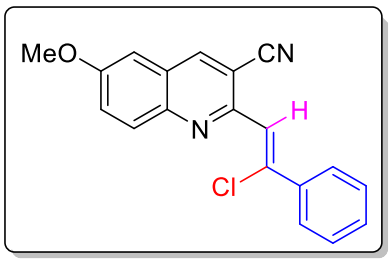
IR (KBr, cm−1) 1609, 2212, 2923; HRMS (ESI) m/z calcd for $C_{19}H_{14}ClN_2$ $[M+H]^+$ 305.0840 found 305.0849.

2-(2-Chloro-2-phenylvinyl)-7-methyl-quinoline-3-carbonitrile (2i).



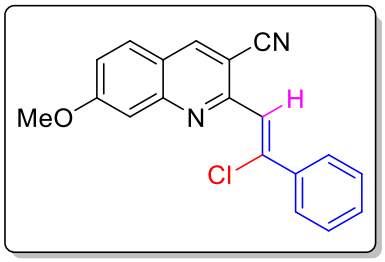
light brown solid; yield 133.8 mg, 88%; mp 127−128 °C; R_f = 0.30 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.62 (s, 3H), 7.35−7.48 (m, 4H), 7.52 (s, 1H), 7.76−7.82 (m, 3H), 7.99 (s, 1H), 8.52 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 22.1, 106.4, 116.9, 121.6, 123.0, 127.2, 127.4, 128.5, 128.7, 129.9, 130.6, 137.9, 140.3, 142.0, 144.0, 148.5, 153.6 ppm; IR (KBr, cm−1) 1614, 2217, 2927; HRMS (ESI) m/z calcd for $C_{19}H_{14}ClN_2$ $[M+H]^+$ 305.0840 found 305.0842.

2-(2-Chloro-2-phenylvinyl)-6-methoxy-quinoline-3-carbonitrile (2j).



white solid; yield 147.2 mg, 92%; mp 162−163 °C; R_f = 0.25 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.97 (s, 3H), 7.11 (s, 1H), 7.44 (d, J = 4.8Hz, 3H), 7.50 (s, 1H), 7.54 (d, J = 2.4 Hz, 1H), 7.81 (d, J = 4.5 Hz, 2H), 8.09 (d, J = 9.3 Hz, 1H), 8.45 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.8, 104.7, 107.5, 117.1, 120.3, 121.7, 121.9, 127.2, 128.5, 128.9, 130.0, 137.9, 140.3, 141.7, 150.5, 154.2, 163.5 ppm; IR (KBr, cm−1) 1601, 2223, 2914; HRMS (ESI) m/z calcd for $C_{19}H_{14}ClN_2O$ $[M+H]^+$ 321.0789 found 321.0794.

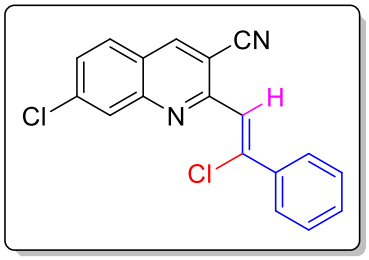
2-(2-Chloro-2-phenylvinyl)-7-methoxy-quinoline-3-carbonitrile (2k).



white solid; yield 142.4 mg, 89%; mp 167−168 °C; R_f = 0.25 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 4.01 (s, 3H), 7.28−7.32 (m, 1H), 7.44 (t, J = 3.3 Hz, 3H), 7.49 (d, J = 2.1 Hz, 1H), 7.50 (s, 1H), 7.75 (d, J = 9.0 Hz, 1H), 7.81 (d, J = 3.9 Hz, 2H), 8.46 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.7, 104.6, 107.5, 117.0, 120.2, 121.6, 121.8, 127.1, 128.4, 128.8, 129.2, 129.8, 137.8, 141.5,

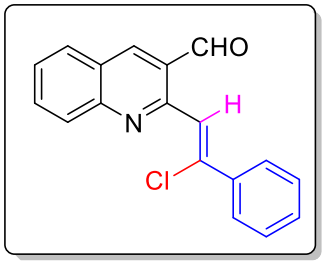
150.4, 154.1, 163.4 ppm; IR (KBr, cm−1) 1596, 2218, 2924; HRMS (ESI) m/z calcd for $C_{19}H_{14}ClN_2O$ $[M+H]^+$ 321.0789, found 321.0797.

7-Chloro-2-(2-chloro-2-phenylvinyl)quinoline-3-carbonitrile (2l).



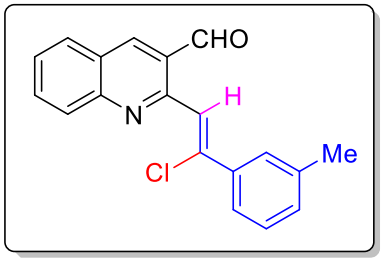
white solid; yield 137.7 mg, 85%; mp 124−125 °C; R_f = 0.50 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.44−7.46 (m, 3H), 7.52 (s, 1H), 7.62 (d, *J* = 8.7 Hz, 1H), 7.82 (t, *J* = 4.5 Hz, 3H), 8.20 (s, 1H), 8.55 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 107.6, 116.4, 121.0, 123.2, 127.2, 128.6, 128.8, 128.9, 129.4, 130.1, 137.7, 139.1, 141.3, 142.2, 148.6, 154.6 ppm; IR (KBr, cm−1) 1616, 2231, 2928; HRMS (ESI) m/z calcd for $C_{18}H_{11}Cl_2N_2$ $[M+H]^+$ 325.0294, found 325.0289.

2-(2-Chloro-2-phenylvinyl-quinoline-3-carbaldehyde (4a).



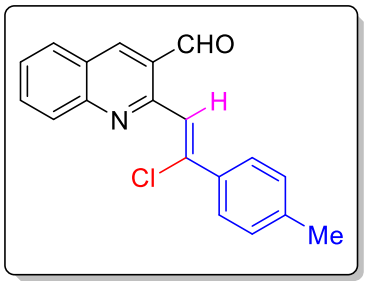
light brown solid; yield 131.8 mg, 90%; mp 123−124 °C; R_f = 0.40 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.44−7.45 (m, 3H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.70 (s, 1H), 7.83−7.90 (m, 3H), 8.01 (d, *J* = 8.1 Hz, 1H), 8.18 (d, *J* = 8.7 Hz, 1H), 8.79 (s, 1H), 10.33 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 122.7, 126.3, 126.8, 127.6, 127.7, 128.5, 129.2, 129.3, 129.7, 132.6, 137.1, 139.0, 139.5, 149.4, 154.7, 190.5 ppm; IR (KBr, cm−1) 1601, 2223, 2914; IR (KBr, cm−1) 1612, 1693, 2936; HRMS (ESI) m/z calcd for $C_{18}H_{13}ClNO$ $[M+H]^+$ 294.0680, found 294.0690.

2-(2-Chloro-2-m-tolylvinyl)quinoline-3-carbaldehyde (4b).



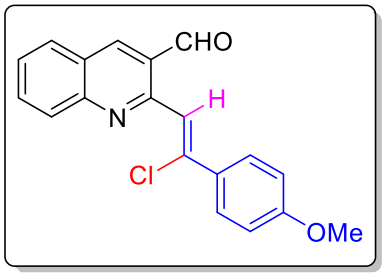
white solid; yield 130.5 mg, 85%; mp 135−136 °C; R_f = 0.40 (05:95 EtOAc/hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.42 (s, 3H), 7.25 (t, *J* = 7.6 Hz, 1H), 7.33 (d, *J* = 7.6 Hz, 1H), 7.61−7.677 (m, 4H), 7.86 (t, *J* = 8.4 Hz, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 8.17 (d, *J* = 8.4 Hz, 1H), 8.77 (s, 1H), 10.32 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.3, 122.4, 124.1, 126.3, 127.5, 127.7, 128.4, 129.2, 129.3, 130.6, 132.6, 137.0, 138.2, 139.3, 149.4, 154.9, 190.5 ppm; IR (KBr, cm−1) 1621, 1687, 2908; HRMS (ESI) m/z calcd for $C_{19}H_{15}ClNO$ $[M+H]^+$ 308.0837, found 308.0844.

3.3.1.15 ***2-(2-Chloro-2-p-tolylvinyl)quinoline-3-carbaldehyde (4c).***



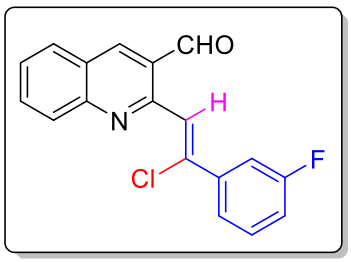
white solid; yield 130.5 mg, 85%; mp 125–126 °C; R_f = 0.40 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.39 (s, 3H), 7.58–7.73 (m, 5H), 7.84 (s, 2H), 7.96 (d, *J* = 5.4 Hz, 1H), 8.16 (d, *J* = 6.9 Hz, 1H), 8.74 (s, 1H), 10.30 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 21.1, 121.6, 126.2, 126.7, 127.6, 127.6, 129.1, 129.3, 132.5, 134.2, 139.2, 139.2, 139.3, 140.0, 149.3, 154.9, 190.6 ppm; IR (KBr, cm−1) 1587, 1695, 2915; HRMS (ESI) m/z calcd for $C_{19}H_{15}ClNO$ $[M+H]^+$ 308.0837, found 308.0839.

2-[2-Chloro-2-(4-methoxy-phenyl)vinyl]quinoline-3-carbaldehyde (4d).



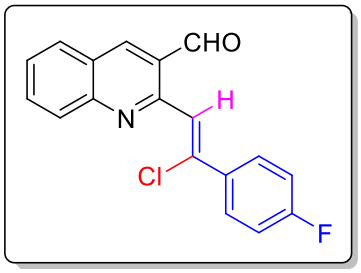
white solid; yield 135.7 mg, 84%; mp 154–155 °C; R_f = 0.30 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.96 (s, 3H), 7.12 (t, *J* = 7.8 Hz, 2H), 7.65 (s, 1H), 7.83 (t, *J* = 6.3 Hz, 3H), 7.97 (d, *J* = 8.1 Hz, 1H), 8.16 (d, *J* = 8.1 Hz, 1H), 8.73 (s, 1H), 10.29 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.6, 115.6, 122.8, 126.3, 127.7, 127.8, 128.8, 128.9, 129.2, 132.7, 137.7, 140.0, 149.3, 154.3, 161.8, 165.1, 190.3 ppm; IR (KBr, cm−1) 1614, 1696, 2932; HRMS (ESI) m/z calcd for $C_{19}H_{15}ClNO_2$ $[M+H]^+$ 324.0786, found 324.0788.

2-(2-chloro-2-(3-fluorophenyl)vinyl)quinoline-3-carbaldehyde (4e).



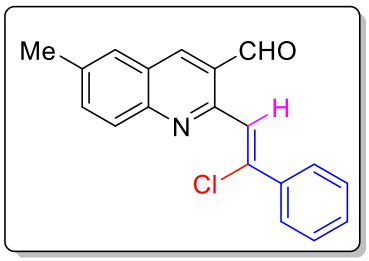
white solid; yield 141.5 mg, 91%; mp 156–157 °C; R_f = 0.40 (05:95 EtOAc/hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.00–7.05 (m, 1H), 7.30–7.34 (m, 1H), 7.43–7.46 (m, 1H), 7.55 (t, *J* = 8.4 Hz, 2H), 7.65 (s, 1H), 7.76–7.80 (m, 1H), 789 (d, *J* = 8.0 Hz, 1H), 8.08 (d, *J* = 8.4 Hz, 1H), 8.65 (s, 1H), 10.20 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 114.1 (d, *J* = 23.6 Hz), 116.6 (d, *J* = 21.1 Hz), 112.5 (d, *J* = 2.9 Hz), 123.8, 126.3, 127.6, 127.8, 129.2(d, *J* = 5.7 Hz), 130.0 (d, *J* = 8.3 Hz), 132.7, 137.3(d, *J* = 2.8 Hz), 139.4(d, *J* = 7.8 Hz), 140.2, 149.3, 154.0, 161.4, 163.8, 190.4 ppm; IR (KBr, cm−1) 1608, 1690, 2931; HRMS (ESI) m/z calcd for $C_{18}H_{12}ClFNO$ $[M+H]^+$ 312.0586, found 312.0592.

2-[2-Chloro-2-(4-fluoro-phenyl)vinyl]quinoline-3-carbaldehyde (4f).



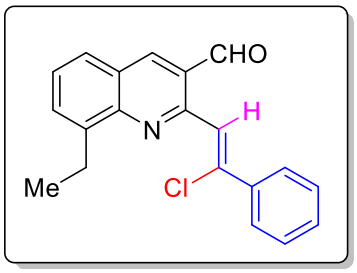
white solid; yield 136.8 mg, 88%; mp 137–138 °C; R_f = 0.40 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.12 (t, *J* = 8.4 Hz, 2H), 7.64 (t, *J* = 7.8 Hz, 2H), 7.79–7.89 (m, 3H), 7.99 (d, *J* = 8.1 Hz, 1H), 8.17 (d, *J* = 8.7 Hz, 1H), 8.75 (s, 1H), 10.30 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 115.5 (d, *J* = 21.6 Hz), 122.8, 126.4, 127.7, 129.0 (d, *J* = 8.4 Hz), 129.4, 132.8, 133.5(d, *J* = 3.3 Hz), 137.9, 140.2, 149.5, 154.5, 162.0, 165.3, 190.6 ppm; IR (KBr, cm−1) 1613, 1695, 2922; HRMS (ESI) m/z calcd for $C_{18}H_{12}ClFNO$ $[M+H]^+$ 312.0586, found 312.0589.

2-(2-Chloro-2-phenylvinyl)-6-methyl-quinoline-3-carbaldehyde (4h).



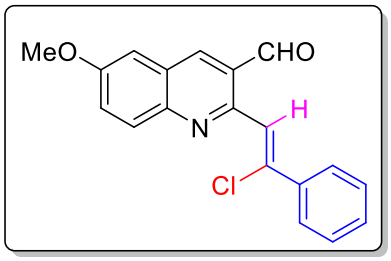
white solid; yield 133.5 mg, 87%; mp 147–148 °C; R_f = 0.40 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.59 (s, 3H), 7.42–7.46 (m, 4H), 7.68 (s, 1H), 7.84 (t, *J* = 7.2 Hz, 3H), 7.94 (s, 1H), 8.68 (s, 1H), 10.28 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 22.2, 122.9, 124.4, 126.9, 127.0, 128.3, 128.4, 128.9, 129.6, 130.0, 137.2, 138.8, 139.2, 143.7, 149.6, 154.7 ppm, 190.57; IR (KBr, cm−1) 1594, 1691, 2906; HRMS (ESI) m/z calcd for $C_{19}H_{15}ClNO$ $[M+H]^+$ 308.0837, found 308.0839.

2-(2-Chloro-2-phenylvinyl)-8-ethyl-quinoline-3-carbaldehyde (4i).



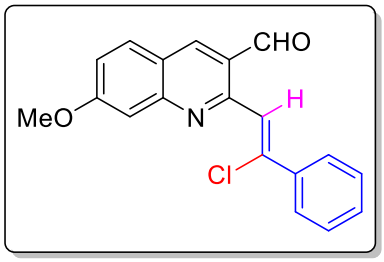
light yellow solid; yield 133.2 mg, 83%; mp 101–102 °C; R_f = 0.45 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.40 (t, *J* = 7.5 Hz, 3H), 3.36 (q, *J* = 7.2 Hz, 2H), 7.45 (d, *J* = 6.9 Hz, 3H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.71 (s, 1H), 7.80–7.89 (m, 4H), 8.68 (s, 1H), 10.33 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 15.1, 24.4, 123.0, 126.1, 127.0, 127.2, 127.5, 128.4, 129.5, 131.0, 137.9, 138.1, 141.1, 141.2, 143.6, 147.7, 152.5, 191.1 ppm; IR (KBr, cm−1) 1586, 1689, 2924; HRMS (ESI) m/z calcd for $C_{19}H_{15}ClNO$ $[M+H]^+$ 322.0993, found 322.0997.

3.3.1.22 ***2-(2-Chloro-2-phenylvinyl)-6-methoxy-quinoline-3-carbaldehyde (4j).***



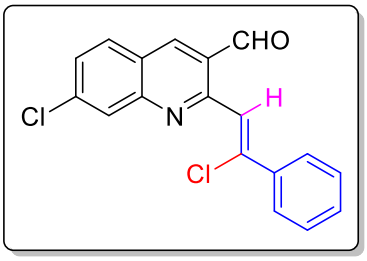
white solid; yield 140.5 mg, 87%; mp 163–164 °C; R_f = 0.30 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$): δ 3.96 (s, 3H), 7.21 (d, *J* = 1.8 Hz, 1H), 7.43–7.53 (m, 4H), 7.66 (s, 1H), 7.82 (d, *J* = 3.9 Hz, 2H), 8.05 (d, *J* = 9.0 Hz, 1H), 8.65 (s, 1H), 10.31 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 55.6, 106.1, 122.8, 125.7, 126.9, 127.6, 127.8, 128.5, 129.7, 130.7, 137.2, 137.7, 138.7, 145.8, 152.4, 158.6, 190.7 ppm; IR (KBr, cm−1) 1619, 1691, 2926; HRMS (ESI) m/z calcd for $C_{19}H_{15}ClNO_2$ $[M+H]^+$ 324.0786, found 324.0785.

2-(2-Chloro-2-phenylvinyl)-7-methoxy-quinoline-3-carbaldehyde (4k).



white solid; yield 134 mg, 83%; mp 169–170 °C; R_f = 0.30 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 4.02 (s, 3H), 7.31 (d, *J* = 9.3 Hz, 1H), 7.45 (s, 4H), 7.72 (s, 1H), 7.88 (t, *J* = 7.5 Hz, 3H), 8.75 (s, 1H), 10.27 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 56.1, 106.3, 121.8, 125.8, 127.1, 128.6, 129.9, 130.6, 137.0, 139.6, 139.9, 150.6, 154.9, 163.9, 189.9 ppm; IR (KBr, cm−1) 1591, 1687, 2933; HRMS (ESI) m/z calcd for $C_{19}H_{15}ClNO_2$ $[M+H]^+$ 324.0786, found 324.0790.

7-Chloro-2-(2-chloro-2-phenylvinyl)-quinoline-3-carbaldehyde (4l).



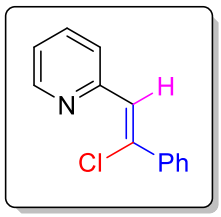
white solid; yield 132.4 mg, 81%; mp 129–130 °C; R_f = 0.35 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.43 (t, *J* = 1.5 Hz, 3H), 7.56 (d, *J* = 7.2 Hz, 1H), 7.67 (s, 1H), 7.81–7.83 (m, 2H), 7.90 (d, *J* = 8.7 Hz, 1H), 8.15 (s, 1H), 8.71 (s, 1H), 10.29 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 122.3, 124.7, 126.9, 127.7, 128.4, 128.5, 128.8, 129.9, 130.4, 137.0, 138.8, 139.2, 139.5, 149.6, 155.7, 190.1 ppm; IR (KBr, cm−1) 1594, 1693, 2911; HRMS (ESI) m/z calcd for $C_{18}H_{11}Cl_2NO$ $[M+H]^+$ 328.0290, found 328.0299.

General procedure for synthesis of hydrochlorination of other ethynylated azaheterocycles (6a–6f).

To a solution of compound (**5a–5f**) (0.5 mmol) in 3 equiv $POCl_3$ and stirred at 80 °C under aerobic condition. After completion of the reaction, chilled water was poured into the reaction mixture and extracted with ethyl acetate. The organic layer was washed with water, brine and dried over anhydrous sodium sulphate (Na_2SO_4). The solvent was evaporated under

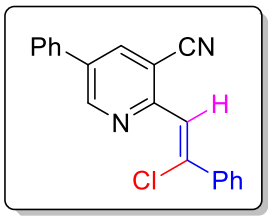
vacuum to give the corresponding product (**6a–6f**). The product was further recrystallized from ethanol.

2-(2-chloro-2-phenylvinyl)pyridine (6a).



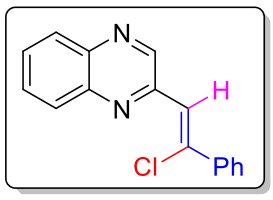
yellow liquid; yield 89.2 mg, 83%; R_f = 0.35 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.12 (t, *J* = 8.4 Hz, 2H), 7.49 (s, 1H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.80 (t, *J* = 7.8 Hz, 1H), 7.94 (d, *J* = 8.1 Hz, 1H), 8.21(d, *J* = 8.4 Hz, 1H), 8.30 (d, *J* = 8.7 Hz, 2H), 8.61 (d, *J* = 10.5 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 120.5, 124.0, 126.3, 129.2, 130.0, 131.1, 135.4, 136.6, 140.1, 149.6, 154.5 ppm; IR (KBr, cm−1) 1617, 2936; HRMS (ESI) m/z calcd for $C_{13}H_{11}ClN$ $[M+H]^+$ 216.0575, found 216.0583.

2-(2-chloro-2-phenylvinyl)-5-phenylnicotinonitrile (6b).



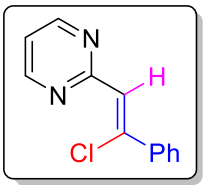
brown solid; yield 142.4 mg, 90%; mp 161–162 °C; R_f = 0.25 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.46–7.48 (m, 3H), 7.50–7.55 (m, 3H), 7.62 (d, *J* = 7.2 Hz, 2H), 7.69 (s, 1H), 7.80 (d, *J* = 3.6 Hz, 2H), 8.15 (d, *J* = 8.4 Hz, 1H), 9.12 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 111.3, 114.0, 126.8, 127.2, 128.2, 128.5, 128.6, 129.0, 129.2, 129.7, 134.1, 137.3, 138.7, 151.4, 153.7 ppm; IR (KBr, cm−1) 1584, 2207, 2906; HRMS (ESI) m/z calcd for $C_{25}H_{19}N_2O$ $[M+H]^+$ 317.0840, found 317.0853.

2-(2-chloro-2-phenylvinyl)quinoxaline (6c).



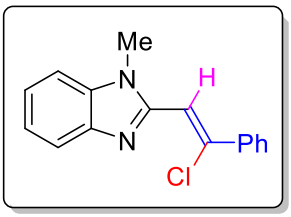
yellow gummy; yield 101.6 mg, 77%; R_f = 0.30 (05:95 EtOAc/hexane); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.37 (t, *J* = 7.2 Hz, 1H), 7.44–7.47 (m, 3H), 7.48 (s, 1H), 7.51–7.54 (m, 3H), 7.65 (s, 1H), 8.09 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 119.5, 121.4, 126.9, 127.2, 128.3, 128.4, 128.5, 129.3, 131.5, 133.1, 135.8, 136.4, 142.8, 145.8 ppm; IR (KBr, cm−1) 1628, 1638, 2913; HRMS (ESI) m/z calcd for $C_{13}H_{11}ClN$ $[M+H]^+$ 265.0684, found 265.0697.

2-(2-chloro-2-phenylvinyl)pyrimidine (6d).



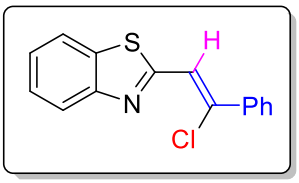
yellow liquid; yield 87.4 mg, 81%; R_f = 0.45 (05:95 EtOAc/hexane); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.13 (q, *J* = 6.6 Hz, 2H), 7.39–7.42 (m, 2H), 7.52 (s, 1H), 7.62 (d, *J* = 7.2 Hz, 1H), 7.66 (t, *J* = 6.6 Hz, 1H), 8.83 (d, *J* = 5.4 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 118.2, 125.4, 127.8, 128.9, 129.6, 129.5, 136.3, 137.9, 153.8, 161.8 ppm; IR (KBr, cm−1) 1594, 1617, 2923; HRMS (ESI) m/z calcd for $C_{12}H_{10}ClN_2$ $[M+H]^+$ 217.0527, found 217.0533.

2-(2-chloro-2-phenylvinyl)-1-methyl-1H-benzo[d]imidazole (6e).



brown solid; yield 112.5 mg, 84%; mp 145–147 °C; R_f = 0.35 (05:95 EtOAc/hexane); ^{1}H NMR (600 MHz, $CDCl_3$) δ 3.75 (s, 3H), 7.18 (t, *J* = 7.8 Hz, 1H), 7.29 (t, *J* = 7.8 Hz, 3H), 7.38 (s, 1H), 7.53 (t, *J* = 7.2 Hz, 1H), 7.70 (d, *J* = 7.8 Hz, 2H), 7.75–7.79 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ30.0, 112.4, 120.1, 126.2, 126.9, 128.0, 128.8, 129.2, 132.4, 133.8, 138.6, 143.3, 147.5, 150.4 ppm; IR (KBr, cm−1) 1628, 2929; HRMS (ESI) m/z calcd for $C_{16}H_{14}ClN_2$ $[M+H]^+$ 269.0840, found 269.0849.

2-(2-chloro-2-phenylvinyl)benzo[d]thiazole (6f).

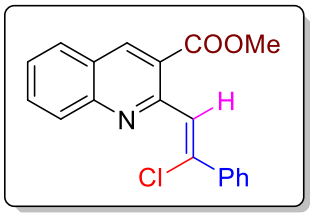


light yelllow solid; yield 117.8 mg, 87%; mp 158–159 °C; R_f = 0.35 (05:95 EtOAc/hexane); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.13 (d, *J* = 7.8 Hz, 1H), 7.19–7.22 (m, 2H), 7.44 (s, 1H), 7.55–7.57 (m, 3H), 7.73 (d, *J* = 10.2 Hz, 1H), 7.77–7.80 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ119.4, 121.5, 125.3, 126.8, 127.8, 128.4, 129.3, 130.6, 131.5, 135.7, 143.9, 150.8, 160.3 ppm; IR (KBr, cm−1) 1636, 2918; HRMS (ESI) m/z calcd for $C_{15}H_{11}ClNS$ $[M+H]^+$ 272.0295, found 272.0303.

Procedure for synthesis of 2-(2-Chloro-2-phenylvinyl)-quinoline-3-carboxylic acid methyl ester (8).

To a solution of compound 2-phenylethynylquinoline-3-carboxylic acid methyl ester **7** (0.5 mmol) in 3 equiv $POCl_3$ and stirred at 80°C under aerobic condition. After completion of the reaction, chilled water was poured into the reaction mixture and extracted with ethyl acetate. The organic layer was washed with water, brine and dried over anhydrous sodium sulphate (Na_2SO_4). The solvent was evaporated under vacuum to give product **8**. The product was washed with hexane and further recrystallized from ethanol.

2-(2-Chloro-2-phenylvinyl)-quinoline-3-carboxylic acid methyl ester (8).

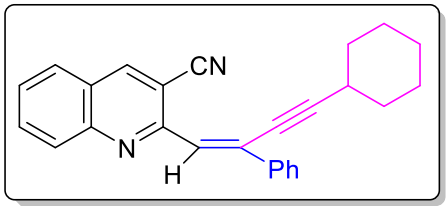


white solid; yield 143.7 mg, 89%; mp 119–120 °C; R_f = 0.20 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ3.96 (s, 3H), 7.41 (d, *J* = 7.2 Hz, 1H), 7.62 (t, *J* = 7.5 Hz, 1H), 7.80 (s, 1H), 7.83 (d, *J* = 7.2 Hz, 2H), 7.92 (d, *J* = 8.4 Hz, 1H), 8.18 (d, *J* = 8.4 Hz, 1H), 8.84 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ52.6, 123.8, 125.2, 125.9, 127.0, 12.5, 128.3, 128.5, 122.2, 129.3, 131.9, 136.1, 138.2, 140.0, 148.6, 153.8, 166.4 ppm; IR (KBr, cm^{-1}): 1723, 2917, 3085; HRMS (ESI) m/z calcd for $C_{19}H_{14}ClNO_2$ $[M+H]^+$ 324.0786, found 324.0795.

General procedure for palladium-catalyzed Sonogashira coupling reaction of 2a.

A mixture of 2-(2-chloro-2-phenylvinyl)quinoline-3-carbonitrile **2a** (0.20 mmol), ethynylcyclohexane (0.24 mmol), $PdCl_2$ (5 mol %), PPh_3 (10 mol %), CH_3CN (2 mL) and TEA (0.3 mmol) was stirred under N_2 at 80 °C for 2 h (as monitored by TLC). After completion of reaction, the reaction mixture was concentrated in vacuo and residue was purified by column chromatography on silica gel using EtOAc/hexane as eluent to afford product **9**.

***2-(4-cyclohexyl-2-phenyl-but-1-en-3-ynyl)-quinoline-3-carbonitrile (9)*.**

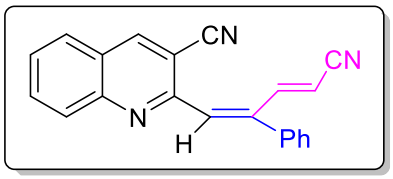


red solid; yield 59.3 mg, 82%; mp 137–138 °C; R_f = 0.30 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.25–1.39 (m, 2H), 1.49–1.65 (m, 4H), 1.69–1.76 (m, 2H), 1.87–1.93 (m, 2H), 2.69–2.77 (m, 1H), 7.36–7.45 (m, 3H), 7.61 (t, *J* = 5.4 Hz, 2H), 7.83–7.88 (m, 4H), 8.15 (d, *J* = 8.7 Hz, 1H), 8.53 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ24.8, 25.8, 30.3, 32.3, 79.1, 105.4, 107.4, 107.0, 117.0, 124.9, 127.1, 127.1, 127.8, 128.4, 128.9, 131.4, 132.6, 138.9, 142.3, 142.4, 148.4, 154.2 ppm; IR (KBr, cm^{-1}): 2213, 2231, 3034; HRMS (ESI) m/z calcd for $C_{26}H_{23}N_2$ $[M+H]^+$ 363.1856, found 363.1867.

General procedure for palladium-catalyzed Heck reaction of 2a.

A mixture of 2-(*β*-chloro-*β*-phenylvinyl)quinoline-3-carbonitrile **2a** (0.20 mmol), acrylonitrile (0.40 mmol), $PdCl_2$ (2.5 mol %), BINAP (2.5 mol %), DMA (1 mL) and CH_3COONa (0.40 mmol) was stirred under N_2 at 130 °C for 2 h (as monitored by TLC). After completion of reaction, the mixture was cooled and extracted with ethyl acetate and purified by column chromatography on silica gel using EtOAc/hexane as eluent to afford product **10**.

***2-(4-cyano-2-phenyl-buta-1,3-dienyl)-quinoline-3-carbonitrile (10)*.**

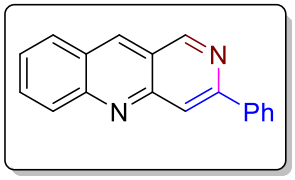


brown solid; yield 49.1 mg, 80%; mp 106–107 °C; R_f = 0.30 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.14 (t, *J* = 8.4 Hz, 2H), 7.47 (s, 1H), 7.68 (t, *J* = 7.5 Hz, 1H), 7.79–7.90 (m, 6H), 8.19 (d, *J* = 8.7 Hz, 2H), 8.58 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 107.4, 115.6, 115.9, 116.9, 121.5, 125.0, 128.0, 128.5, 129.3, 129.4, 129.9, 133.1, 134.1, 139.6, 142.7, 148.5, 153.6, 162.2, 165.5 ppm; IR (KBr, cm^{-1}): 2214, 2221, 2852; HRMS (ESI) m/z calcd for $C_{21}H14N_3$ $[M+H]^+$ 308.1182, found 308.1189.

General procedure for synthesis of 3-Phenylbenzo[b][1,6]naphthyridine (11).

To a solution of 2-(2-Chloro-2-phenylvinyl-quinoline-3-carbaldehyde **(4a)** (0.2 mmol) in EtOH (2 mL) were added K_2CO_3 (0.30 mmol) and saturated with 5 mmol aq NH_3. The reaction mixture was stirred at refluxed temperature. The reaction completed after 15 min (as monitored by TLC). The reaction mixture allowed to pour in chilled water and precipitate filtered out and dried. Further the product **11** was recrystallized from ethanol.

3-Phenylbenzo[b][1,6]naphthyridine (11).

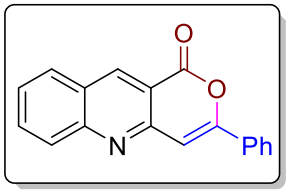


light green solid; yield 47.6 mg, 93%; mp 172–174 °C; R_f = 0.25 (05:95 EtOAc/hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (t, *J* = 7.2 Hz, 1H), 7.49–7.54 (m, 3H), 7.82 (t, *J* = 7.2 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.17–7.22 (m, 3H), 8.37 (s, 1H), 8.81 (s, 1H), 9.50 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 116.3, 120.9, 126.1, 126.8, 127.1, 128.8, 128.8, 129.1, 129.2, 132.4, 137.0, 138.6, 150.1, 151.8, 153.6, 154.5 IR (KBr, cm−1) 1441, 1613, 3052; HRMS (ESI) m/z calcd for $C_{18}H_{13}N_2$ $[M+H]^+$ 257.1073, found 257.1081.

General procedure for synthesis of 3-Phenyl-1H-pyrano[4,3-b]quinolin-1-one (12).

To a solution of 2-(2-Chloro-2-phenylvinyl)-quinoline-3-carboxylic acid methyl ester **(6)** (0.2 mmol) in 2 mL MeOH was added 10% aq KOH and stirred at 80 °C. After completion of the reaction, monitored by TLC, the reaction mixture was pour in chilled water and precipitate filtered out and dried. The product **12** was recrystallized from ethanol.

3-Phenyl-1H-pyrano[4,3-b]quinolin-1-one (12).

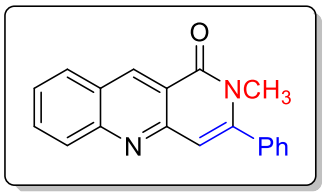


green solid; yield 47.5 mg, 87%; mp 129–131 °C; R_f = 0.35 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36 (s, 1H), 7.45–7.64 (m, 4H), 7.87–8.02 (m, 4H), 8.15 (d, *J* = 8.4 Hz, 1H), 9.17 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 103.2, 115.4, 125.6, 127.0, 128.3, 128.9, 130.1, 130.7, 131.2, 133.6, 140.5, 140.7, 151.3, 152.4, 156.9, 161.8, 170.0 ppm; IR (KBr, cm−1) 1705, 2930, 3052; HRMS (ESI) m/z calcd for $C_{19}H_{15}N_2O$ $[M+H]^+$ 274.0863, found 274.0876.

General procedure for synthesis of 13.

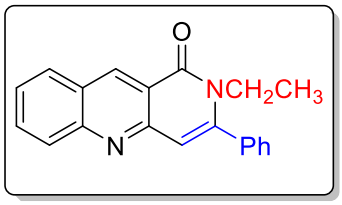
To a solution of compound 2-(2-chloro-2-phenylvinyl)quinoline-3-carbonitrile **2a** (0.20 mmol), in water (2 mL) were added 3 equiv alkyl amine and 2 equiv K_2CO_3. The reaction mixture was heated at 90 °C for 3-9 h under aerobic condition. After completion of the reaction, chilled water was poured into the reaction mixture and extracted with ethyl acetate. The organic layer was washed with water, brine and dried over anhydrous sodium sulphate (Na_2SO_4). The solvent was evaporated under vacuum to give product. The pure product **13(a-d)** were obtained after recrystalization in ethanol.

N-methyl-3-phenyl-2H-benzo[b][1,6]naphthyridin-1-one (13a).



light brown solid yield 51.4 mg, 90%; mp 108–109 °C; R_f = 0.35 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.45 (s, 3H), 6.83 (s, 1H), 7.46–7.59 (m, 6H), 7.84 (t, *J* = 7.5 Hz, 1H), 8.03–8.14 (m, 2H), 9.31 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 34.0, 109.2, 119.6, 126.1, 126.6, 128.5, 128.6, 128.7, 129.3, 129.4, 132.3, 135.7, 138.5, 148.3, 151.1, 151.7, 163.8 ppm; IR (KBr, cm−1) 1664, 2917, 3023; HRMS (ESI) m/z calcd for $C_{19}H_{15}N_2O$ $[M+H]^+$ 287.1179, found 287.1183.

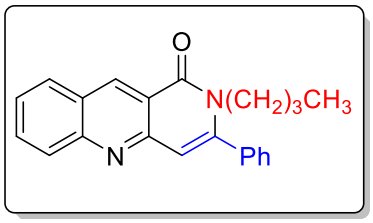
N-ethyl-3-phenylbenzo[b][1,6]naphthyridin-1(2H)-one (13b).



light yellow solid yield 49.8 mg, 83%; mp 97–98 °C; R_f = 0.35 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.35 (t, *J* = 7.2 Hz, 3H), 3.71 (q, *J* = 7.2 Hz, 2H), 6.96 (s, 1H), 7.42 (d, *J* = 6.6 Hz, 4H), 7.68 (t, *J* = 81 Hz, 1H), 7.81 (d, *J* = 6.9 Hz, 3H), 7.95 (d, *J* = 8.4 Hz, 1H), 8.88 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.5, 36.5, 110.5, 114.0, 125.7, 126.5,

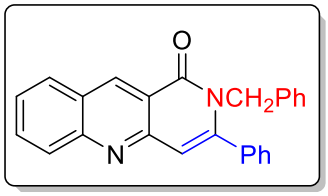
126.8, 128.4, 128.6, 129.0, 129.1, 132.0, 134.2, 138.8, 151.1, 151.4, 152.8, 160.7 ppm; IR (KBr, cm−1) 1657, 2923, 3007; HRMS (ESI) m/z calcd for $C_{19}H_{15}N_2O$ $[M+H]^+$ 301.1335, found 301.1343.

N-butyl-3-phenylbenzo[b][1,6]naphthyridin-1(2H)-one (13c).



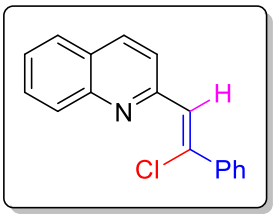
light green solid yield 50.5 mg, 77%; mp 90–91 °C; R_f = 0.25 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ0.74 (t, *J* = 7.2 Hz, 3H), 0.85–0.97 (m, 2H), 1.12-1.19 (m, 2H), 3.97 (t, *J* = 8.1 Hz, 2H), 6.77 (s, 1H), 7.50–7.59 (m, 6H), 7.85 (t, *J* = 8.1 Hz, 1H), 8.04 (t, *J* = 8.4 Hz, 1H), 8.12 (d, *J* = 8.7 Hz, 1H), 9.30 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 13.3, 19.7, 30.6, 45.1, 109.5, 109.5, 119.9, 126.1, 126.7, 128.6, 128.8, 129.2, 129.4, 132.4, 135.8, 138.6, 148.2, 151.2, 151.7, 163.4 ppm; IR (KBr, cm−1) 1661, 2913, 3012; HRMS (ESI) m/z calcd for $C_{22}H_{21}N_2O$ $[M+H]^+$ 329.1654 found 329.1646.

N-benzyl-3-phenyl-2H-benzo[b][1,6]naphthyridin-1-one (13d).



green solid; yield 58.6 mg, 81%; mp 121–122 °C; R_f = 0.25 (05:95 EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ5.26 (s, 2H), 6.81 (s, 1H), 6.92 (d, *J* = 3.3 Hz, 2H), 7.18 (t, *J* = 2.7 Hz, 3H), 7.28 (s, 1H), 7.35–7.44 (m, 4H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.86 (t, *J* = 7.2 Hz, 1H), 8.04 (d, *J* = 8.1 Hz, 1H), 8.13 (d, *J* = 8.7 Hz, 1H), 9.35 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ48.4, 110.1, 119.8, 126.2, 126.7, 126.8, 127.1, 128.4, 128.7, 128.9, 129.2, 129.5, 132.5, 135.5, 137.3, 139.0, 148.3, 151.3, 151.8, 163.9 ppm; IR (KBr, cm−1) 1659, 2923, 3016; HRMS (ESI) m/z calcd for $C_{25}H_{19}N_2O$ $[M+H]^+$ 363.1497, found 363.1496.

2-(2-chloro-2-phenylvinyl)quinoline (17).

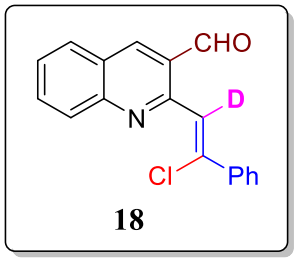


yellow liquid; yield 108.6 mg, 82%; R_f = 0.30 (05:95 EtOAc/hexane); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.27 (d, *J* = 7.8 Hz, 1H), 7.34–7.38 (m, 2H), 7.51 (s, 1H), 7.63 (t, *J* = 7.2 Hz, 1H), 7.80–7.83 (m, 3H), 7.85–7.88 (m, 2H), 8.15 (s, 1H), 8.24 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 120.4, 124.0, 126.4, 127.4, 127.9, 128.2, 128.3, 129.4, 129.8, 130.4, 131.2, 139.9, 146.2, 150.0, 154.7 ppm; IR (KBr, cm−1) 1603, 2923; HRMS (ESI) m/z calcd for $C_{17}H_{13}ClN$ $[M+H]^+$ 266.0731, found 266.0738.

General procedure for synthesis of *2-(2-chloro-2-phenylvinyl-1-d)quinoline-3-carbaldehyde (18)*.

To a solution of compound 2-phenylethynylquinoline-3-carbaldehyde (**3a**) (0.25 mmol) in 3 equiv $POCl_3$ and stirred at 80 °C under aerobic condition. After completion of the reaction, 1 mL D_2O was poured into the reaction mixture and extracted with ethyl acetate. The organic layer was washed with water, brine and dried over anhydrous sodium sulphate (Na_2SO_4). The solvent was evaporated under vacuum to give product **18**. The product was further recrystallized from ethanol.

2-(2-chloro-2-phenylvinyl-1-d)quinoline-3-carbaldehyde (18).



18

white solid; yield 67 mg, 91%; mp 156–157 °C; R_f = 0.35 (05:95 EtOAc/hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (t, *J* = 2.8 Hz, 2H), 7.46–7.68 (m, 1H), 7.72 (s, 1H), 7.84–7.90 (m, 3H), 8.01 (d, *J* = 8.0 Hz, 1H), 8.22 (d, *J* = 8.4 Hz, 1H), 8.81 (s, 1H), 10.33 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 122.4, 126.4, 126.9, 127.7, 127.9, 128.3, 128.5, 129.0, 129.4, 129.9, 132.9, 137.0, 139.8, 149.1, 154.7, 190.3 ppm; IR (KBr, cm−1) 1591, 1696, 2923, 3033; HRMS (ESI) m/z calcd for $C_{18}H_{12}DClNO$ $[M+H]^+$ 295.0743, found 295.0739.

Crystal structure and Data of compound (2j):

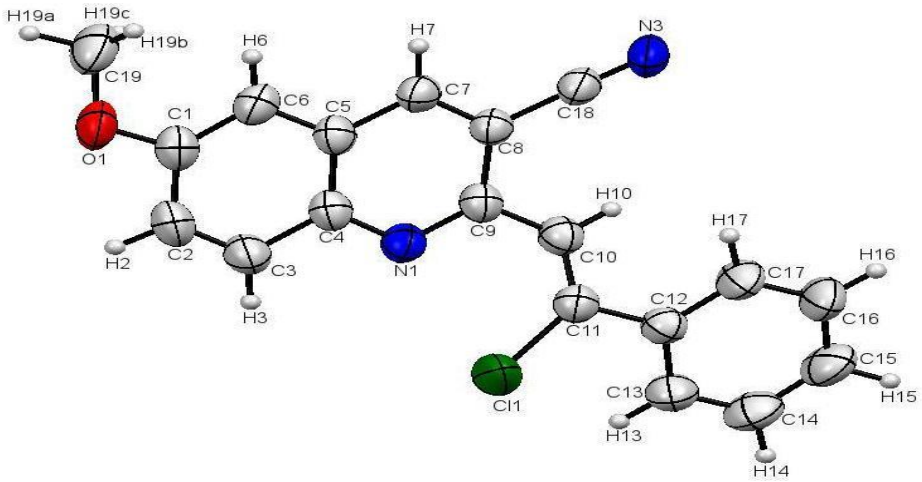


Table S-2: Summary of crystallographic data for compound **2j**.

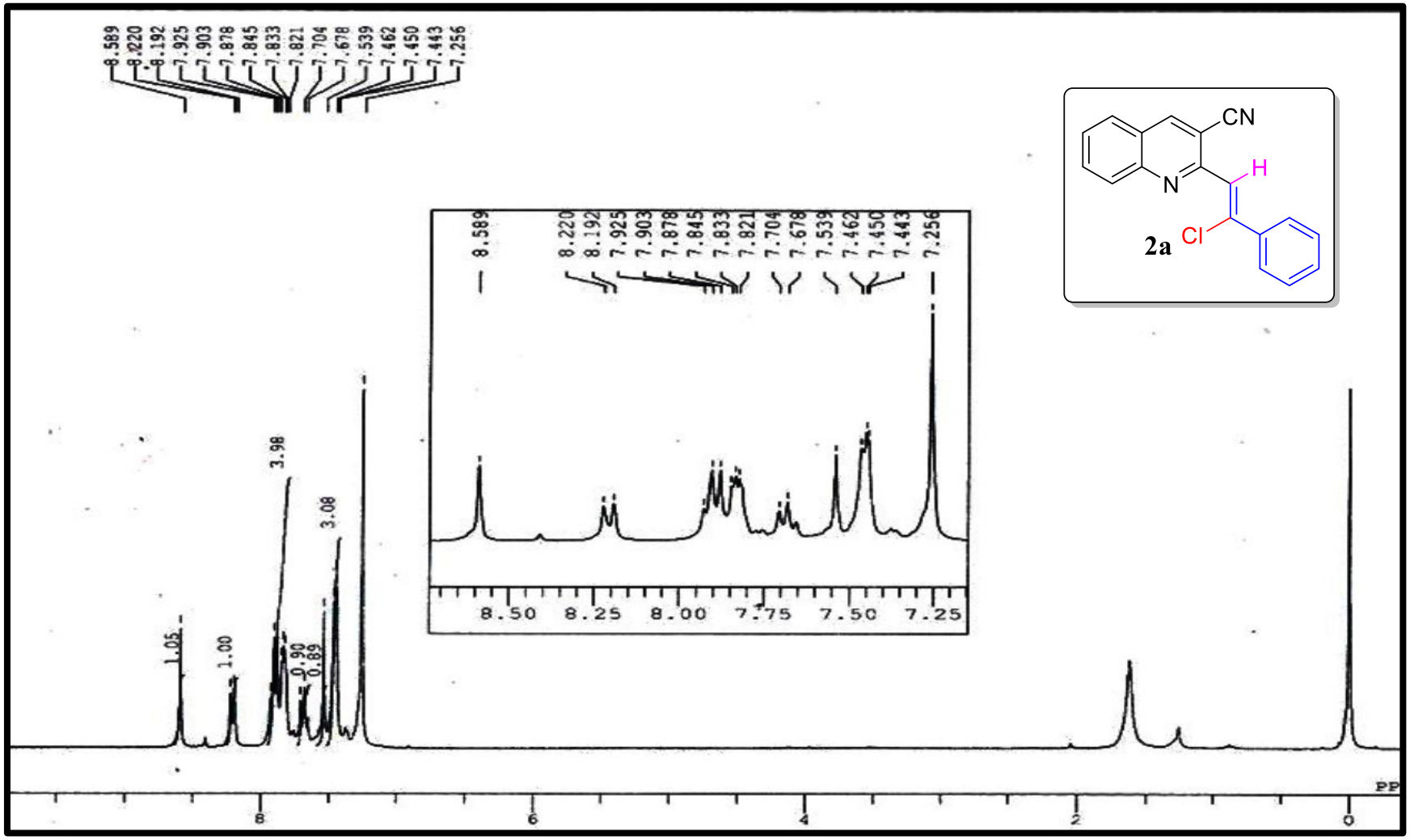
Parameters	**2i**
Compound name	2-(2-Chloro-2-phenylvinyl)-6-methoxy-quinoline-3-carbonitrile

Formula	$C_{19}H_{13}ClN_2O$
M	320
Crystal system	Monoclinic
Temperature	293 K
Space group	P 21/n
a/ Å	7.943 (5)
b/ Å	8.981 (5)
c/ Å	22.131 (5)
α (°)	90 ° (5)
β (°)	96.657 ° (5)
γ (°)	90° (5)
V/ Å^3	1568.1 (14)
Z	4
R (int.)	0.0635
Refinement method	Full-matrix least-squares on F^2
Melting Point	162-163 °C
R Indices (Index ranges)	-10 ≤ h ≤ 10, -12 ≤ k ≤ 12, -30 ≤ l ≤ 28
GoF	0.877
wR_2	0.1738
Wavelength	0.71073 A°
Largest Diff. Peak and Hole (eA^{-3})	0.9264 and -0.288

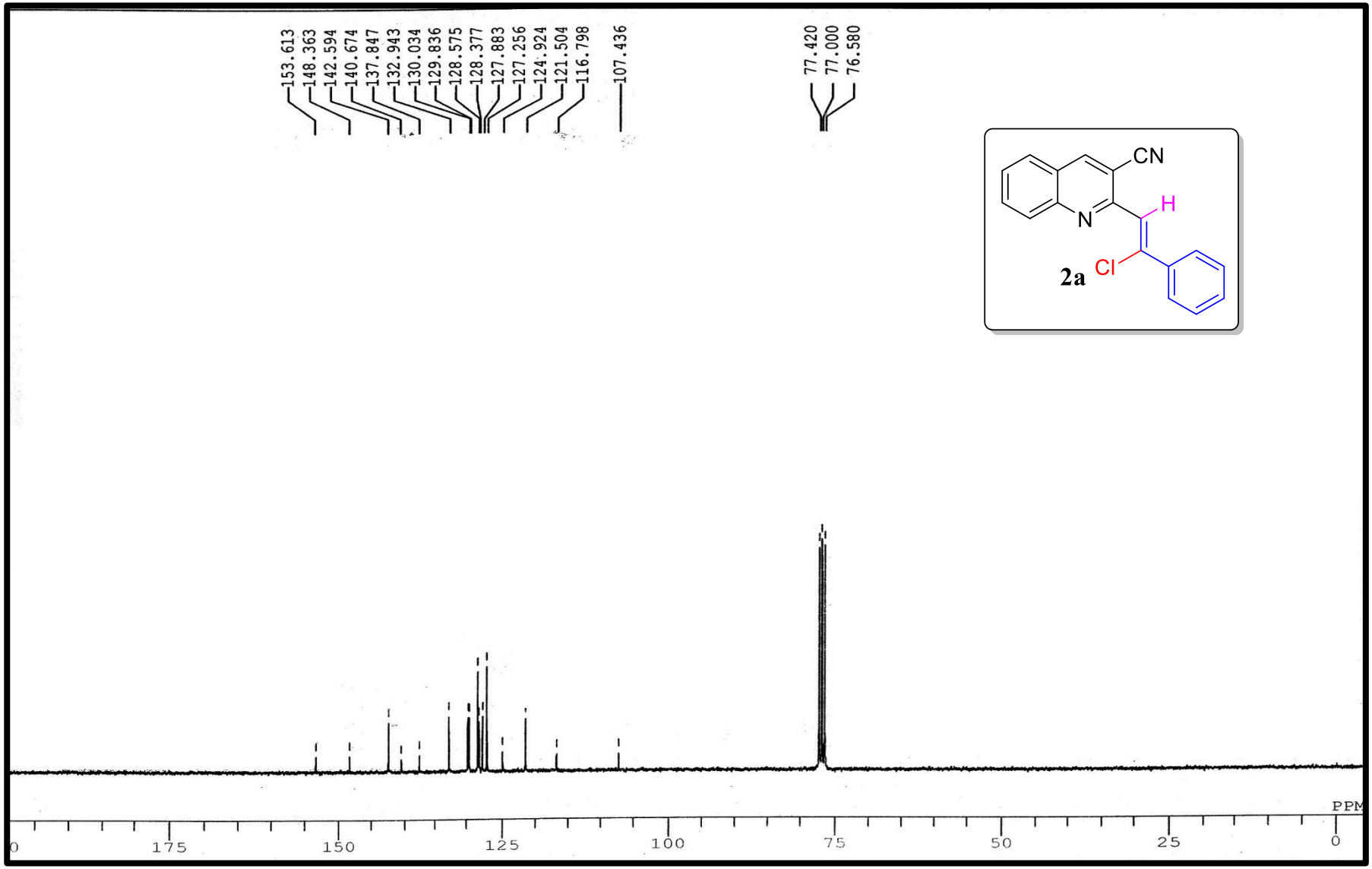
The crystallographic data for compounds **2j** has been deposited at the Cambridge Crystallographic Data Centre. CCDC number **1832991** contain the supplementary crystallographic data's for compound **2j,** respectively. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif .

Spectra (^{1}H & ^{13}C) of compounds

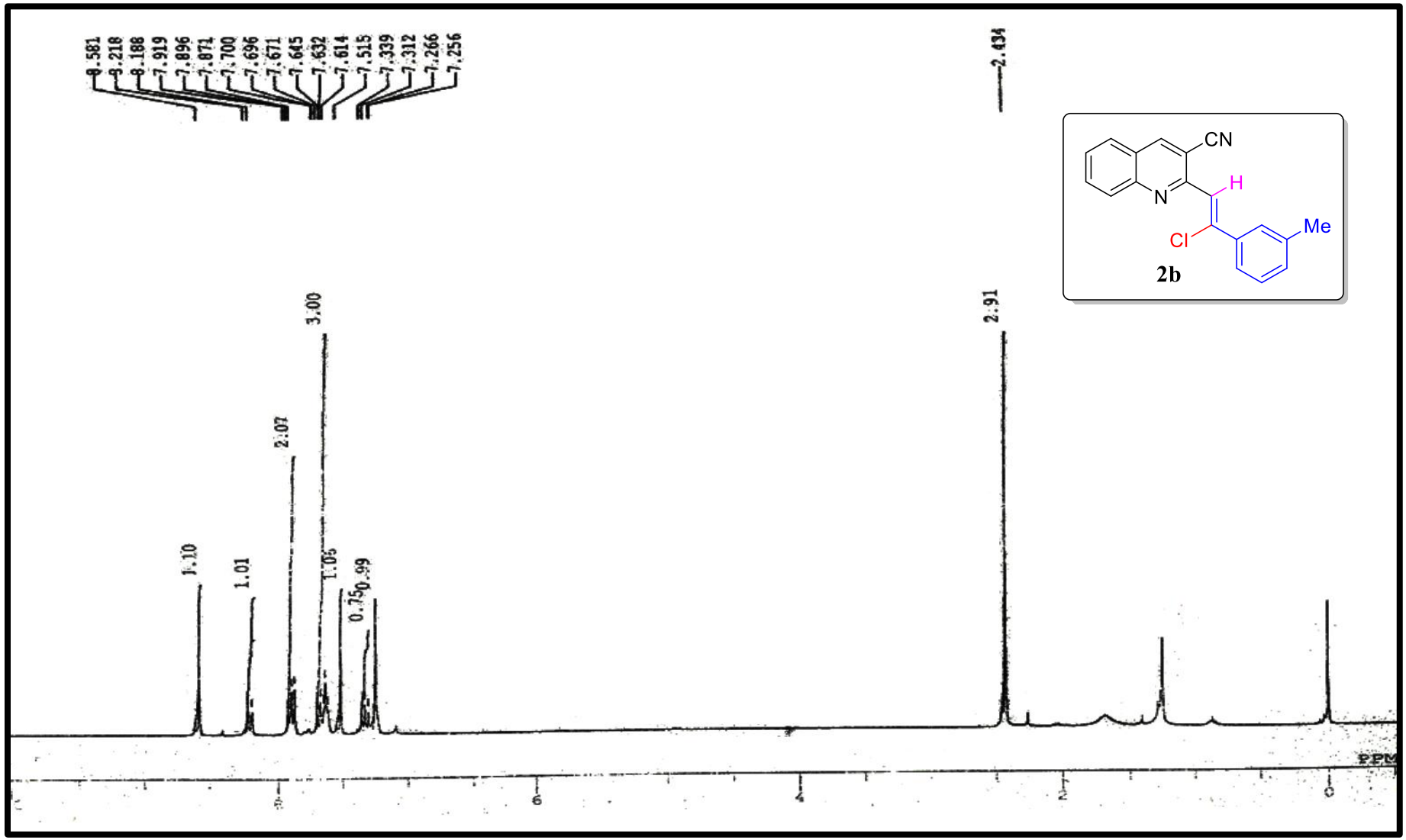
^{1}H spectrum of 2-(2-Chloro-2-phenylvinyl)quinoline-3-carbonitrile (2a)



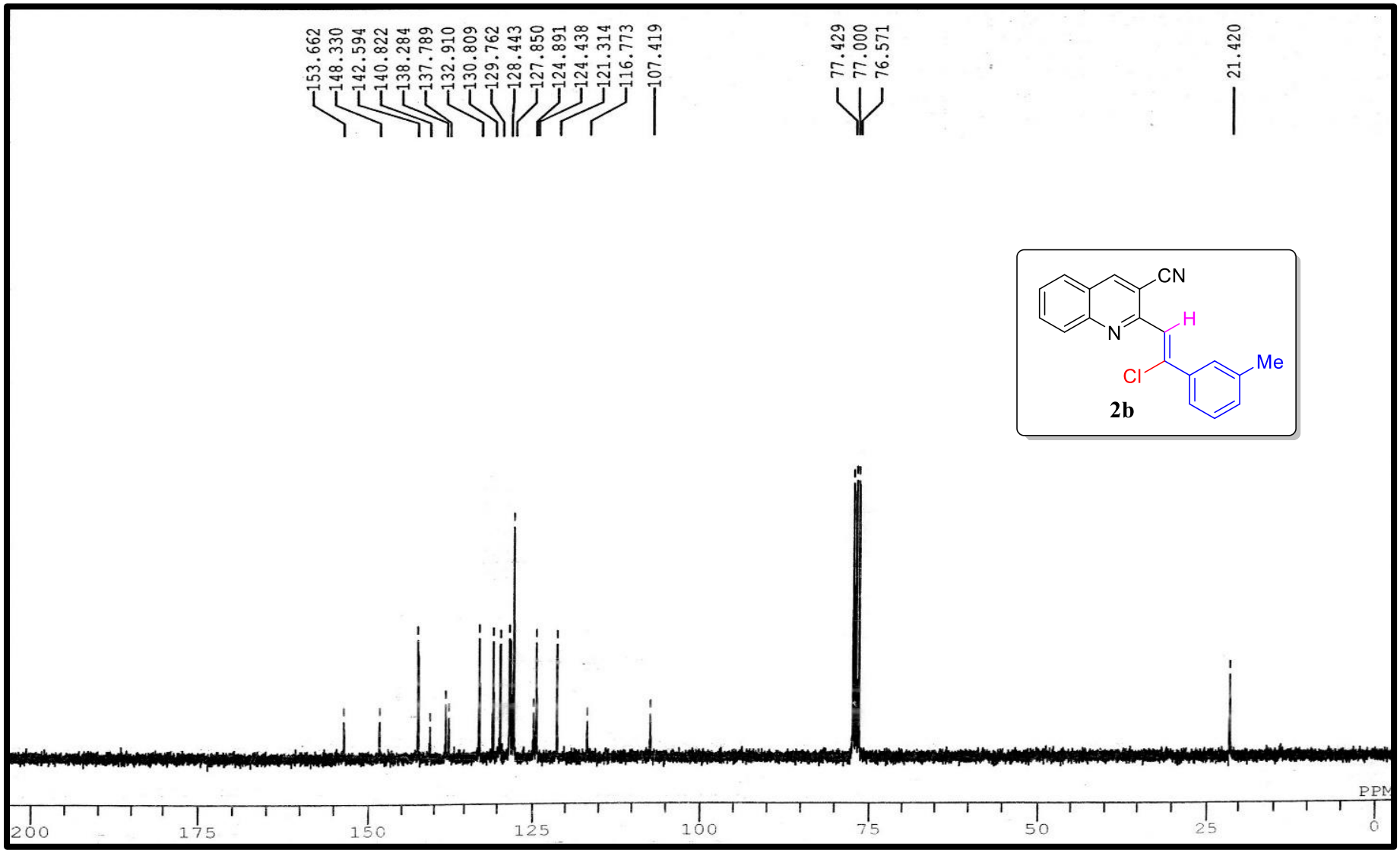
^{13}C NMR spectrum of 2-(2-Chloro-2-phenylvinyl)quinoline-3-carbonitrile (2a)



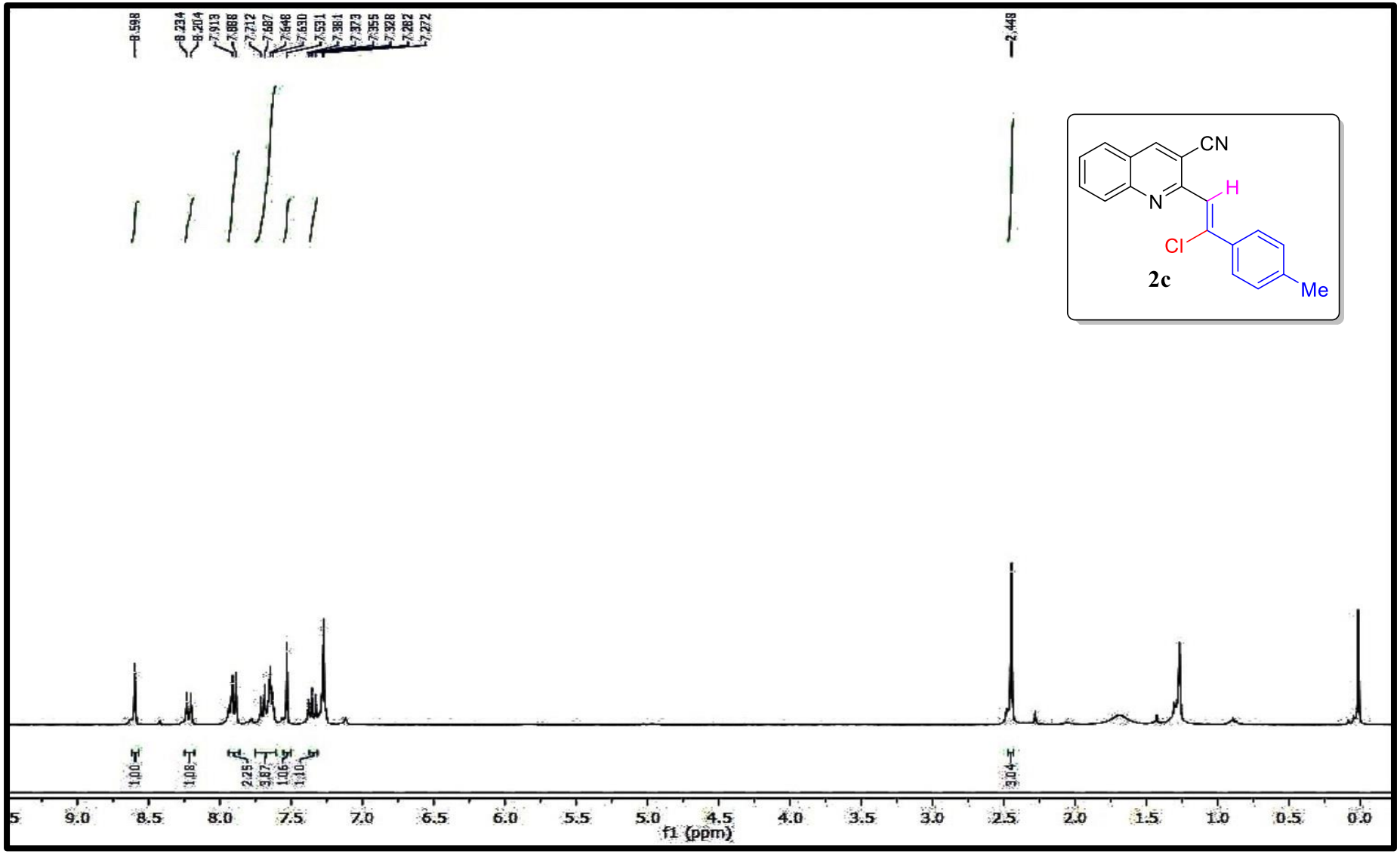
^{1}H spectrum of 2-(2-Chloro-2-m-tolylvinyl)quinoline-3-carbonitrile (2b)



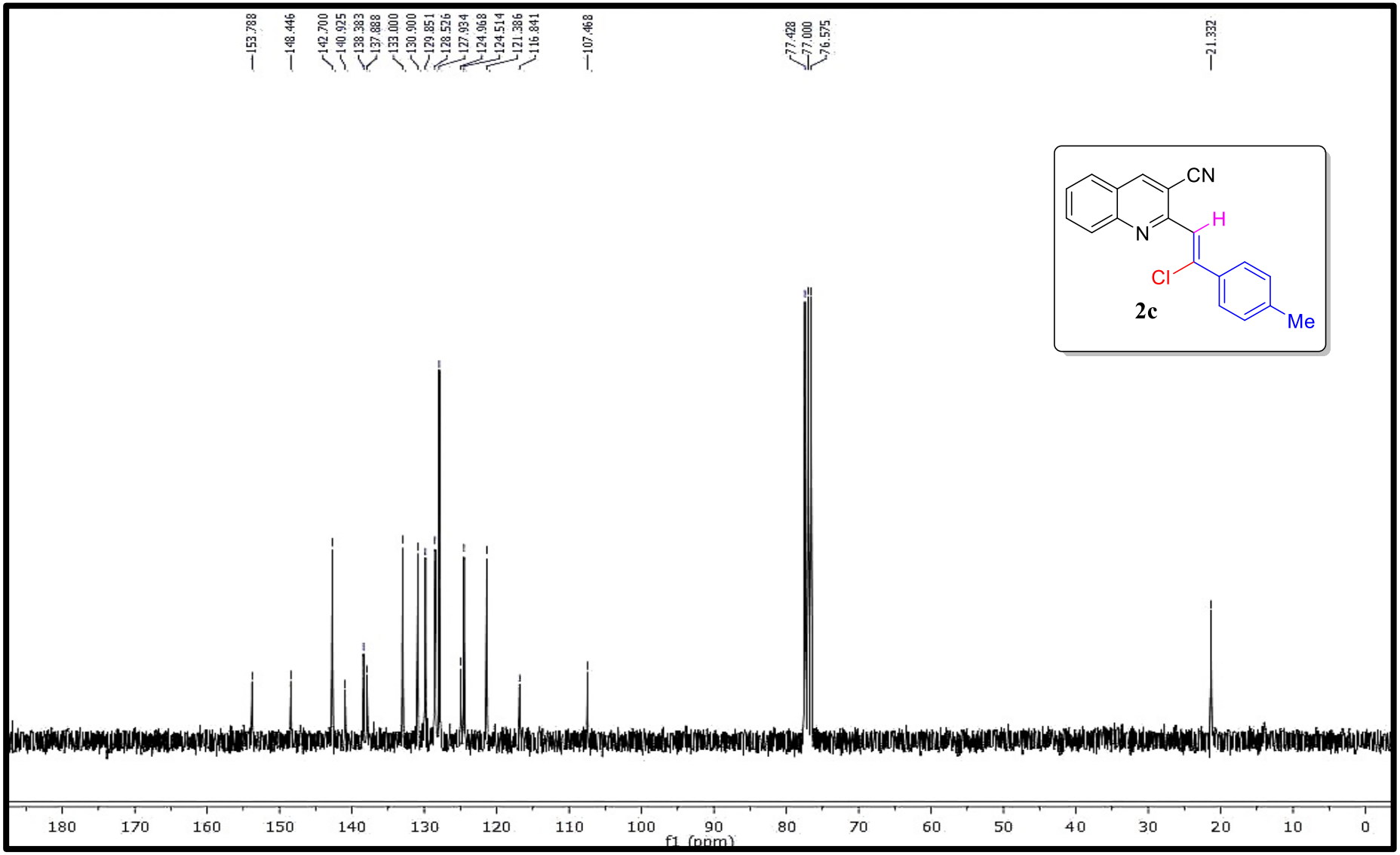
^{13}C NMR spectrum of 2-(2-Chloro-2-m-tolylvinyl)quinoline-3-carbonitrile (2b)



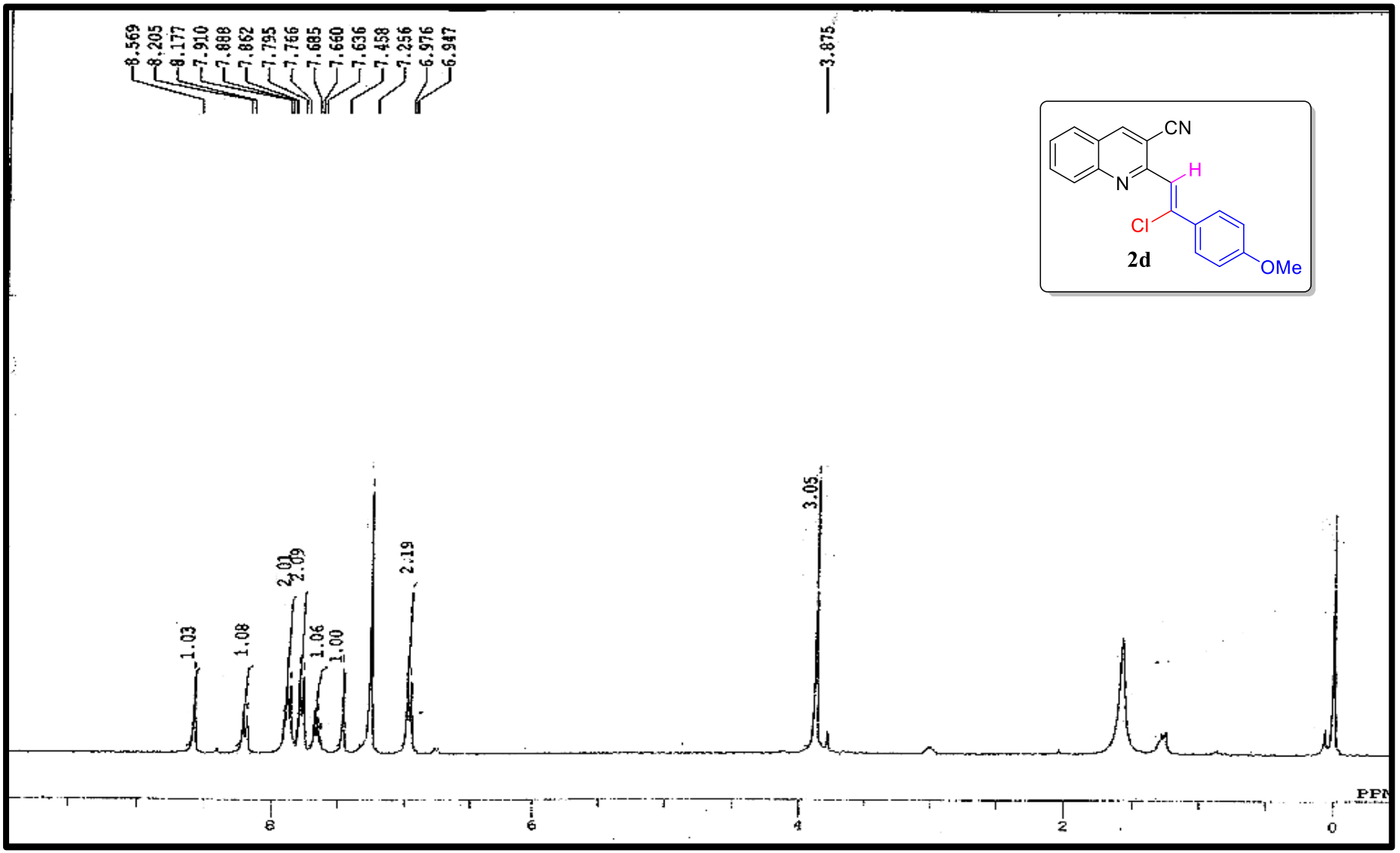
^{1}H NMR spectrum of 2-(2-chloro-2-(p-tolyl)vinyl)quinoline-3-carbonitrile (2c)



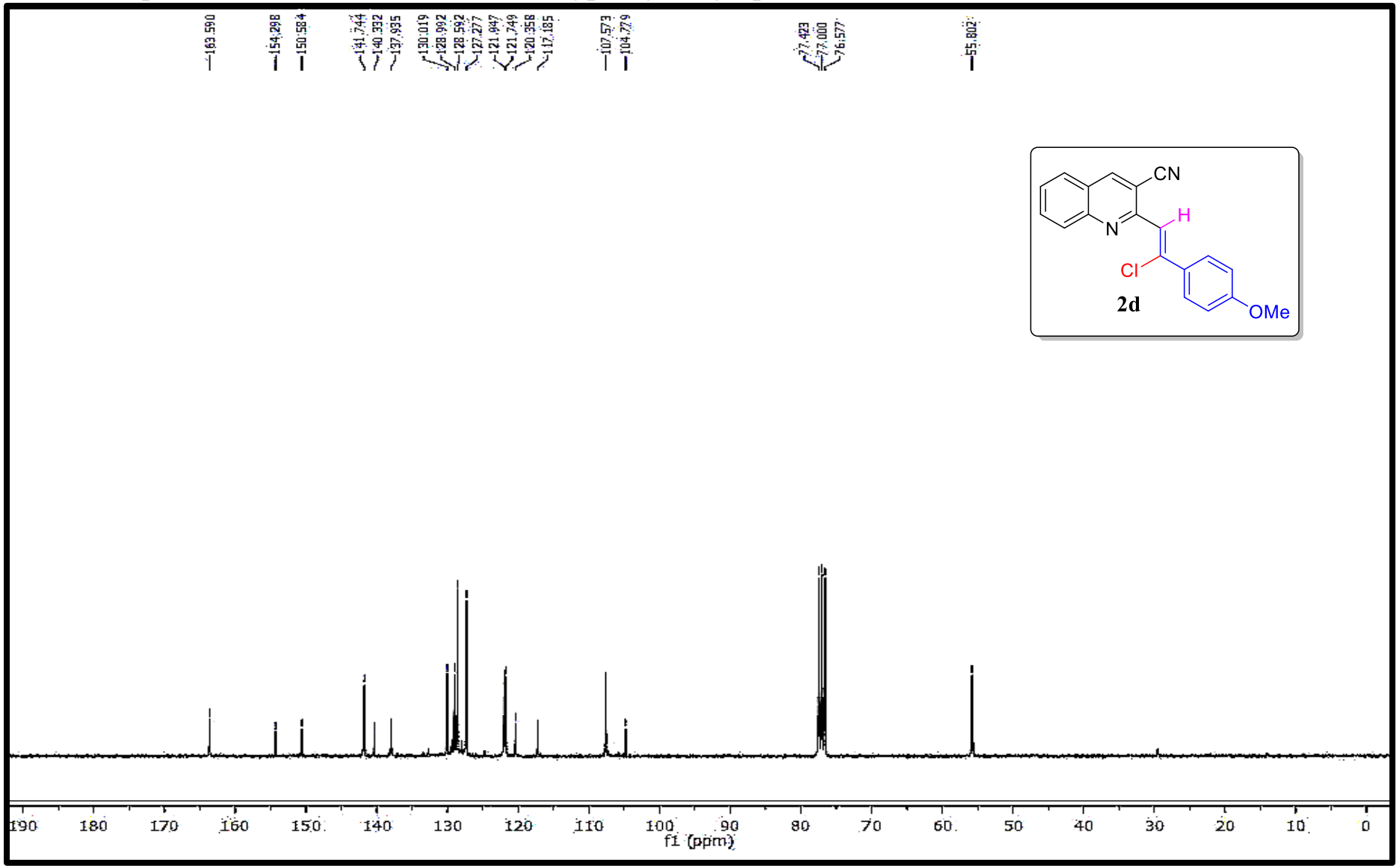
^{13}C NMR spectrum of 2-(2-chloro-2-(p-tolyl)vinyl)quinoline-3-carbonitrile (2c)



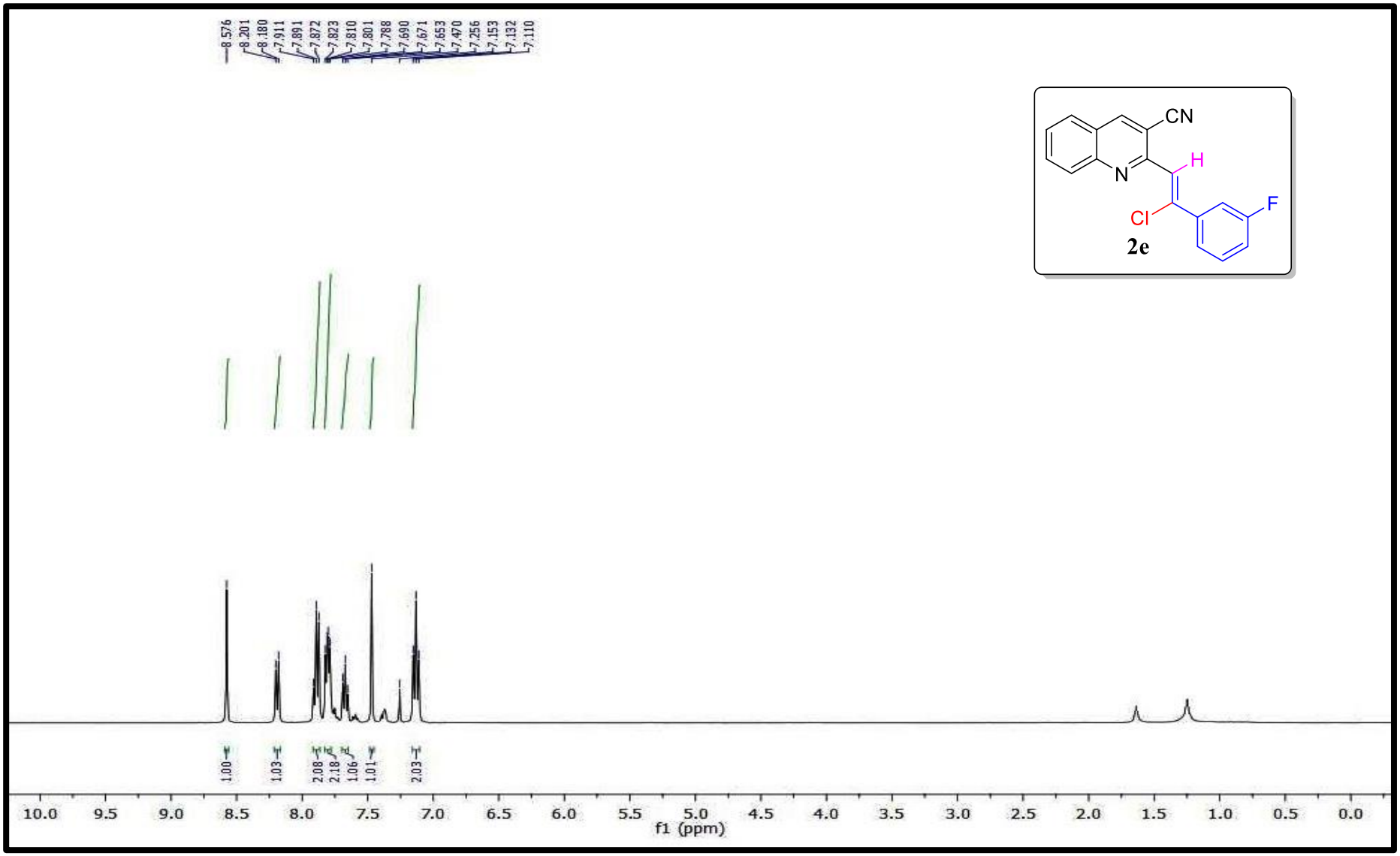
^{1}H spectrum of 2-[2-Chloro-2-(4-methoxyphenyl)vinyl]quinoline-3-carbonitrile (2d)



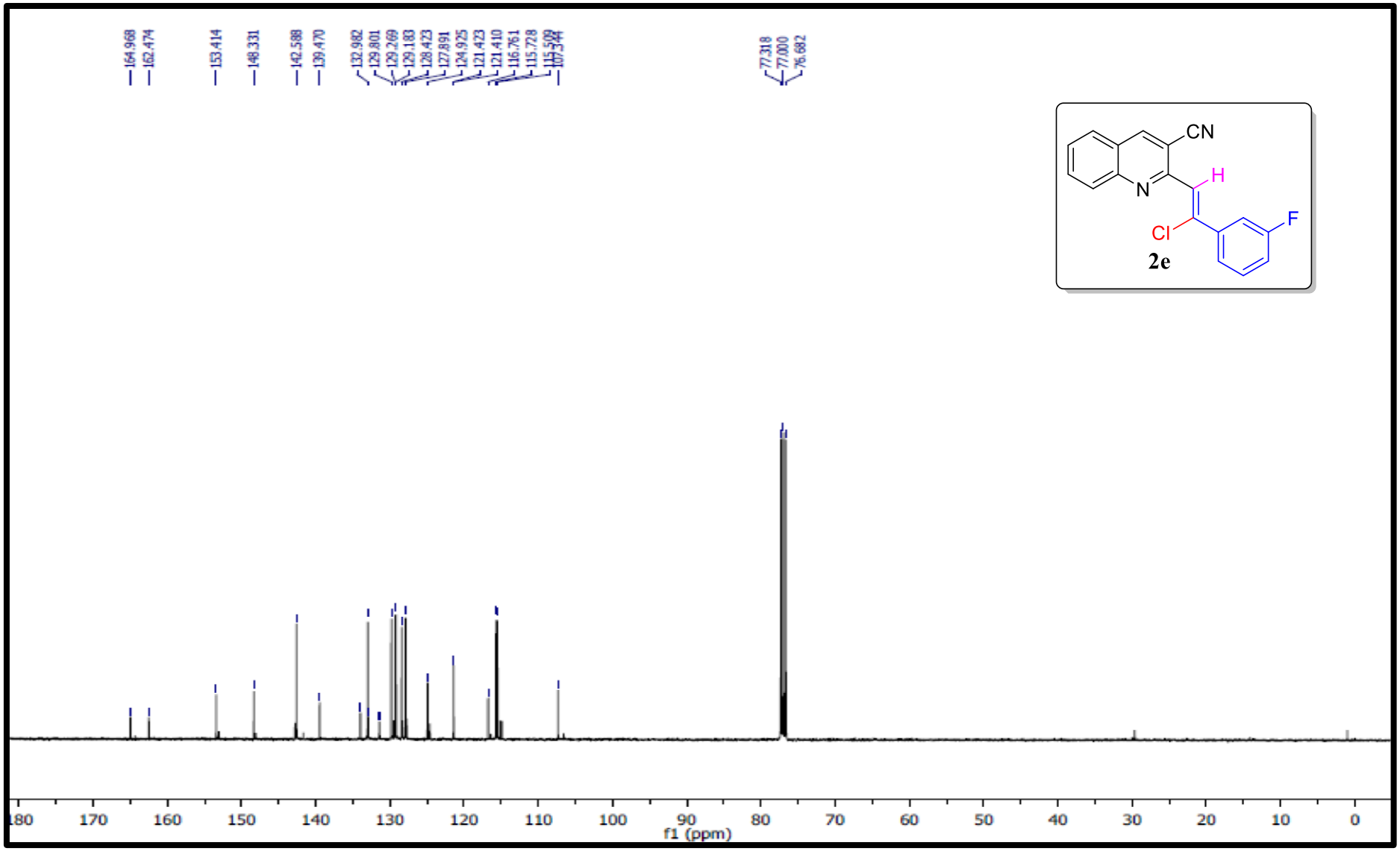
^{13}C NMR spectrum of 2-[2-Chloro-2-(4-methoxyphenyl)vinyl]quinoline-3-carbonitrile (2d)



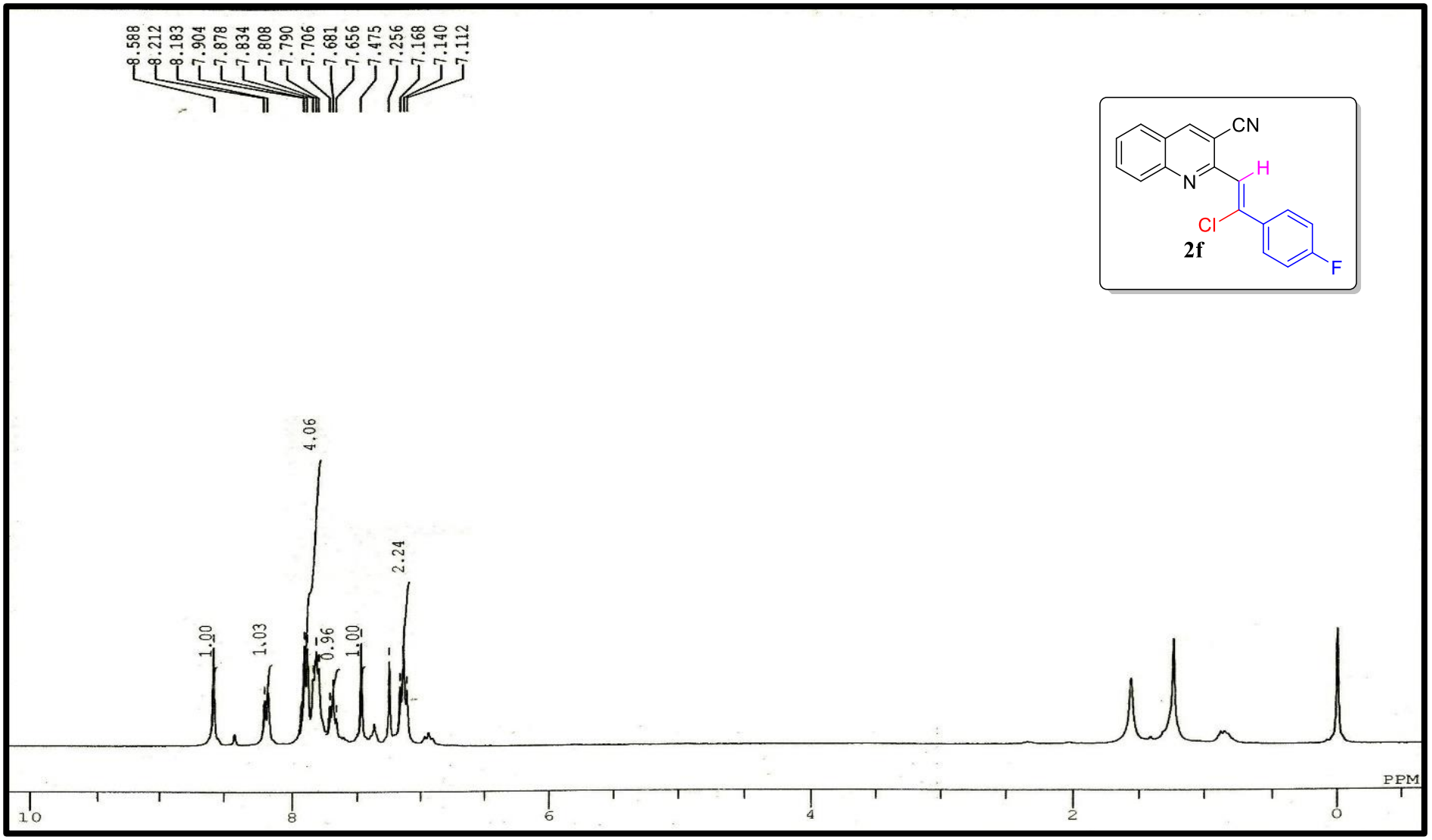
^{1}H spectrum of 2-(2-chloro-2-(3-fluorophenyl)vinyl)quinoline-3-carbonitrile (2e)



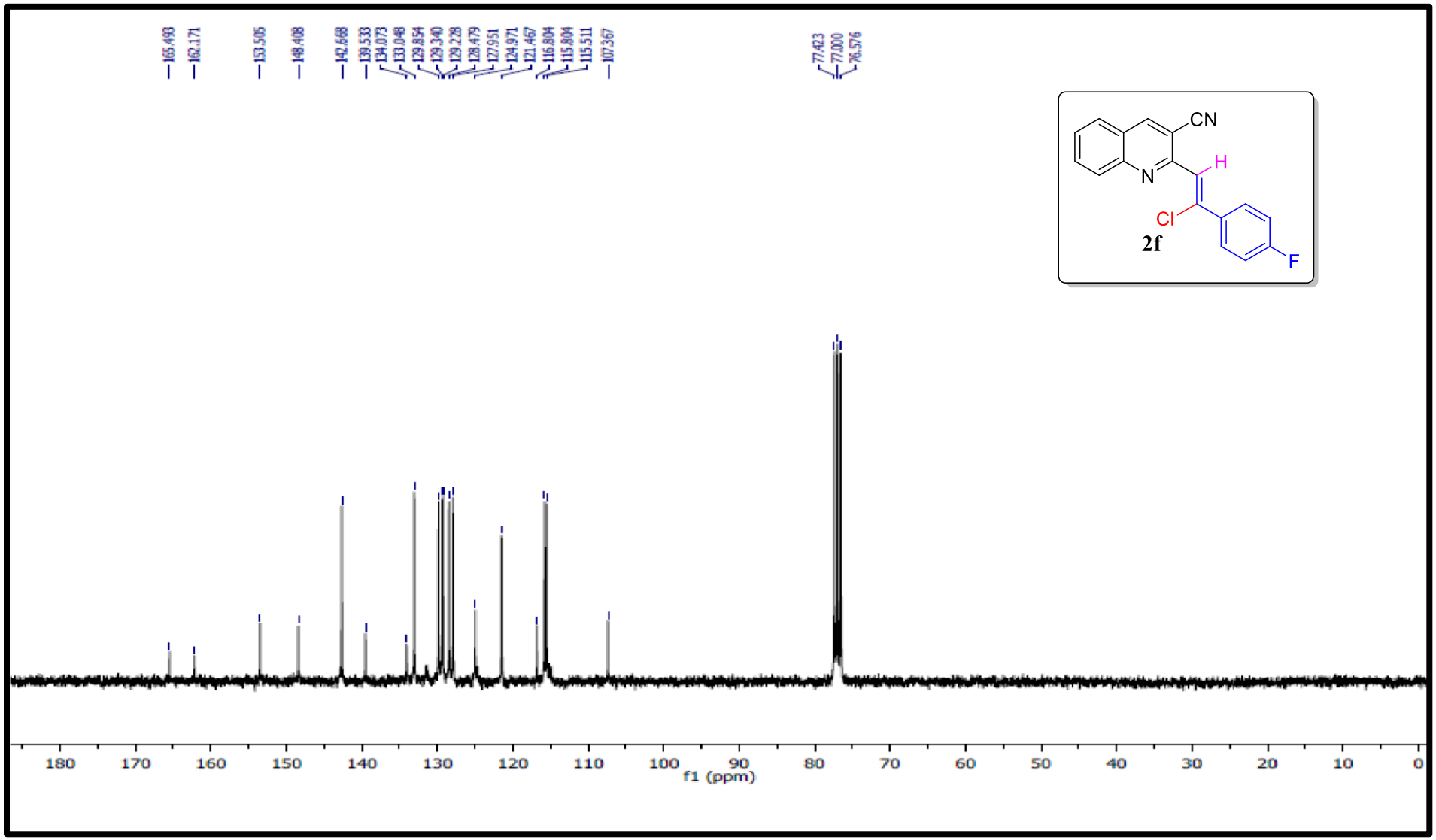
^{13}C NMR spectrum of 2-(2-chloro-2-(3-fluorophenyl)vinyl)quinoline-3-carbonitrile (2e)



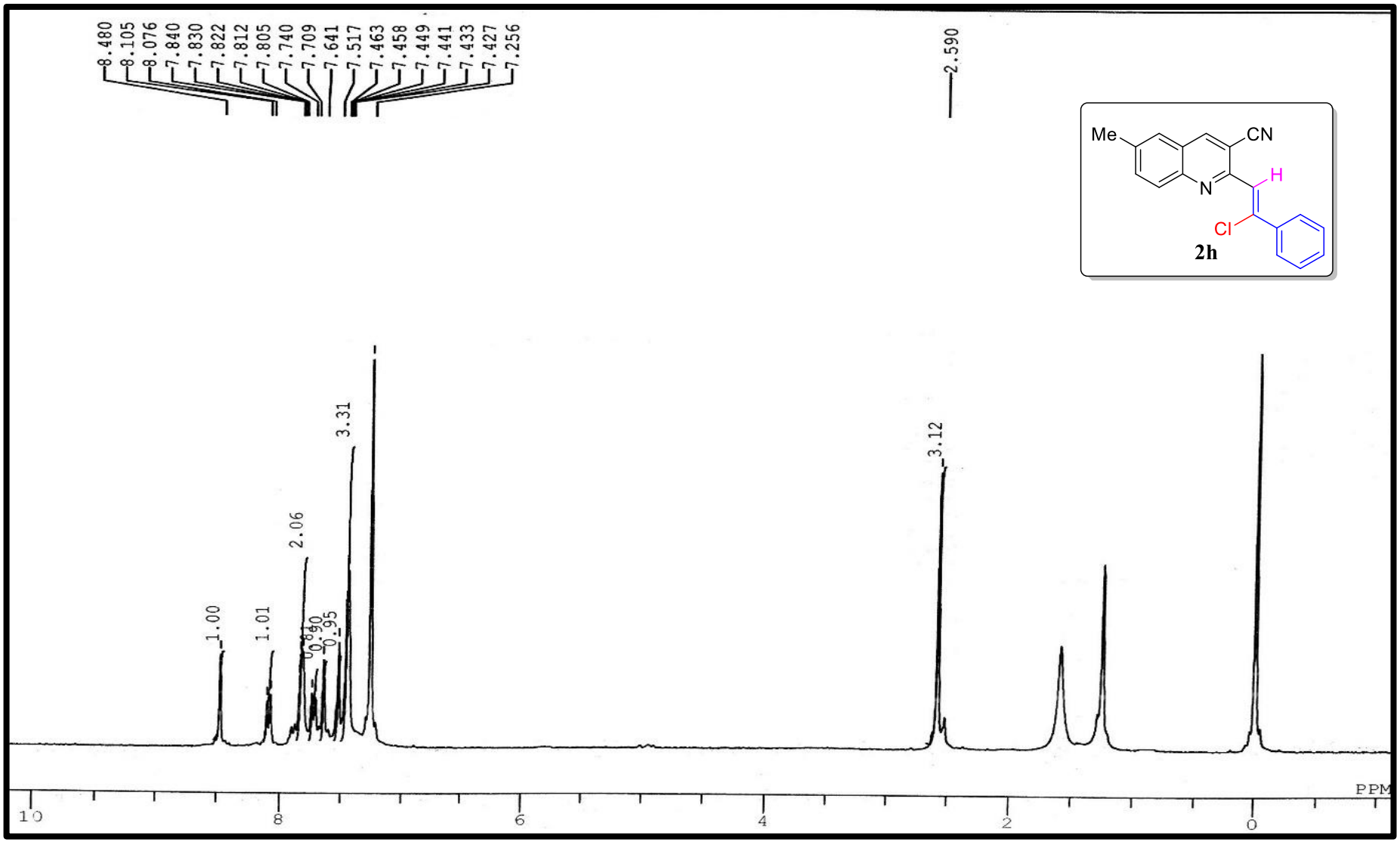
^{1}H and ^{13}C NMR spectrum of 2-[2-Chloro-2-(4-fluoro-phenyl)vinyl]quinoline-3-carbonitrile (2f)



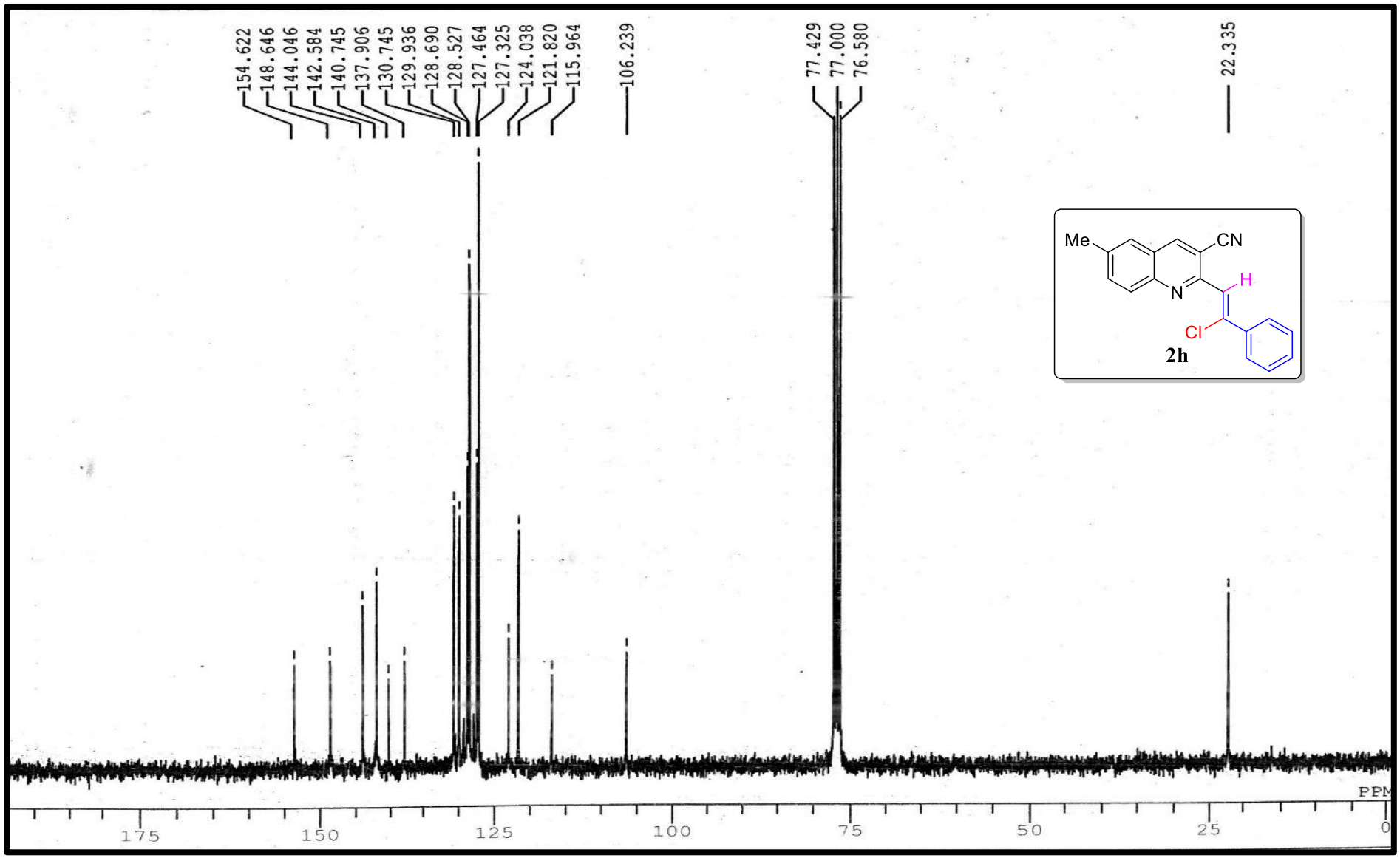
^{13}C NMR spectrum of 2-[2-Chloro-2-(4-fluoro-phenyl)vinyl]quinoline-3-carbonitrile (2f)



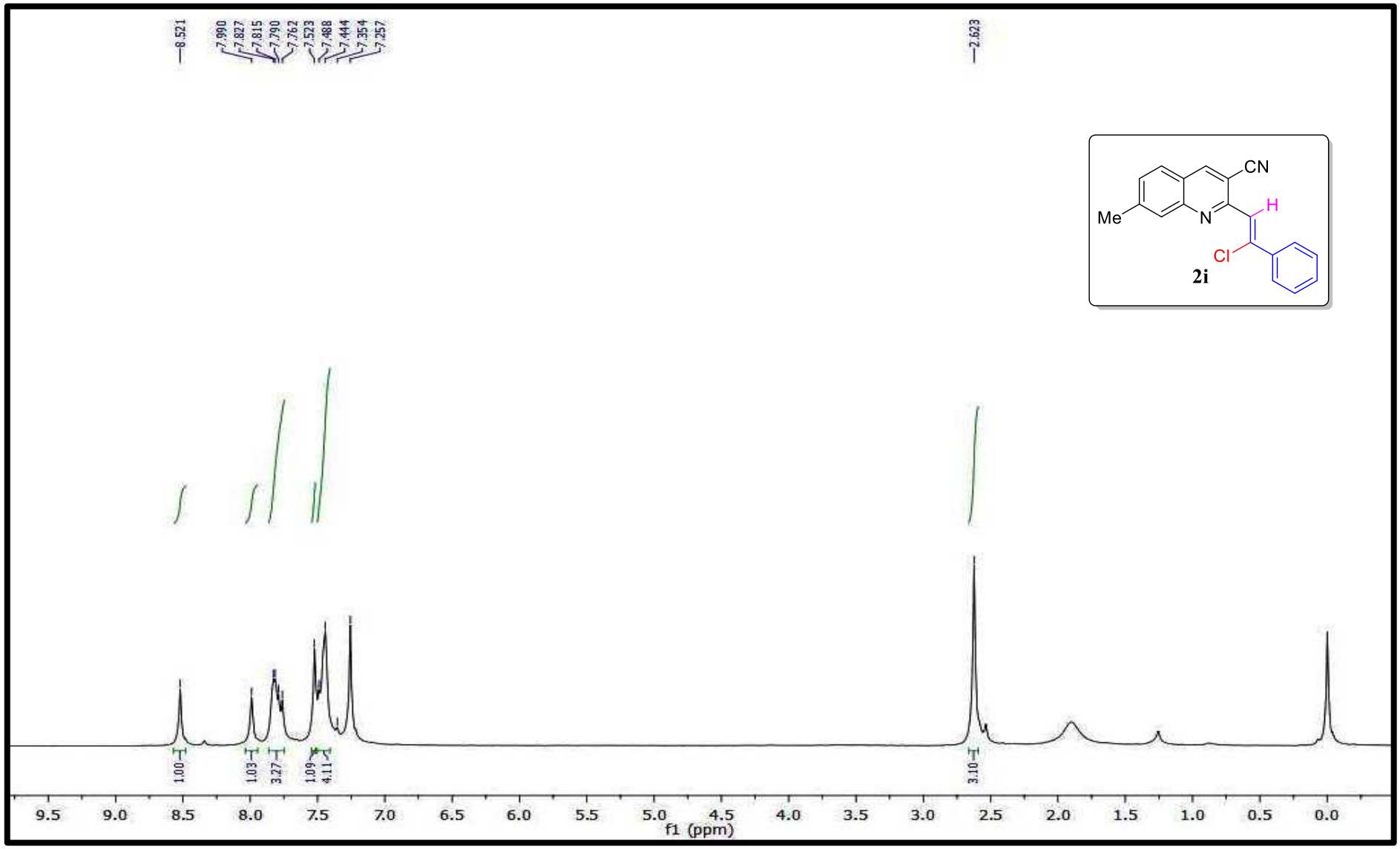
^{1}H and ^{13}C NMR spectrum of 2-(2-Chloro-2-phenylvinyl)6-methyl-quinoline-3-carbonitrile (2h)



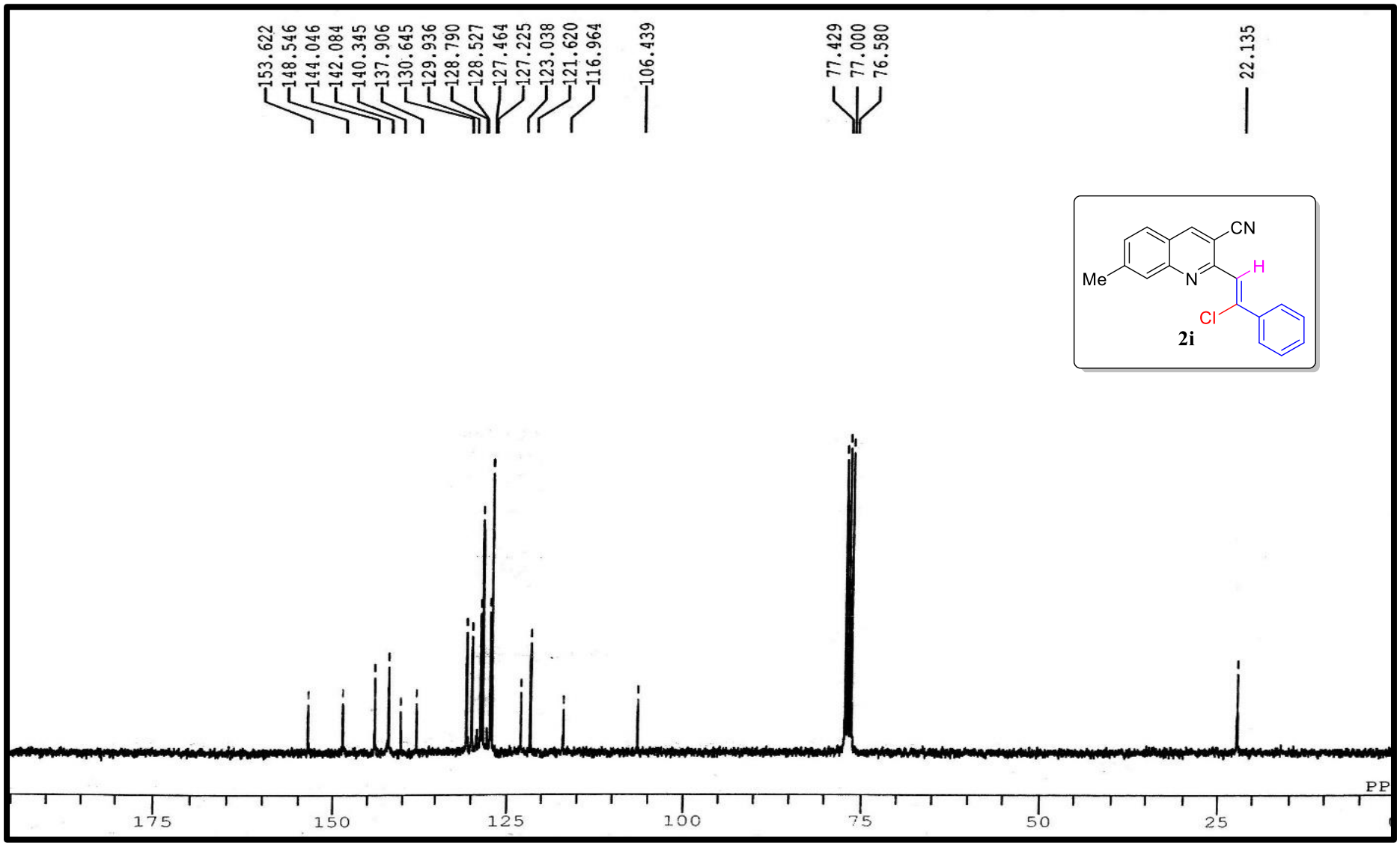
^{13}C NMR spectrum of 2-(2-Chloro-2-phenylvinyl)6-methyl-quinoline-3-carbonitrile (2h)



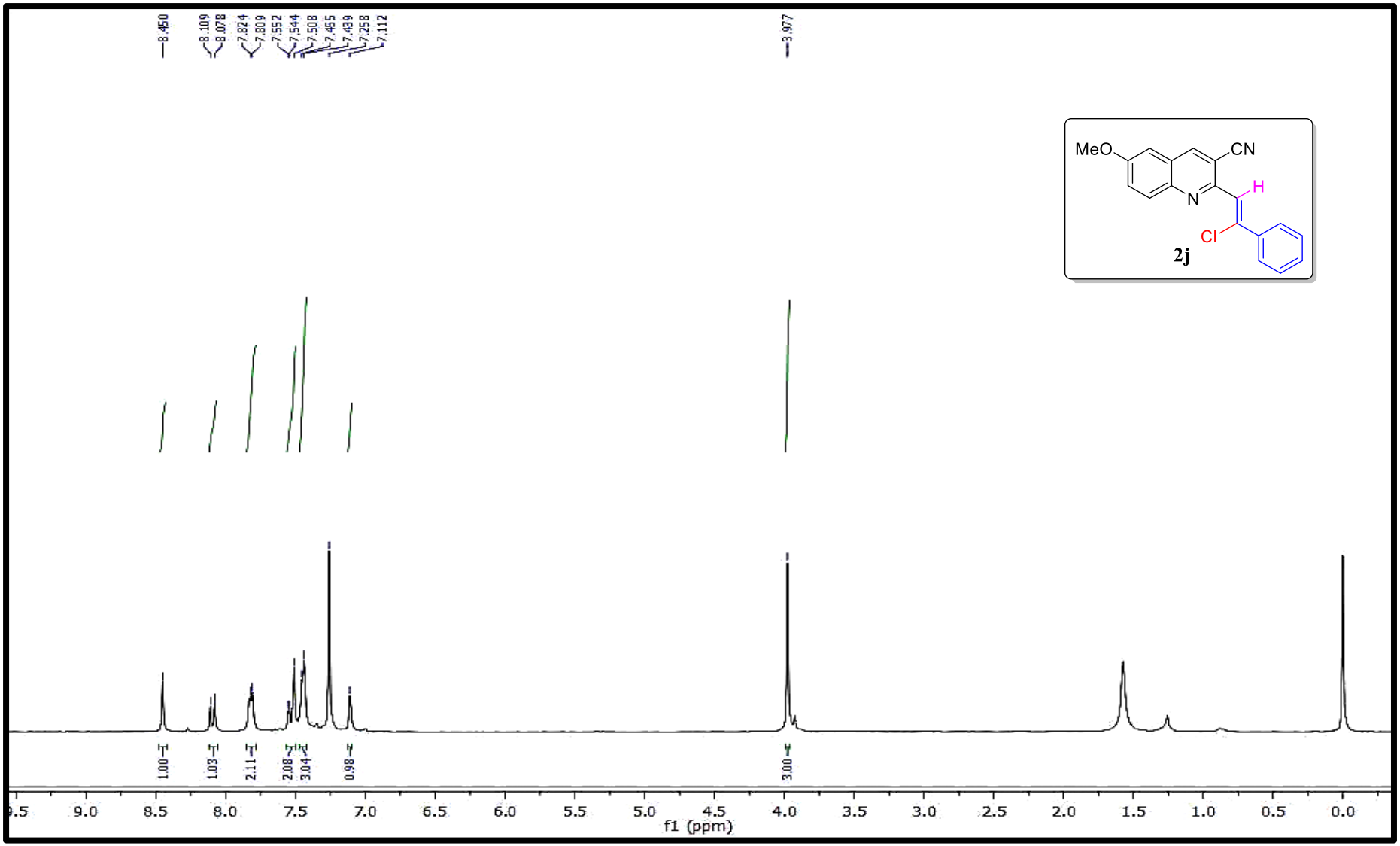
^{1}H spectrum of 2-(2-Chloro-2-phenylvinyl)-7-methyl-quinoline-3-carbonitrile (2i)



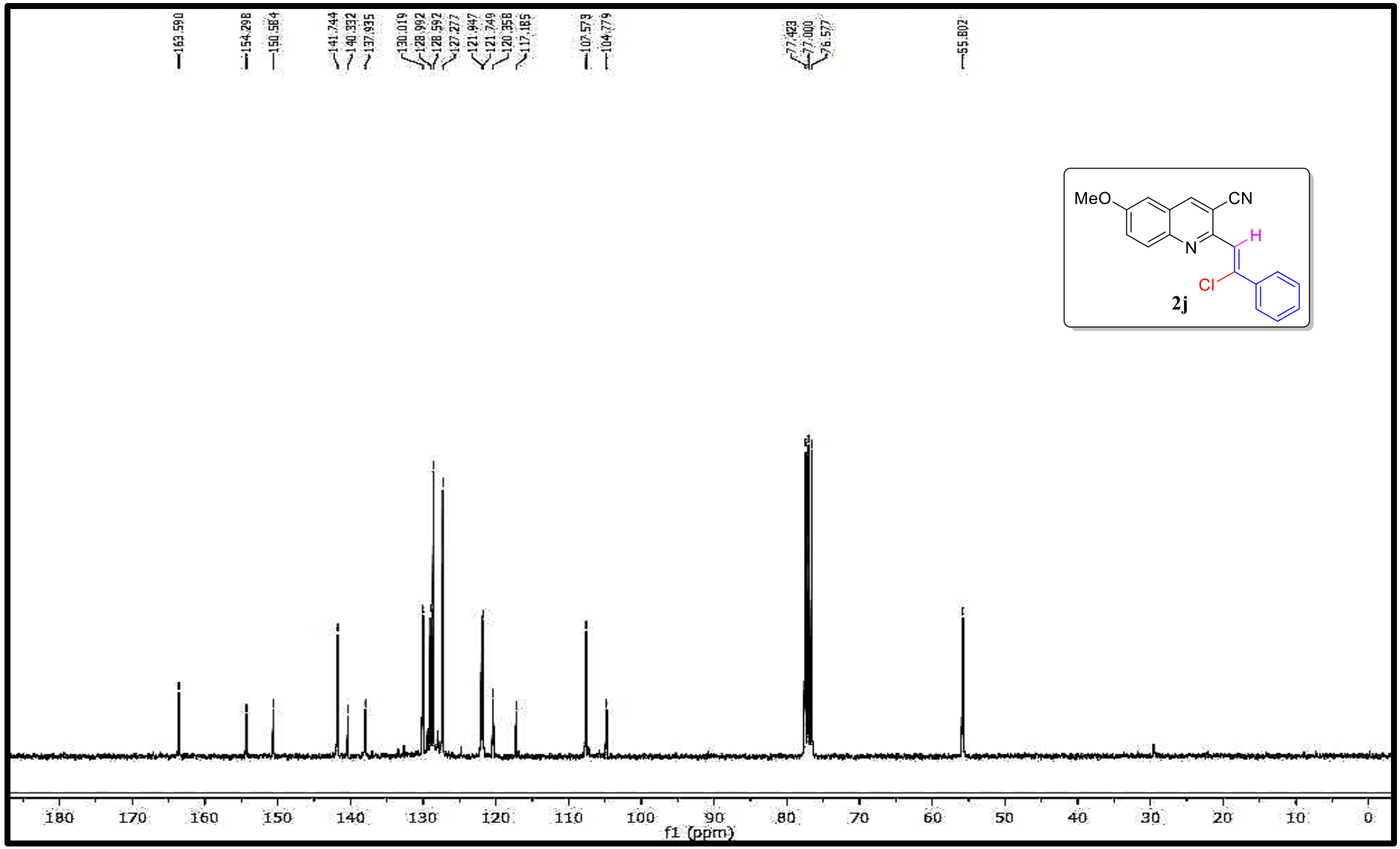
^{13}C NMR spectrum of 2-(2-Chloro-2-phenylvinyl)-7-methyl-quinoline-3-carbonitrile (2i)



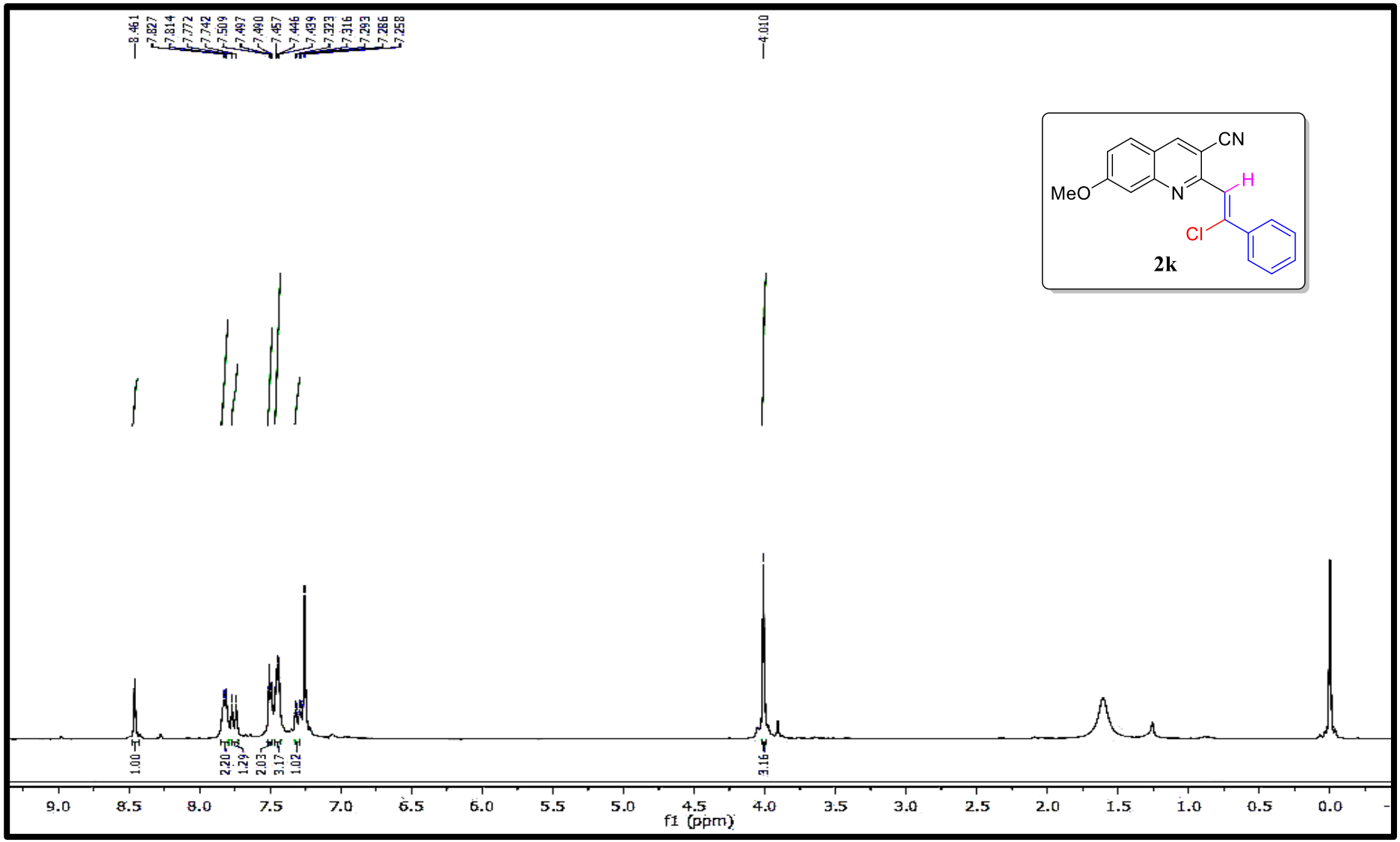
^{1}H and ^{13}C NMR spectrum of 2-(2-Chloro-2-phenylvinyl)-6-methoxy-quinoline-3-carbonitrile (2j)



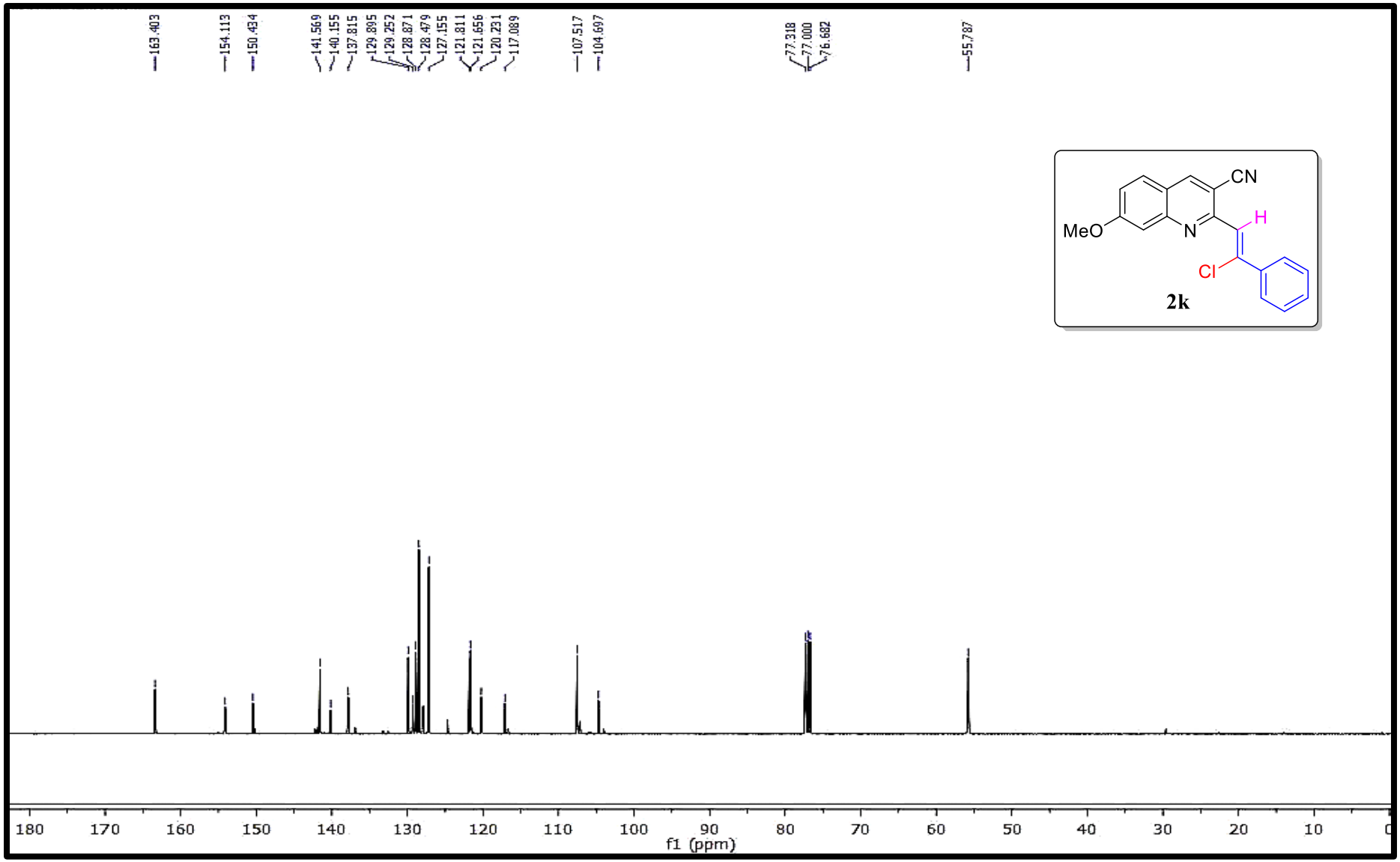
^{13}C NMR spectrum of 2-(2-Chloro-2-phenylvinyl)-6-methoxy-quinoline-3-carbonitrile (2j)



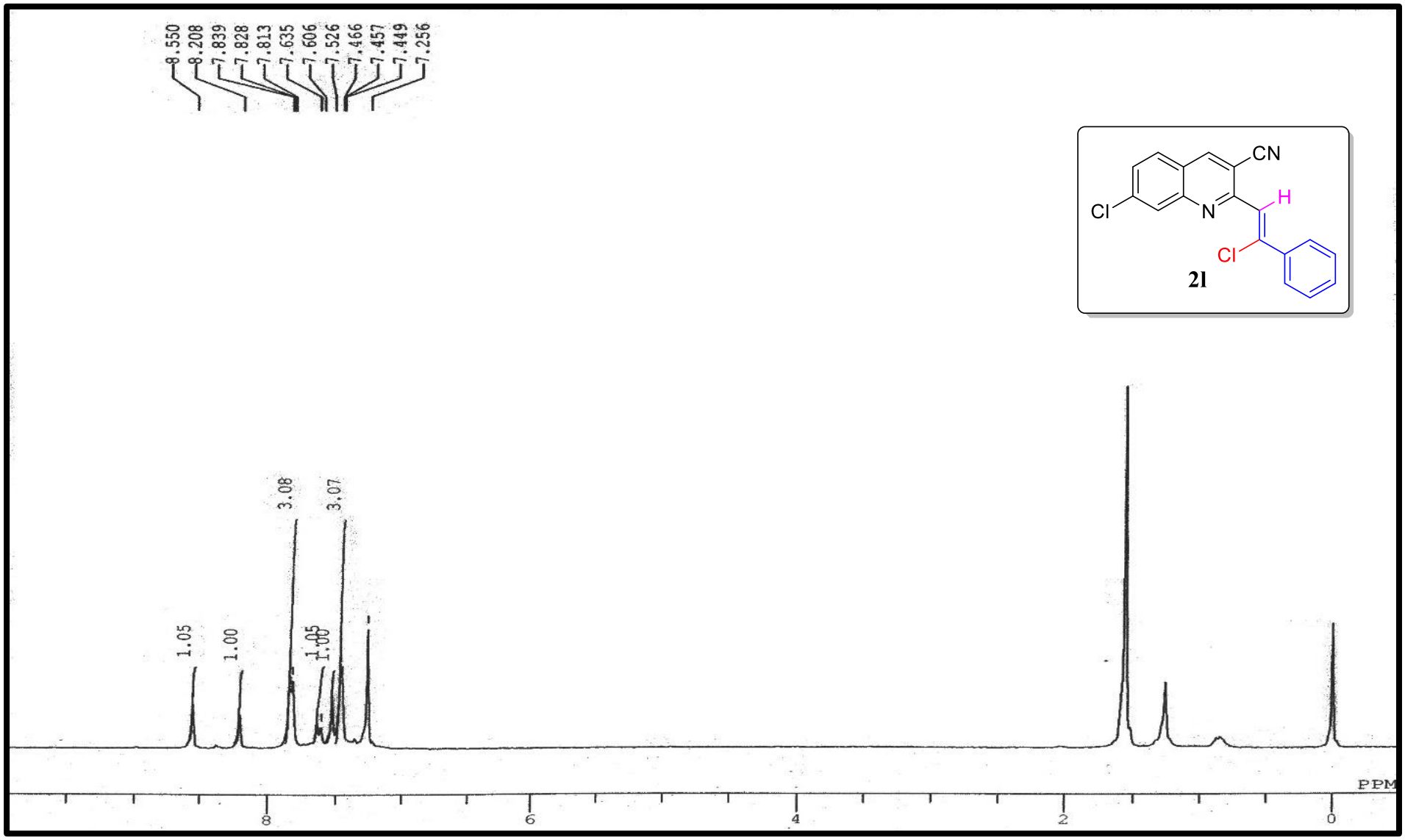
^{1}H and ^{13}C NMR spectrum of 2-(2-Chloro-2-phenylvinyl)-7-methoxy-quinoline-3-carbonitrile (2k)



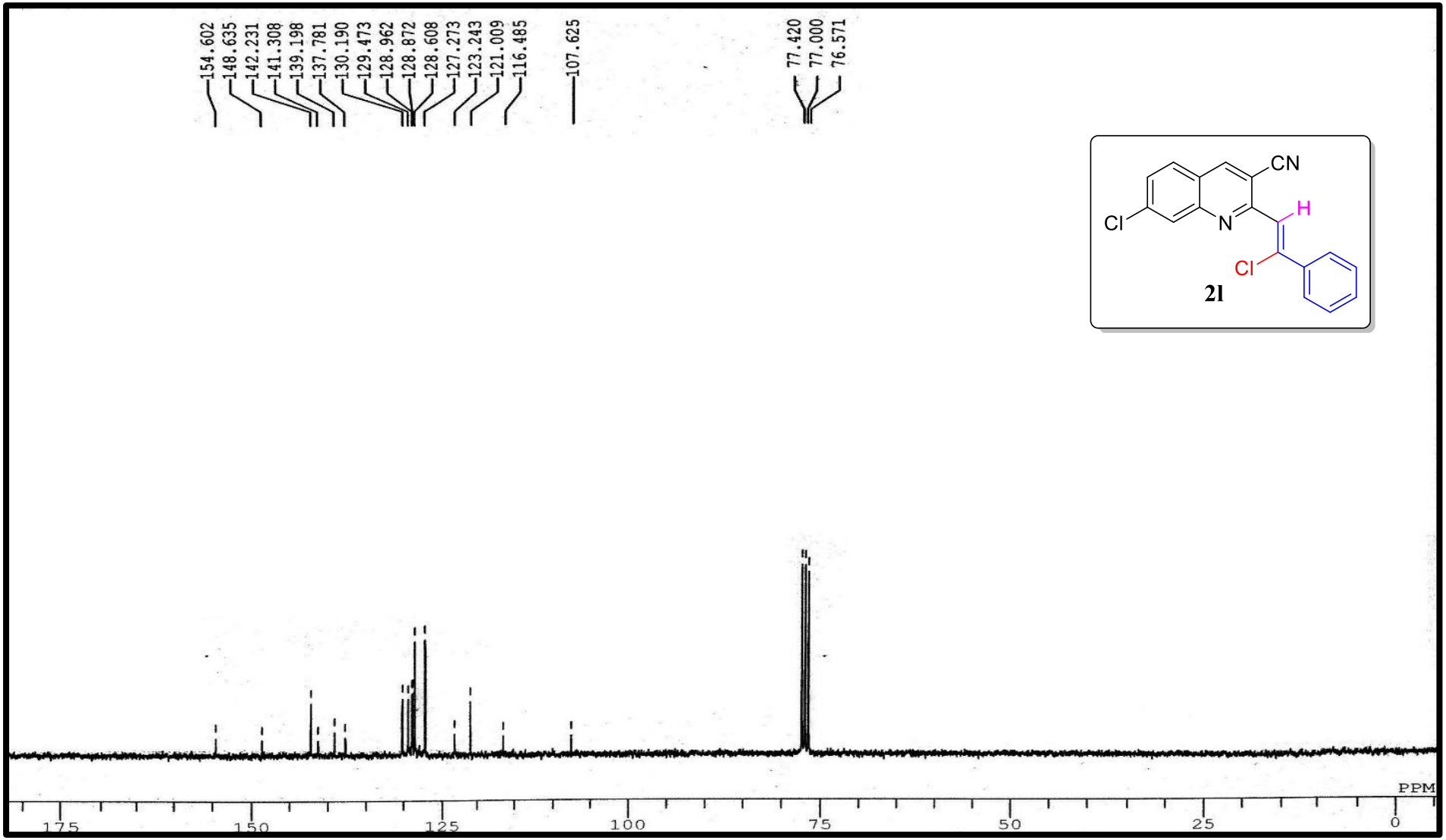
^{13}C NMR spectrum of 2-(2-Chloro-2-phenylvinyl)-7-methoxy-quinoline-3-carbonitrile (2k)



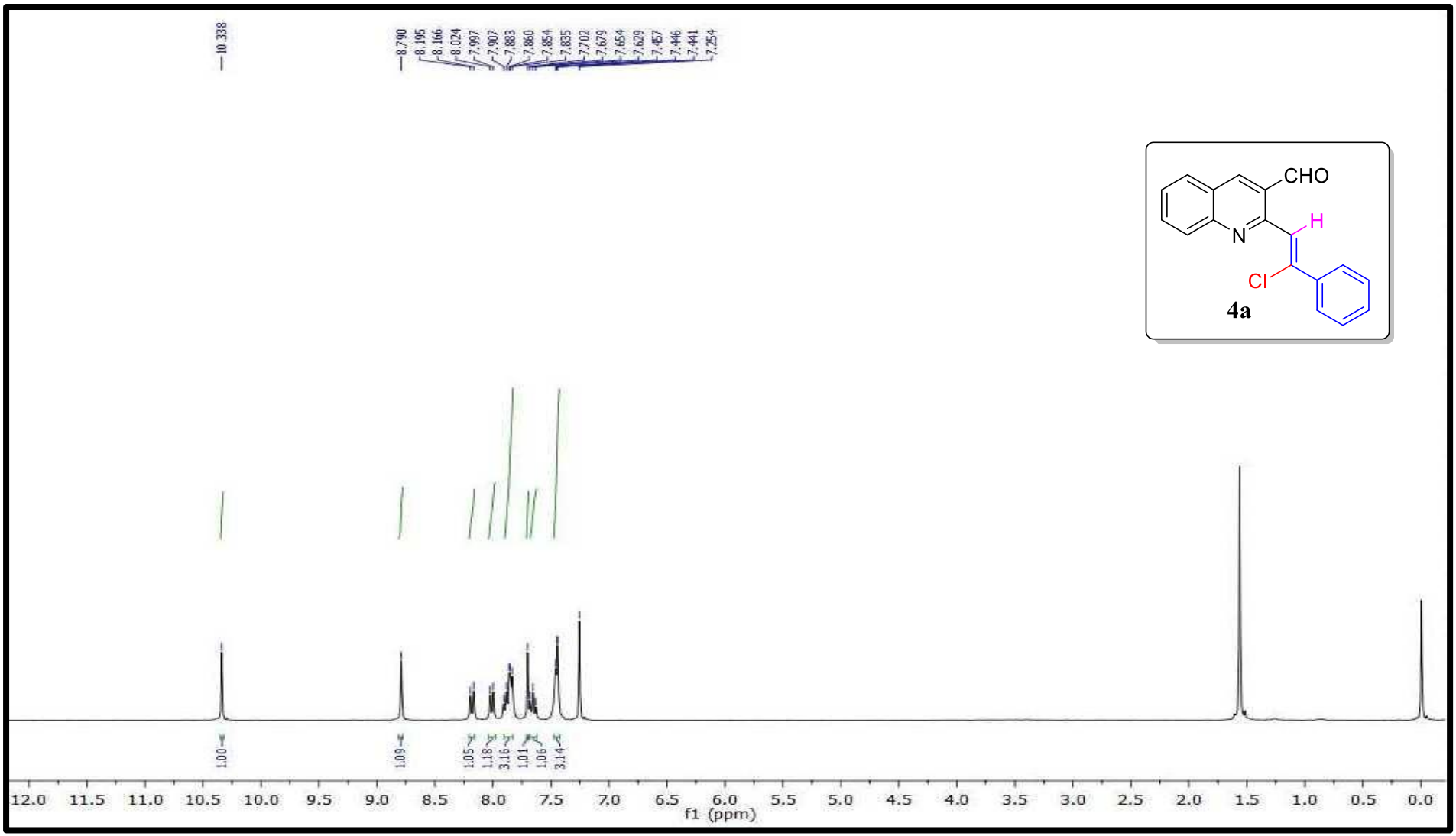
^{1}H spectrum of 7-Chloro-2-(2-chloro-2-phenylvinyl)quinoline-3-carbonitrile (2l)



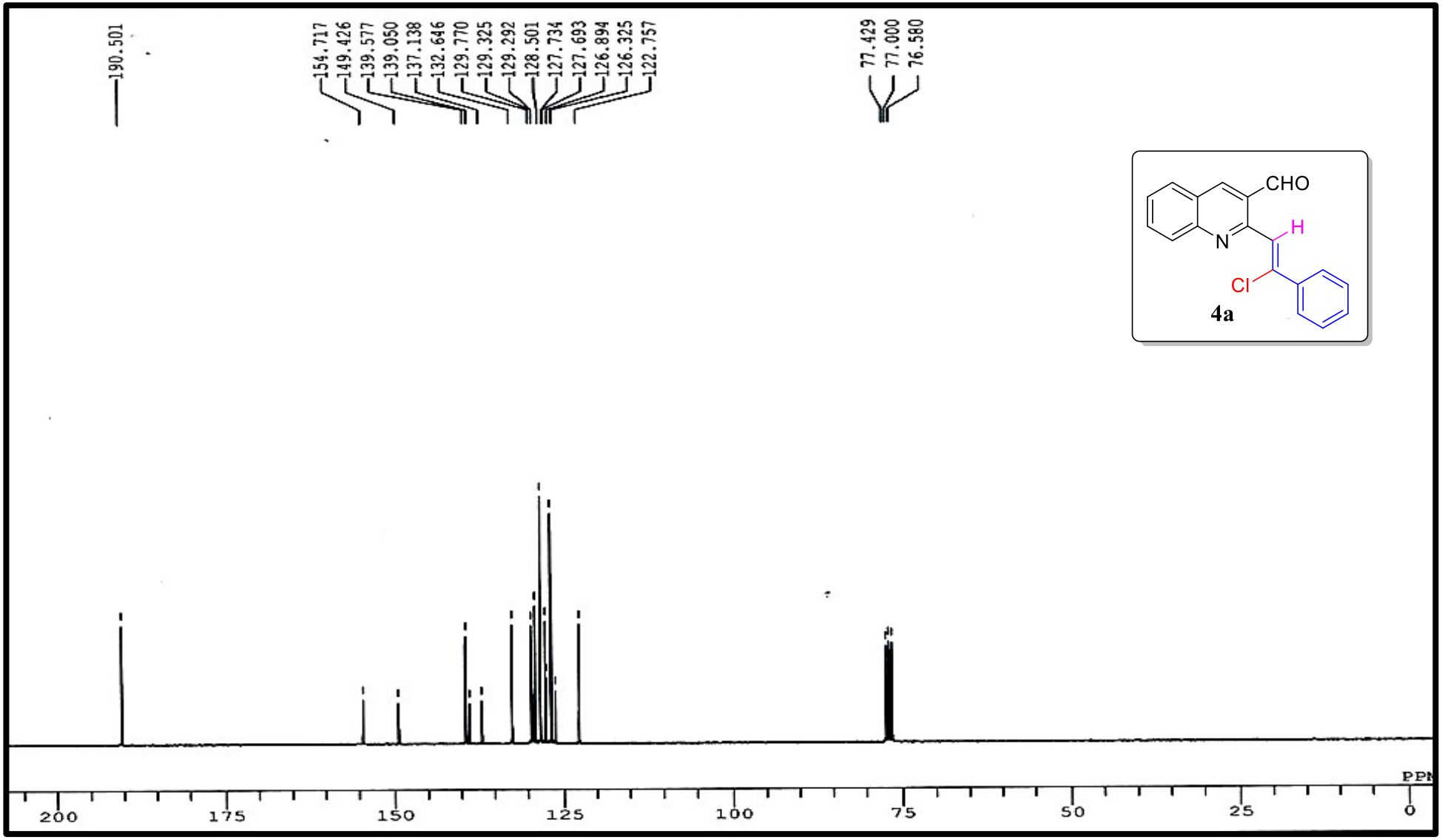
^{13}C NMR spectrum of 7-Chloro-2-(2-chloro-2-phenylvinyl)quinoline-3-carbonitrile (2l)



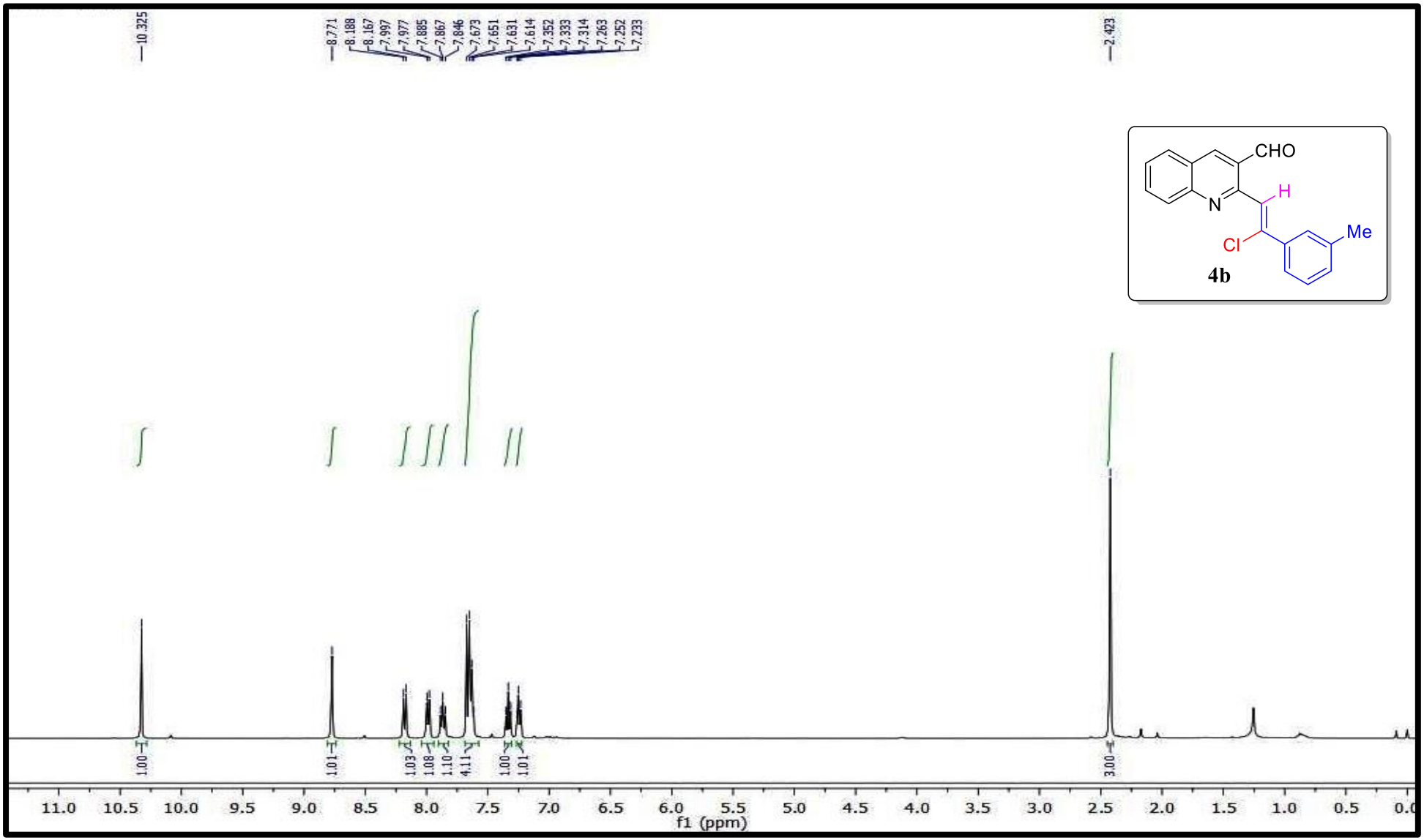
^{1}H spectrum of 2-(2-Chloro-2-phenylvinyl-quinoline-3-carbaldehyde (4a)



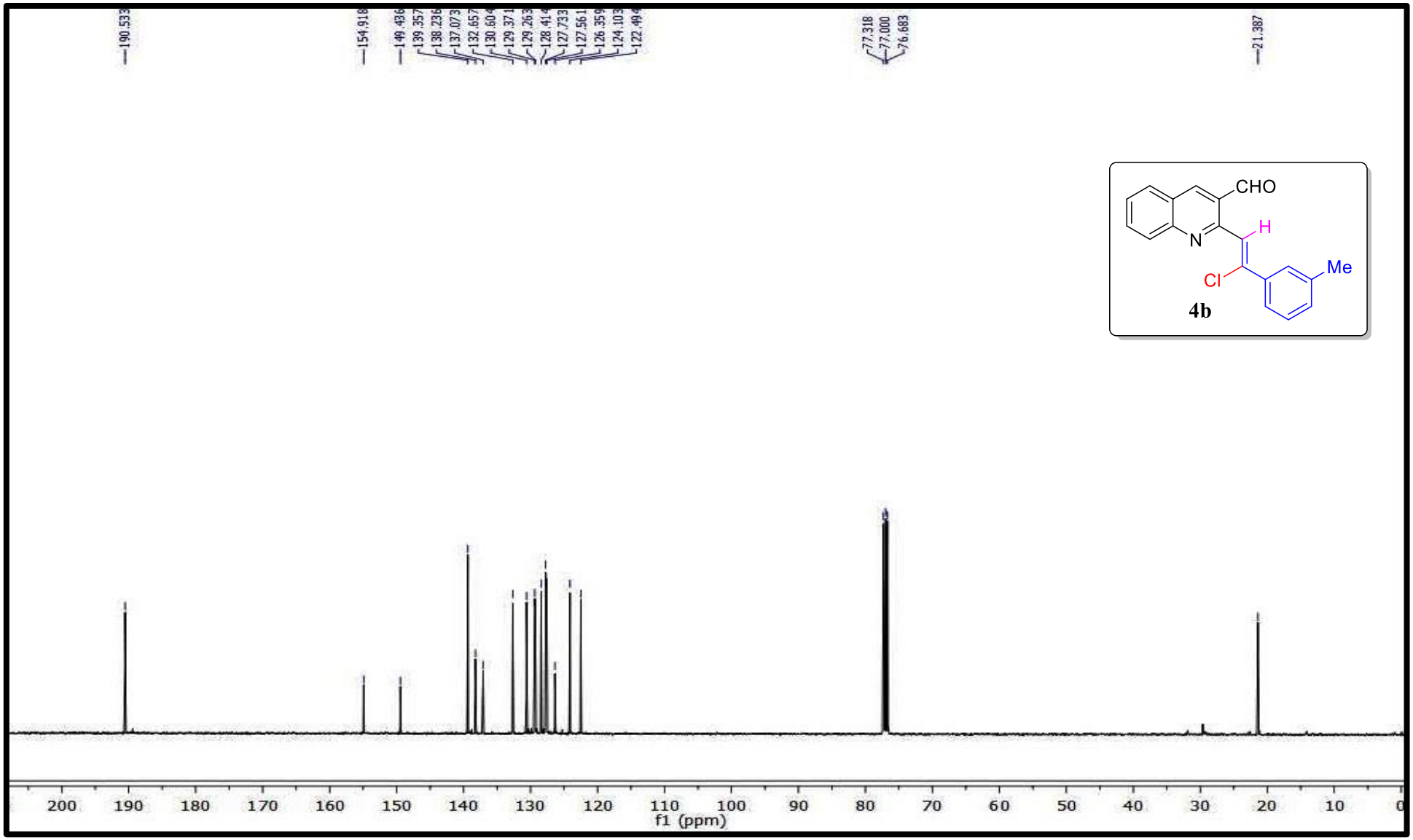
^{13}C NMR spectrum of 2-(2-Chloro-2-phenylvinyl-quinoline-3-carbaldehyde (4a)



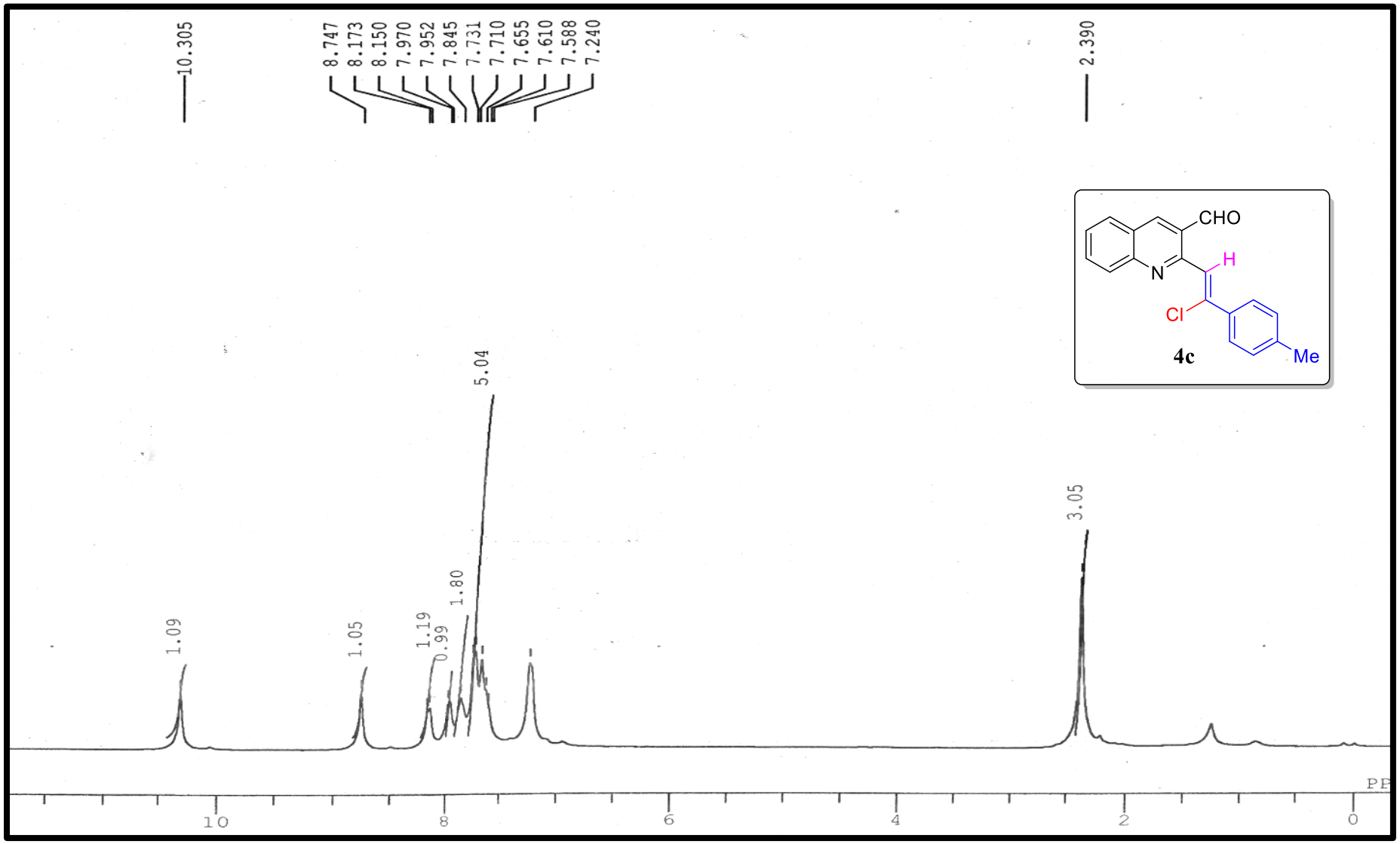
^{1}H and ^{13}C NMR spectrum of 2-(2-Chloro-2-m-tolylvinyl)quinoline-3-carbaldehyde (4b)



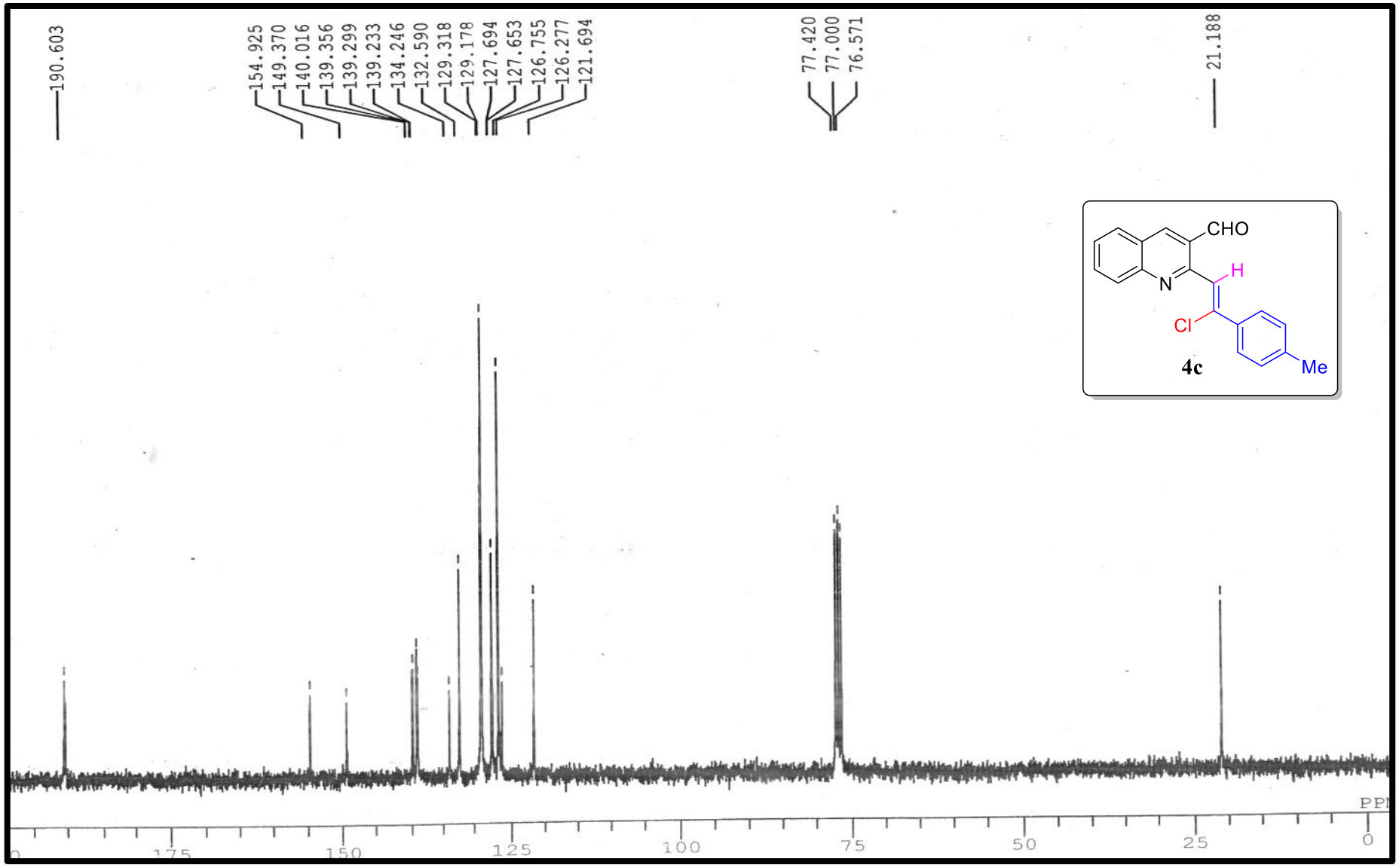
^{13}C NMR spectrum of 2-(2-Chloro-2-m-tolylvinyl)quinoline-3-carbaldehyde (4b)



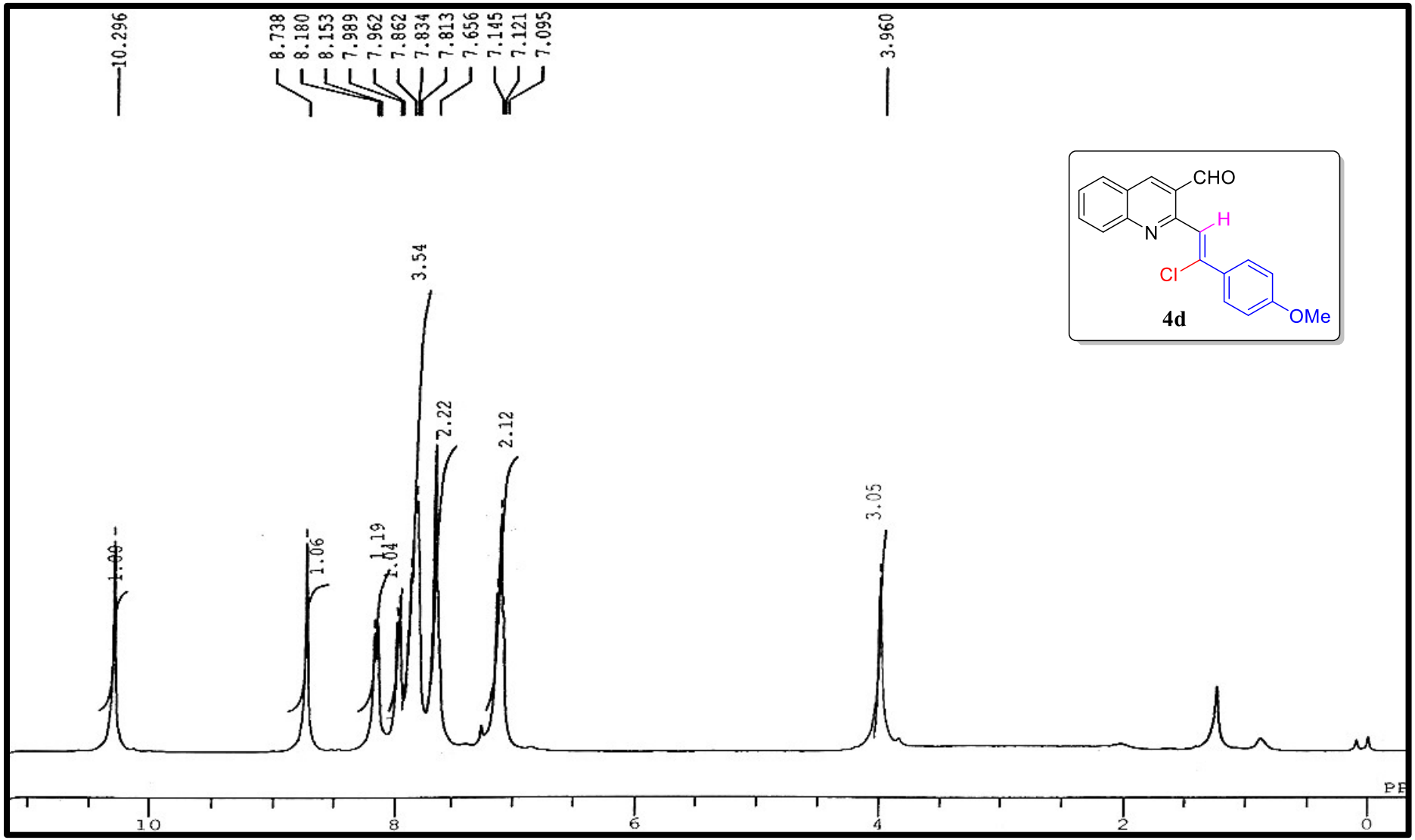
^{1}H spectrum of 2-(2-Chloro-2-p-tolylvinyl)quinoline-3-carbaldehyde (4c)



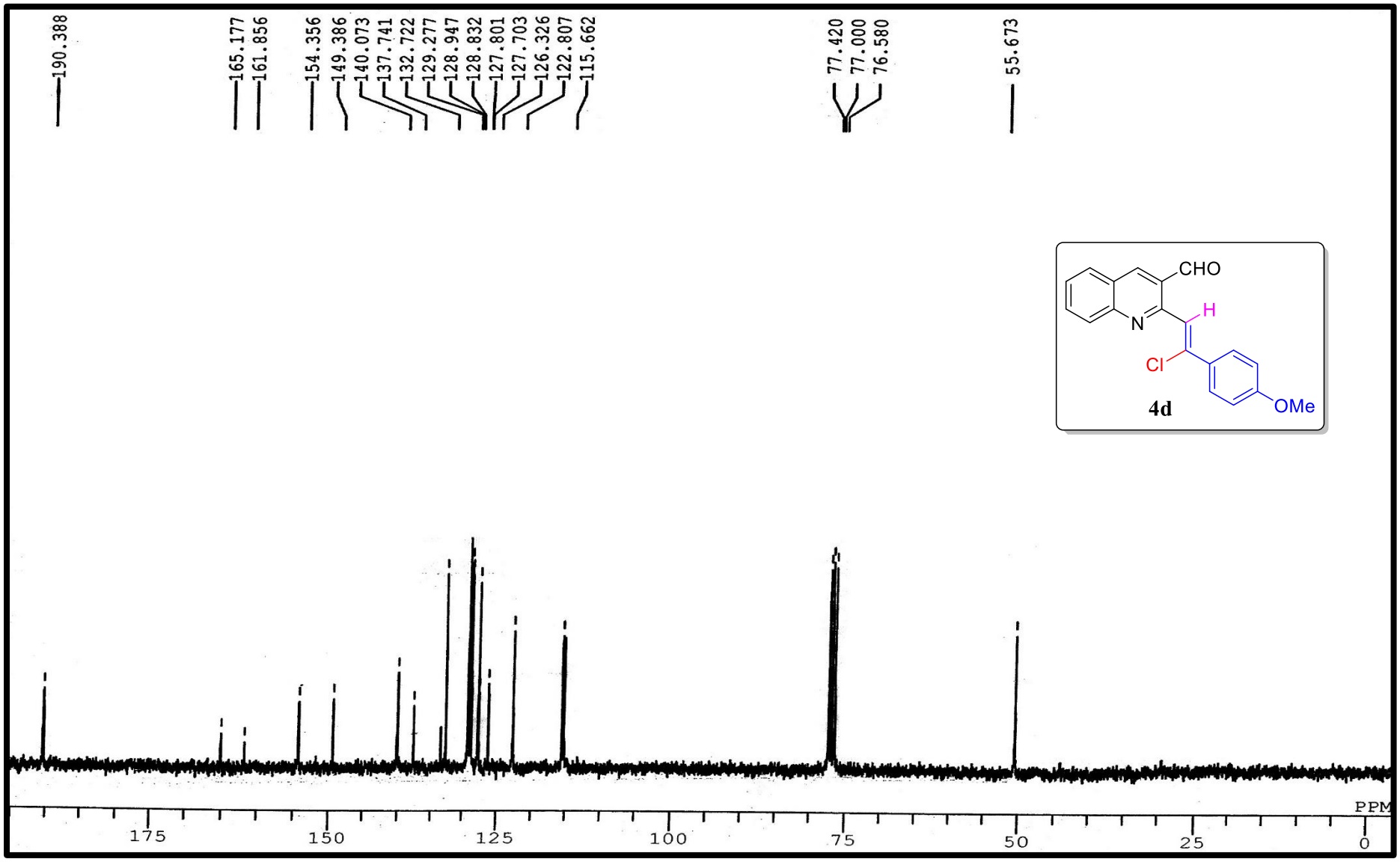
^{13}C NMR spectrum of 2-(2-Chloro-2-p-tolylvinyl)quinoline-3-carbaldehyde (4c)



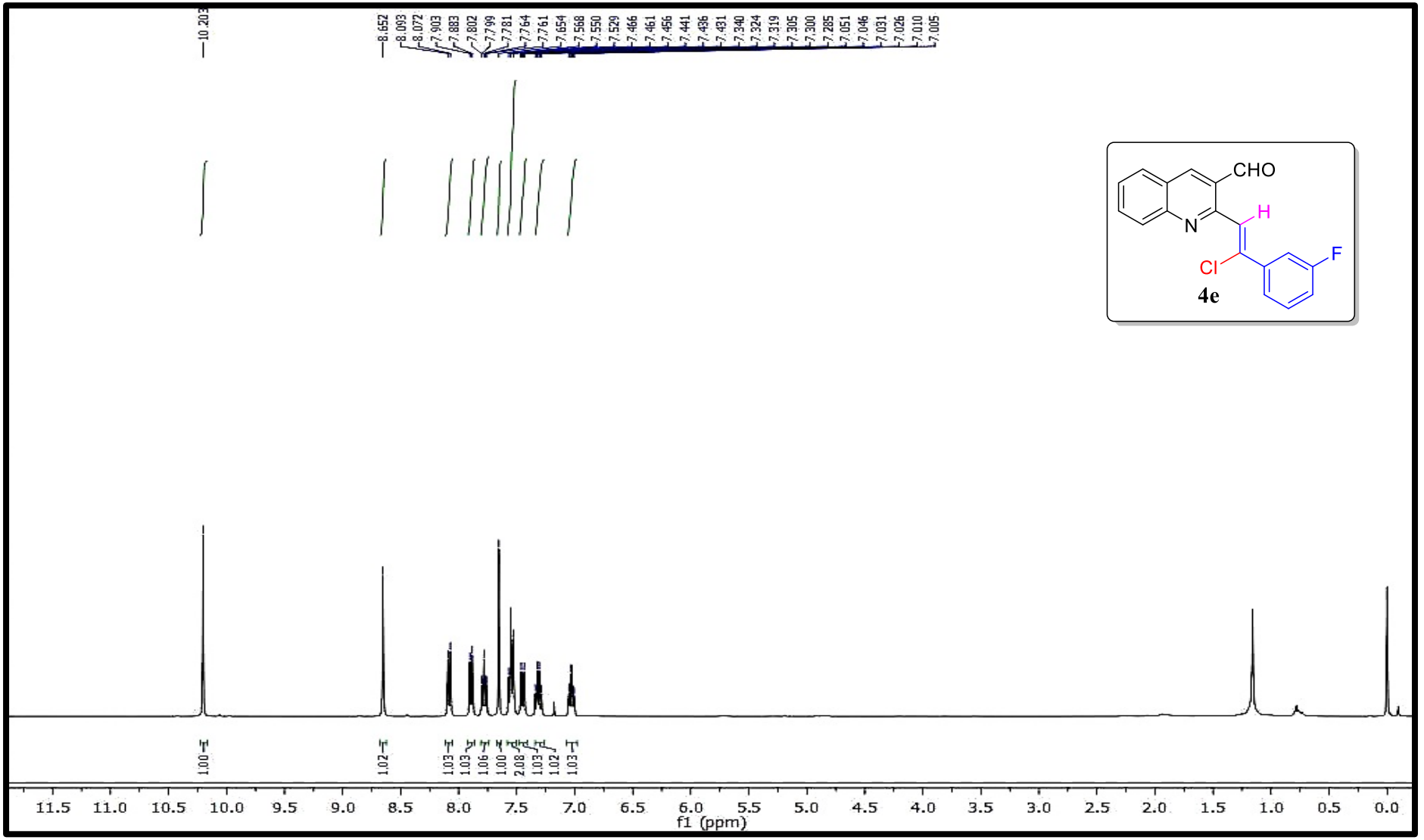
^{1}H and ^{13}C NMR spectrum of 2-[2-Chloro-2-(4-methoxy-phenyl)vinyl]quinoline-3-carbaldehyde (4d)



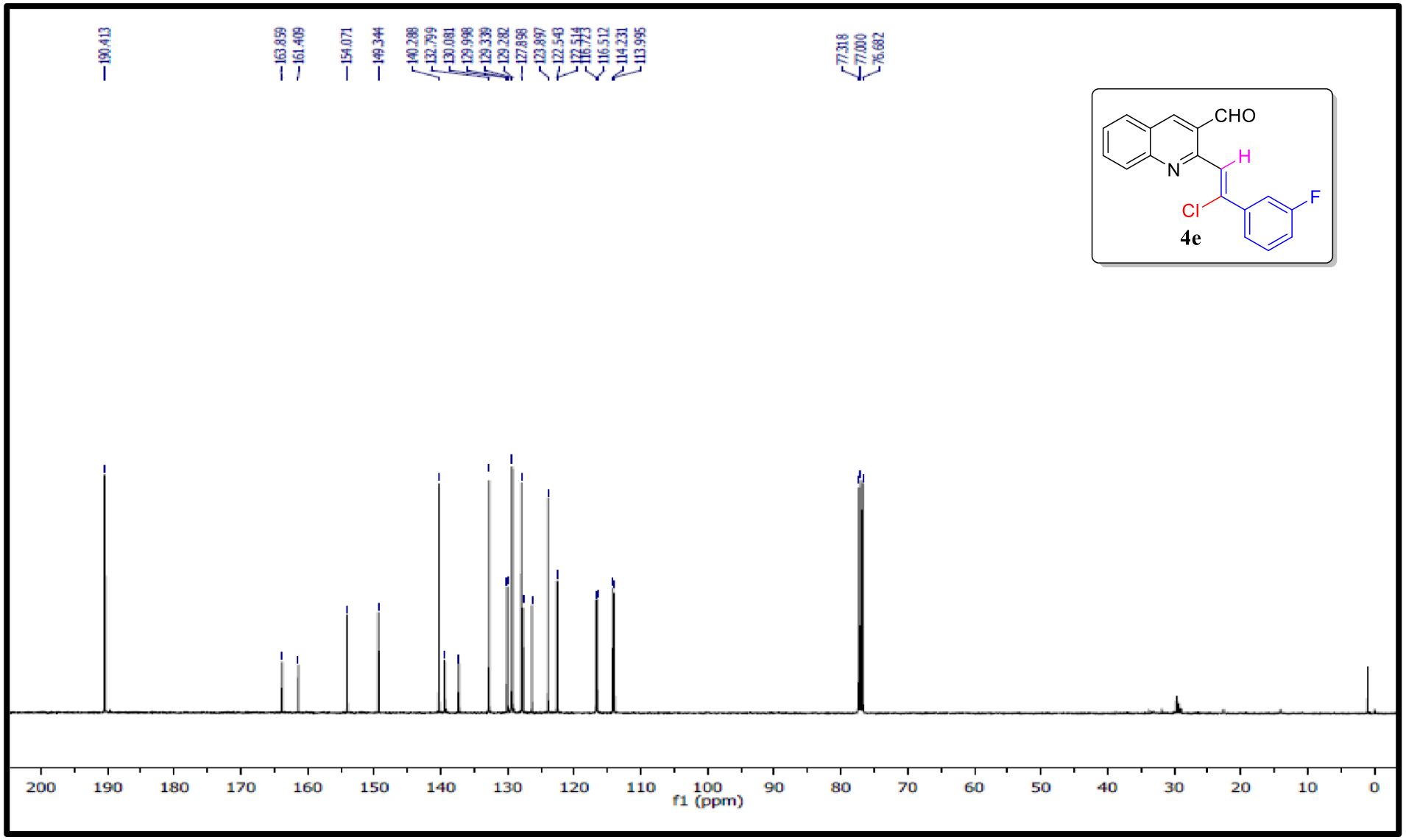
^{13}C NMR spectrum of 2-[2-Chloro-2-(4-methoxy-phenyl)vinyl]quinoline-3-carbaldehyde (4d)



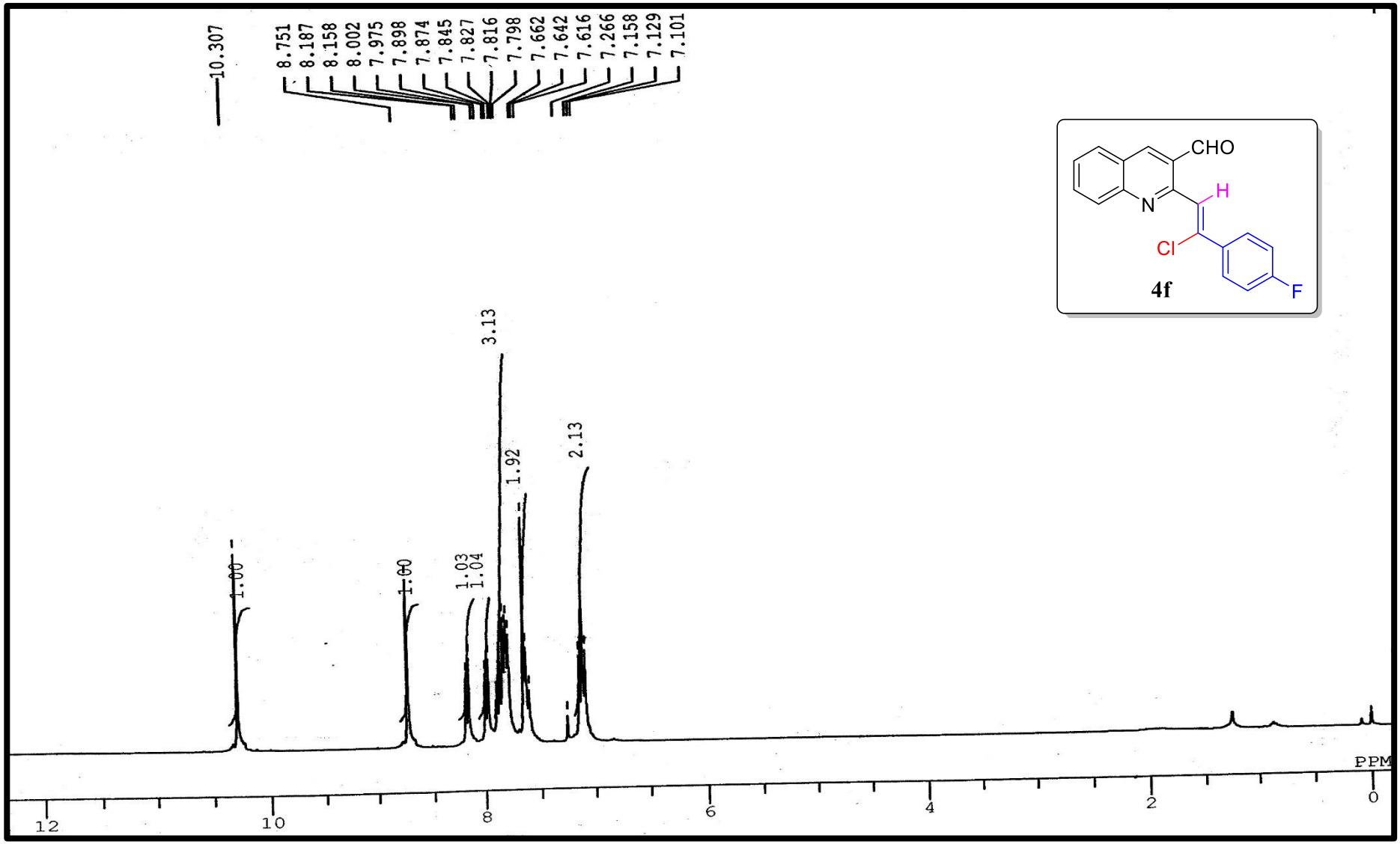
^{1}H spectrum of 2-(2-chloro-2-(3-fluorophenyl)vinyl)quinoline-3-carbaldehyde (4e)



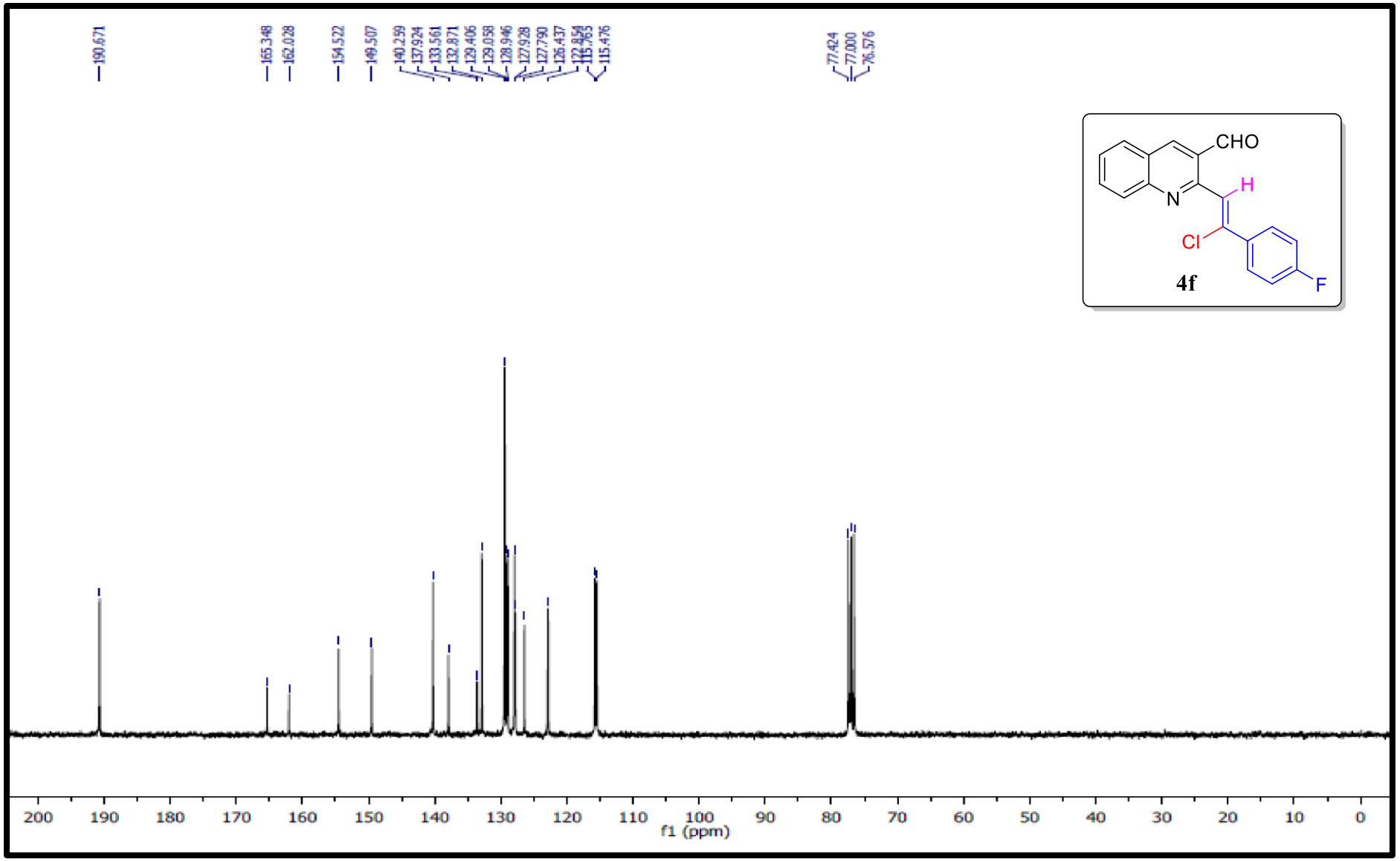
^{13}C NMR spectrum of 2-(2-chloro-2-(3-fluorophenyl)vinyl)quinoline-3-carbaldehyde (4e)



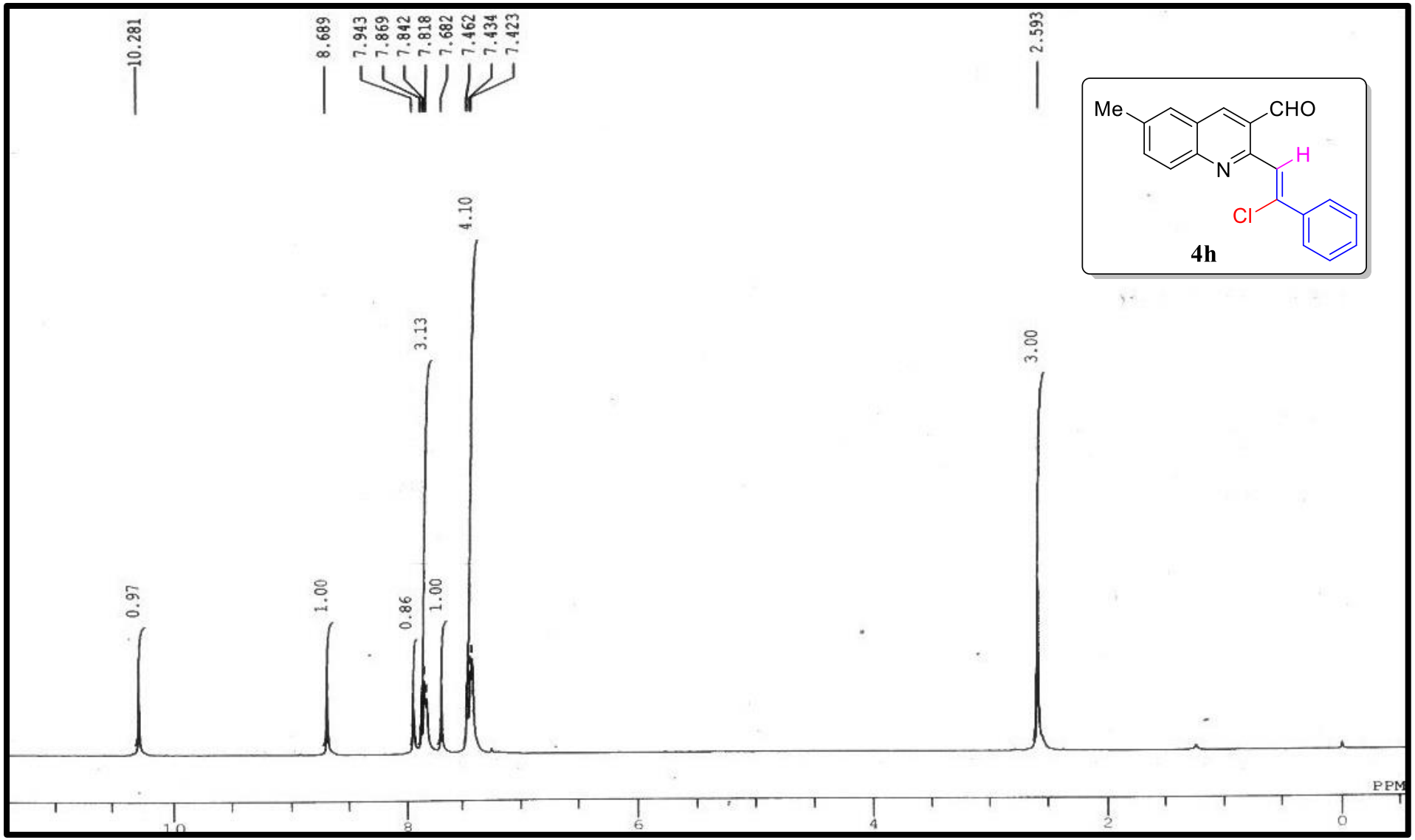
^{1}H NMR spectrum of 2-[2-Chloro-2-(4-fluoro-phenyl)vinyl]quinoline-3-carbaldehyde (4f)



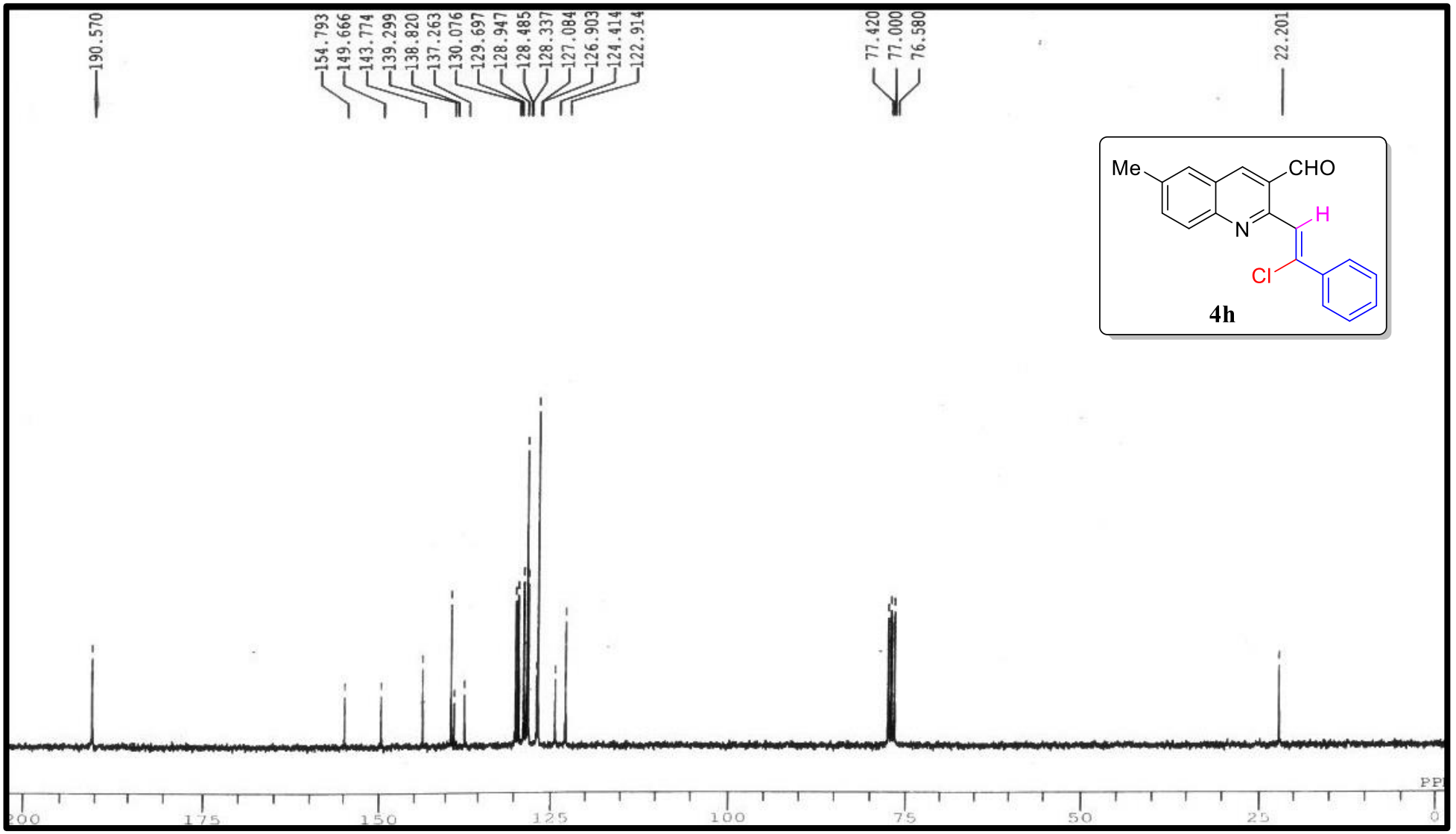
^{13}C NMR spectrum of 2-[2-Chloro-2-(4-fluoro-phenyl)vinyl]quinoline-3-carbaldehyde (4f)



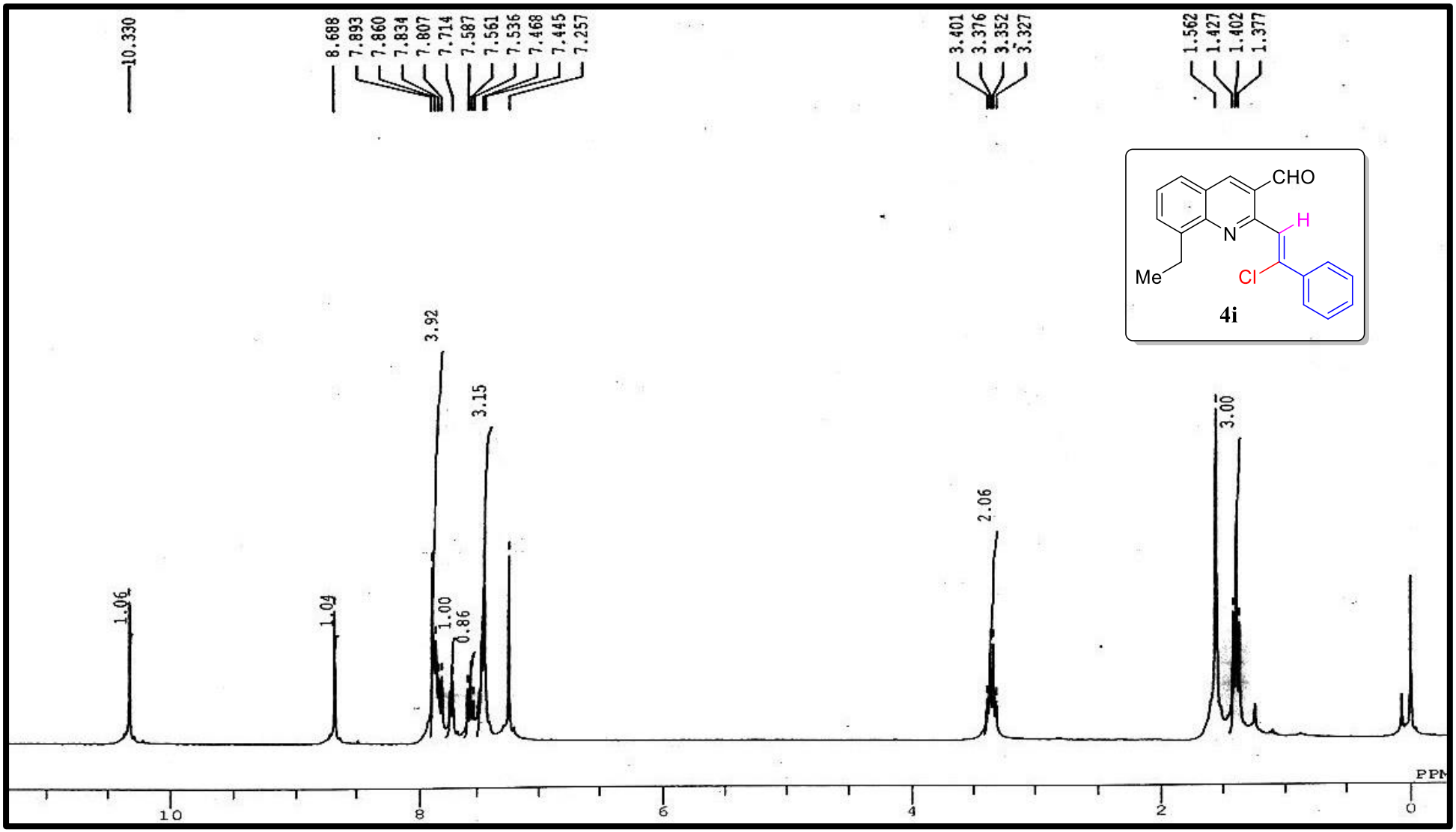
^{1}H and ^{13}C NMR spectrum of 2-(2-Chloro-2-phenylvinyl)-7-methyl-quinoline-3-carbaldehyde (4h)



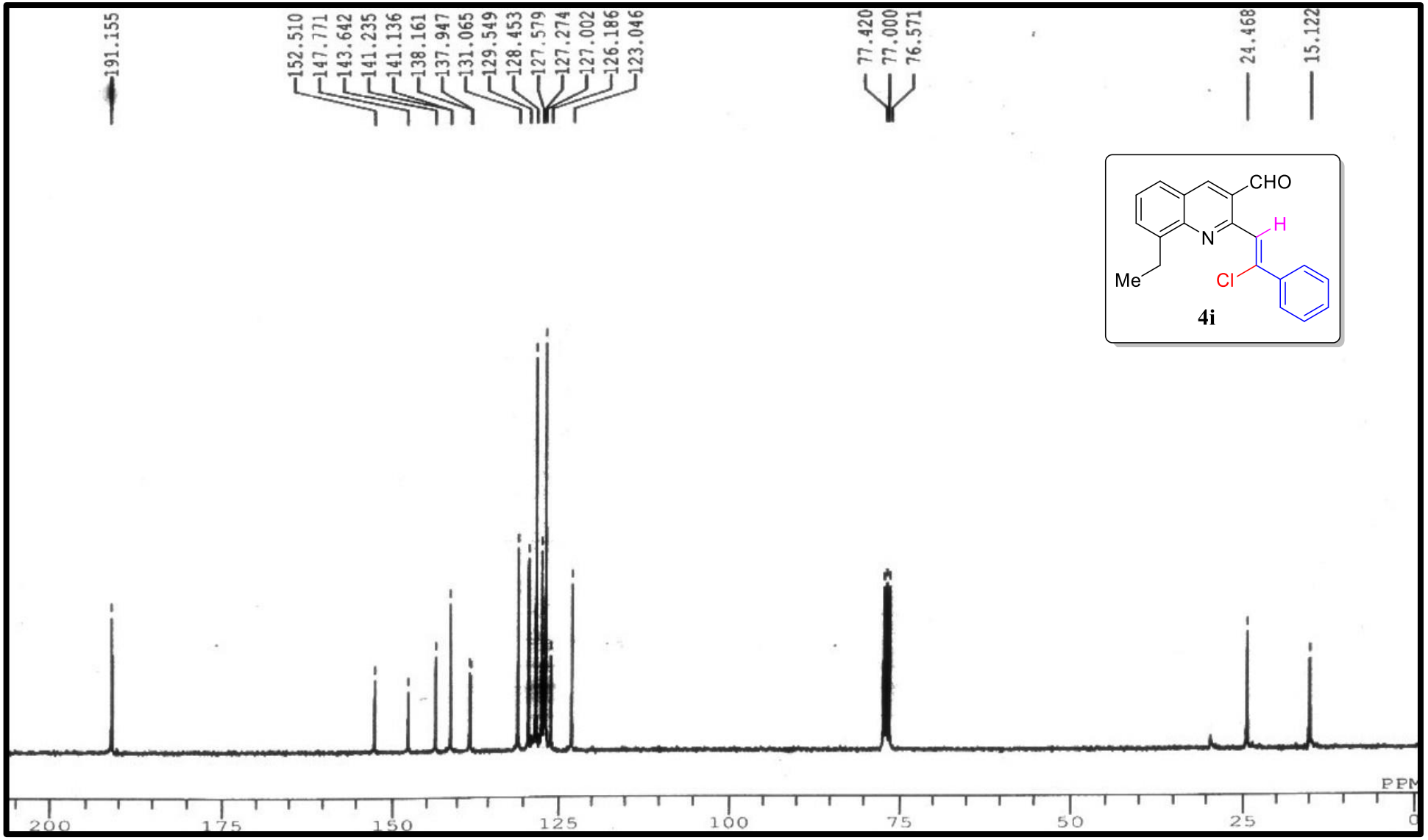
^{13}C NMR spectrum of 2-(2-Chloro-2-phenylvinyl)-7-methyl-quinoline-3-carbaldehyde (4h)



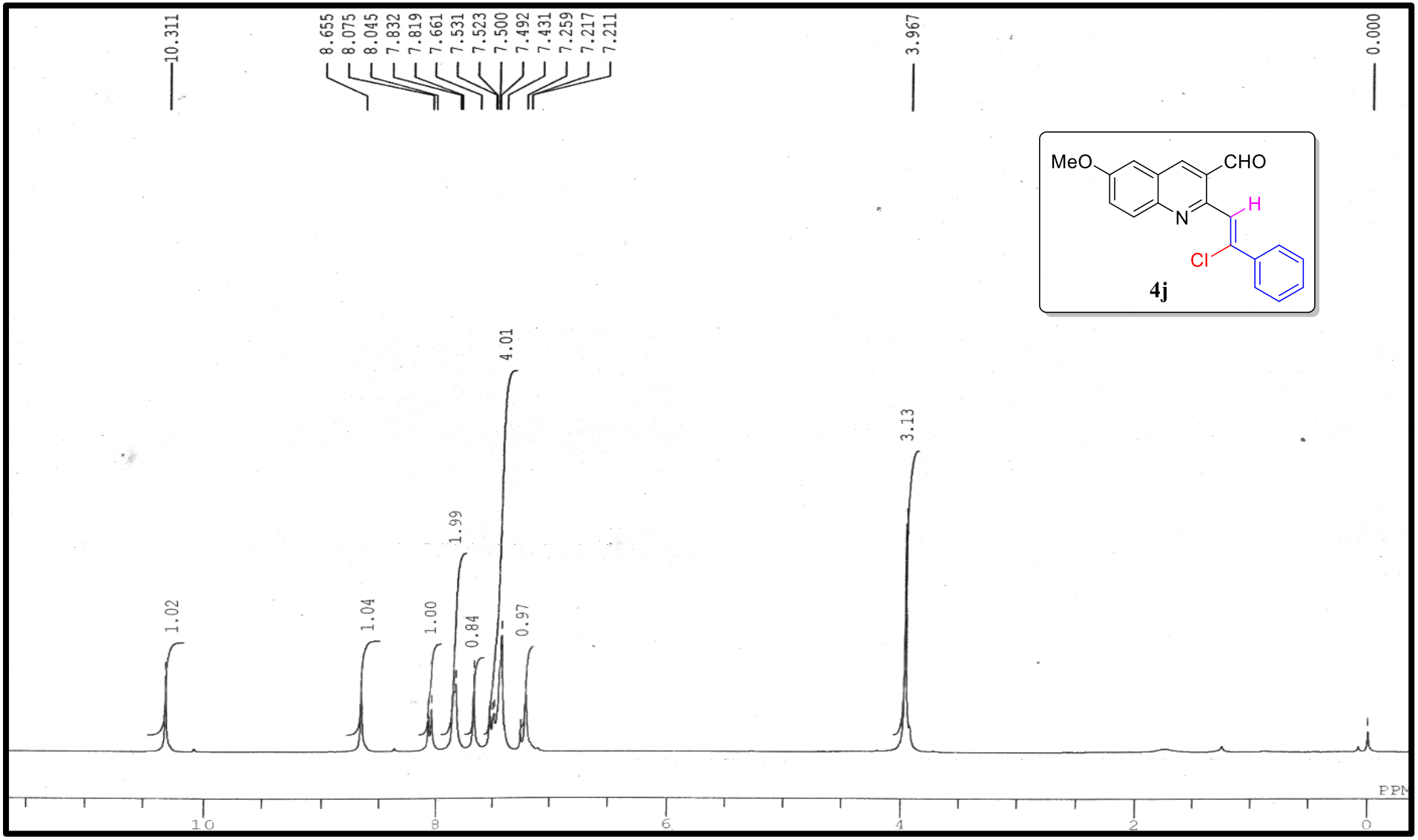
[1]H NMR spectrum of 2-(2-Chloro-2-phenylvinyl)-8-ethyl-quinoline-3-carbaldehyde (4i)



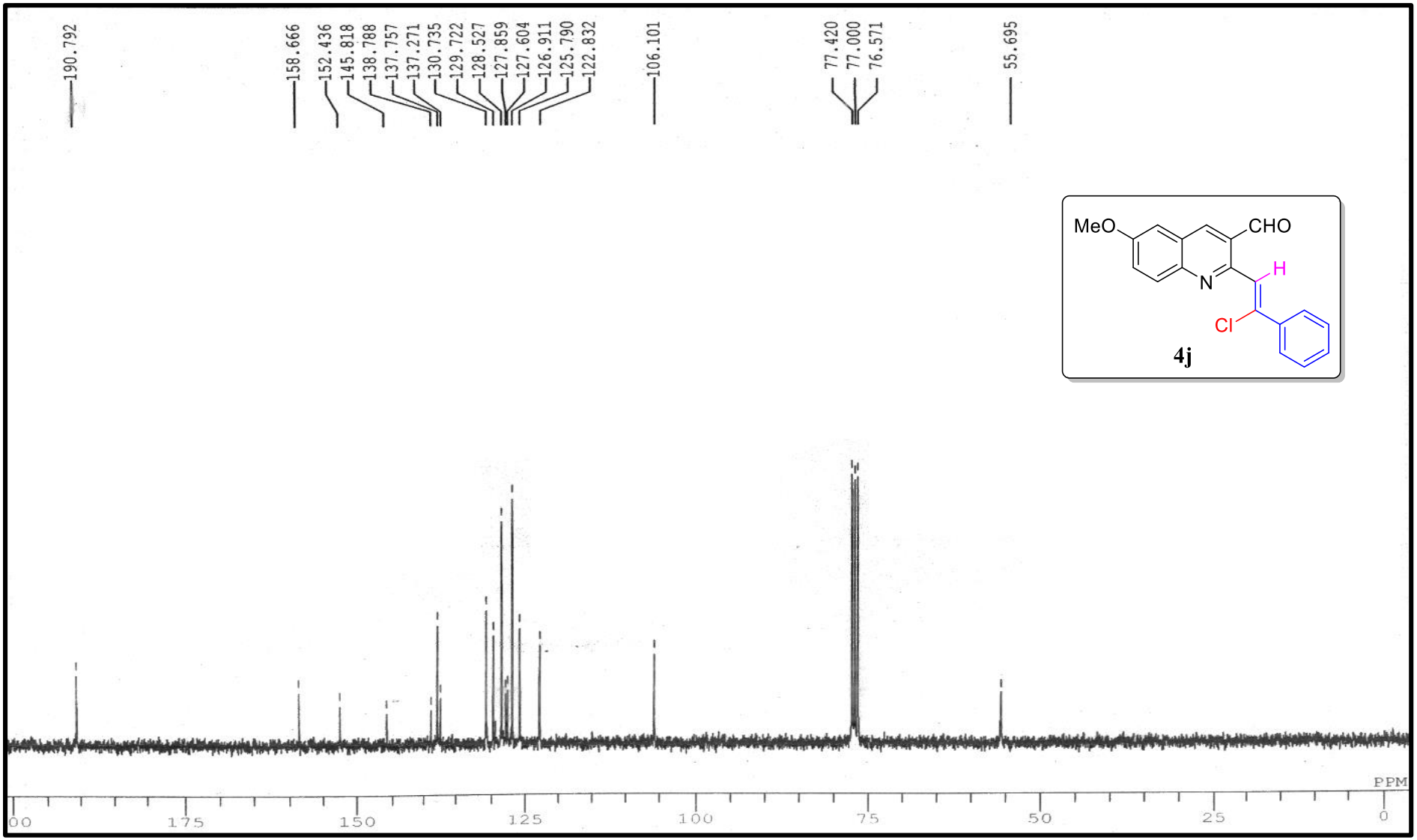
^{13}C NMR spectrum of 2-(2-Chloro-2-phenylvinyl)-8-ethyl-quinoline-3-carbaldehyde (4i)



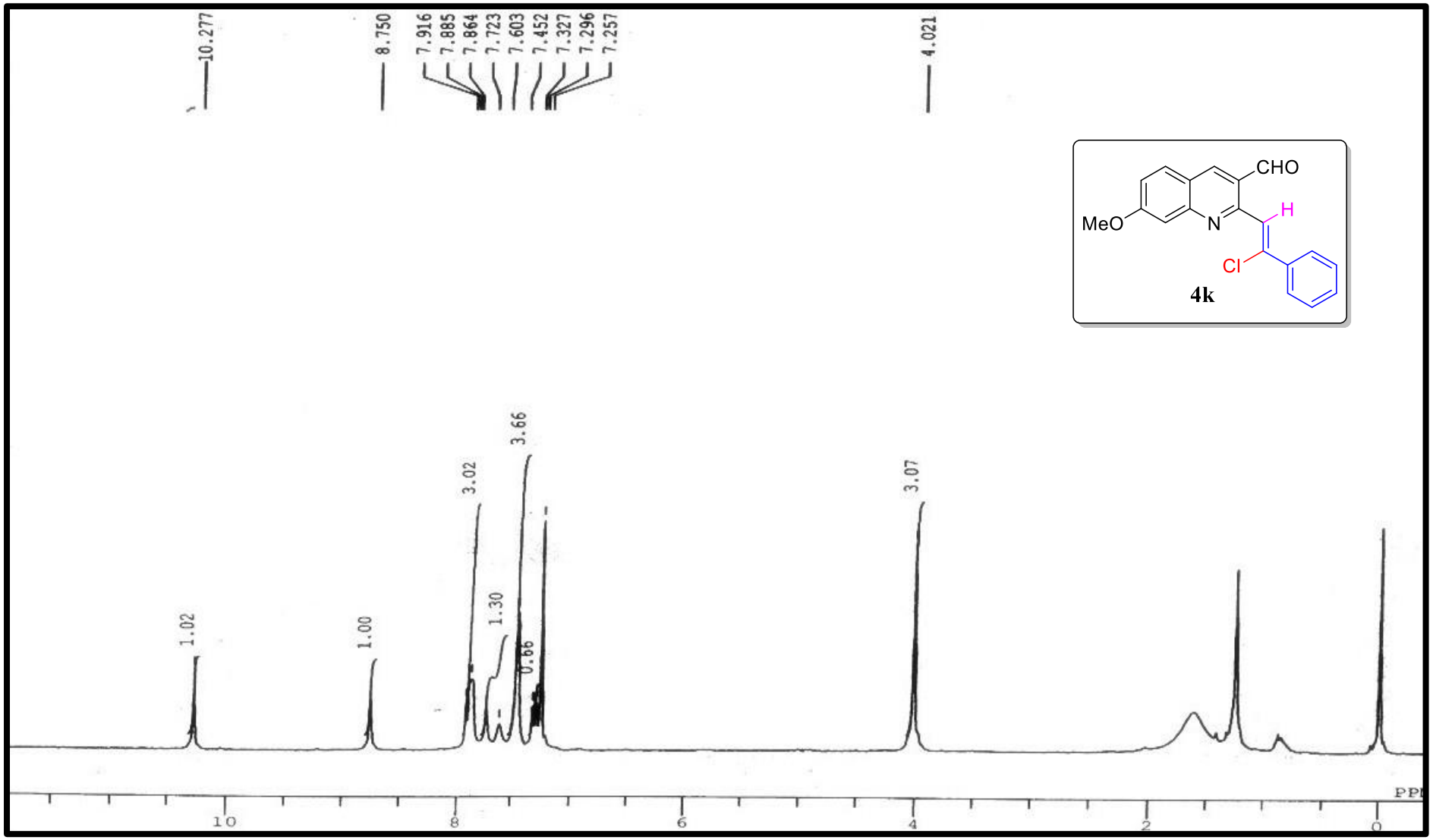
^{1}H NMR spectrum of 2-(2-Chloro-2-phenylvinyl)-6-methoxy-quinoline-3-carbaldehyde (4j)



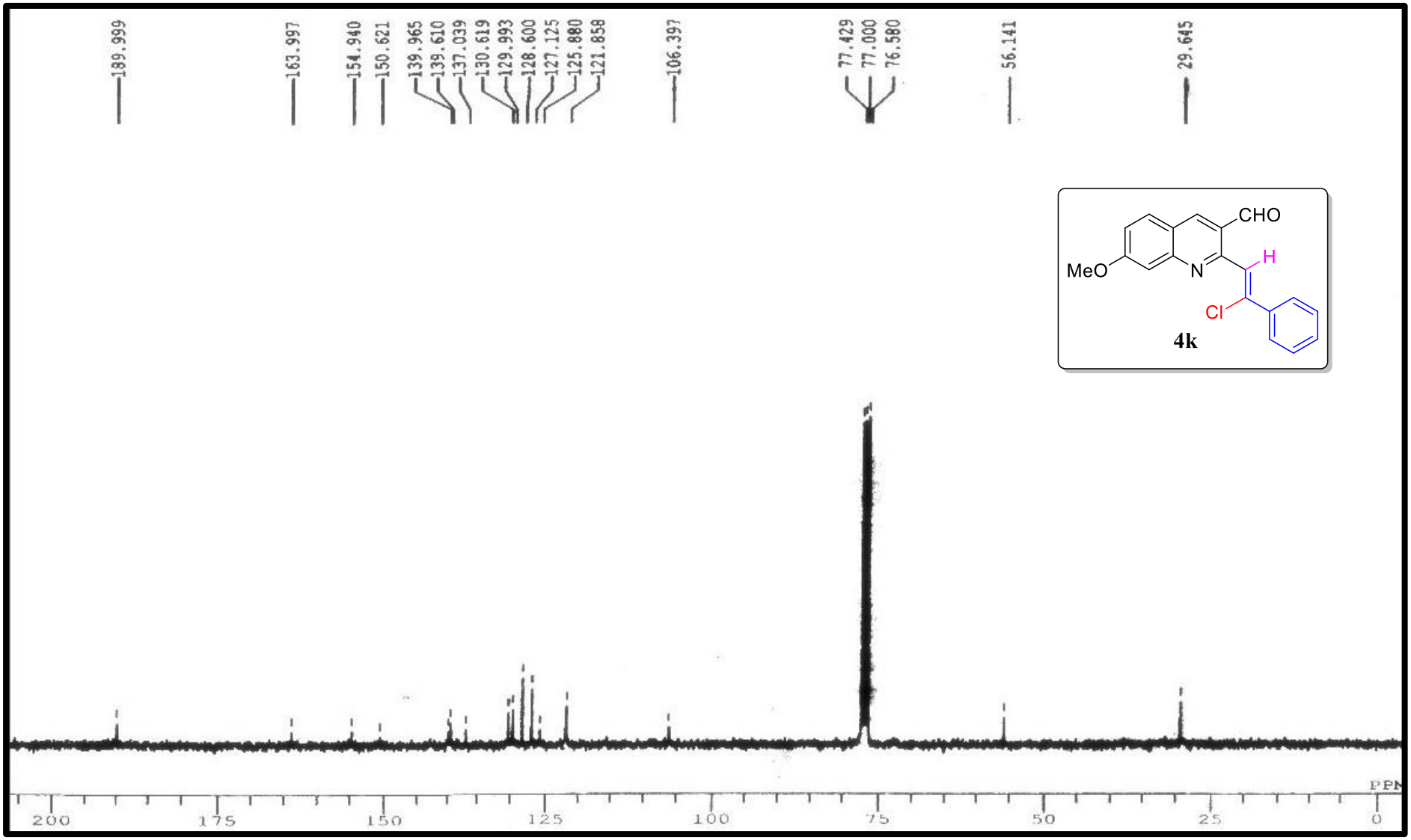
^{13}C NMR spectrum of 2-(2-Chloro-2-phenylvinyl)-6-methoxy-quinoline-3-carbaldehyde (4j).



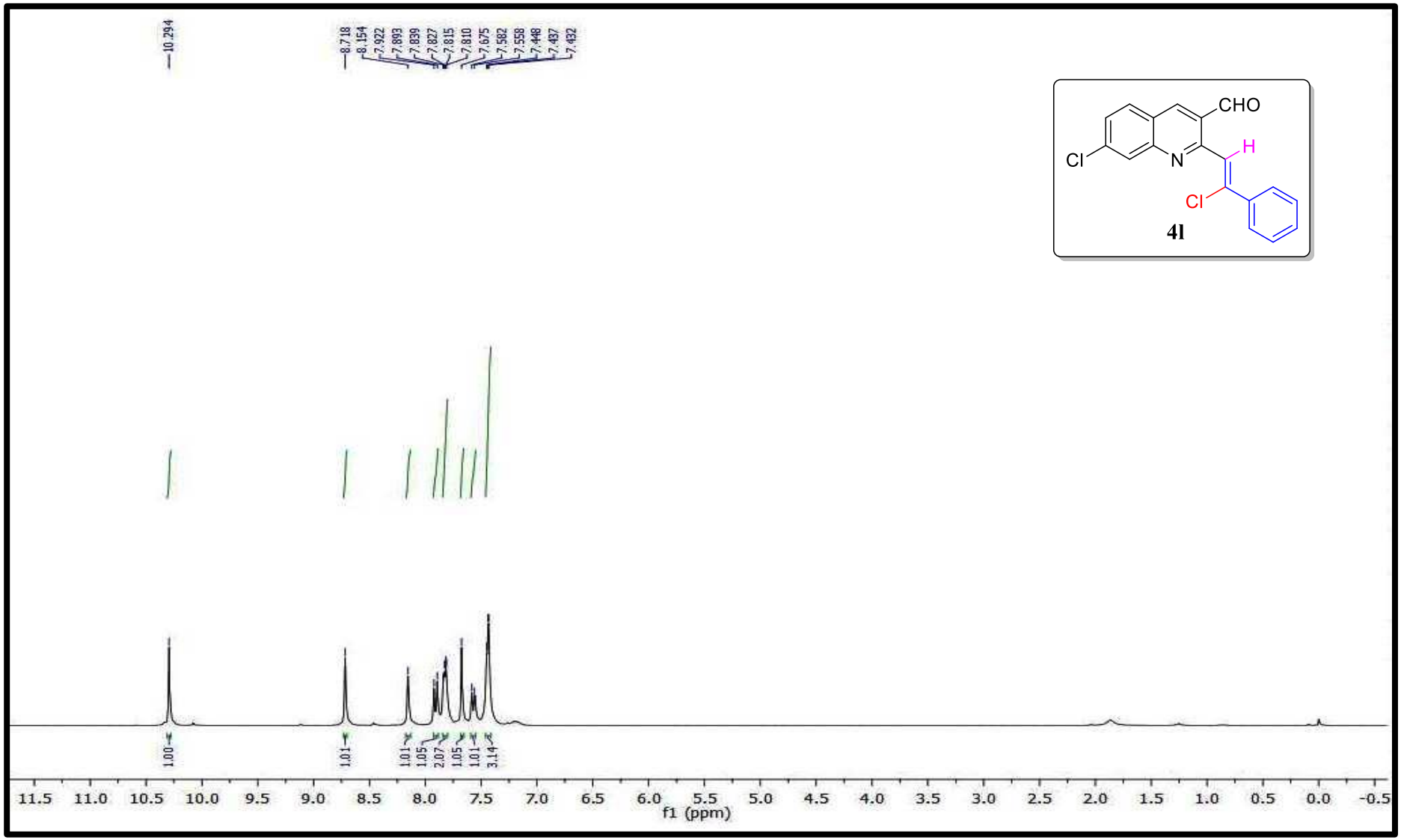
^{1}H NMR spectrum of 2-(2-Chloro-2-phenylvinyl)-7-methoxy-quinoline-3-carbaldehyde (4k)



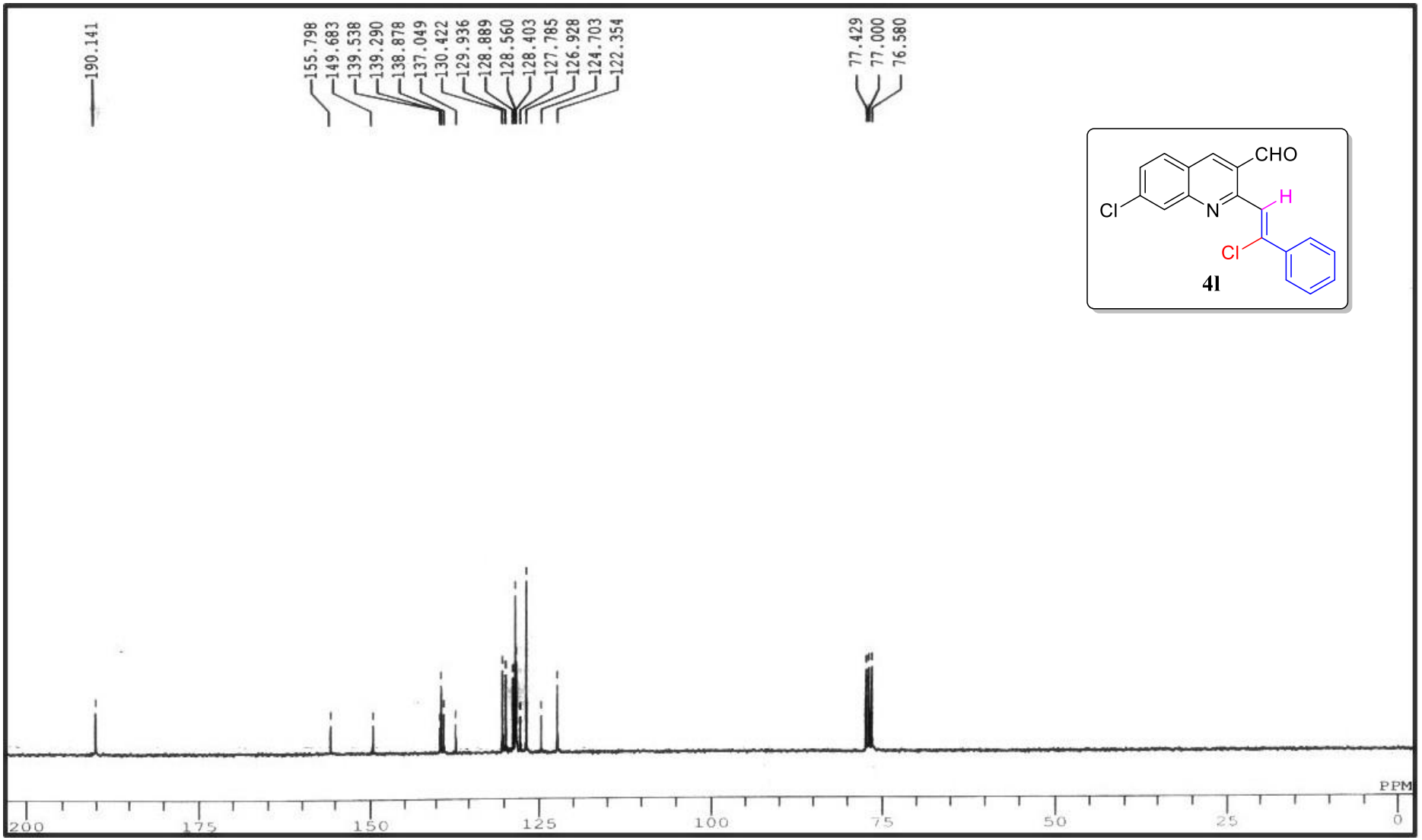
^{13}C NMR spectrum of 2-(2-Chloro-2-phenylvinyl)-7-methoxy-quinoline-3-carbaldehyde (4k)



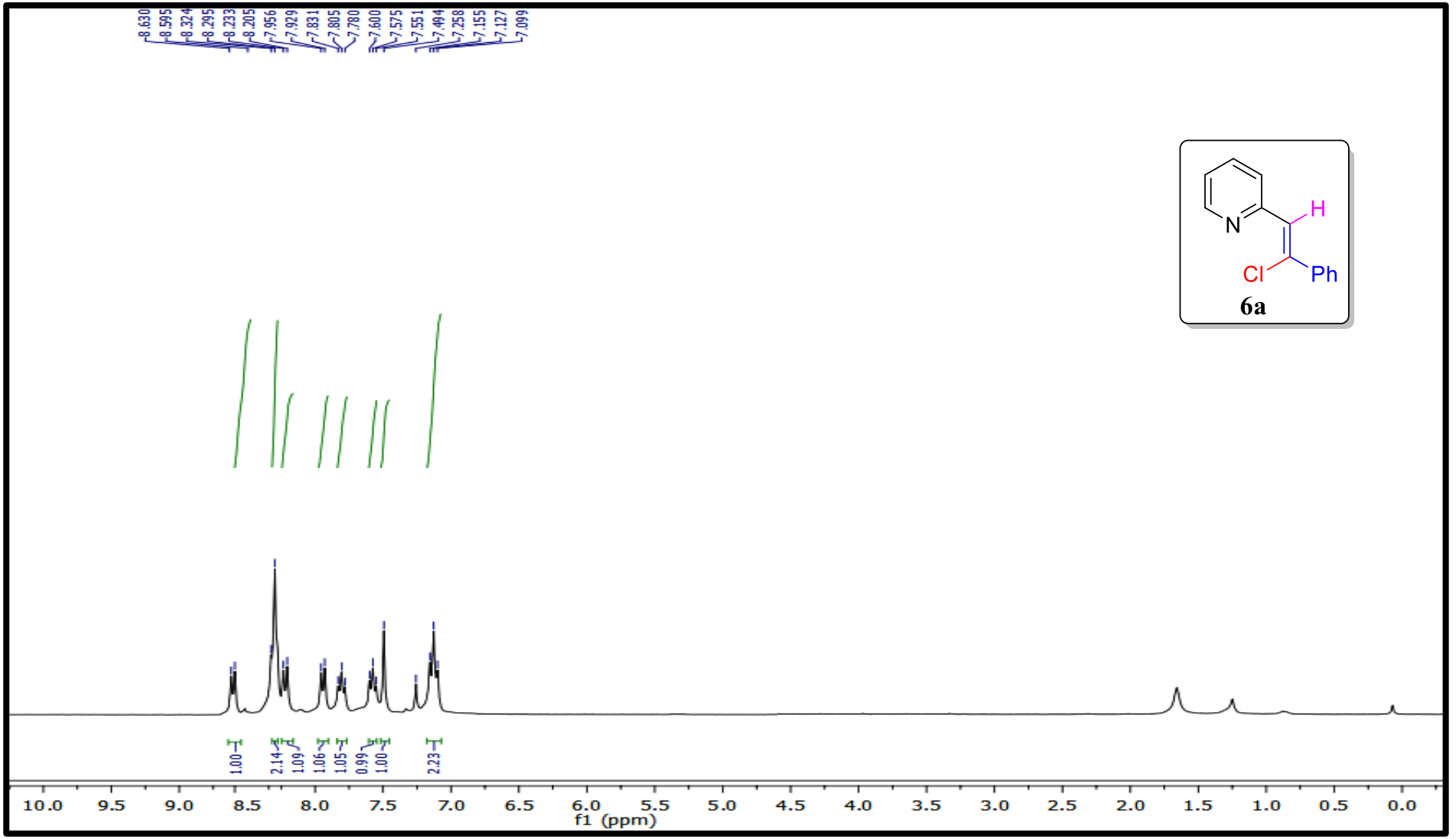
^{1}H NMR spectrum of 7-Chloro-2-(2-chloro-2-phenylvinyl)-quinoline-3-carbaldehyde (4l)



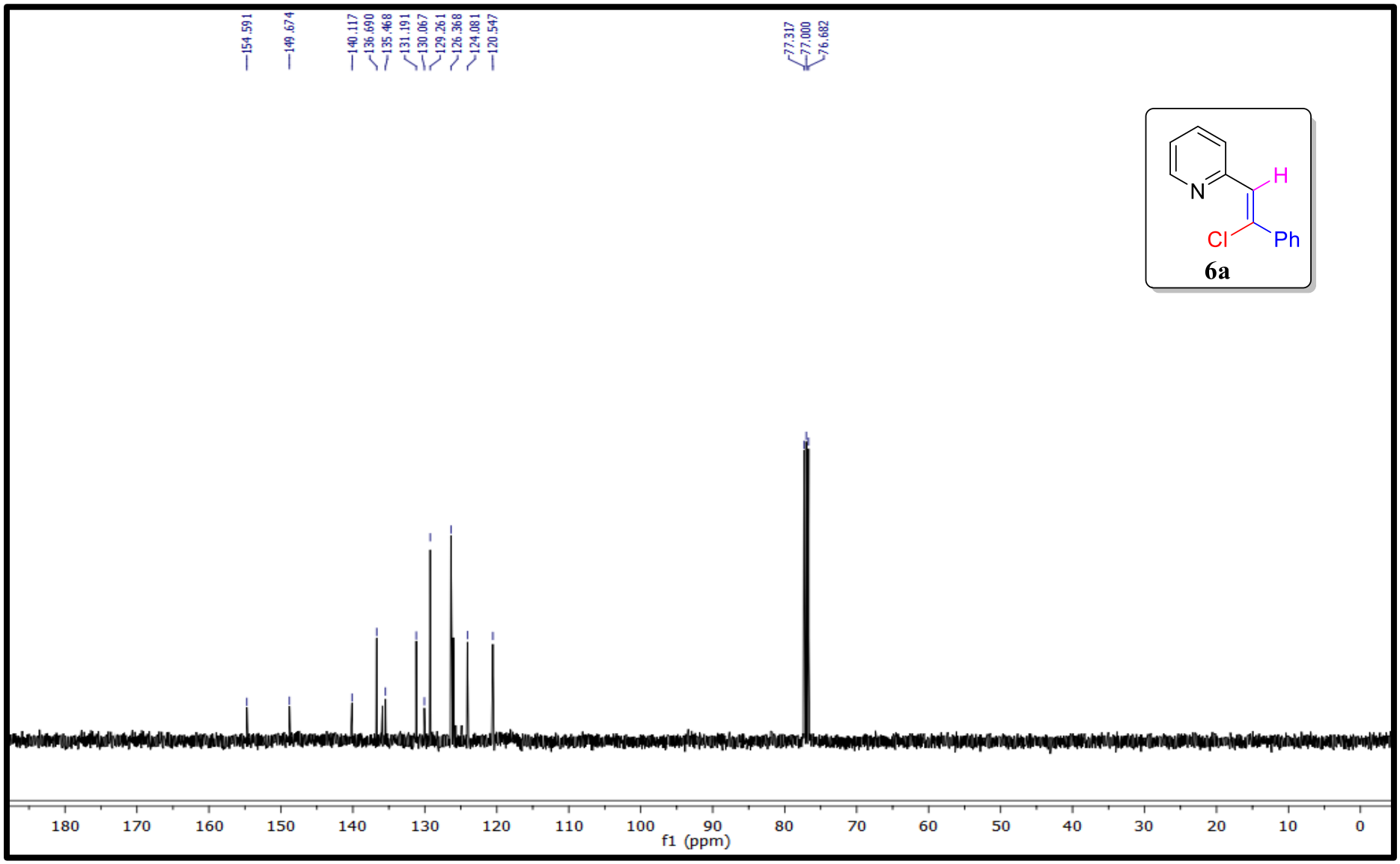
^{13}C NMR spectrum of 7-Chloro-2-(2-chloro-2-phenylvinyl)-quinoline-3-carbaldehyde (4l)



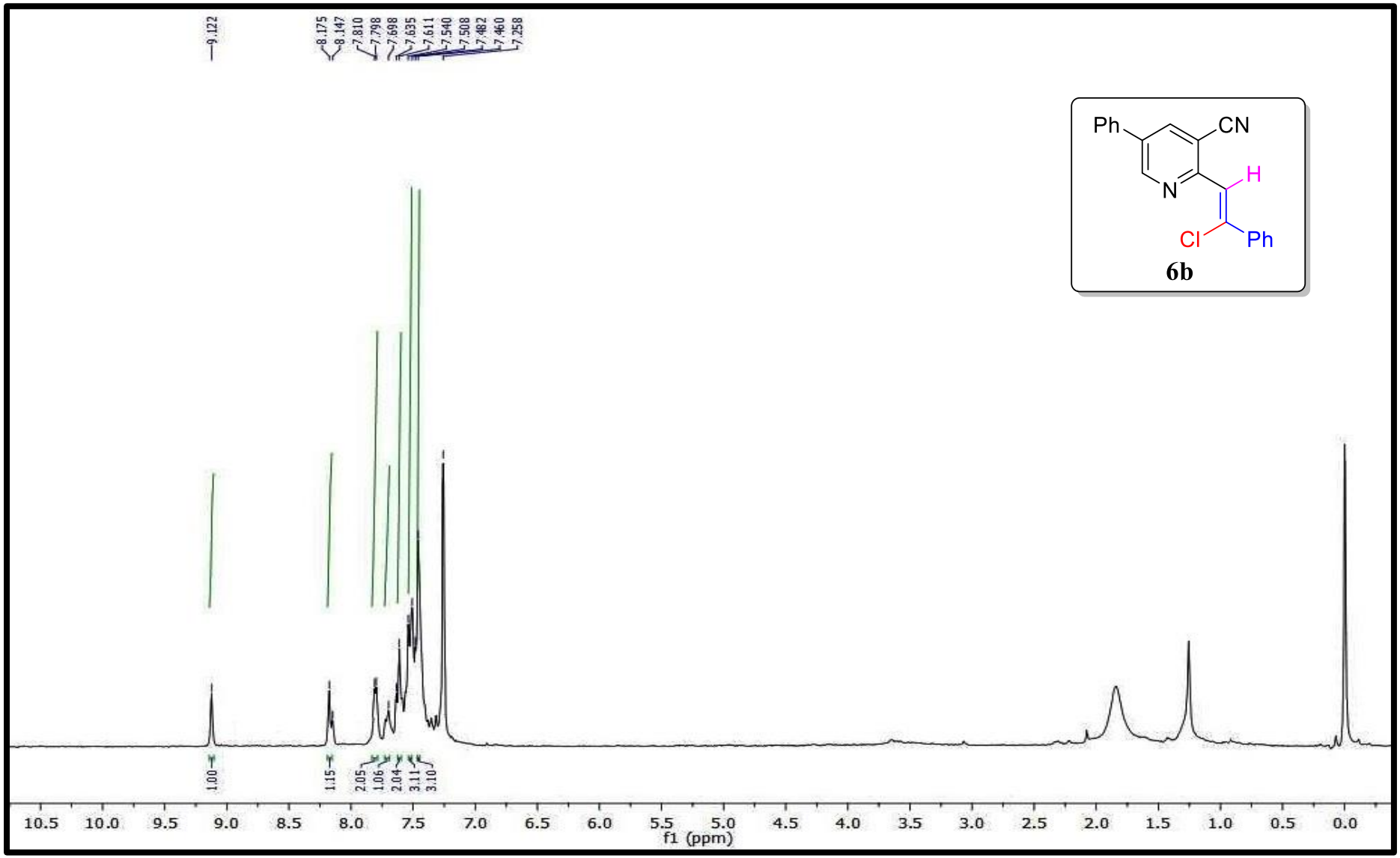
^{1}H and ^{13}C NMR spectrum of 2-(2-chloro-2-phenylvinyl)pyridine (6a)



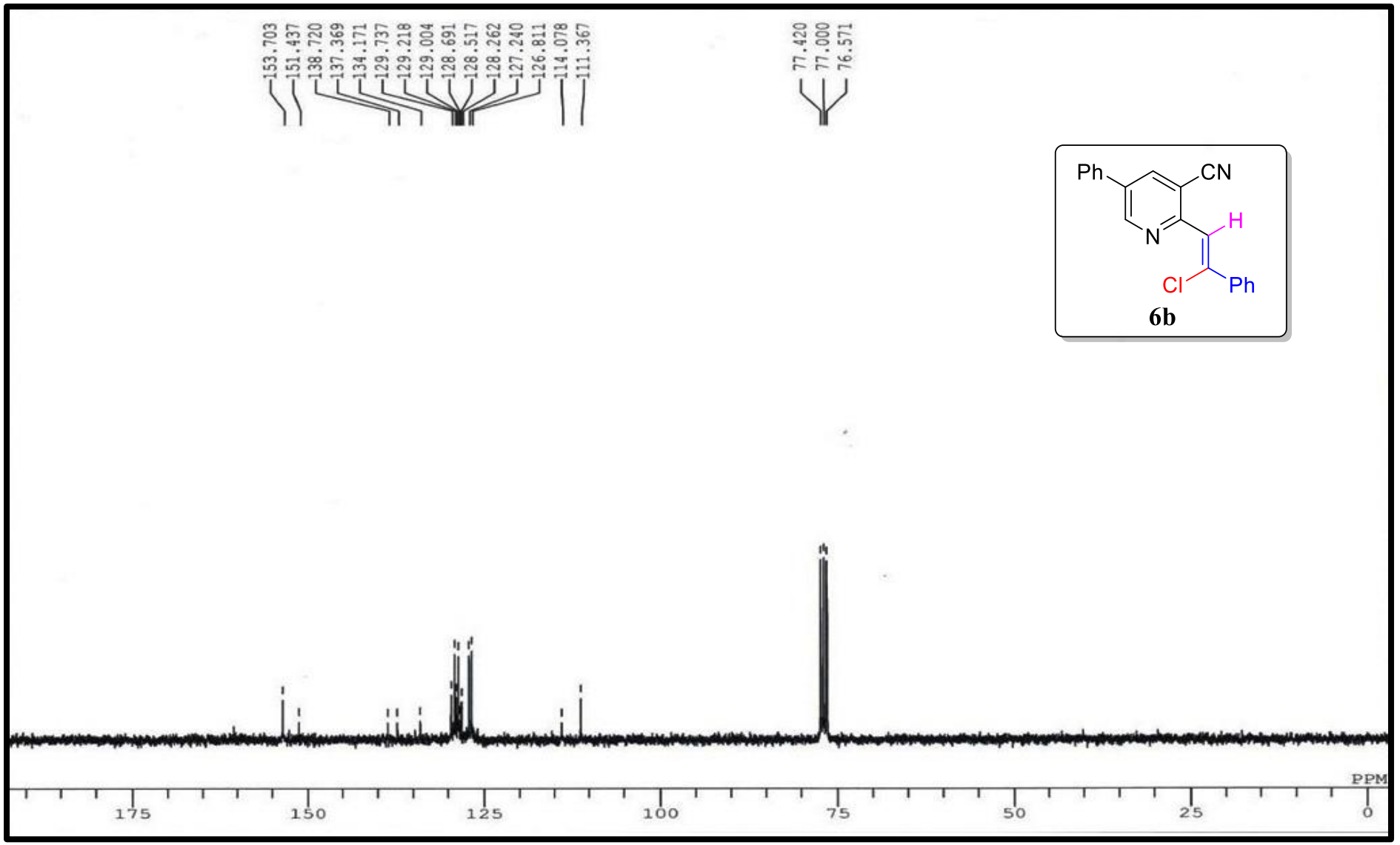
^{13}C NMR spectrum of 2-(2-chloro-2-phenylvinyl)pyridine (6a)



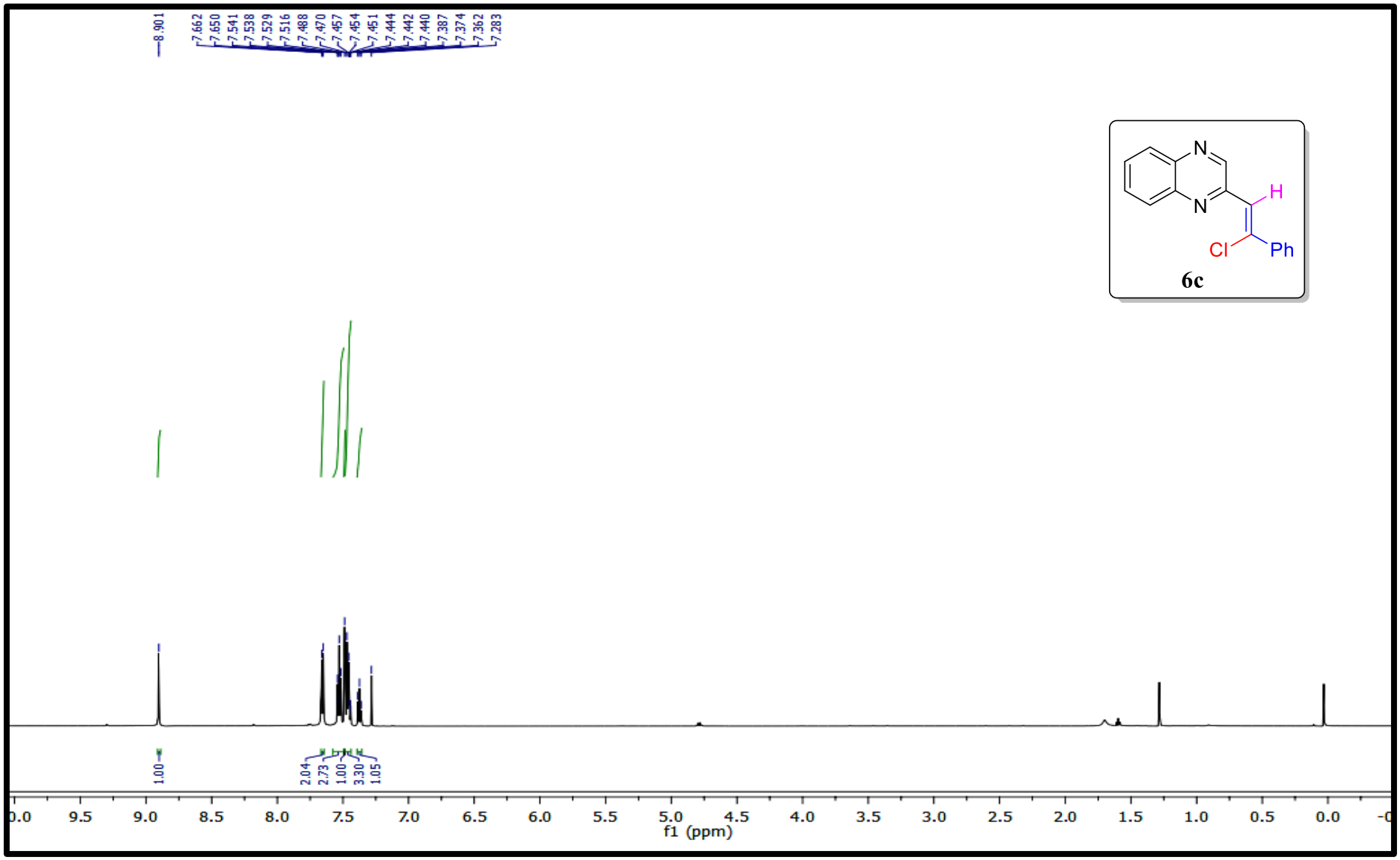
^{1}H NMR spectrum of 2-(2-chloro-2-phenylvinyl)-5-phenylnicotinonitrile (6b)



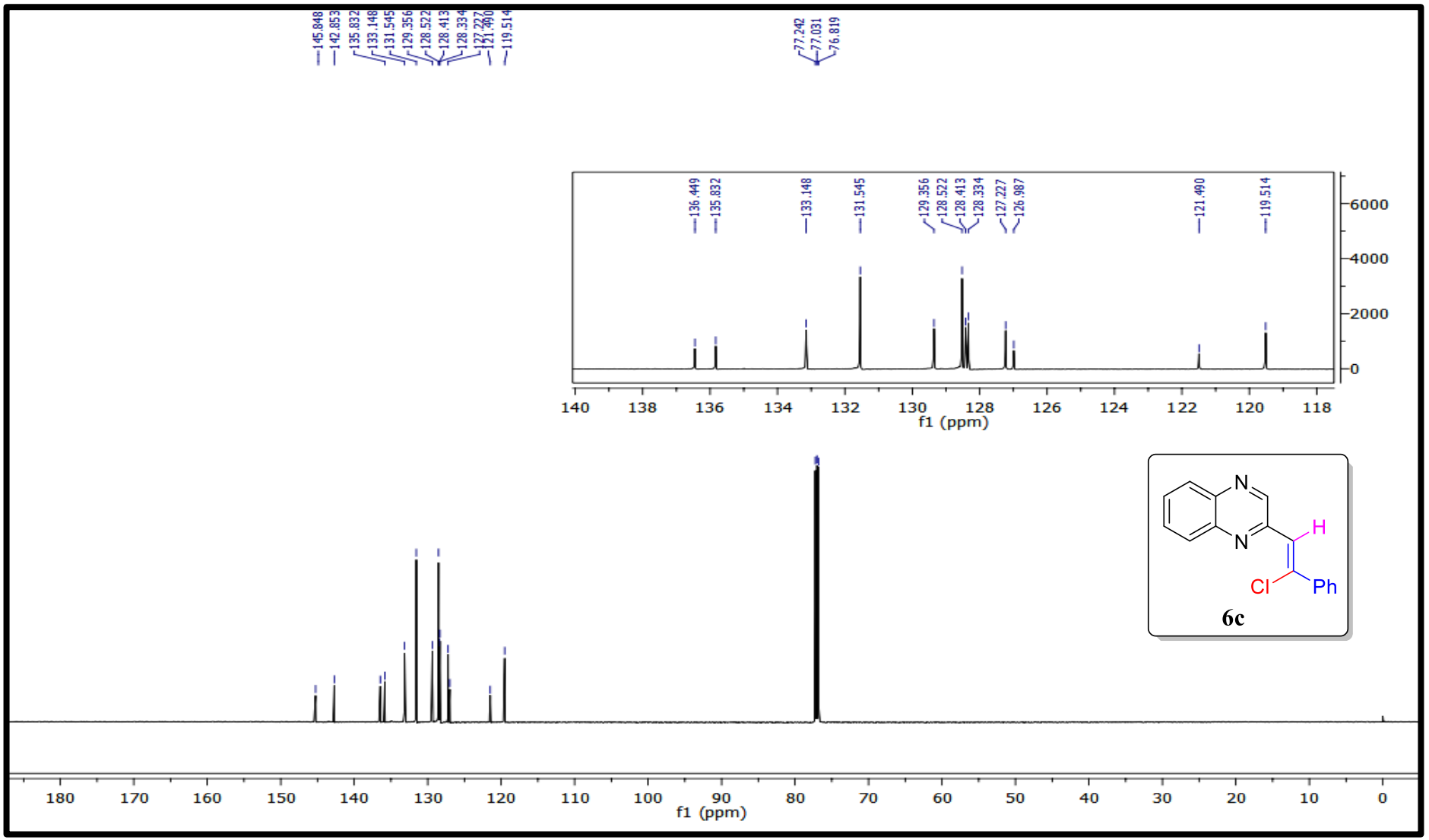
^{13}C NMR spectrum of 2-(2-chloro-2-phenylvinyl)-5-phenylnicotinonitrile (6b)



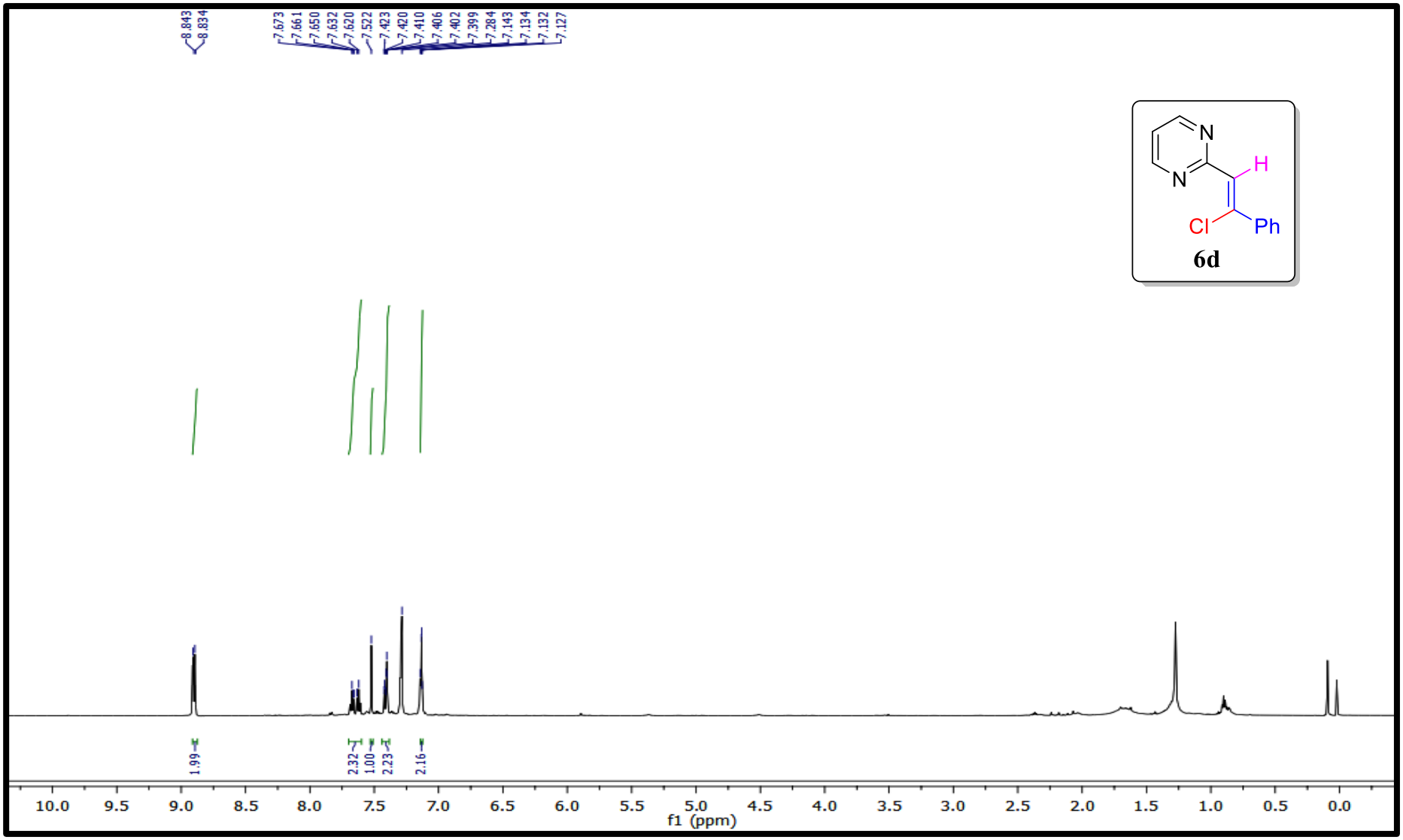
^{1}H spectrum of 2-(2-chloro-2-phenylvinyl)quinoxaline (6c)



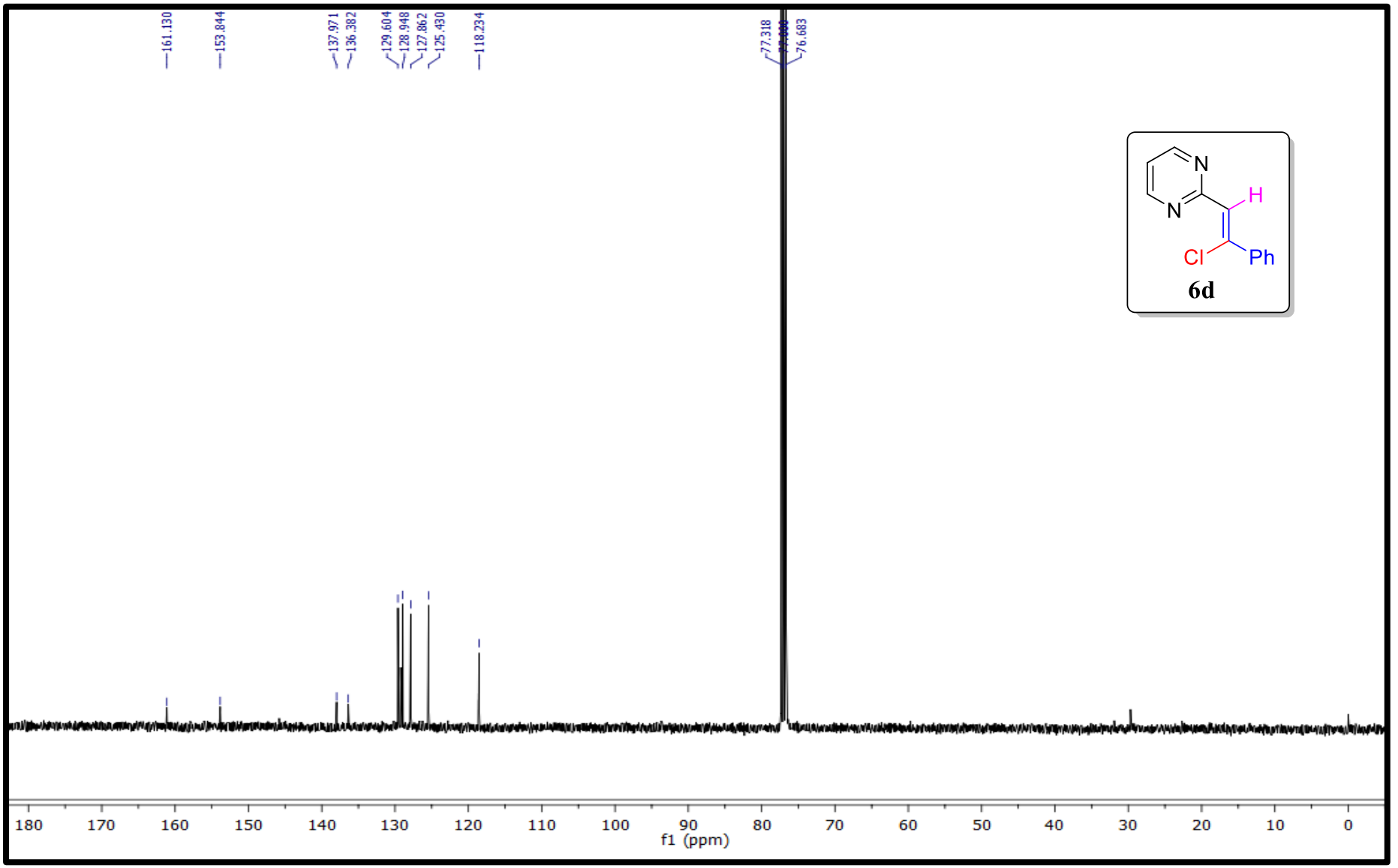
^{13}C NMR spectrum of 2-(2-chloro-2-phenylvinyl)quinoxaline (6c)



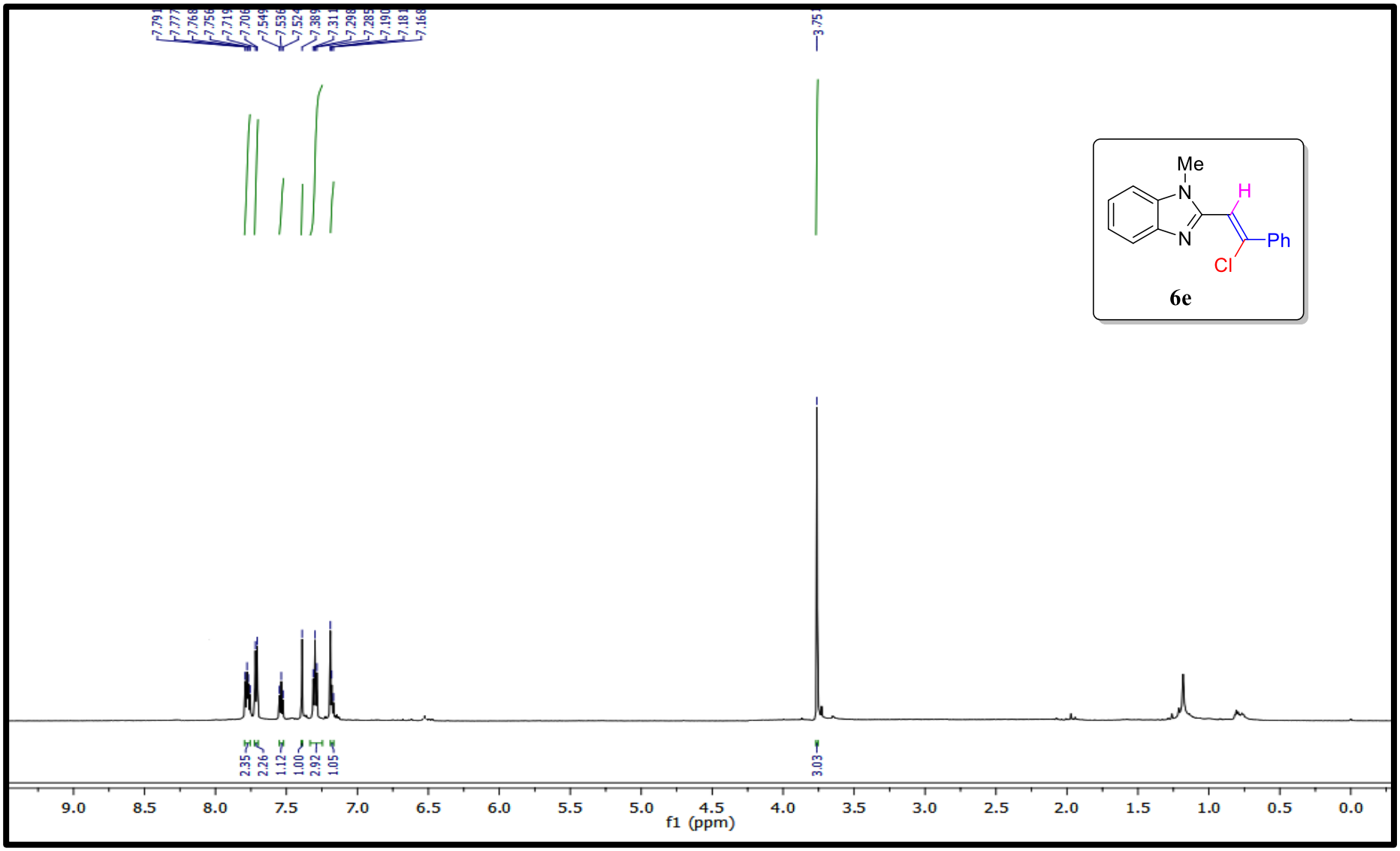
^{1}H NMR spectrum of 2-(2-chloro-2-phenylvinyl)pyrimidine (6d)



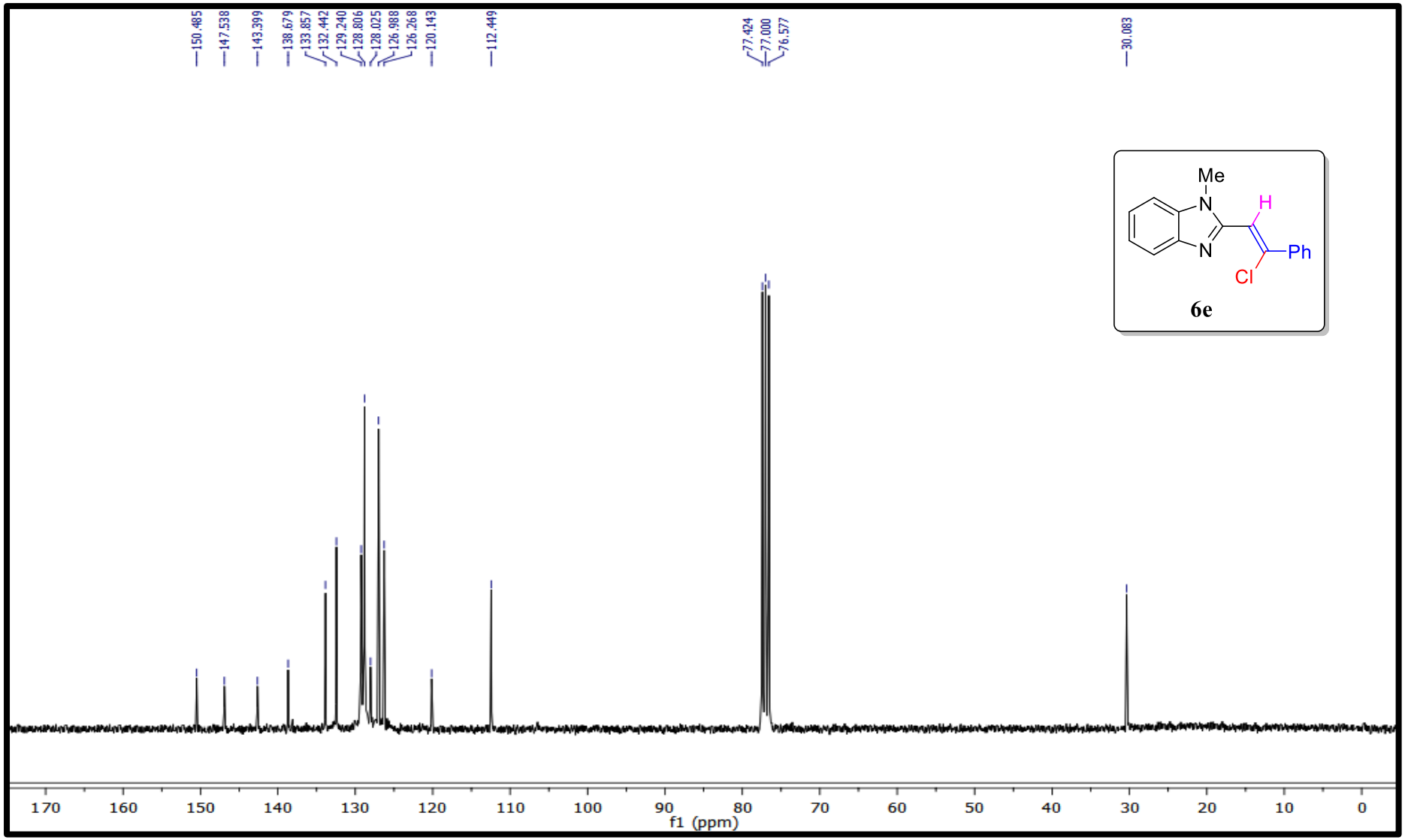
^{13}C NMR spectrum of 2-(2-chloro-2-phenylvinyl)pyrimidine (6d)



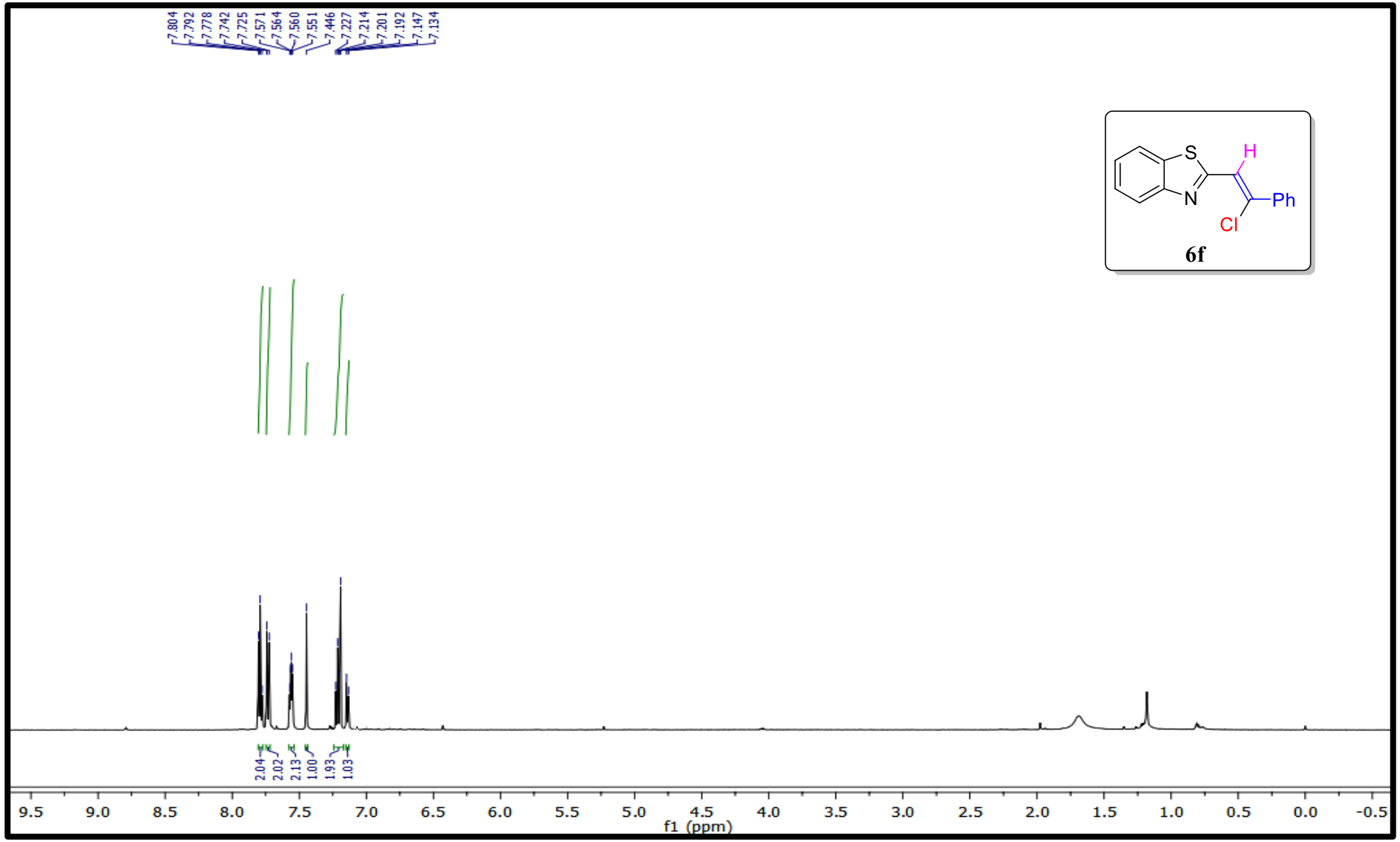
^{1}H NMR spectrum of 2-(2-chloro-2-phenylvinyl)-1-methyl-1H-benzo[d]imidazole (6e)



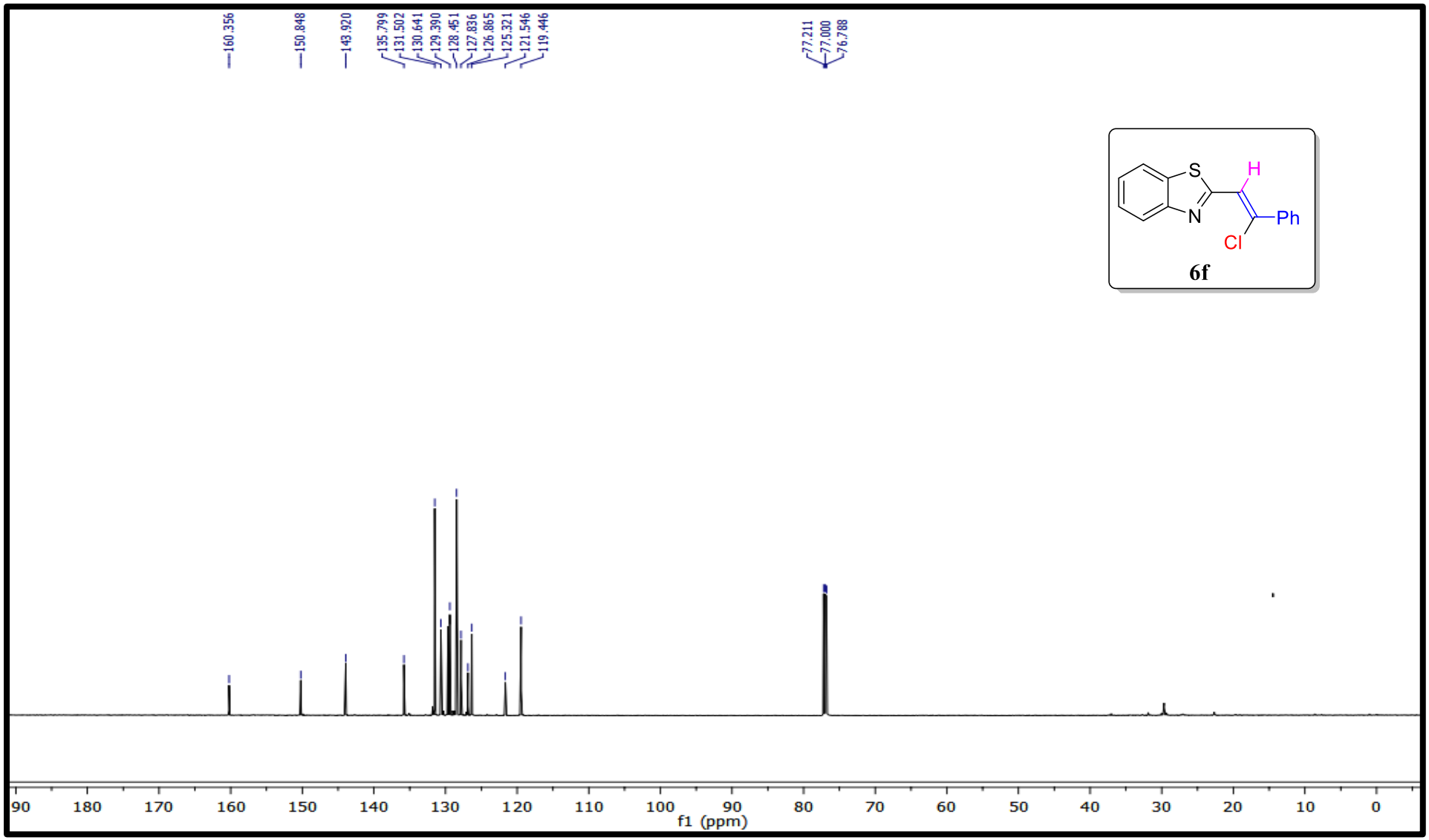
^{13}C NMR spectrum of 2-(2-chloro-2-phenylvinyl)-1-methyl-1H-benzo[d]imidazole (6e)



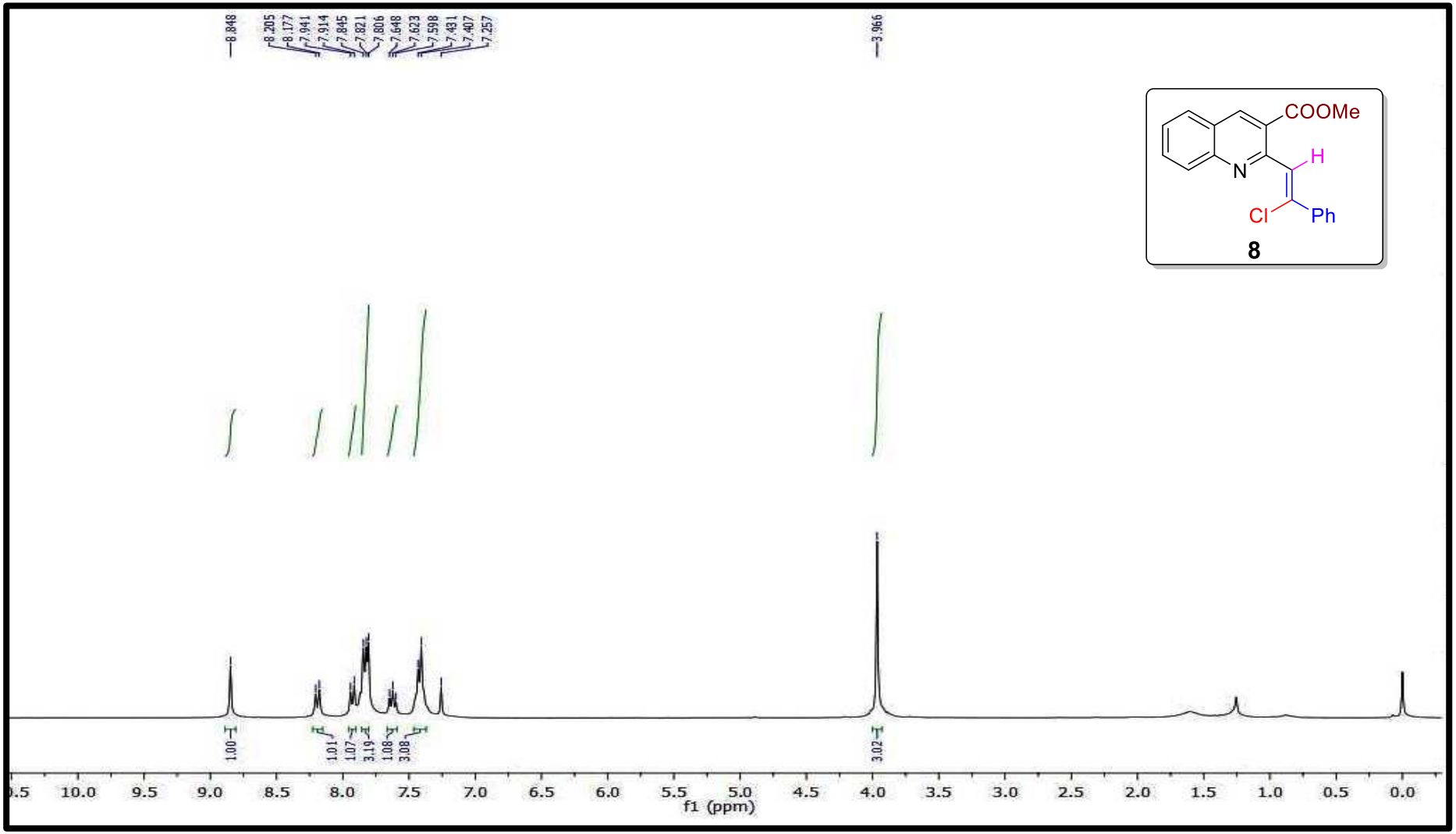
^{1}H NMR spectrum of 2-(2-chloro-2-phenylvinyl)benzo[d]thiazole (6f)



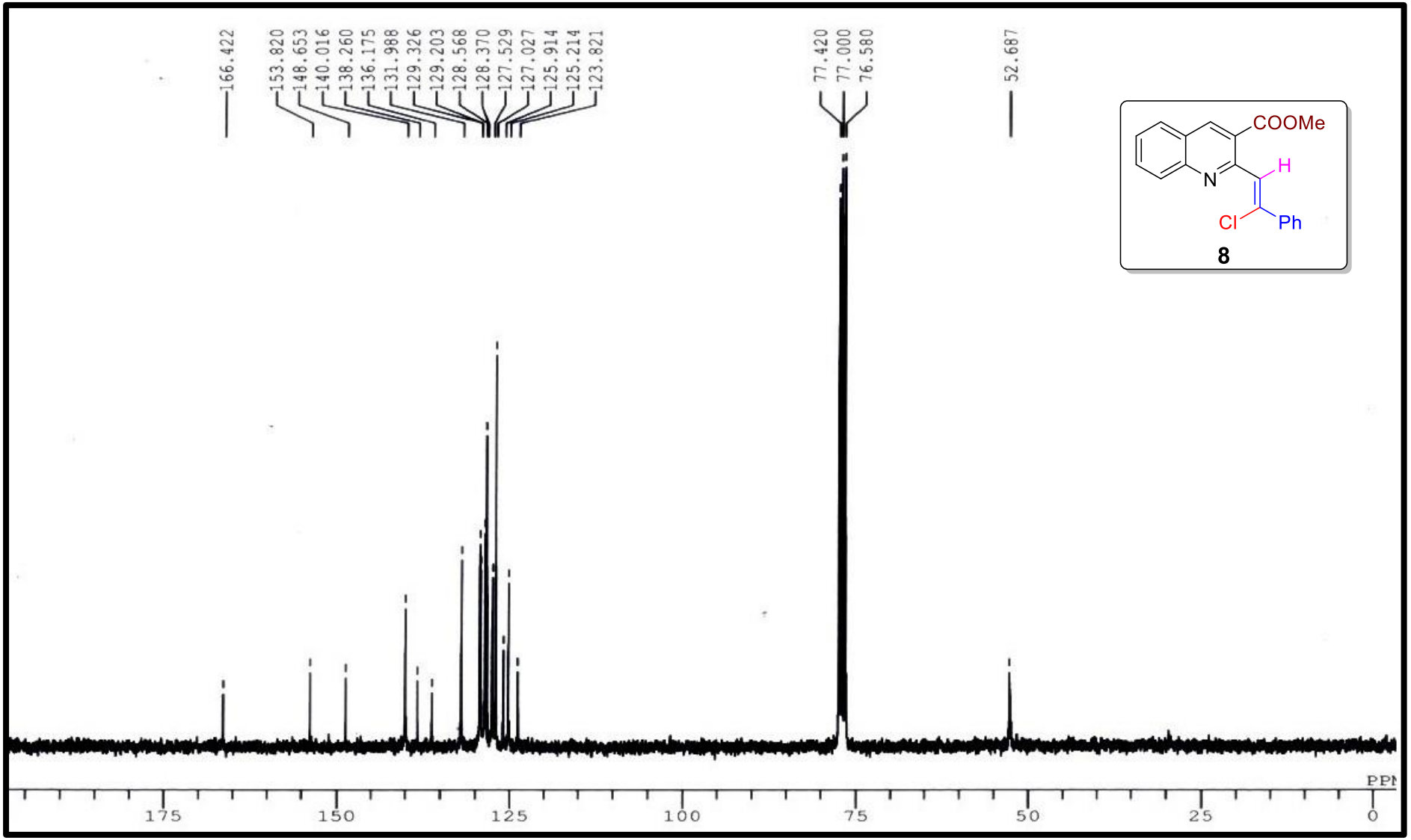
^{1}H NMR spectrum of 2-(2-chloro-2-phenylvinyl)benzo[d]thiazole (6f)



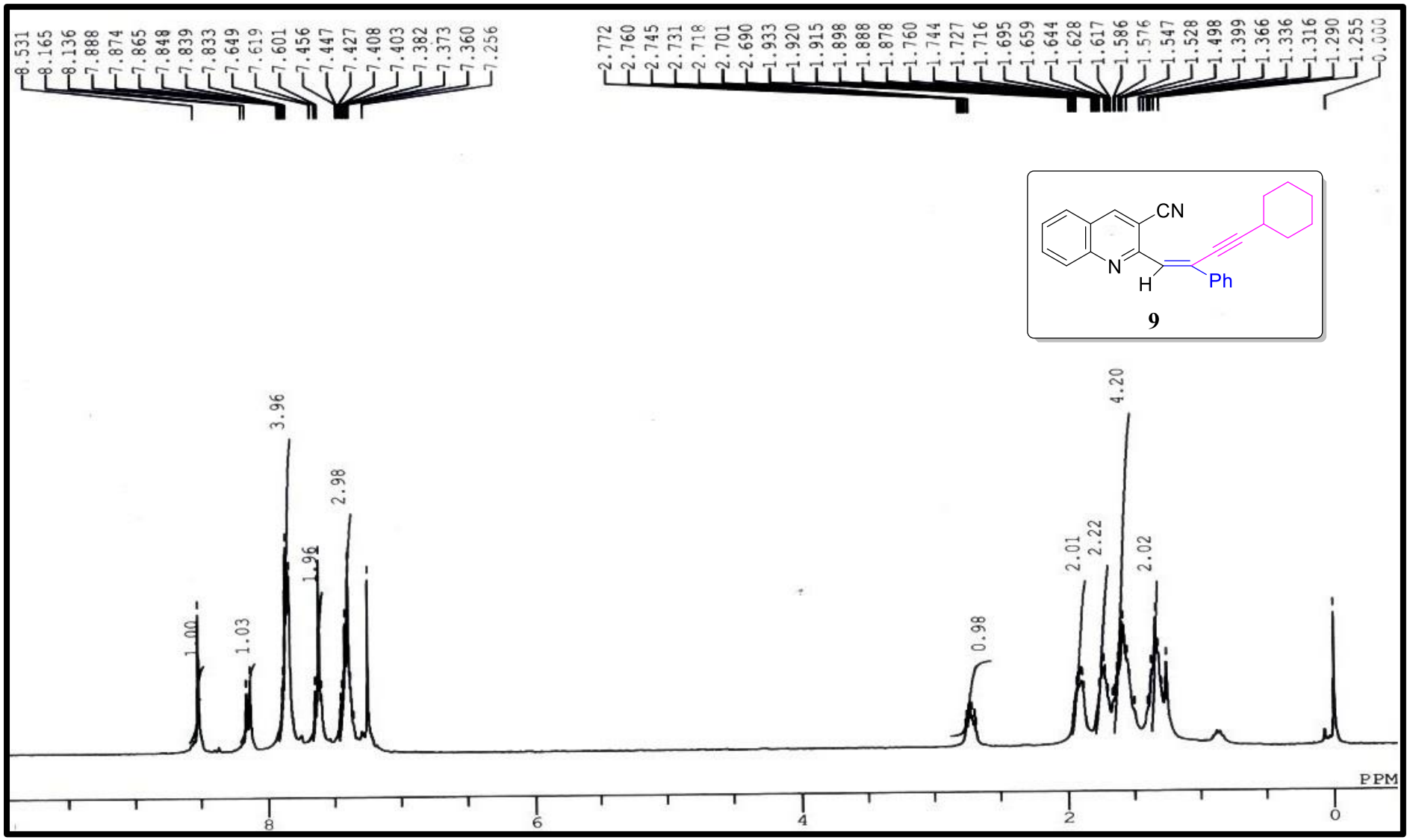
^{1}H NMR spectrum of 2-(2-Chloro-2-phenylvinyl)-quinoline-3-carboxylic acid methyl ester (8)



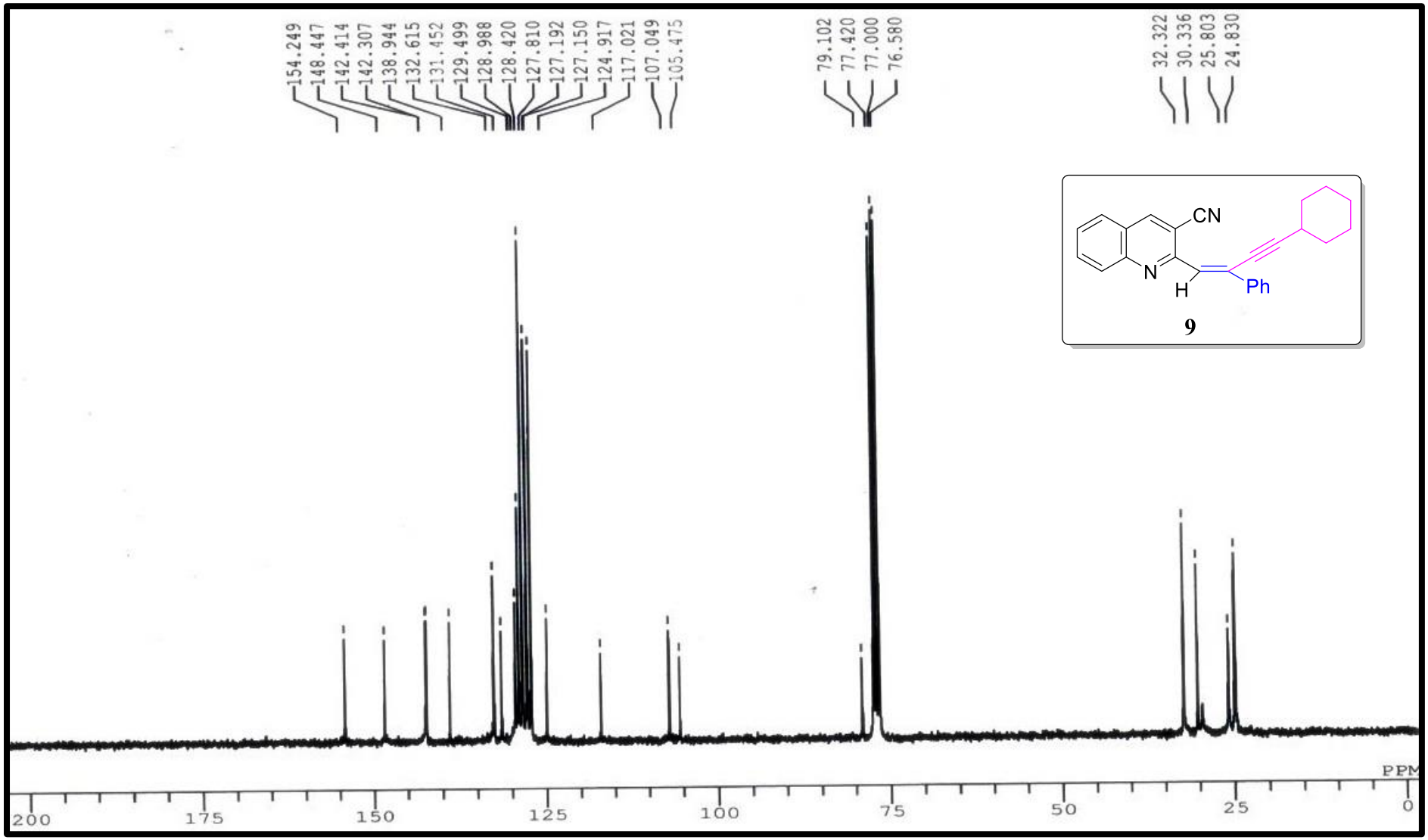
^{13}C NMR spectrum of 2-(2-Chloro-2-phenylvinyl)-quinoline-3-carboxylic acid methyl ester (8)



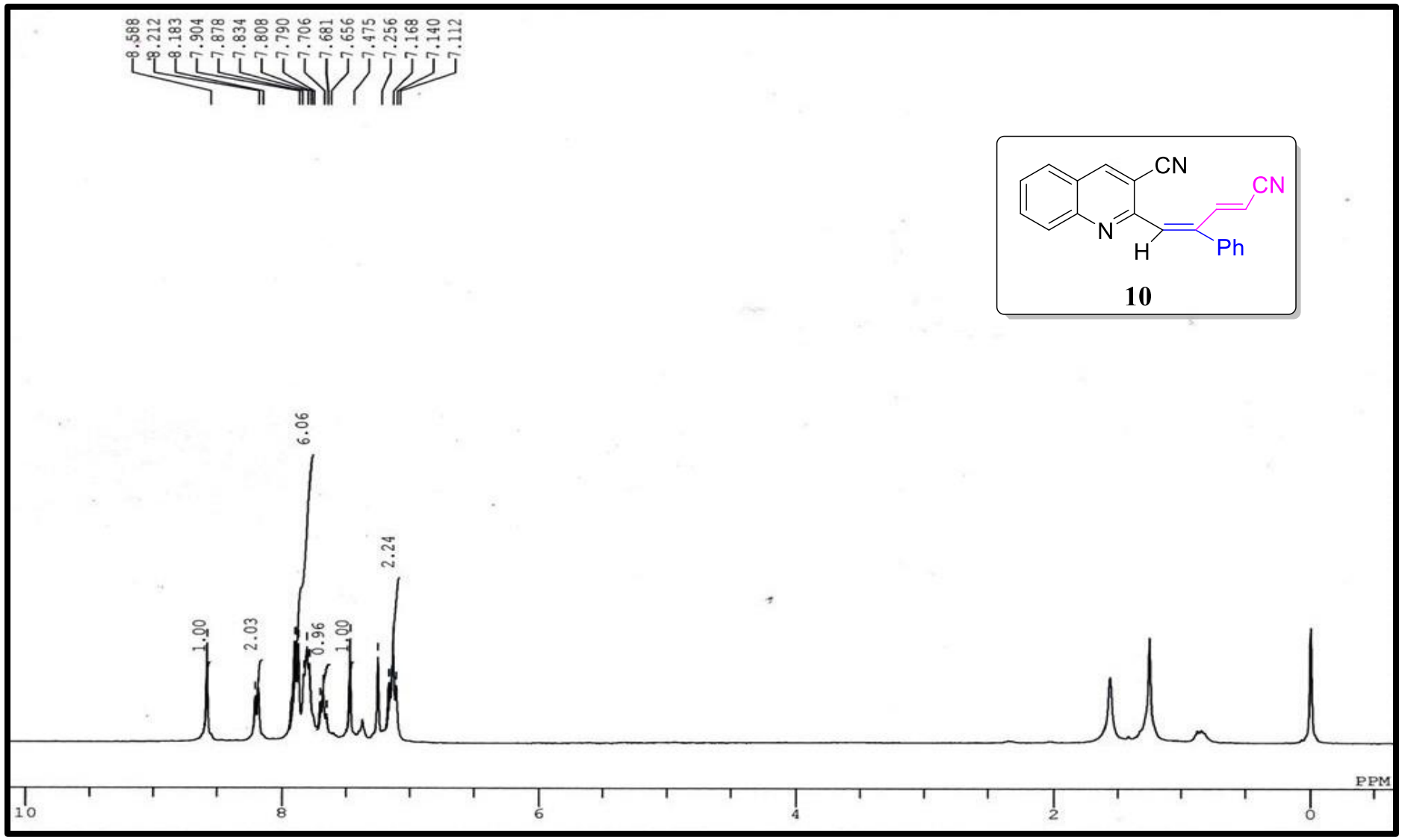
^{1}H NMR spectrum of 2-(4-cyclohexyl-2-phenyl-but-1-en-3-ynyl)-quinoline-3-carbonitrile (9)



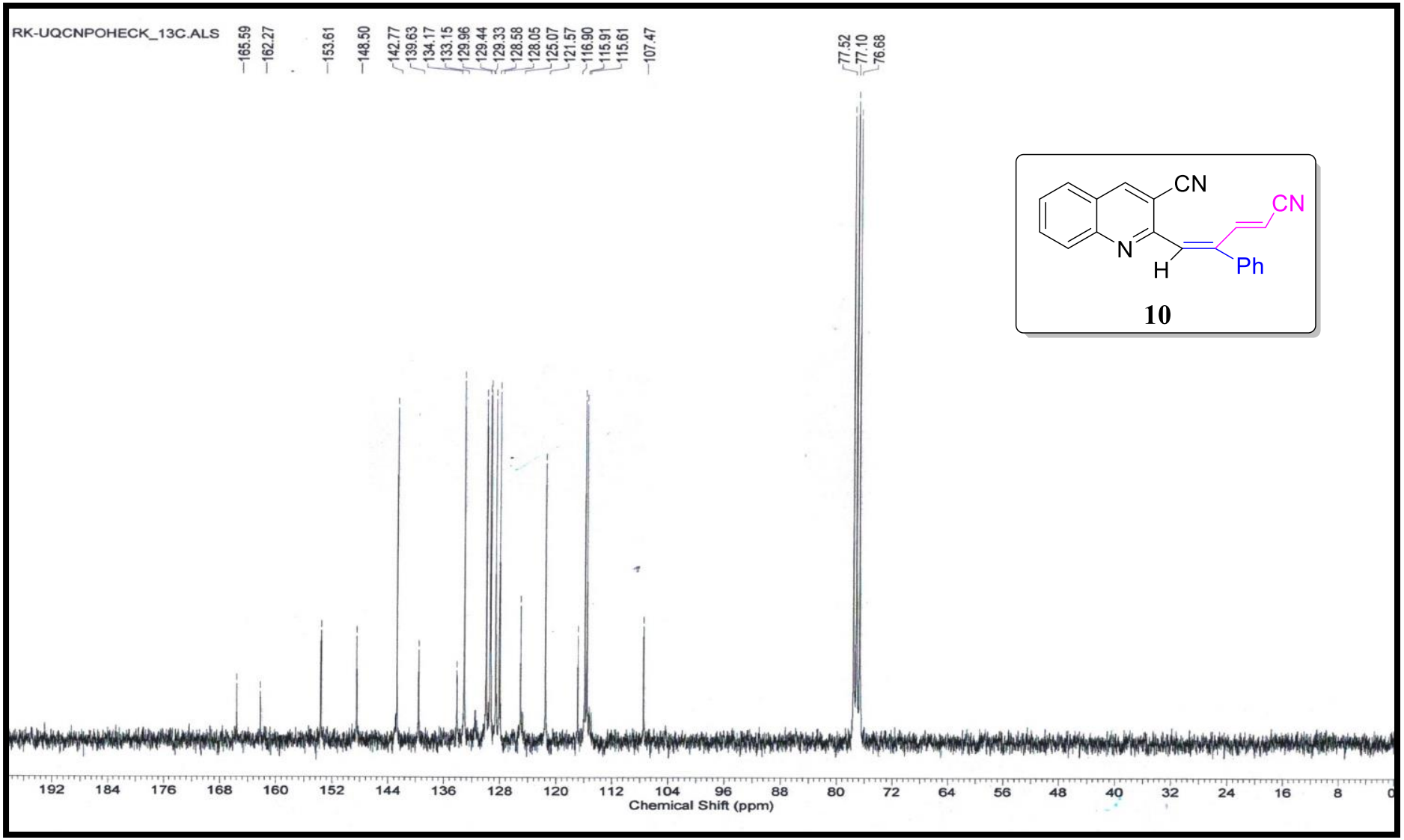
^{13}C NMR spectrum of 2-(4-cyclohexyl-2-phenyl-but-1-en-3-ynyl)-quinoline-3-carbonitrile (9)



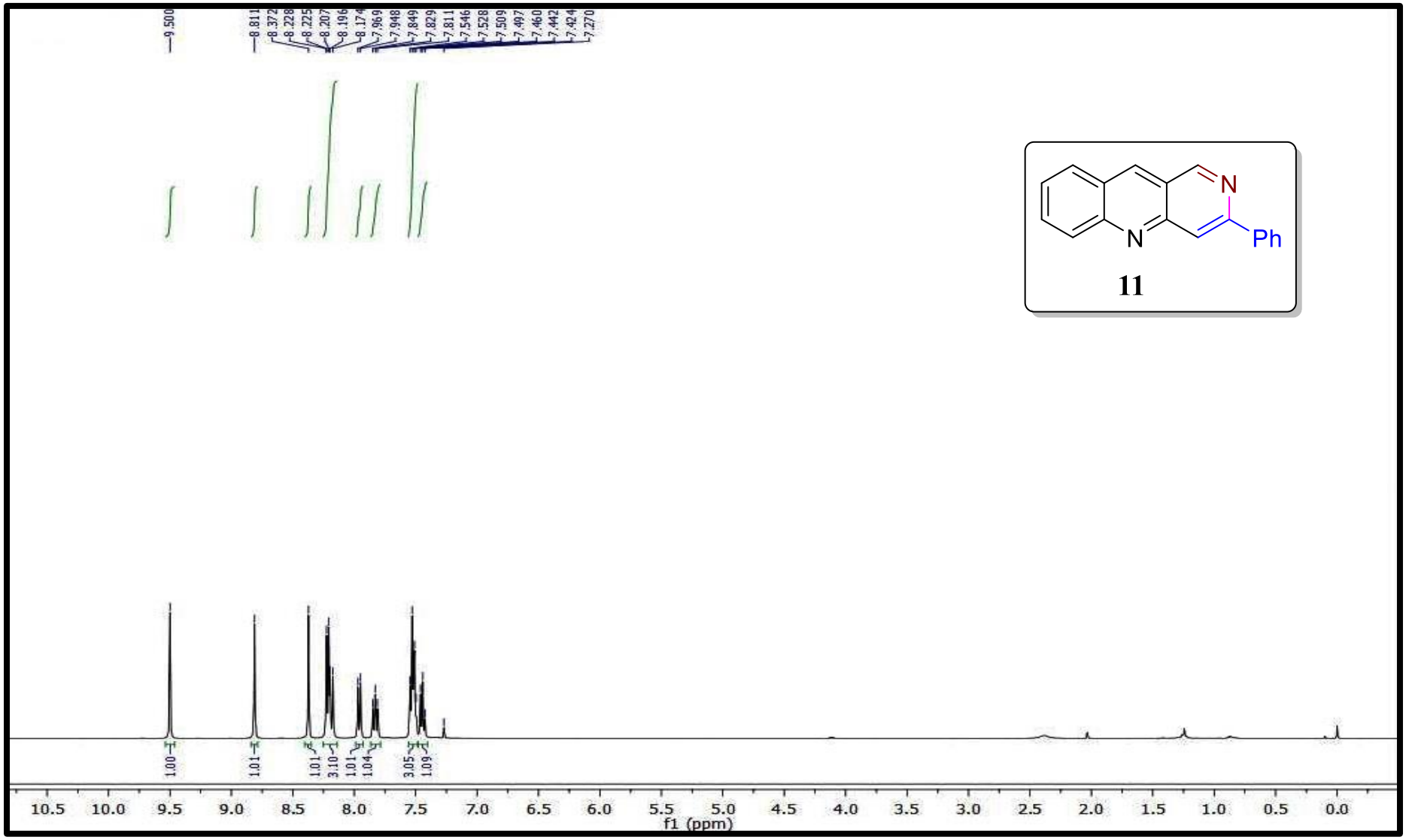
^{1}H NMR spectrum of 2-(4-cyano-2-phenyl-buta-1,3-dienyl)-quinoline-3-carbonitrile (10)



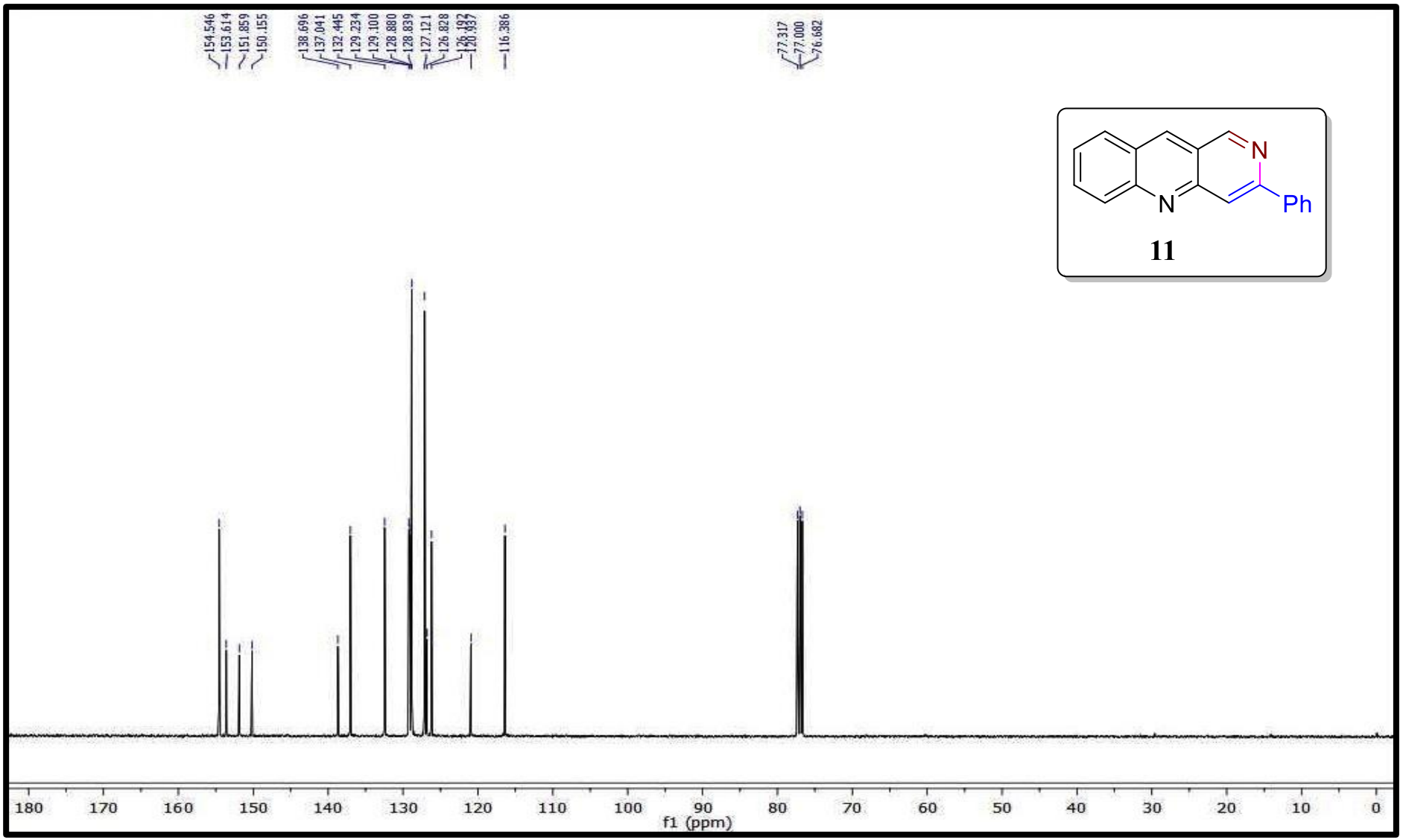
^{13}C NMR spectrum of 2-(4-cyano-2-phenyl-buta-1,3-dienyl)-quinoline-3-carbonitrile (10)



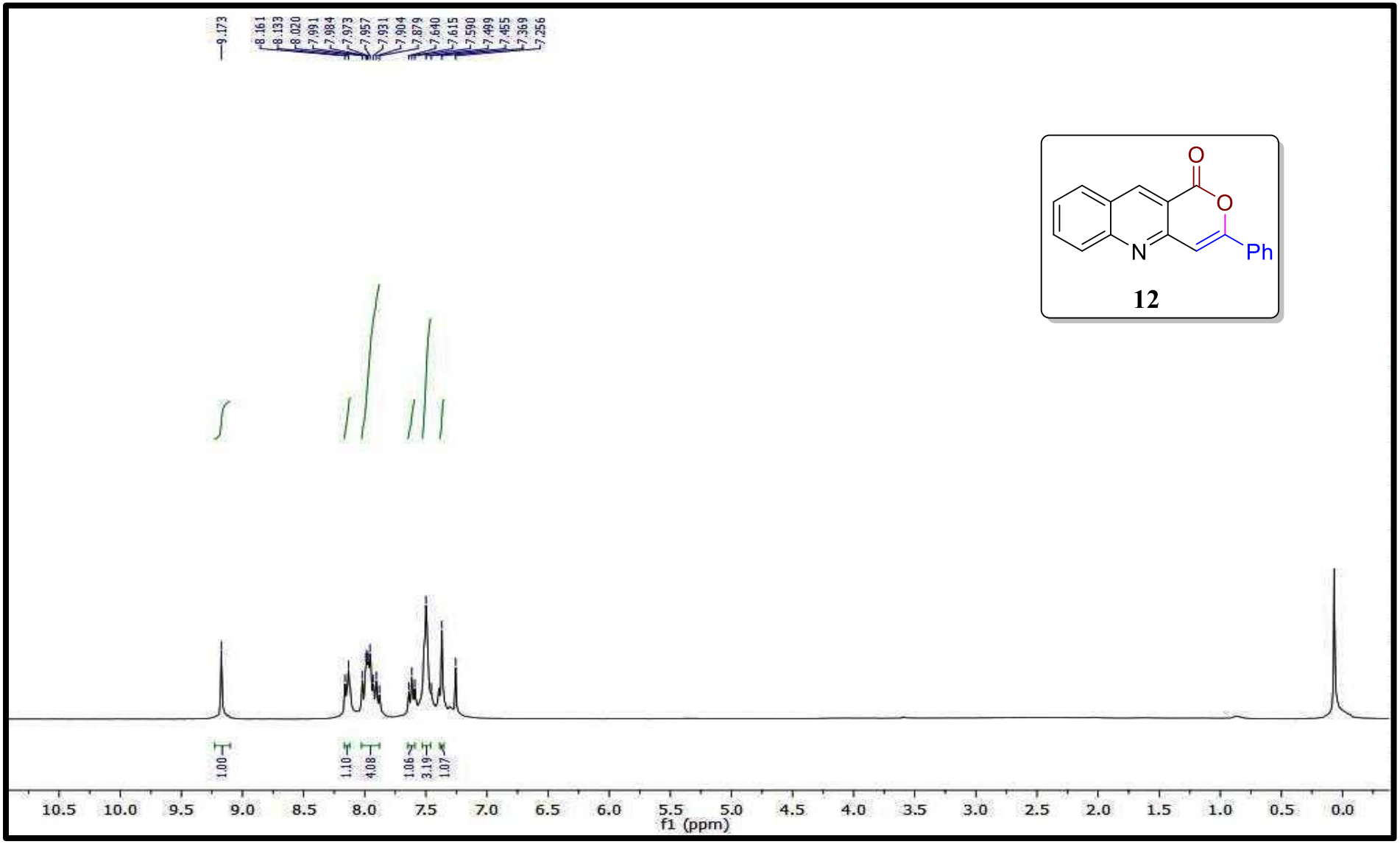
^{1}H NMR spectrum of 3-phenylbenzo[b][1,6]naphthyridine (11)



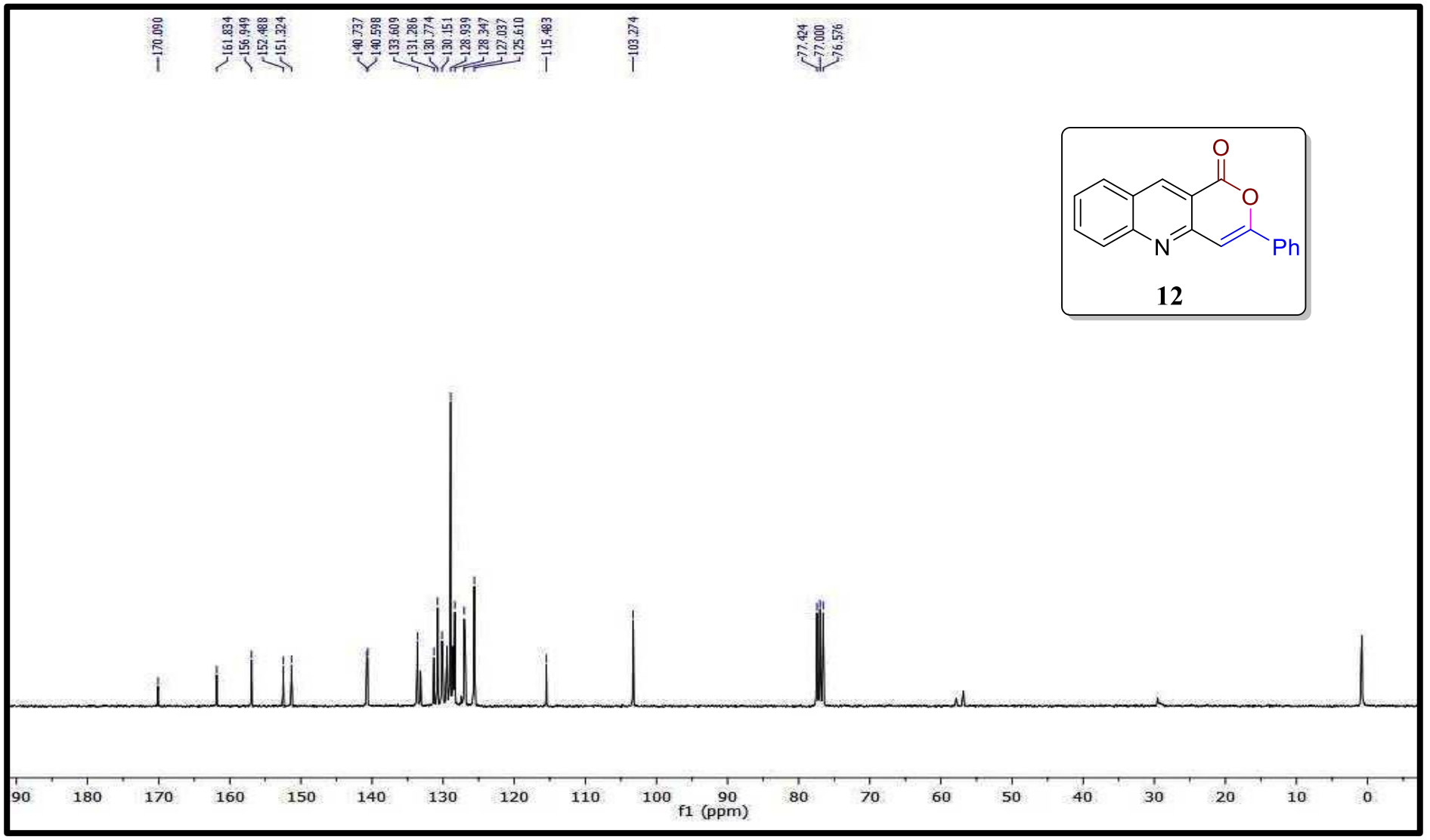
^{13}C NMR spectrum of 3-phenylbenzo[b][1,6]naphthyridine (11)



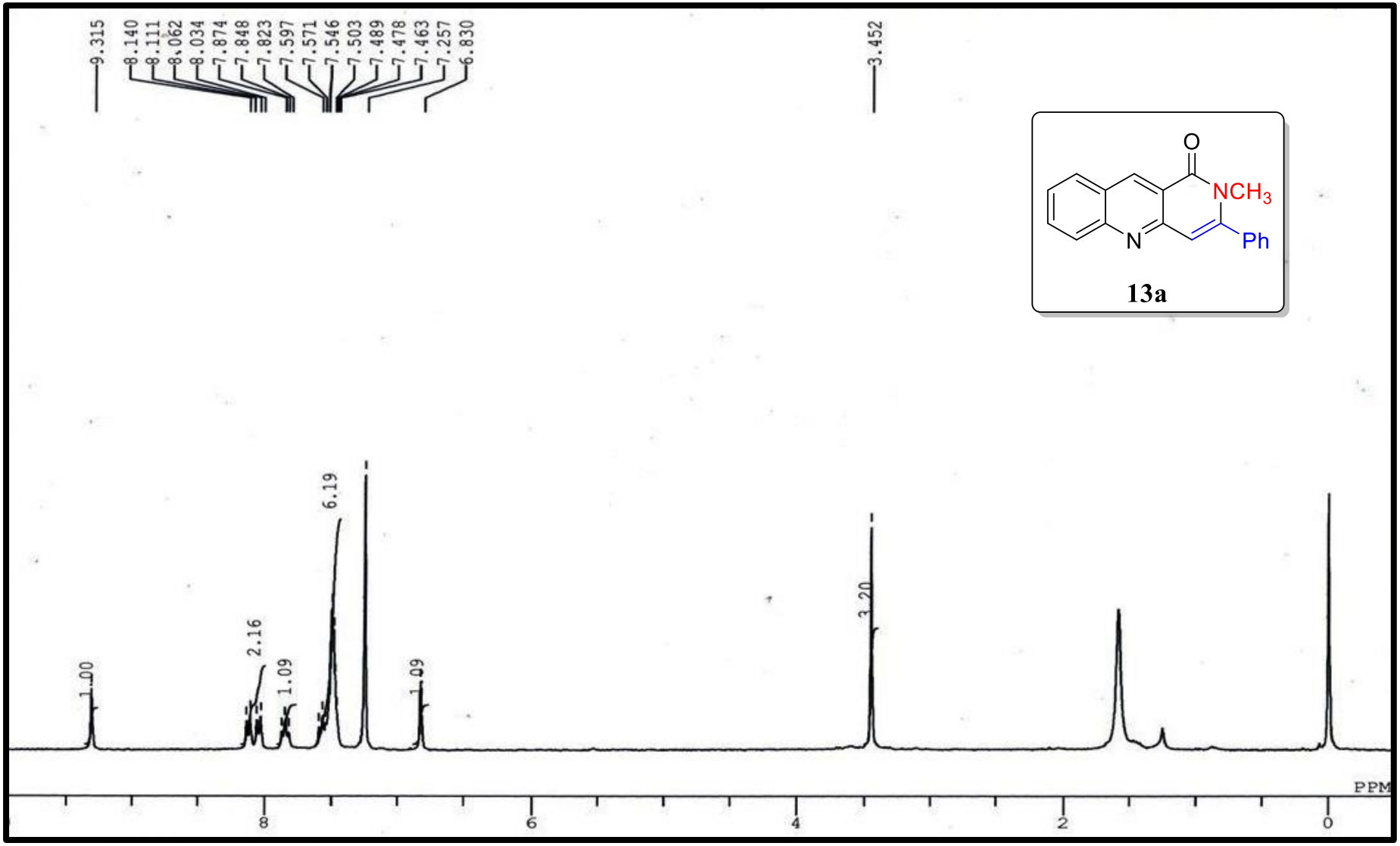
^{1}H NMR spectrum of 3-phenyl-1H-pyrano[4,3-b]quinolin-1-one (12)



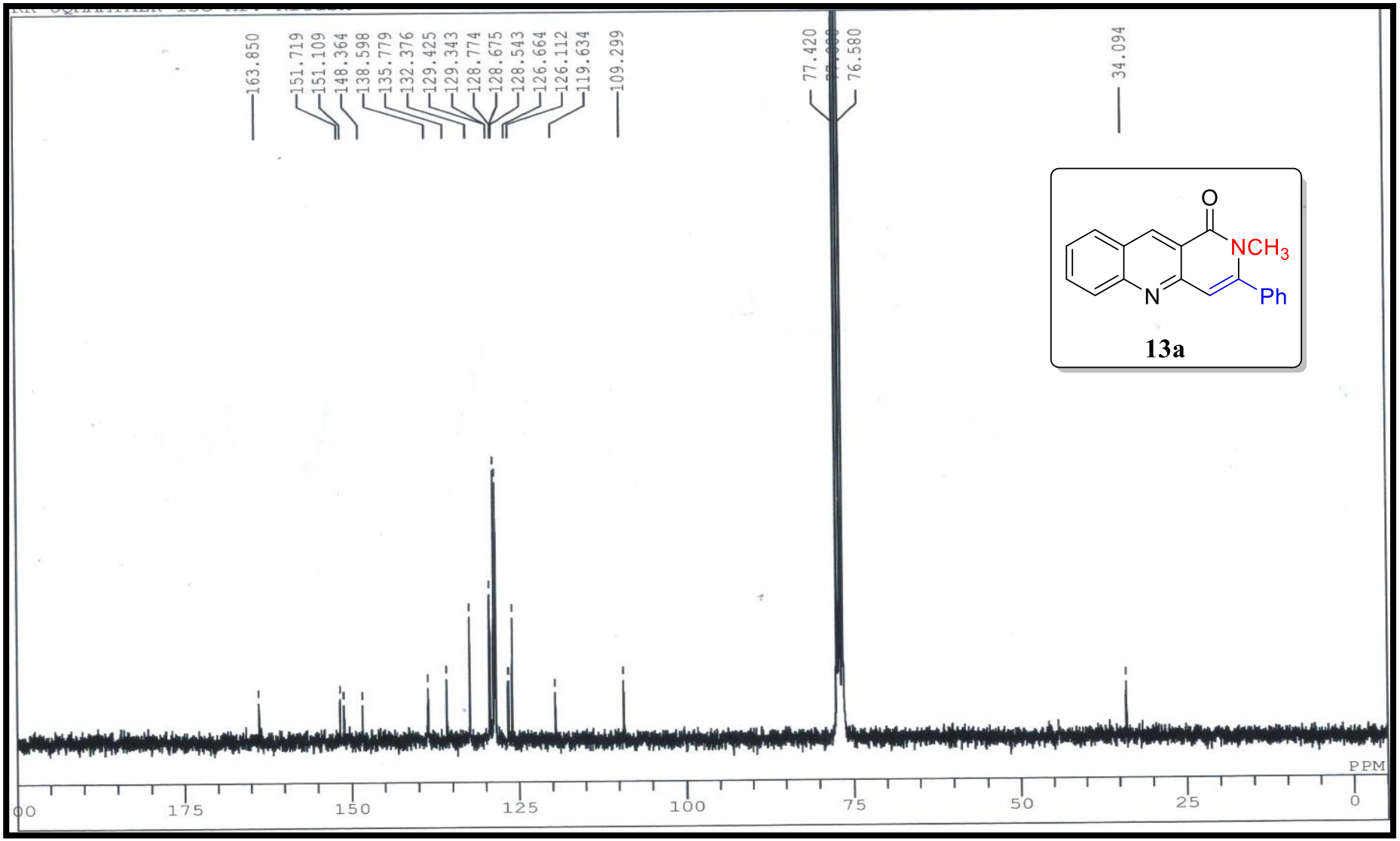
^{13}C NMR spectrum of 3-phenyl-1H-pyrano[4,3-b]quinolin-1-one (12)



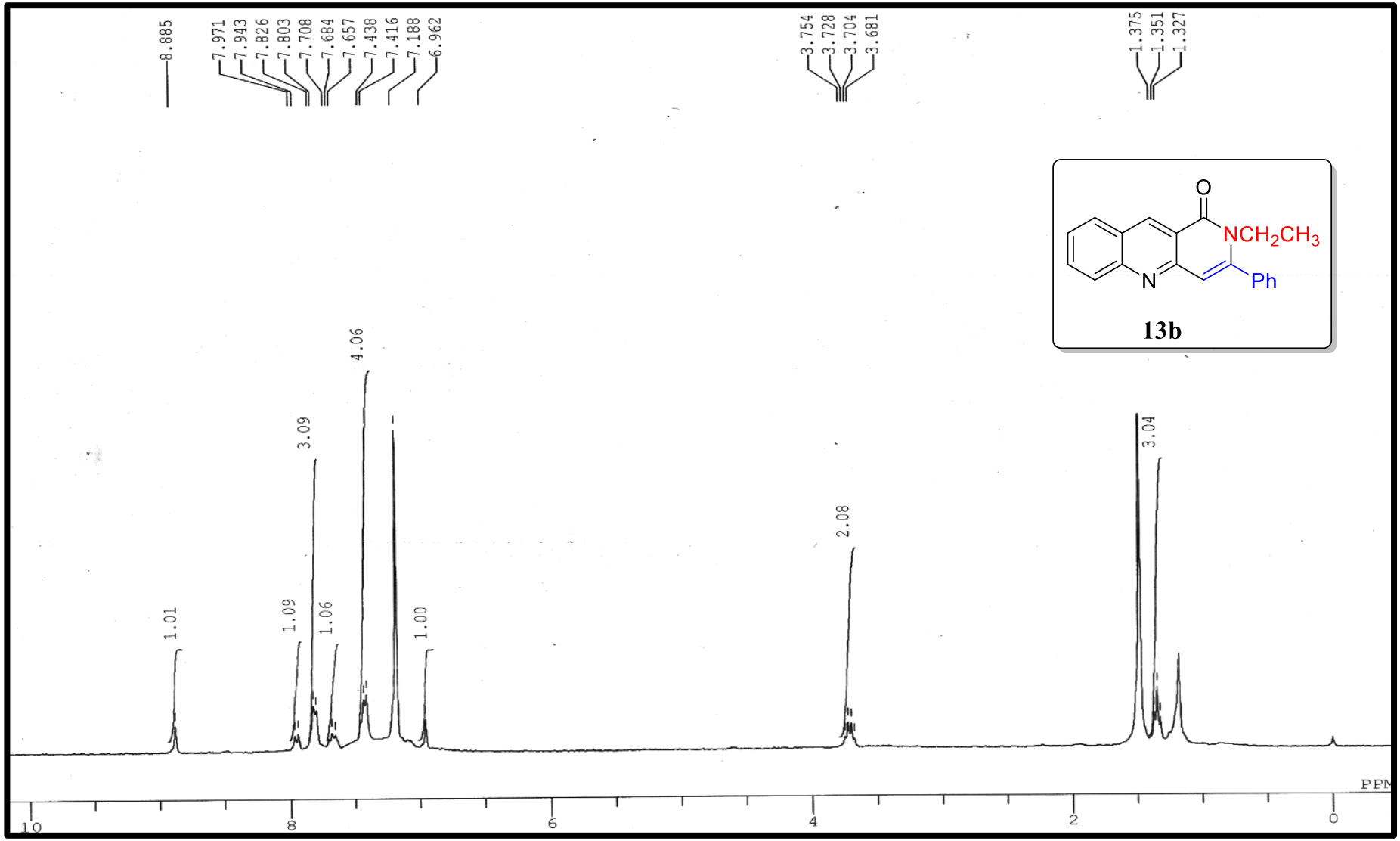
^{1}H NMR spectrum of N-methyl-3-phenyl-2H-benzo[b][1,6]naphthyridin-1-one (13a)



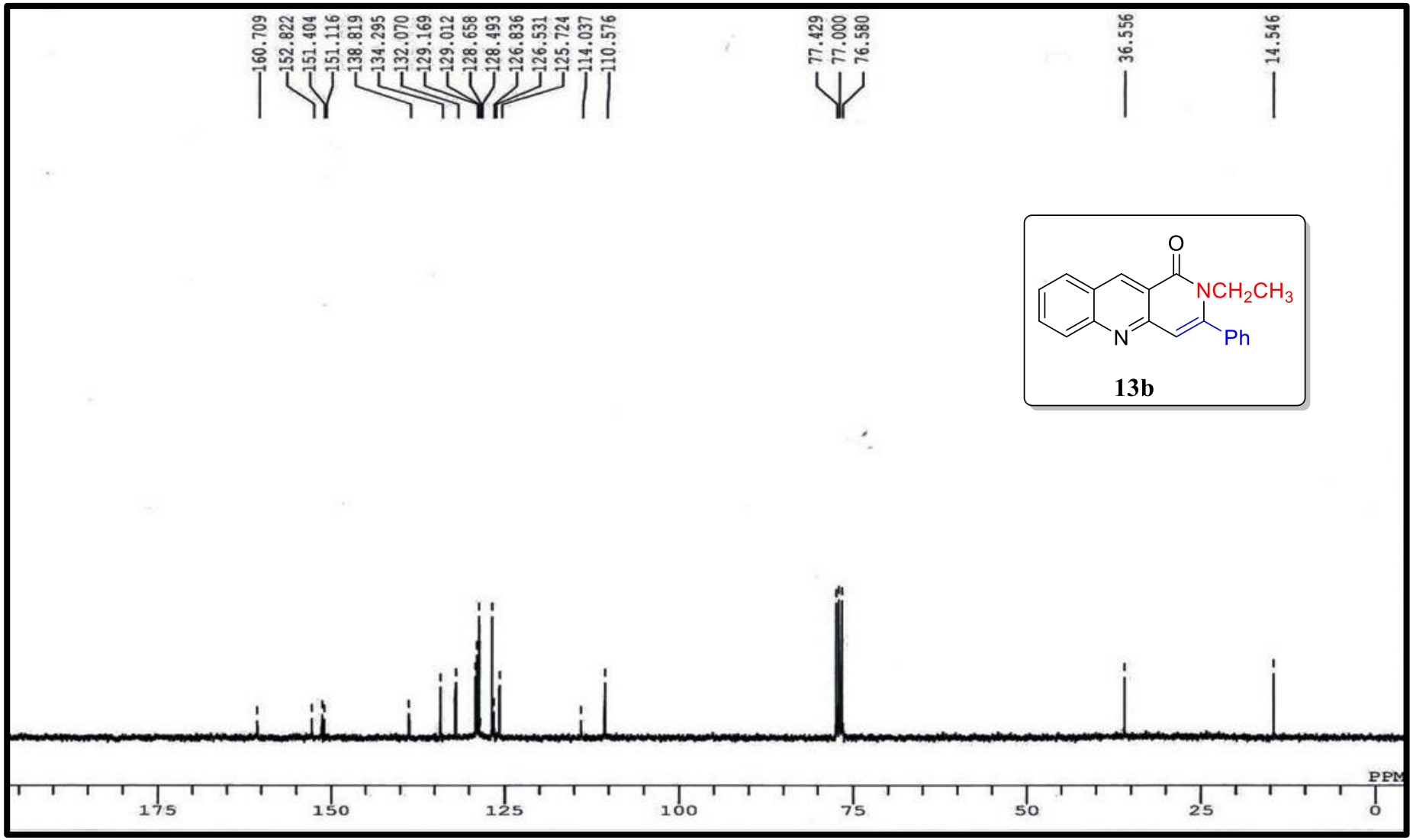
^{13}C NMR spectrum of N-methyl-3-phenyl-2H-benzo[b][1,6]naphthyridin-1-one (13a)



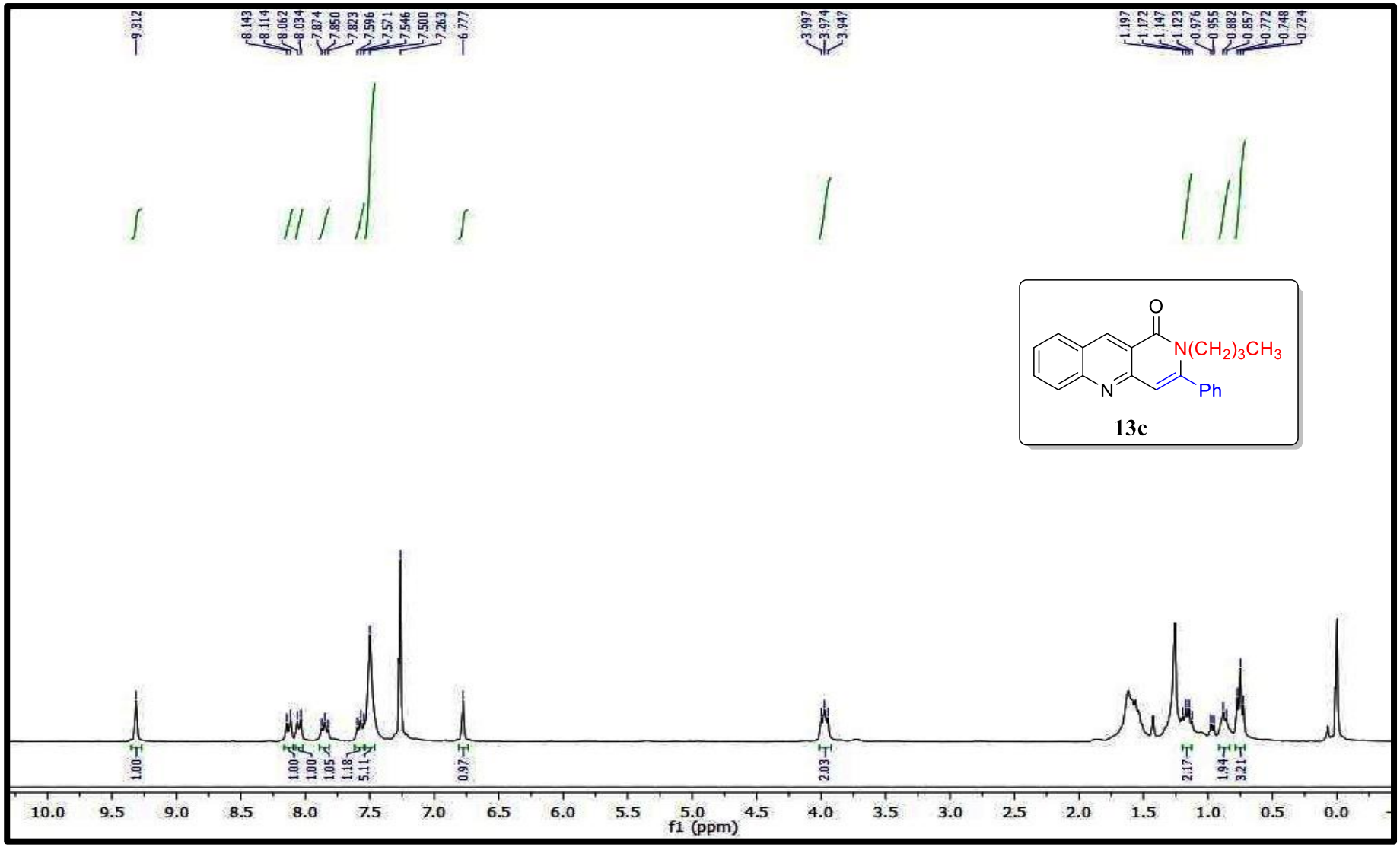
^{1}H and ^{13}C NMR spectrum of N-Ethyl-3-phenylbenzo[b][1,6]naphthyridin-1(2H)-one (13b)



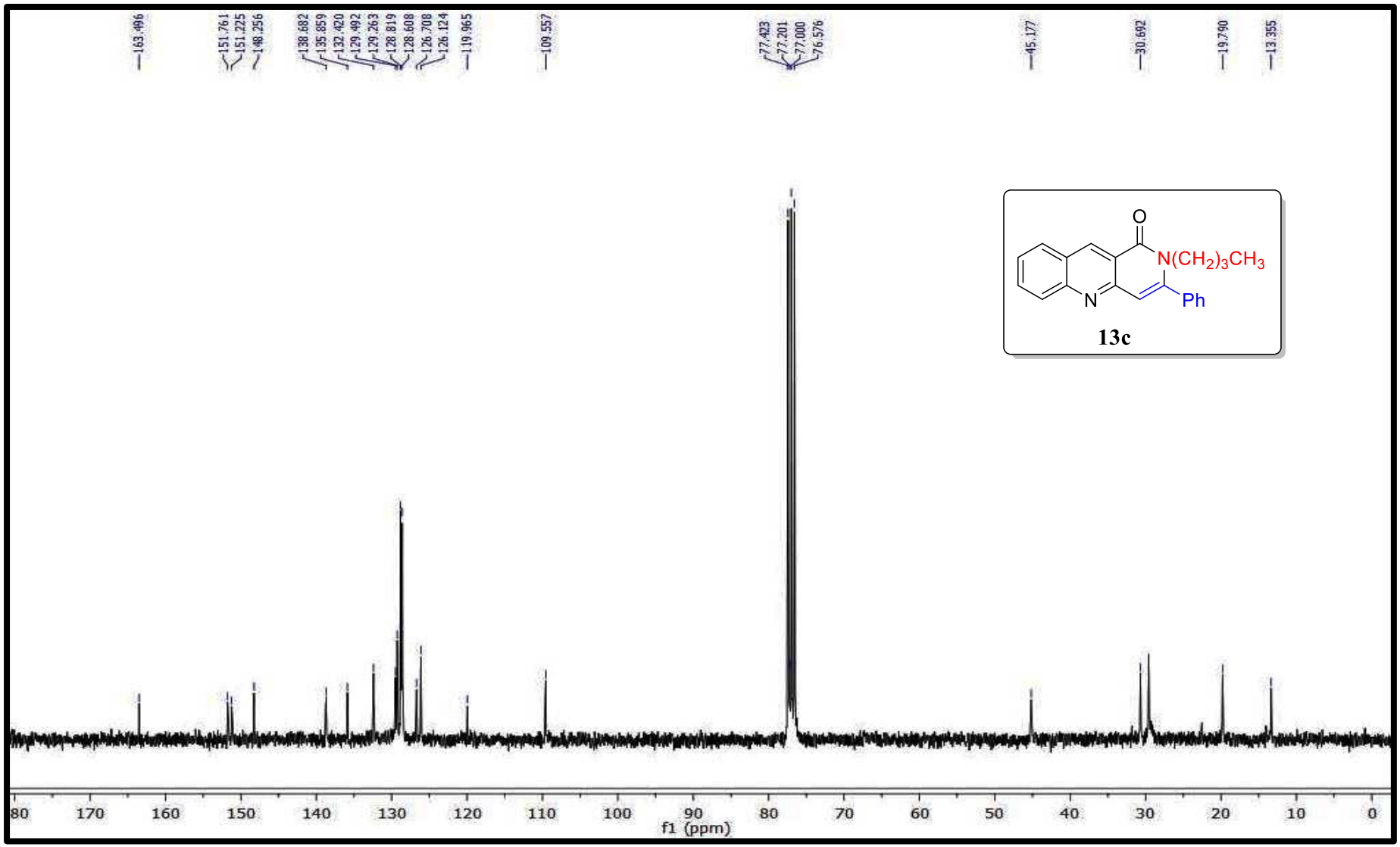
^{13}C NMR spectrum of N-Ethyl-3-phenylbenzo[b][1,6]naphthyridin-1(2H)-one (13b)



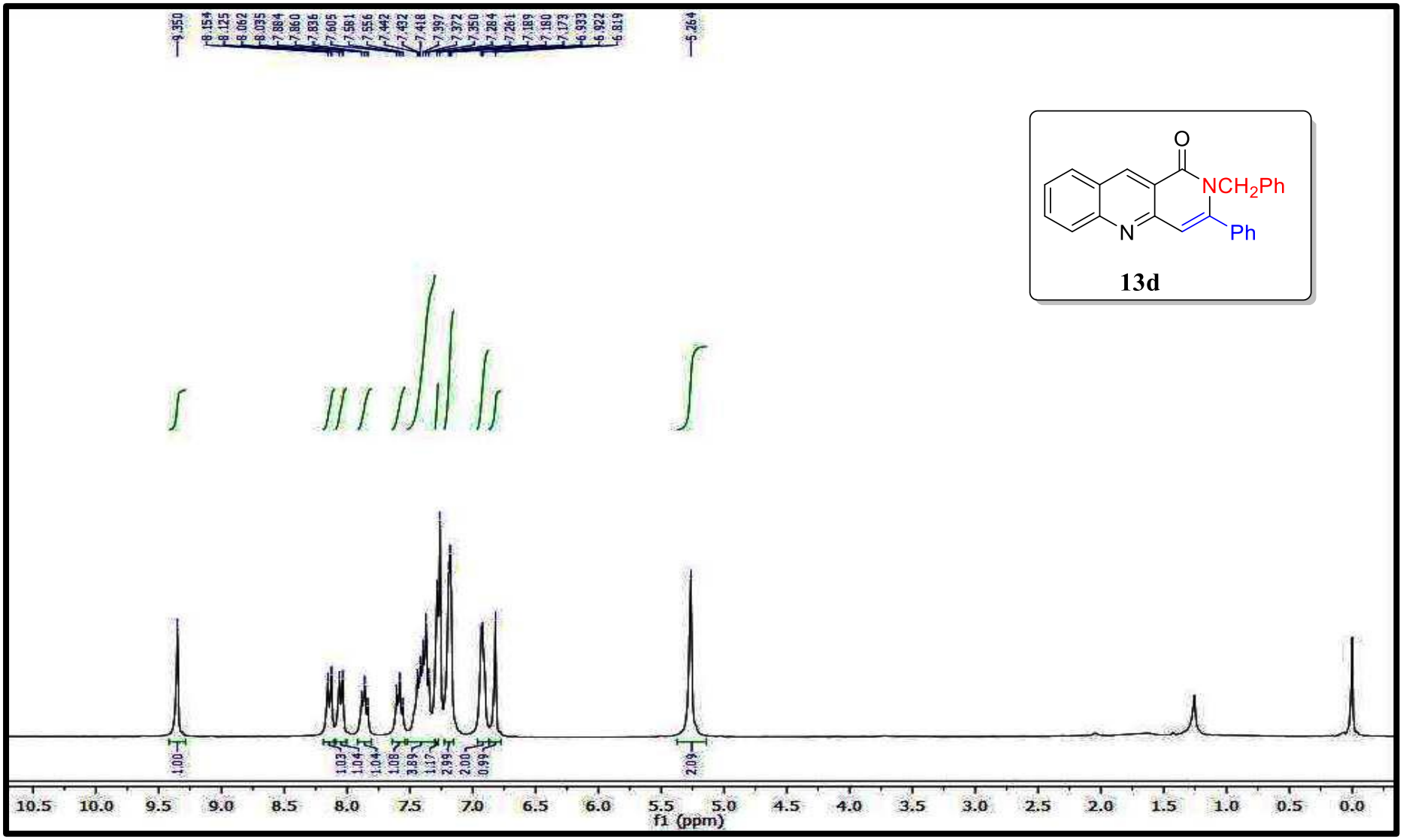
^{1}H NMR spectrum of N-Butyl-3-phenylbenzo[b][1,6]naphthyridin-1(2H)-one (13c)



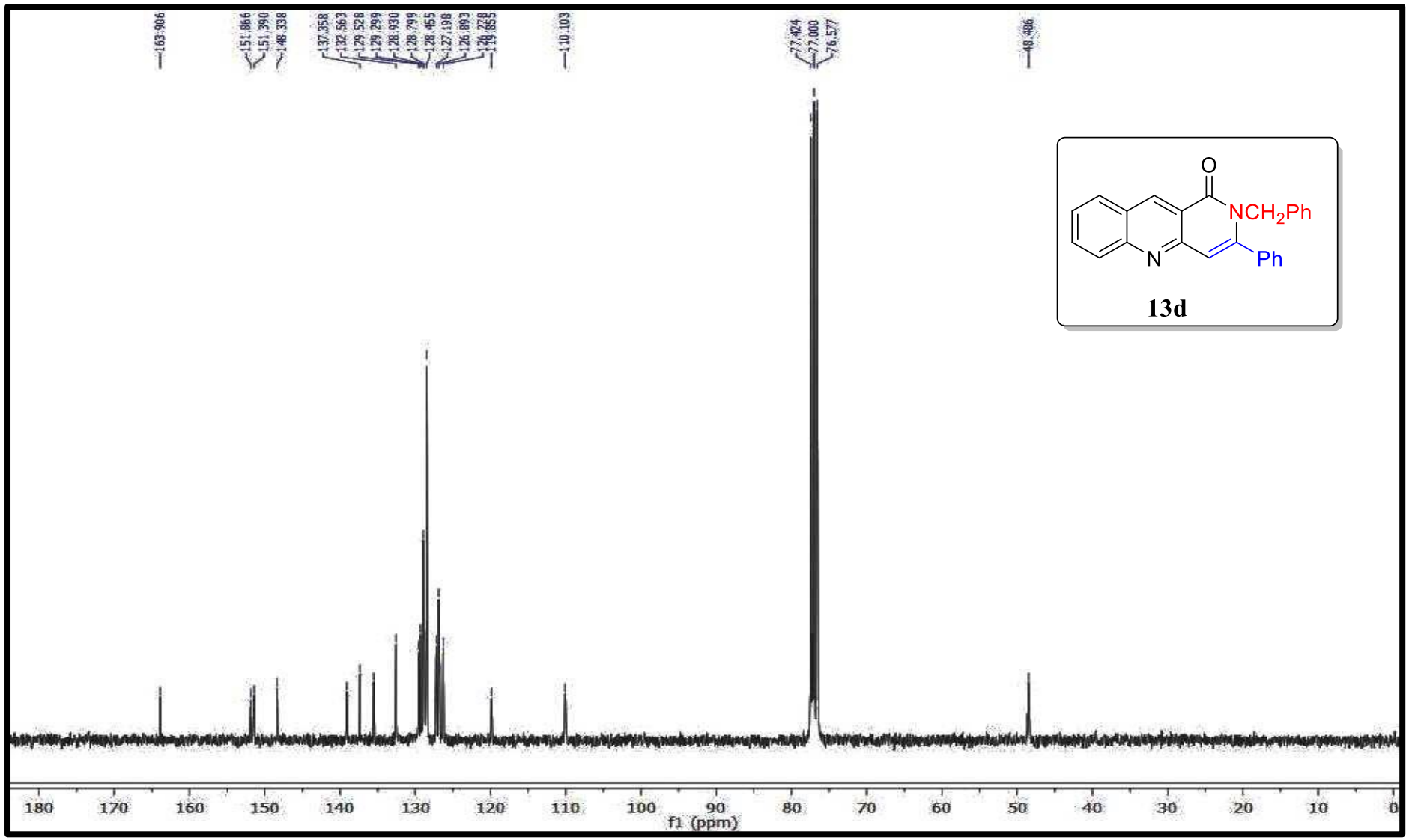
^{13}C NMR spectrum of N-Butyl-3-phenylbenzo[b][1,6]naphthyridin-1(2H)-one (13c)



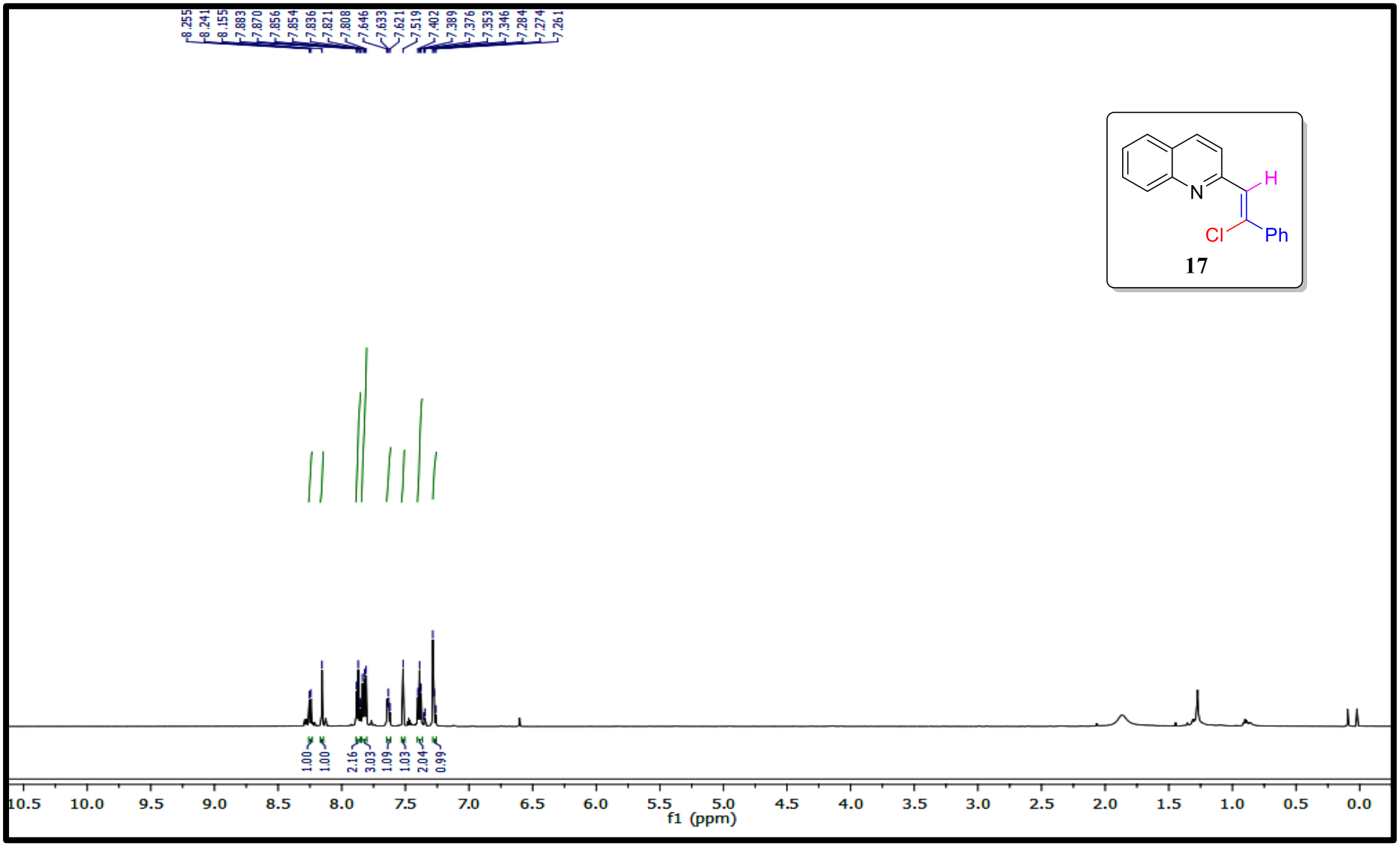
^{1}H NMR spectrum of N-Benzyl-3-phenyl-2H-benzo[b][1,6]naphthyridin-1-one (13d)



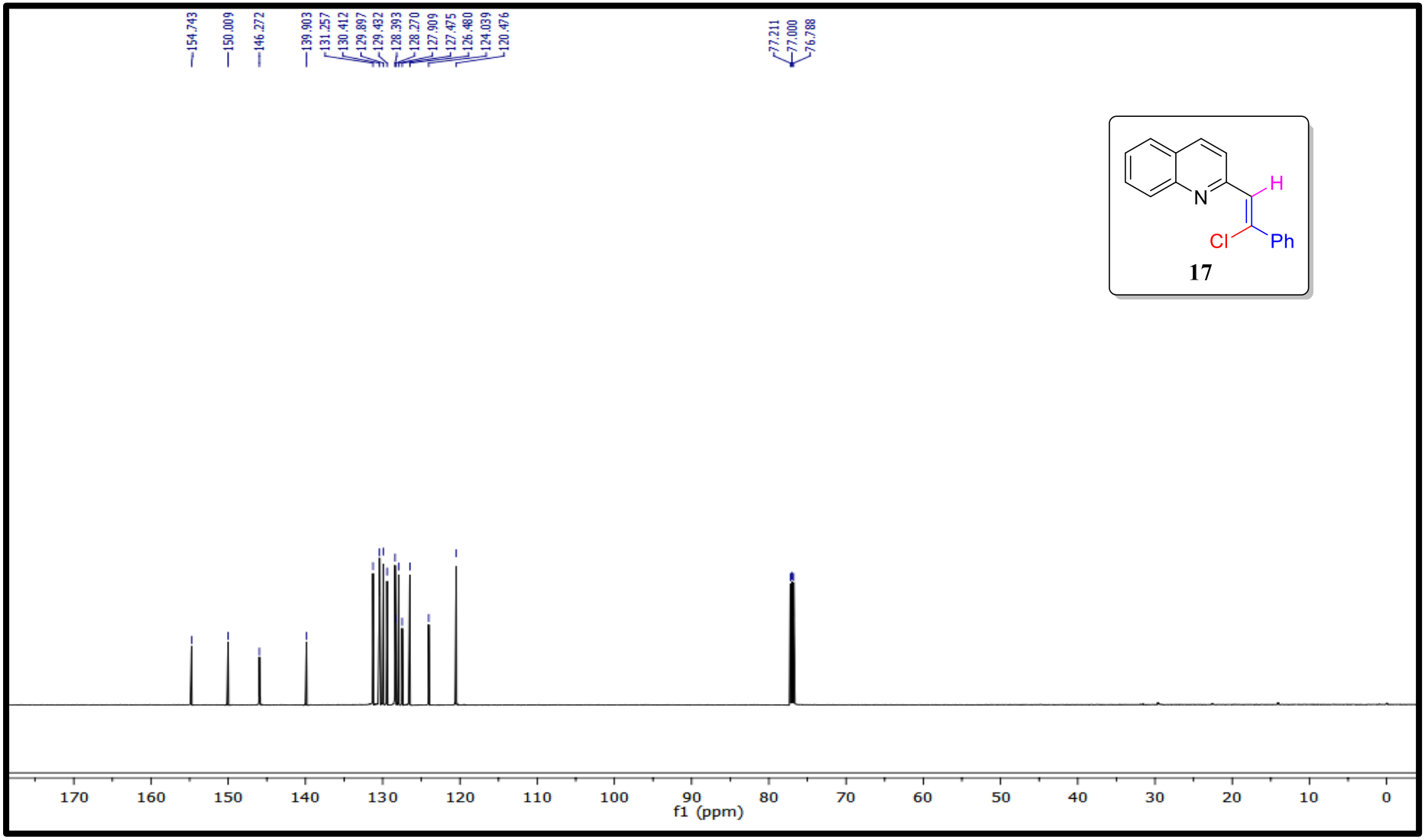
^{13}C NMR spectrum of N-Benzyl-3-phenyl-2H-benzo[b][1,6]naphthyridin-1-one (13d)



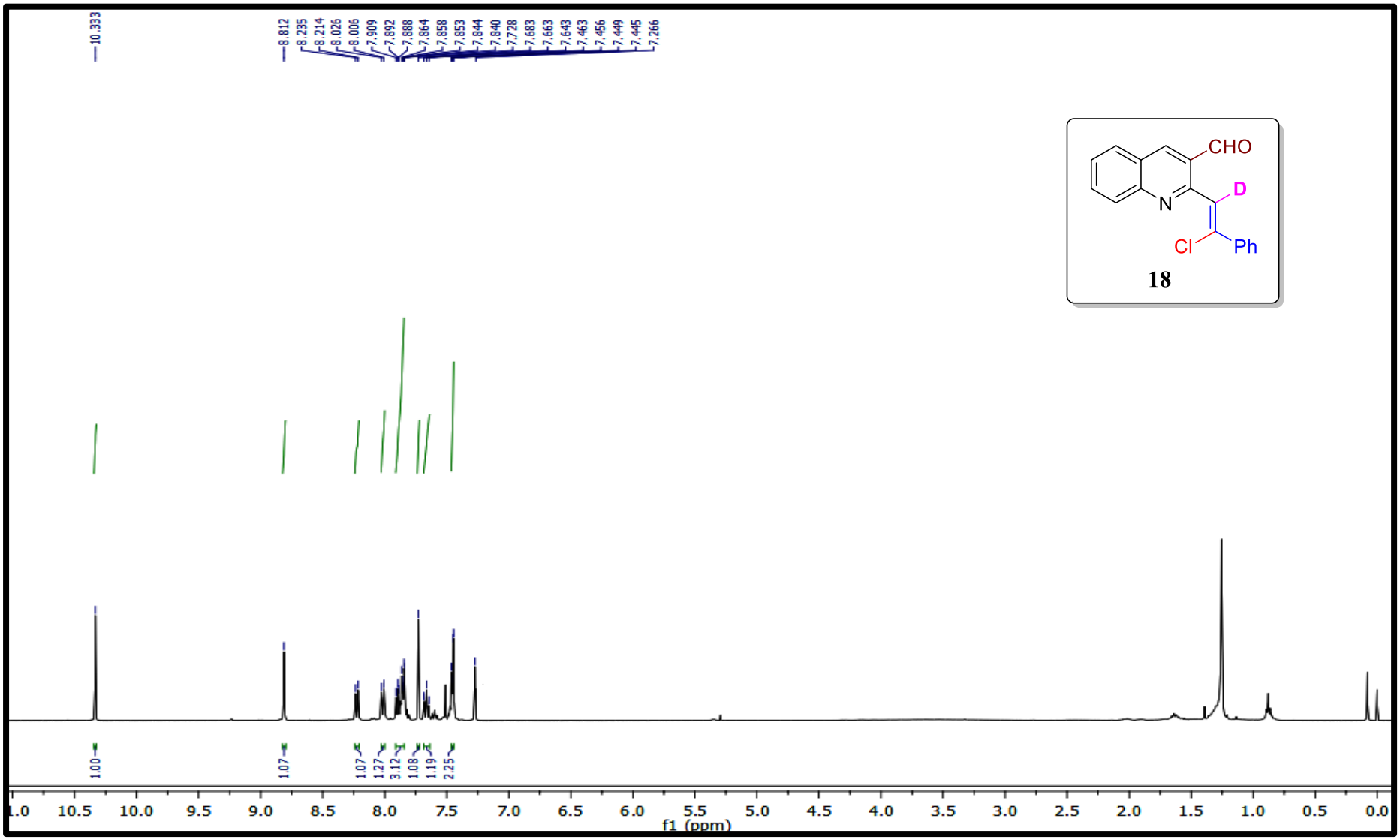
^{1}H NMR spectrum of 2-(2-chloro-2-phenylvinyl)quinoline (17)



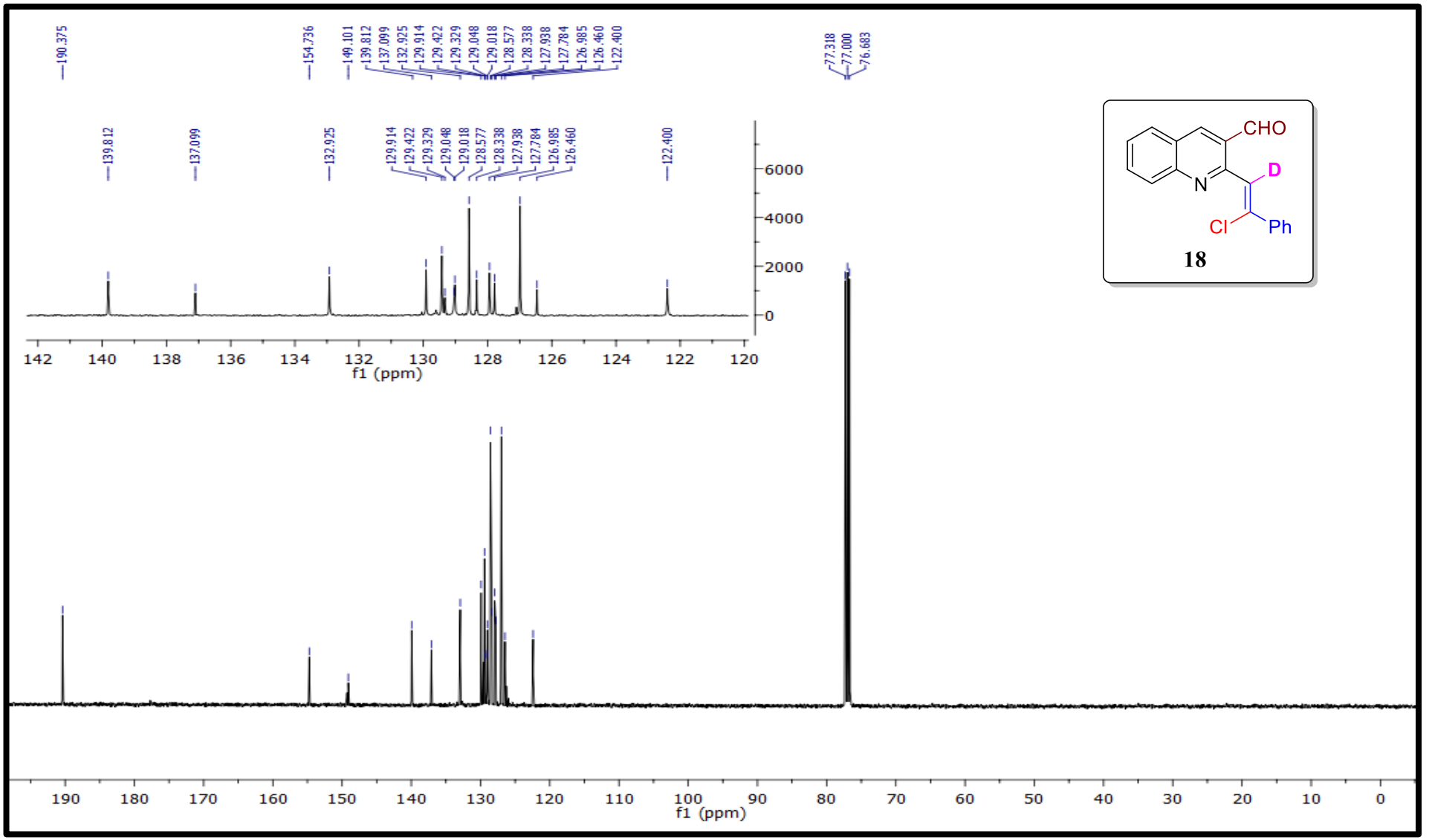
^{13}C NMR spectrum of 2-(2-chloro-2-phenylvinyl)quinoline (17)



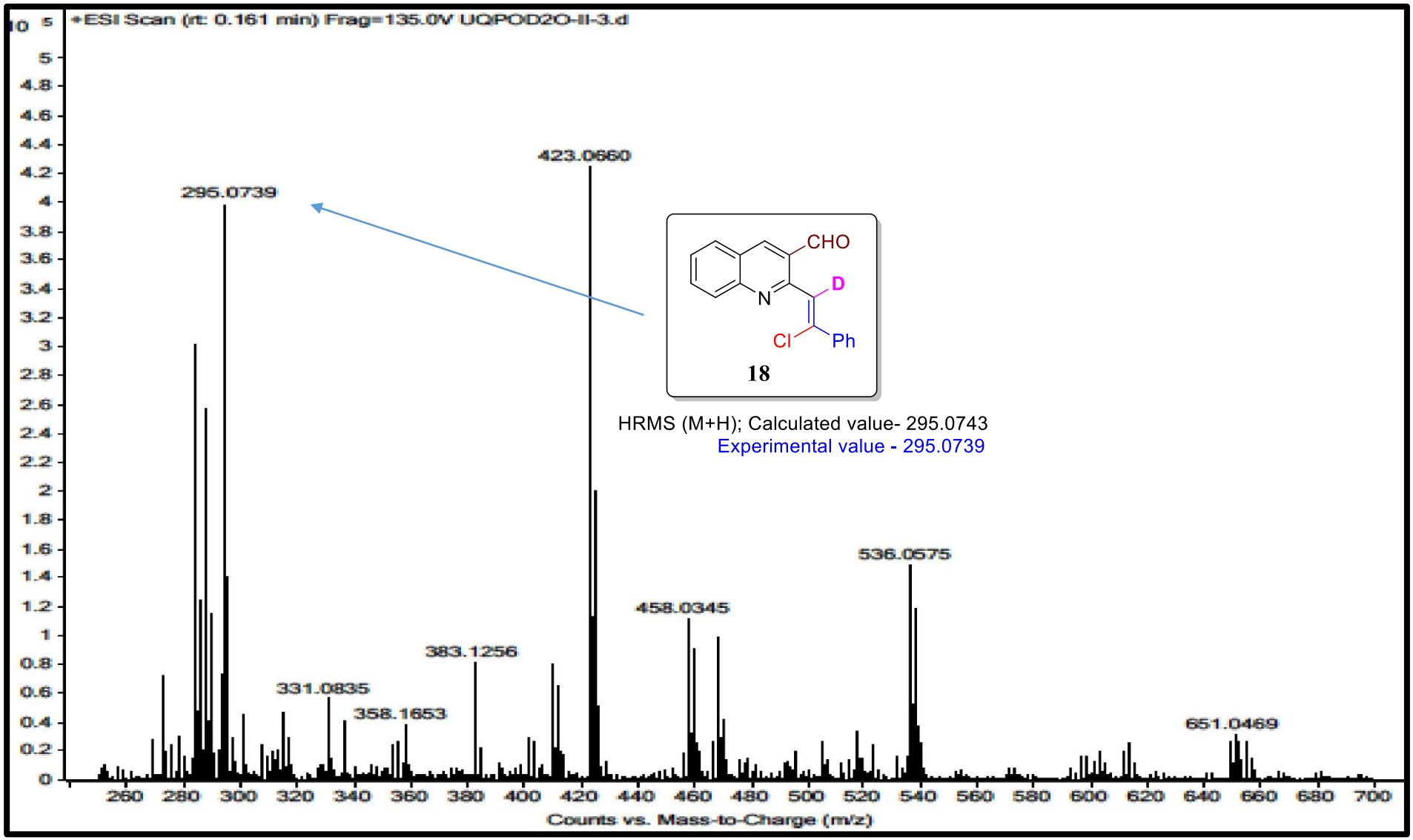
^{1}H NMR spectrum of 2-(2-chloro-2-phenylvinyl-1-d)quinoline-3-carbaldehyde (18)



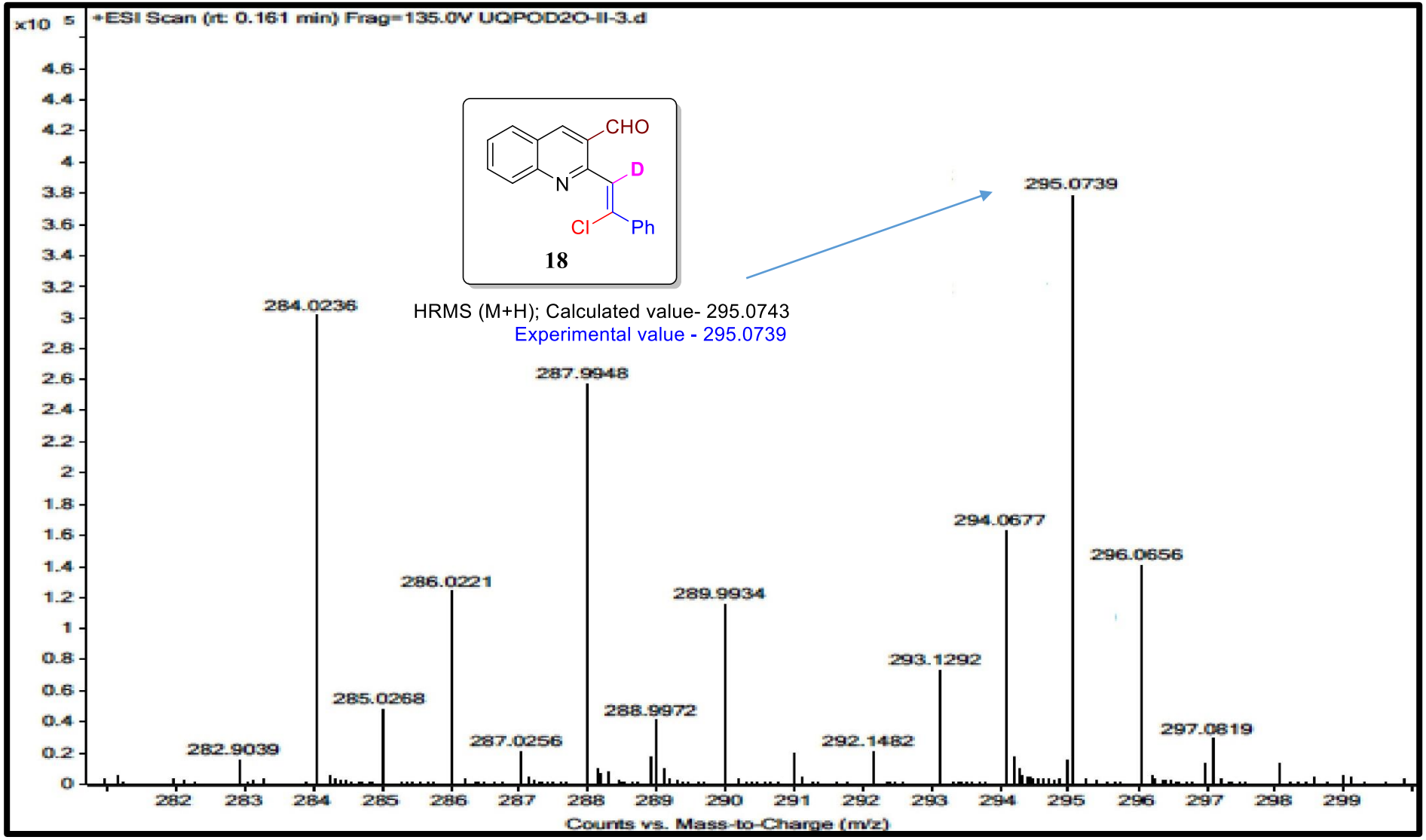
^{13}C NMR spectrum of 2-(2-chloro-2-phenylvinyl-1-d)quinoline-3-carbaldehyde (18)



Full HRMS spectrum of 2-(2-chloro-2-phenylvinyl-1-d)quinoline-3-carbaldehyde (18)

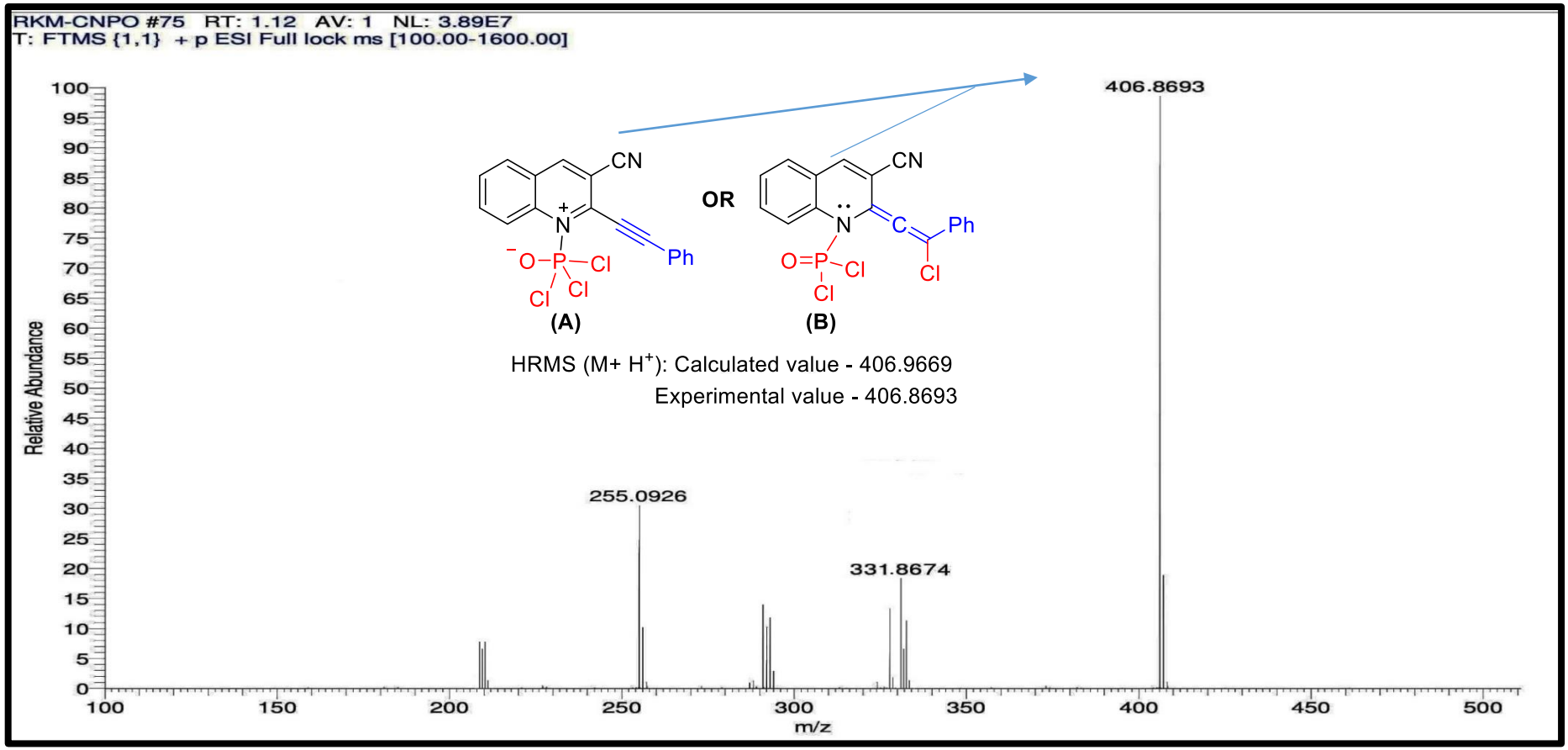


HRMS spectrum of 2-(2-chloro-2-phenylvinyl-1-d)quinoline-3-carbaldehyde (For Isotopic pattern mass) (18)

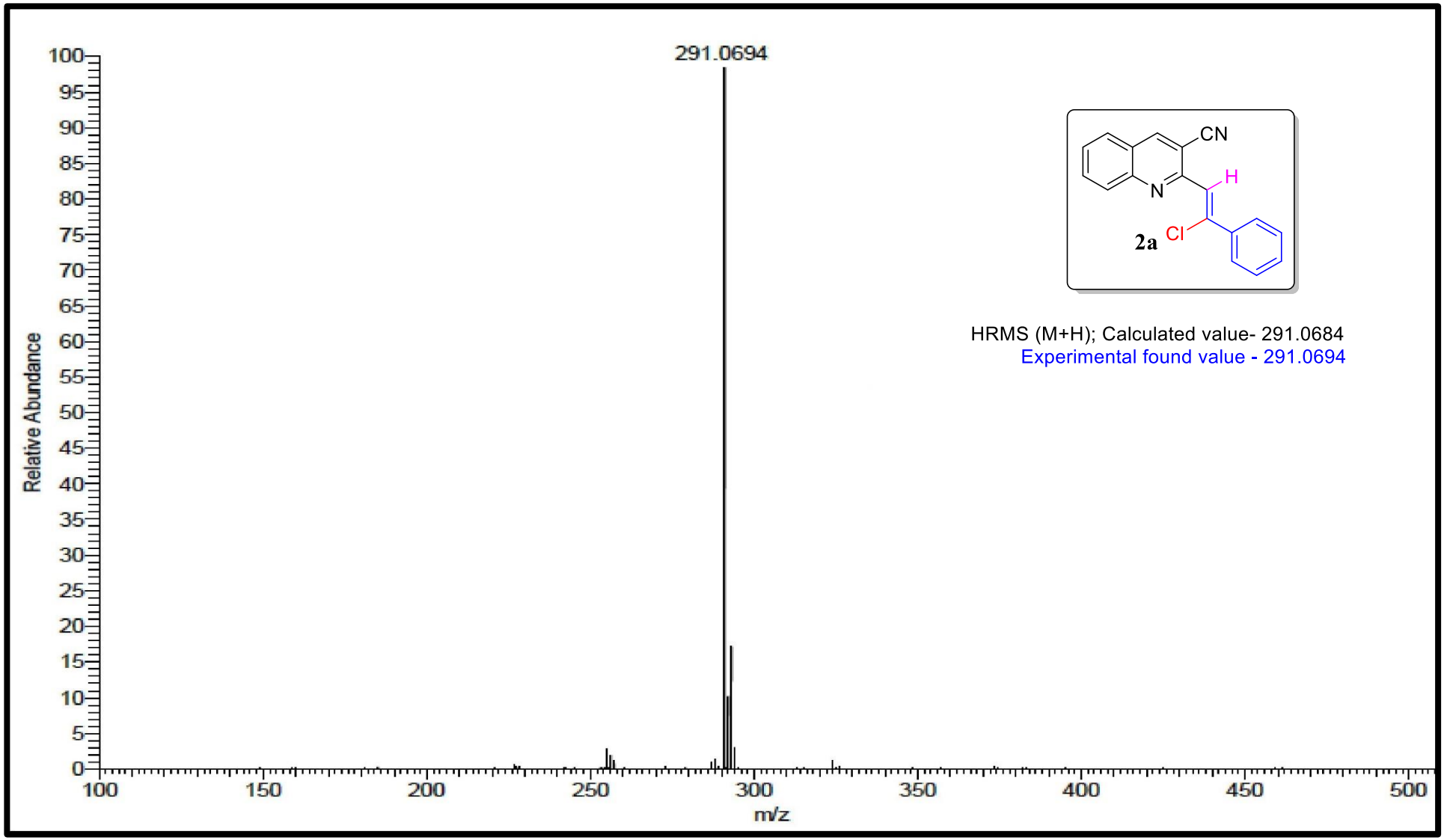


Identification of the reaction intermediates: HRMS spectra after 10 min.

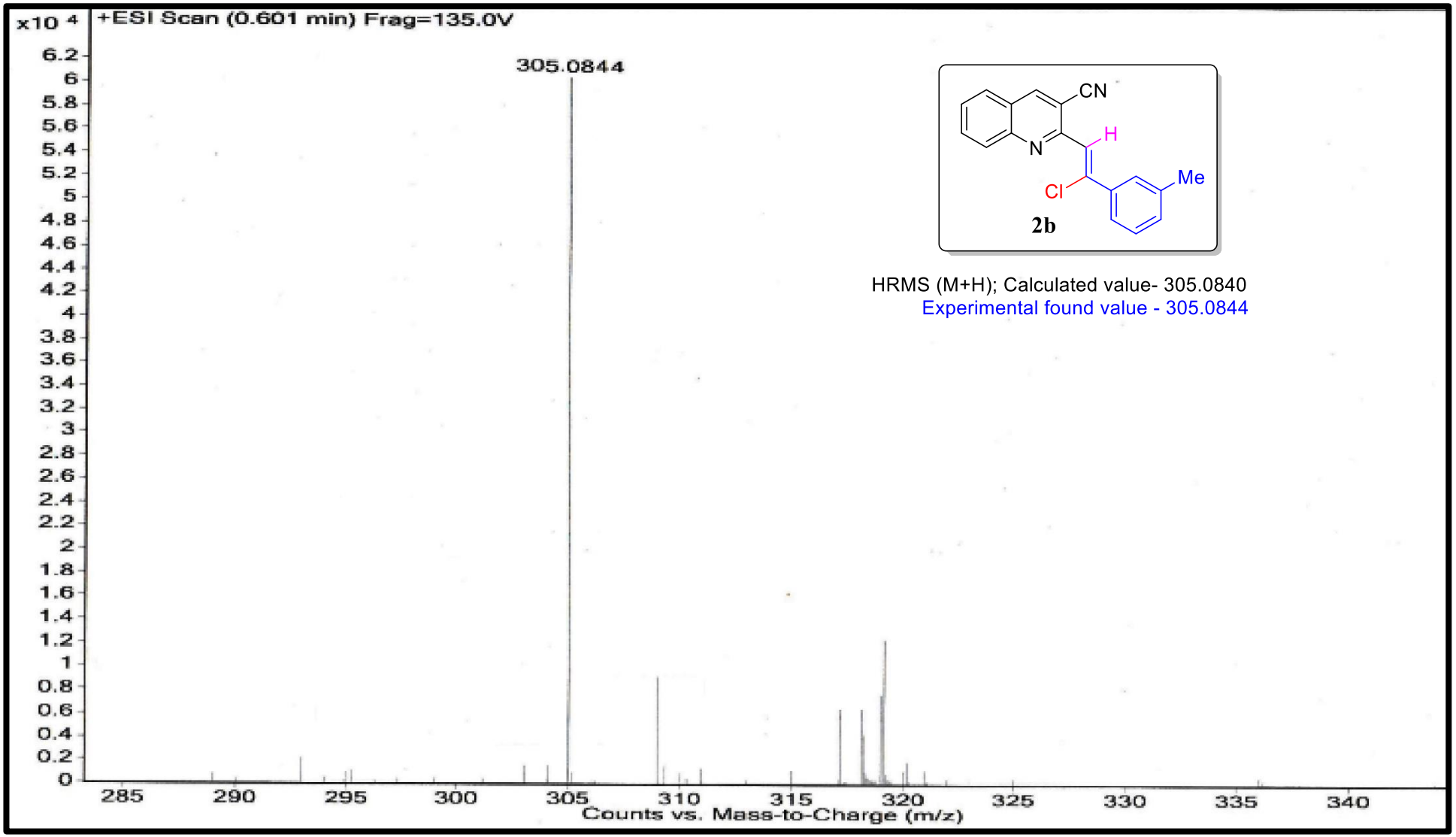
In order to detect the intermediate species involved in the reaction mechanism an HRMS analysis of crude reaction mixture was performed. After stirring the reaction for 10 min. 20 µL reaction mixture was taken out and diluted with HPLC grade acetonitrile. The diluted solution was then injected to run ESI-MS analysis. Intermediates (A) and (B) were detected in the MS analysis as shown below. Based on this reaction experiment, the initial step is likely to suggested that the co-ordination of $POCl_3$ with nitrogen of quinoline ring was proposed. Since both the intermediate have same m/z value that may be the reason the peak remains consistent even after in 50 min of reaction mixture.



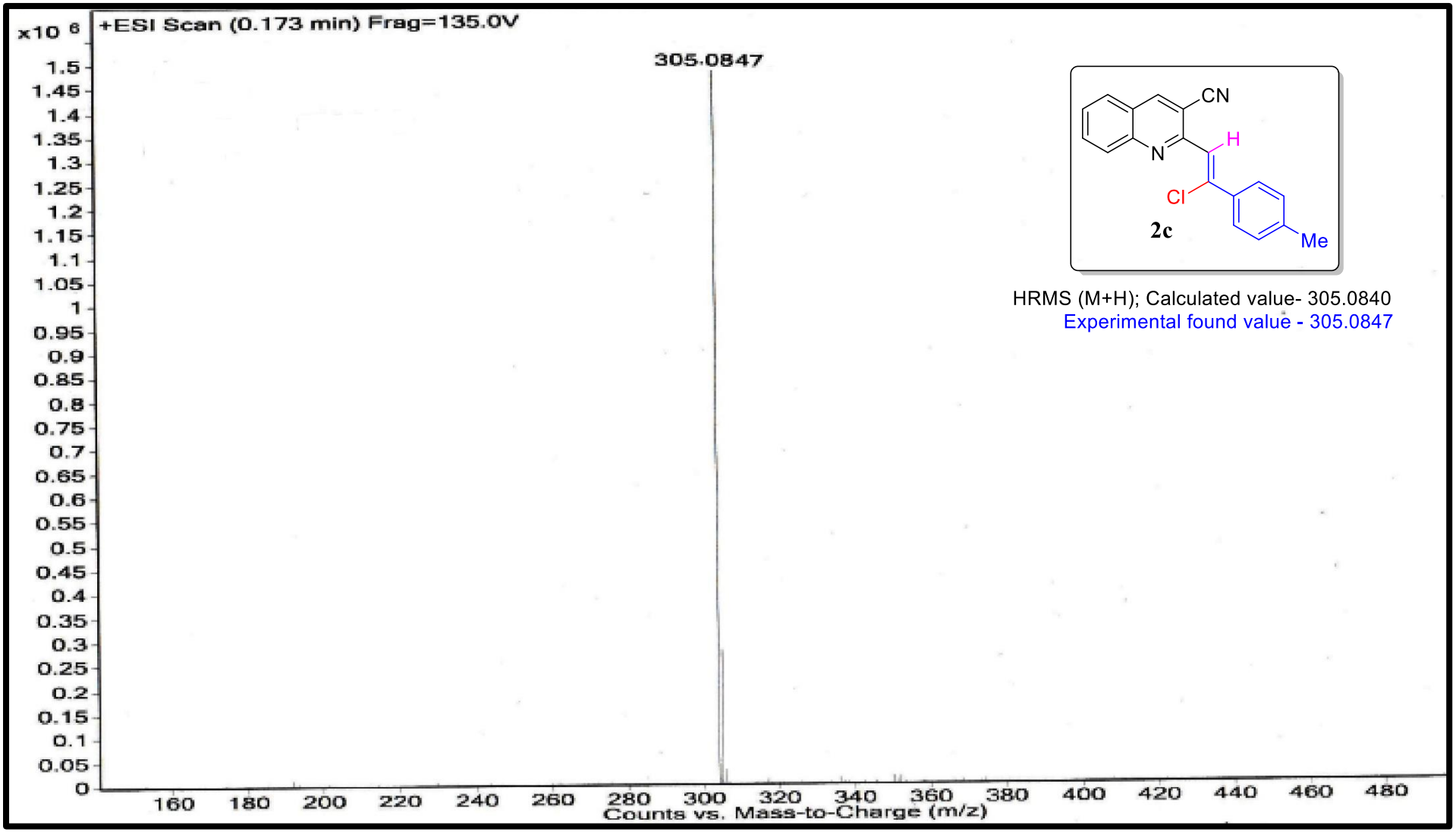
HRMS spectrum of 2-(2-Chloro-2-phenylvinyl)quinoline-3-carbonitrile (2a)



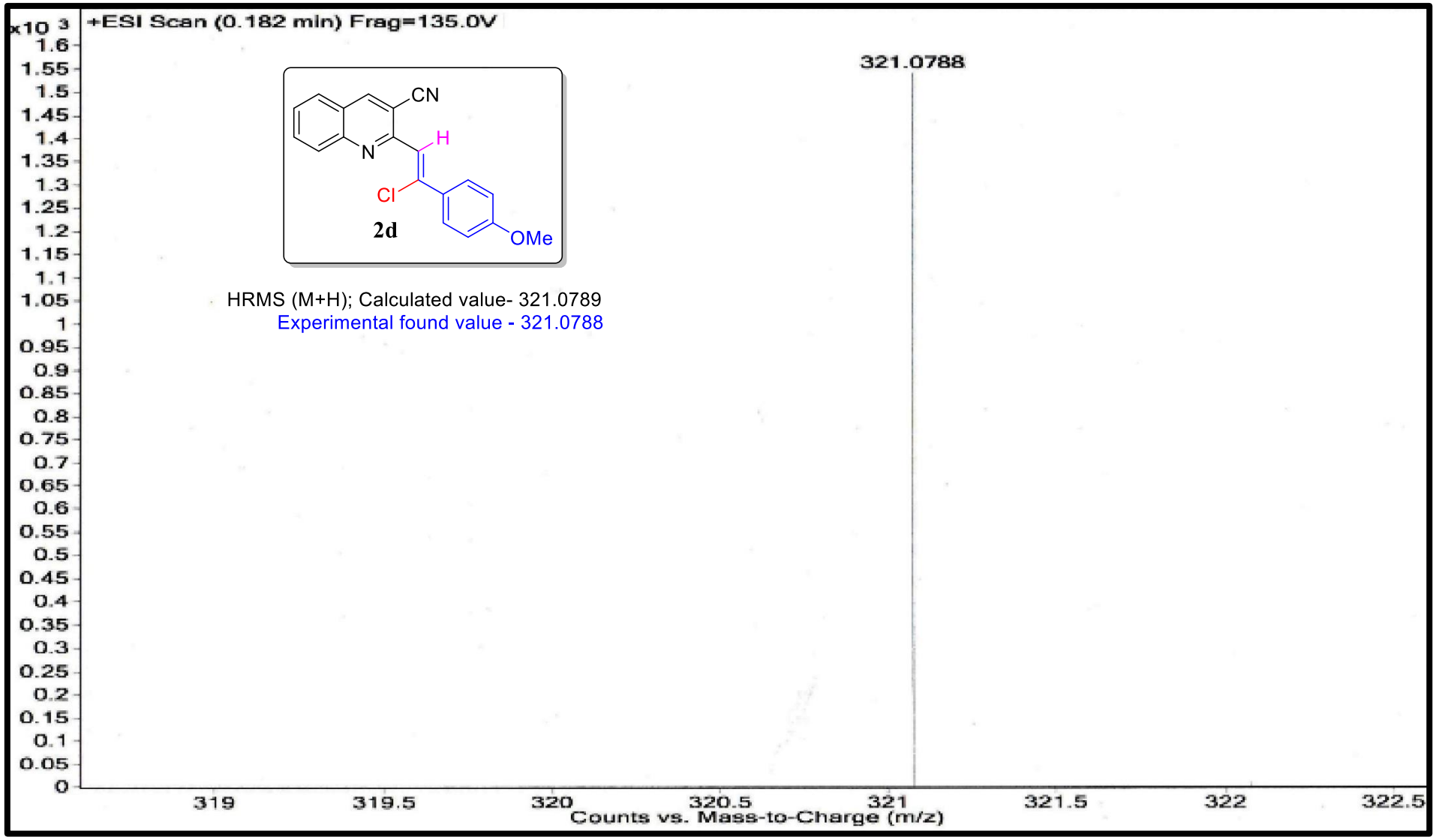
HRMS spectrum of 2-(2-Chloro-2-m-tolylvinyl)quinoline-3-carbonitrile (2b)



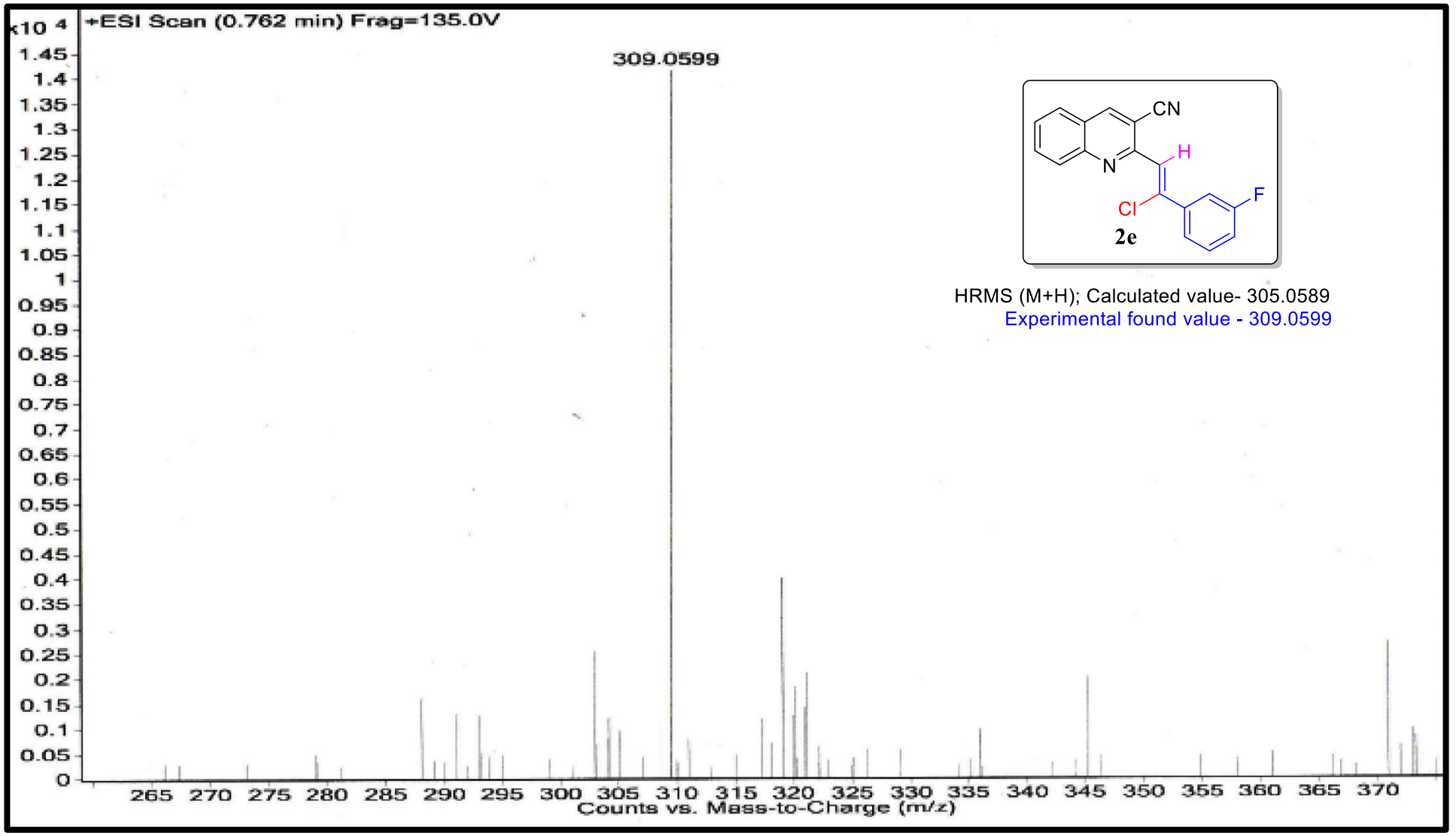
HRMS spectrum of 2-(2-chloro-2-(p-tolyl)vinyl)quinoline-3-carbonitrile (2c).



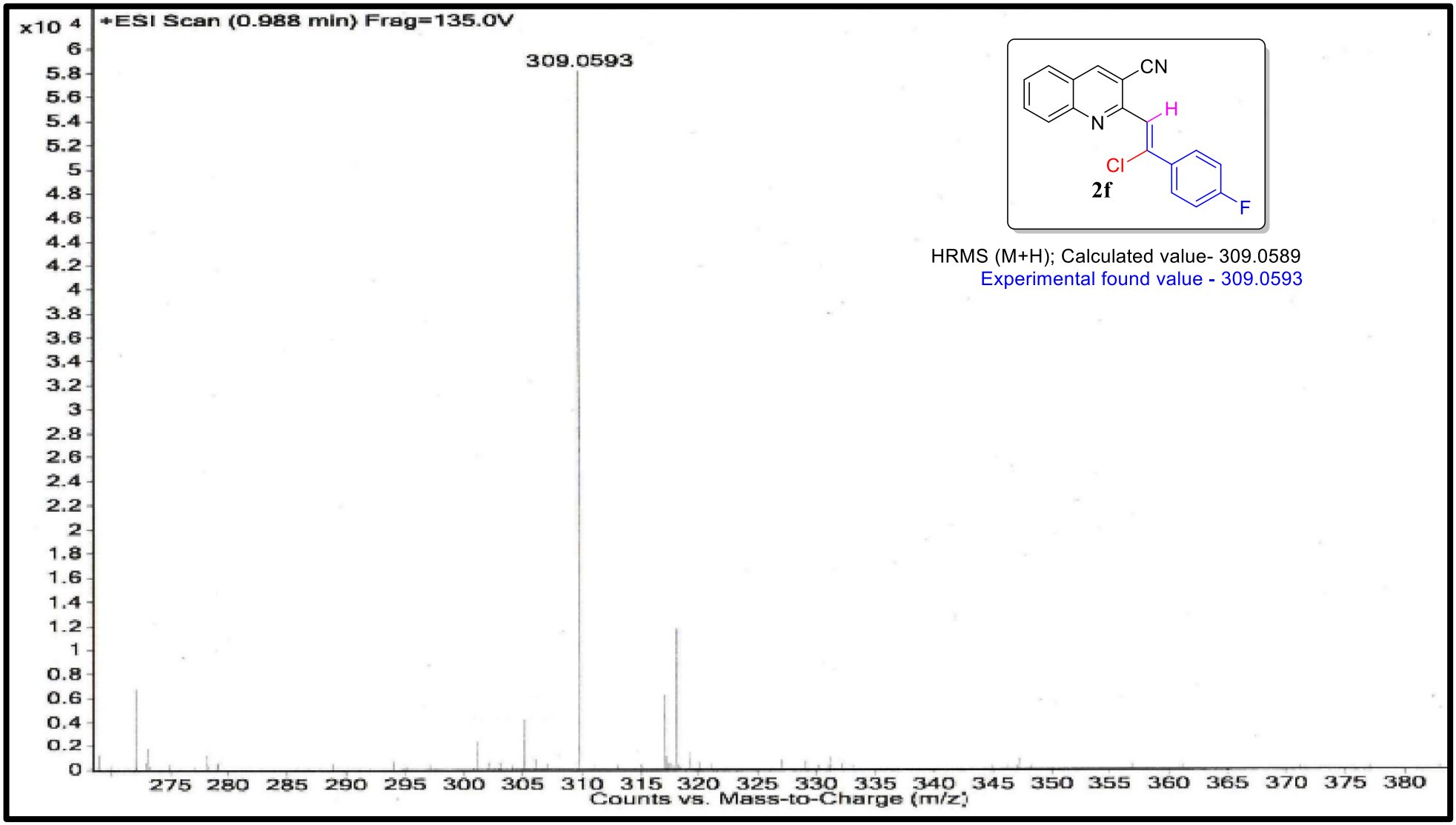
HRMS spectrum of 2-[2-Chloro-2-(4-methoxyphenyl)vinyl]quinoline-3-carbonitrile (2d).



HRMS spectrum of 2-(2-chloro-2-(3-fluorophenyl)vinyl)quinoline-3-carbonitrile (2e).

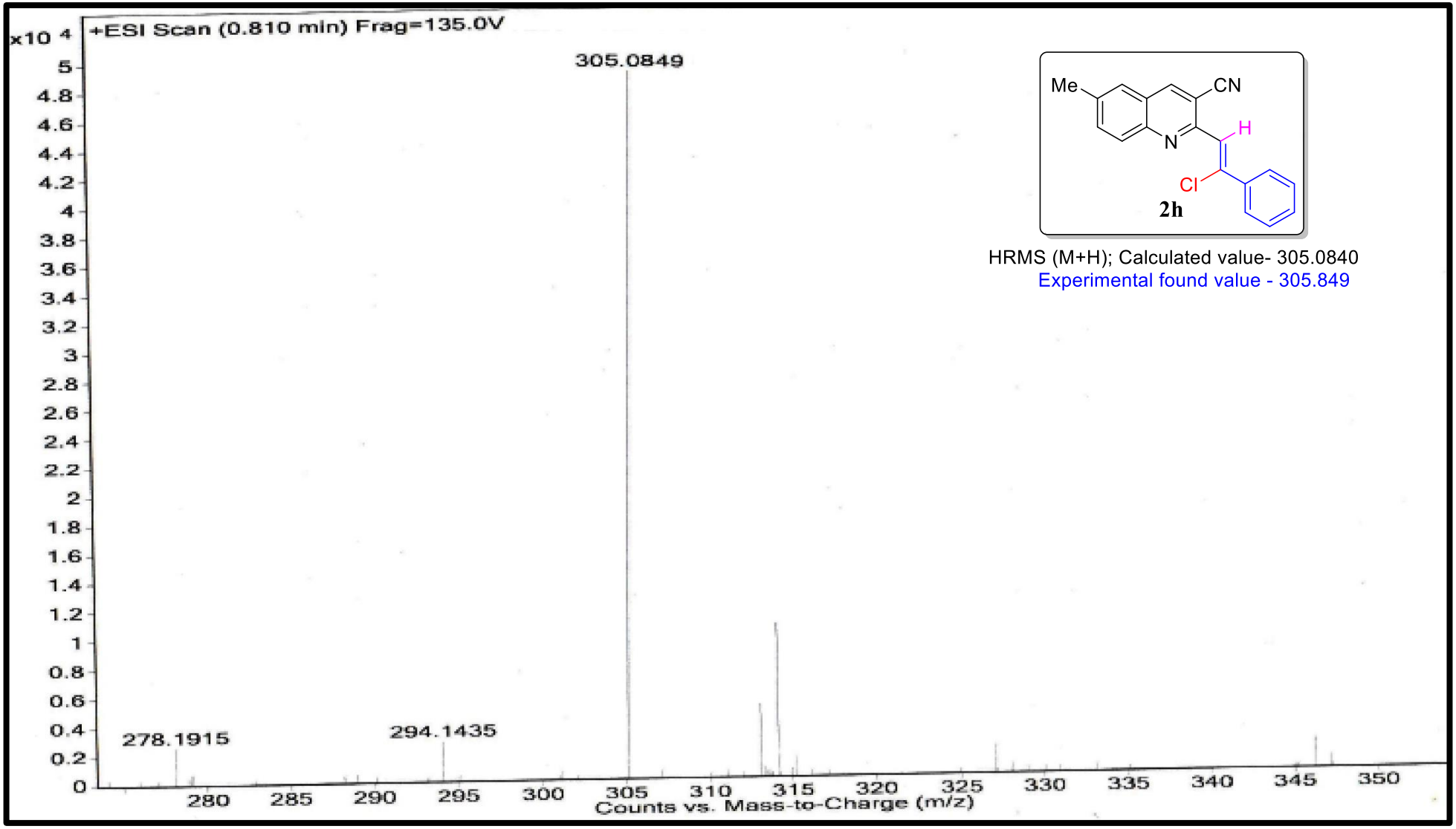


HRMS spectrum of 2-[2-Chloro-2-(4-fluoro-phenyl)vinyl]quinoline-3-carbonitrile (2f)



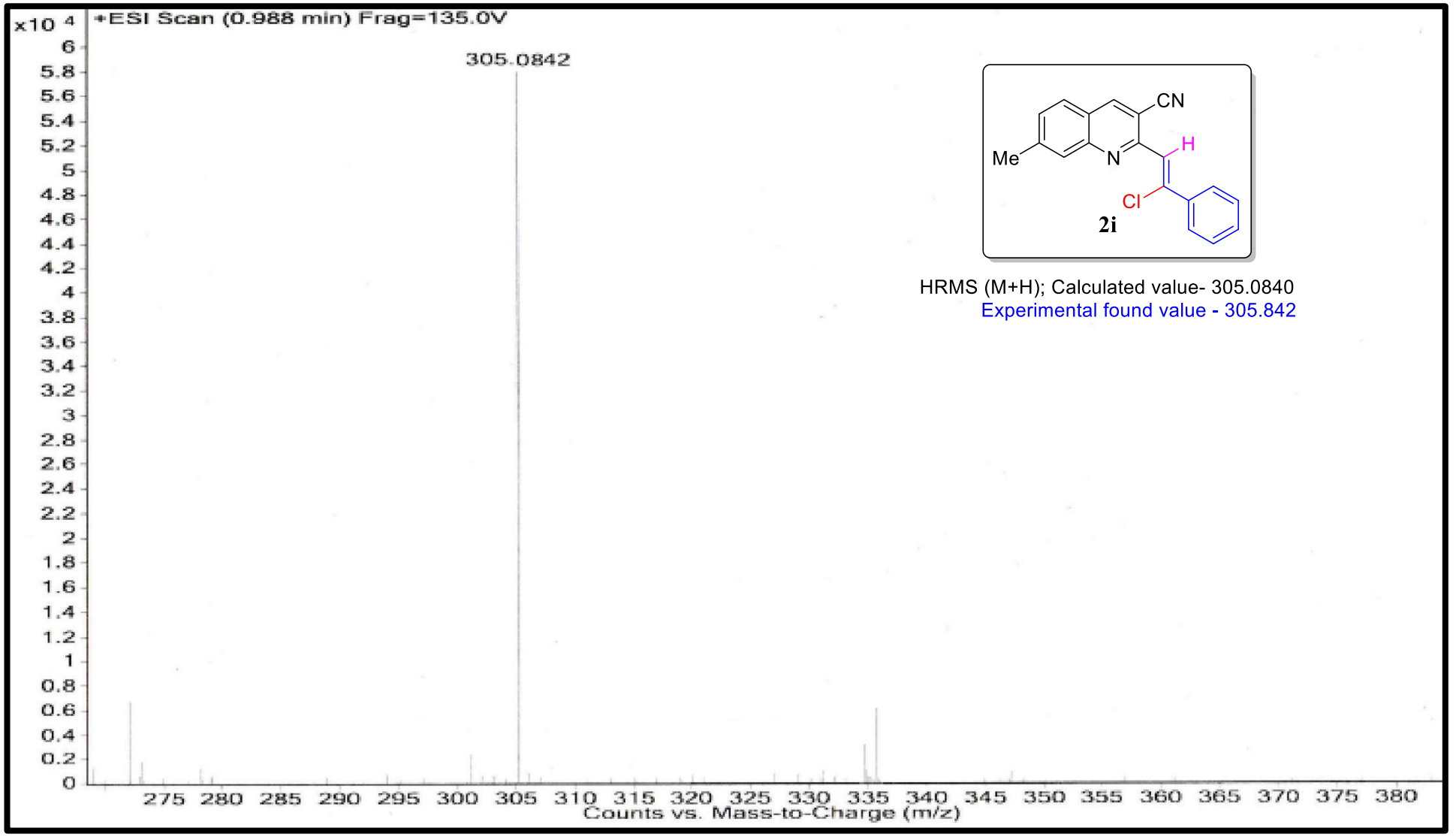
HRMS (M+H); Calculated value- 309.0589
Experimental found value - 309.0593

HRMS spectrum of 2-(2-Chloro-2-phenylvinyl)6-methyl-quinoline-3-carbonitrile (2h)



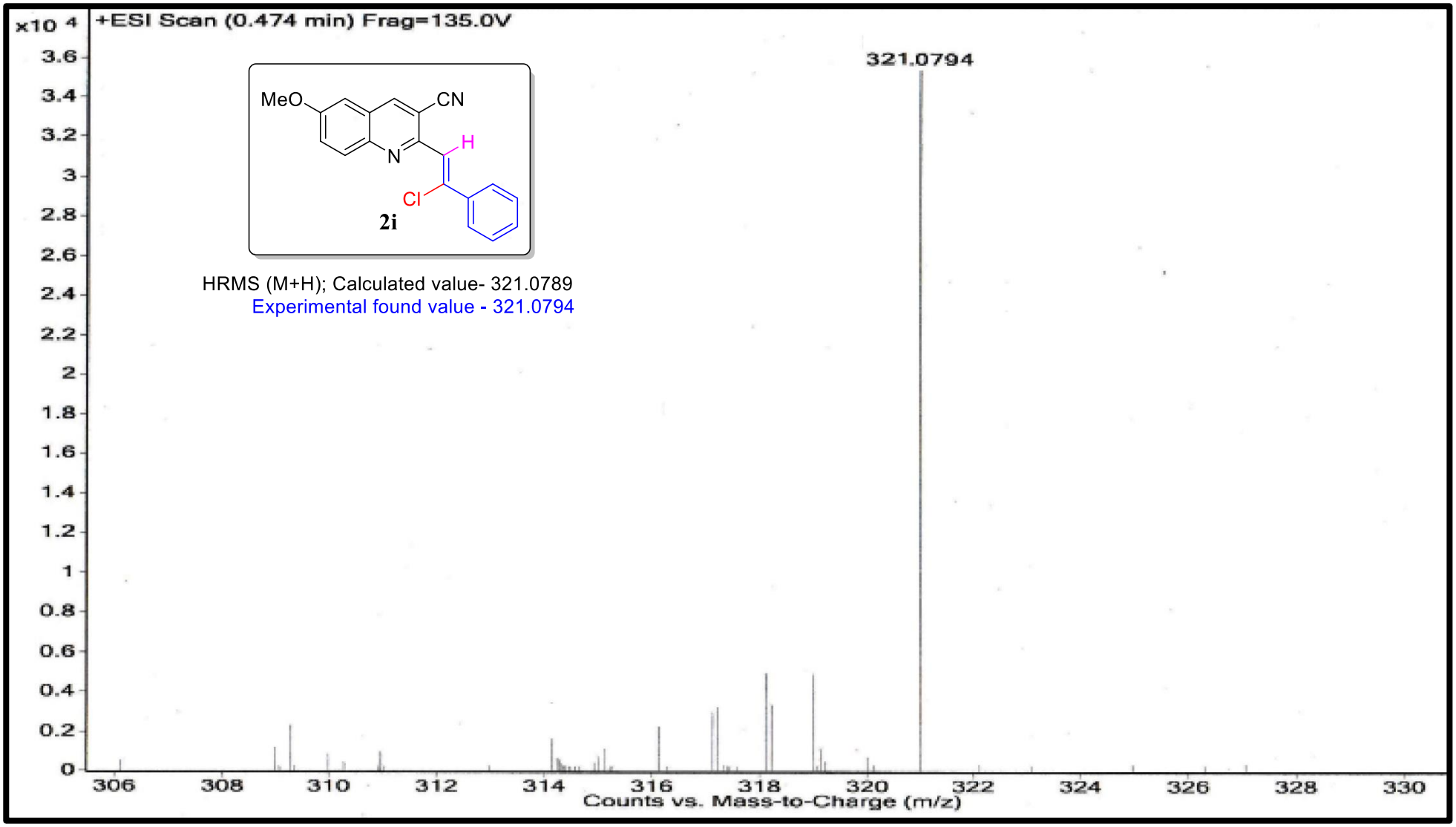
HRMS (M+H); Calculated value- 305.0840
Experimental found value - 305.849

HRMS spectrum of 2-(2-Chloro-2-phenylvinyl)-7-methyl-quinoline-3-carbonitrile (2i)

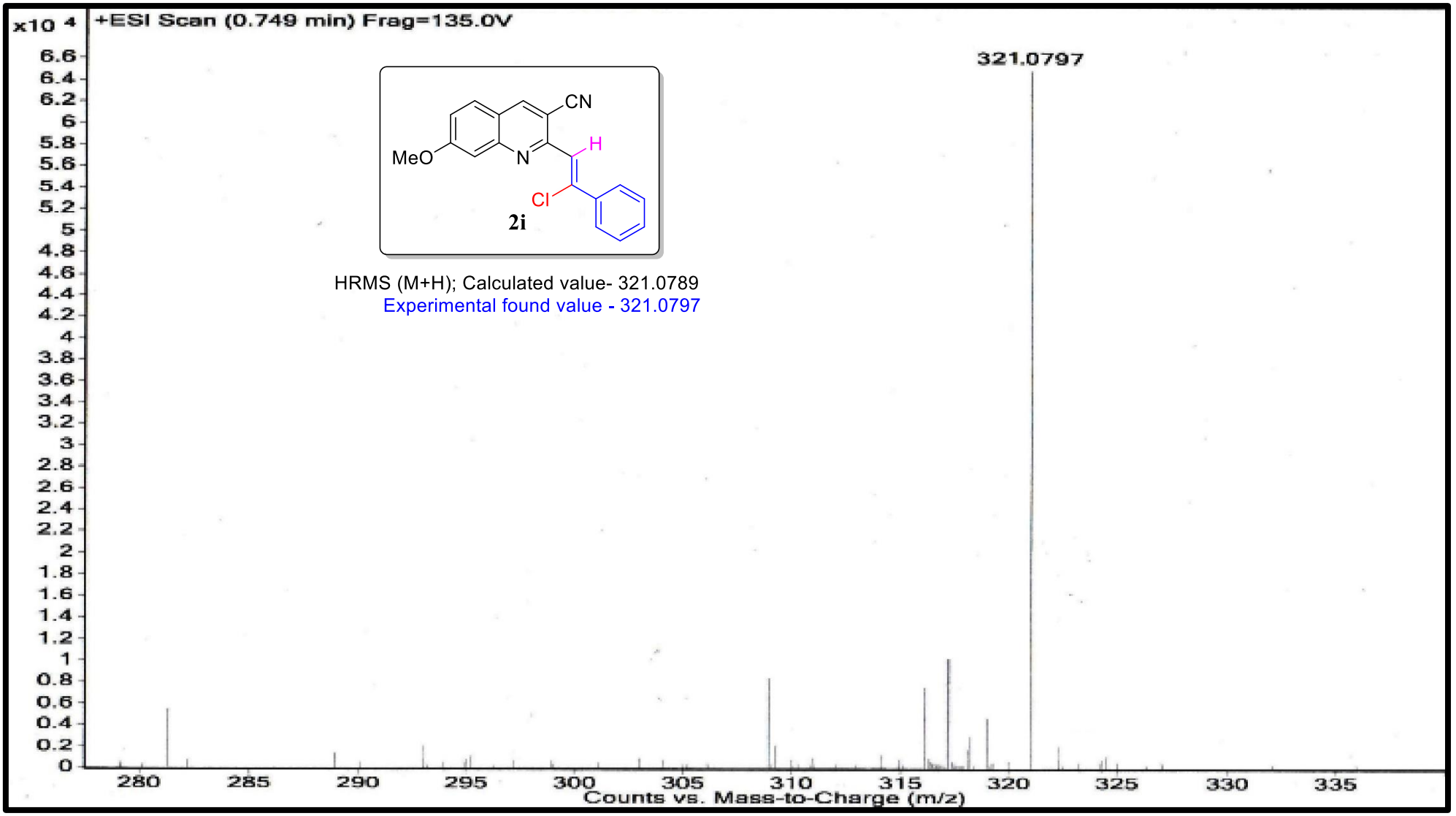


HRMS (M+H); Calculated value- 305.0840
Experimental found value - 305.842

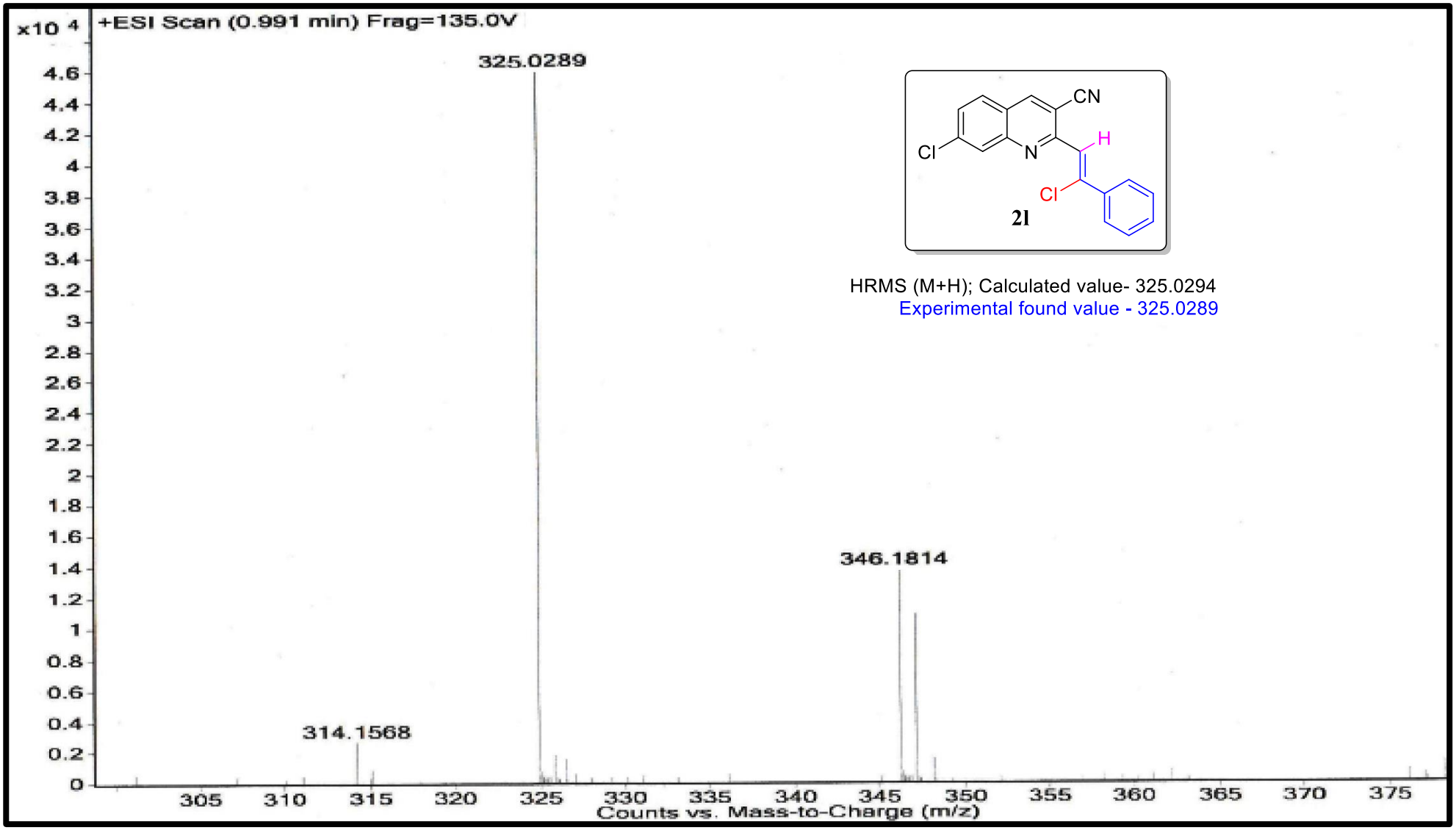
HRMS spectrum of 2-(2-Chloro-2-phenylvinyl)-6-methoxy-quinoline-3-carbonitrile (2j)



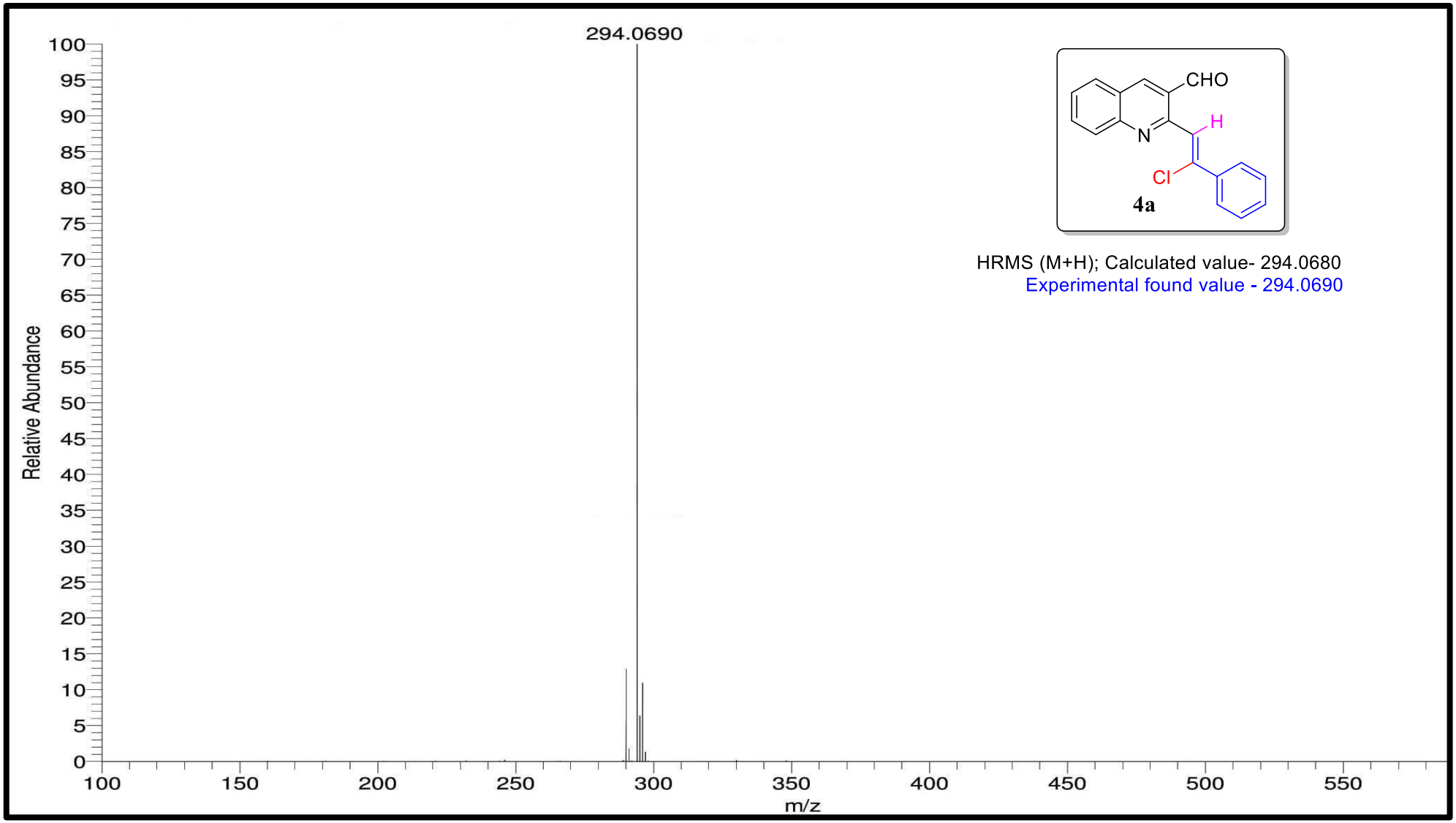
HRMS spectrum of 2-(2-Chloro-2-phenylvinyl)-7-methoxy-quinoline-3-carbonitrile (2k)



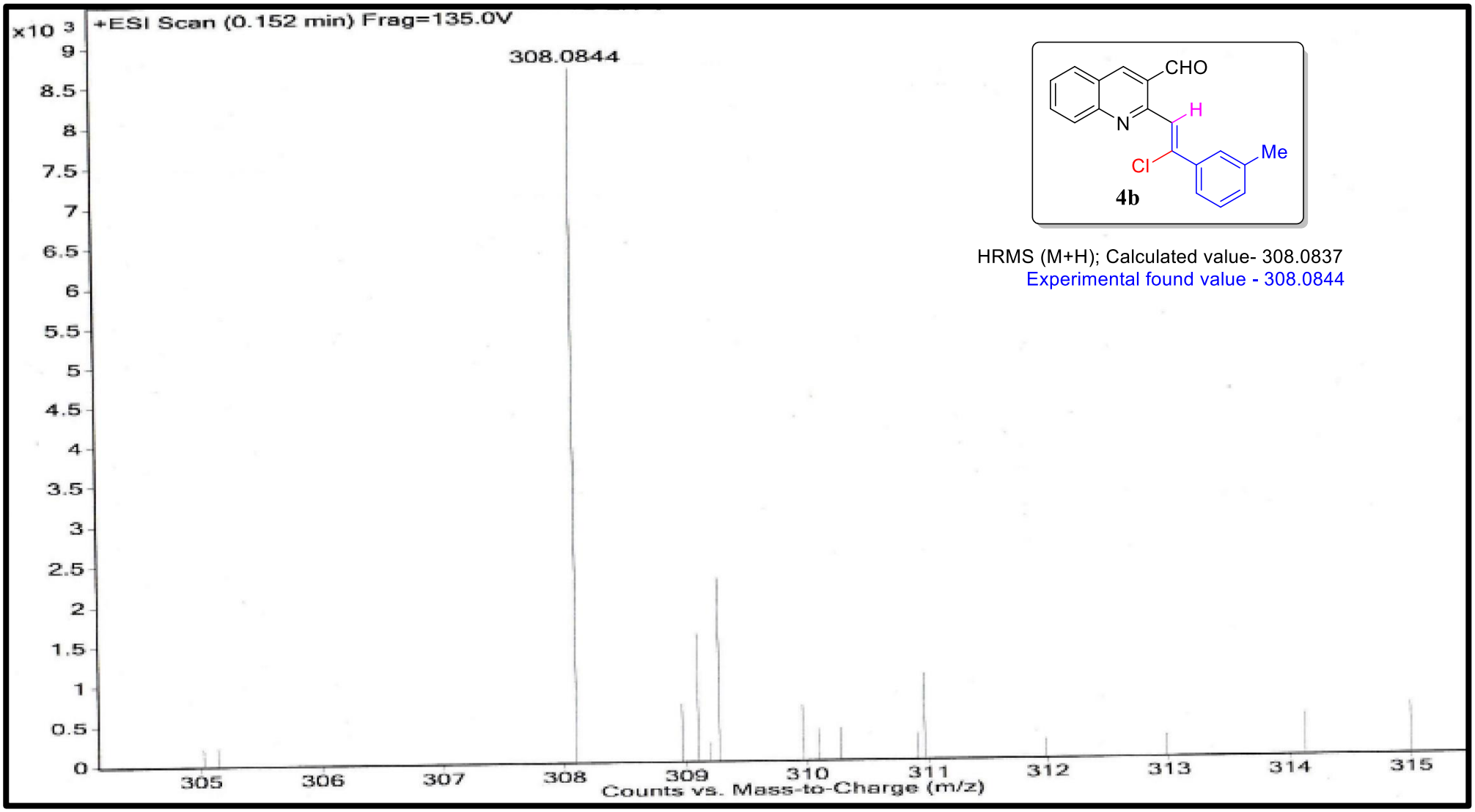
HRMS spectrum of 7-Chloro-2-(2-chloro-2-phenylvinyl)quinoline-3-carbonitrile (2l)



HRMS spectrum of 2-(2-Chloro-2-phenylvinyl-quinoline-3-carbaldehyde (4a)

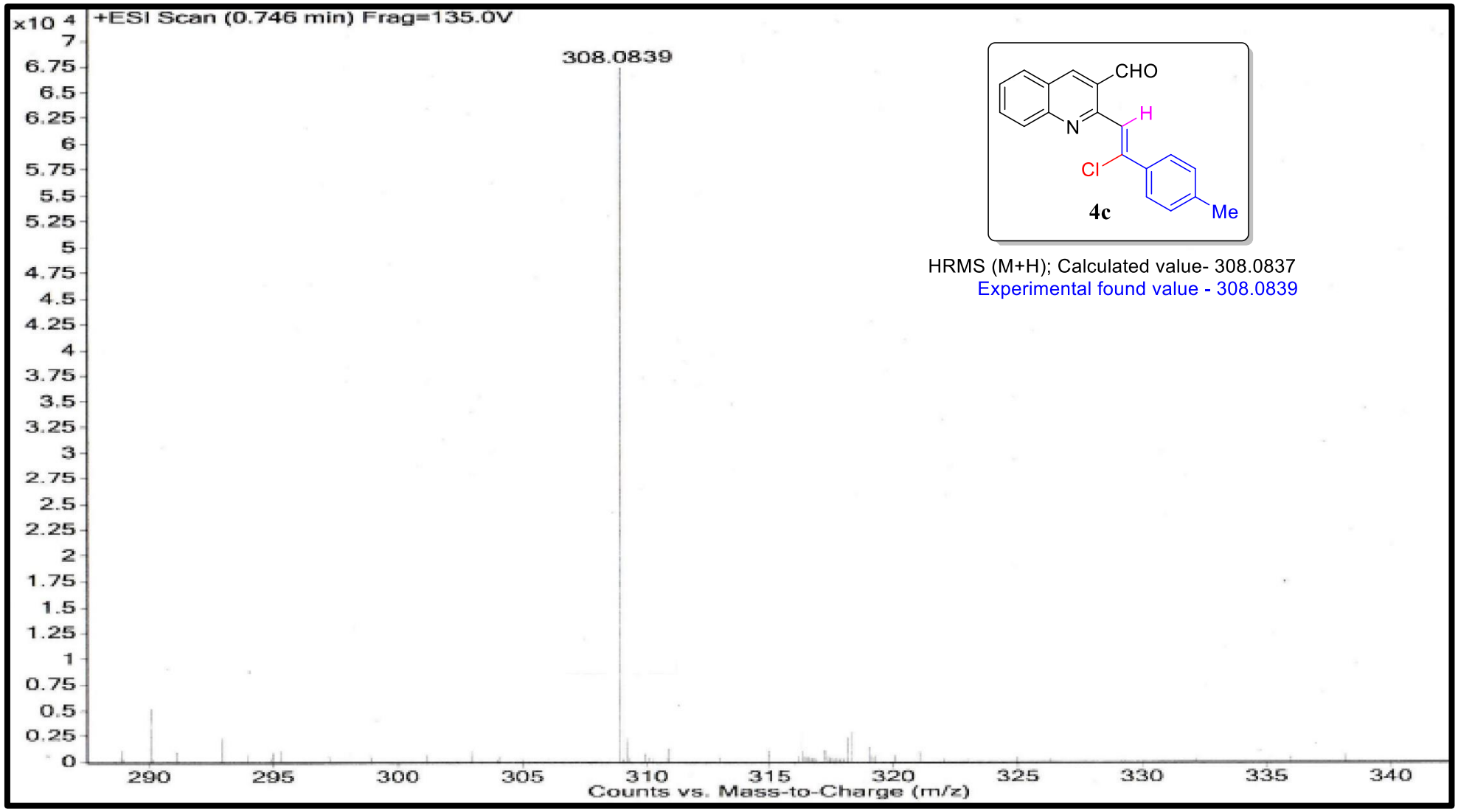


HRMS spectrum of 2-(2-Chloro-2-m-tolylvinyl)quinoline-3-carbaldehyde (4b)



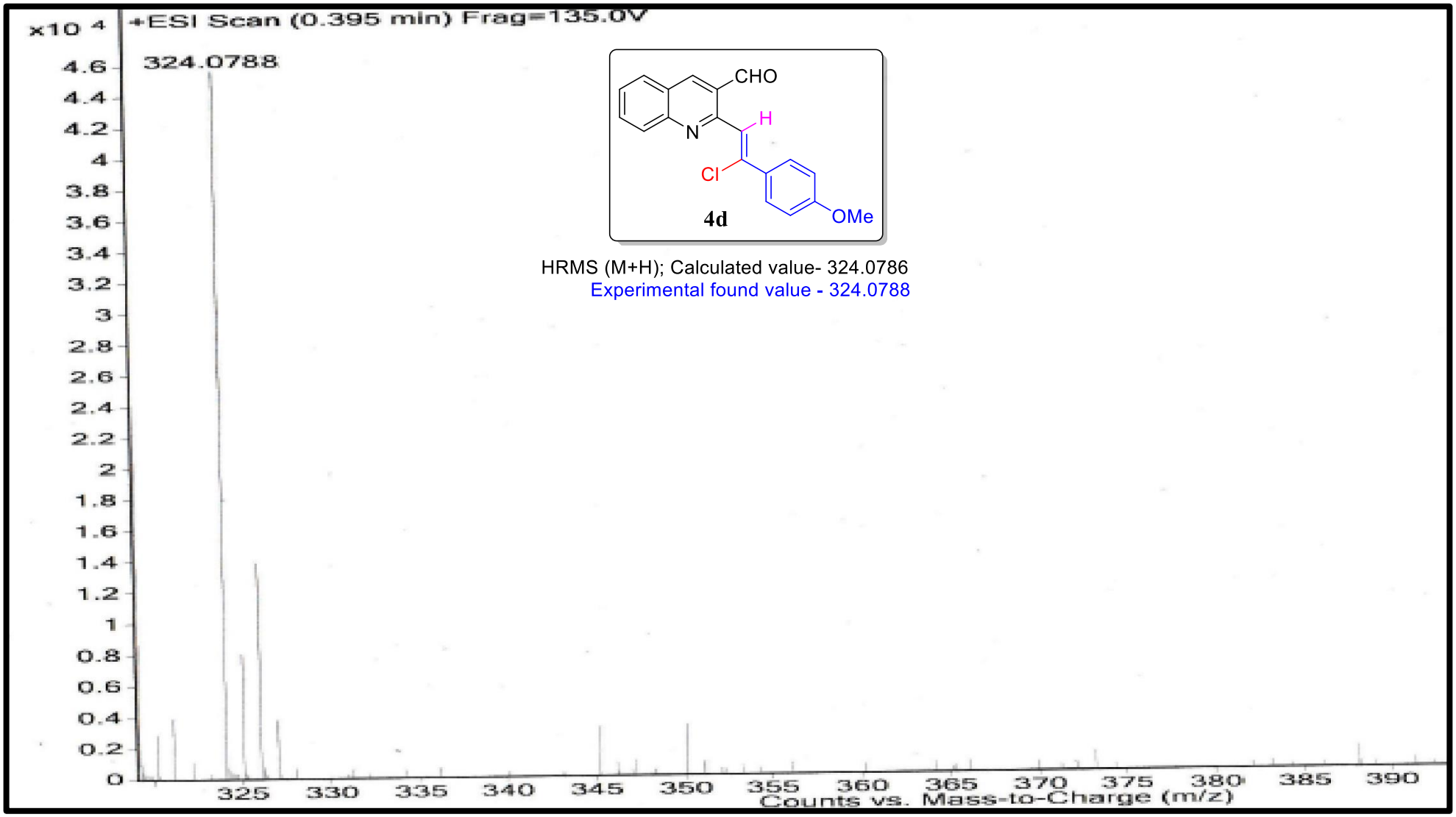
HRMS (M+H); Calculated value- 308.0837
Experimental found value - 308.0844

HRMS spectrum of 2-(2-Chloro-2-p-tolylvinyl)quinoline-3-carbaldehyde (4c)



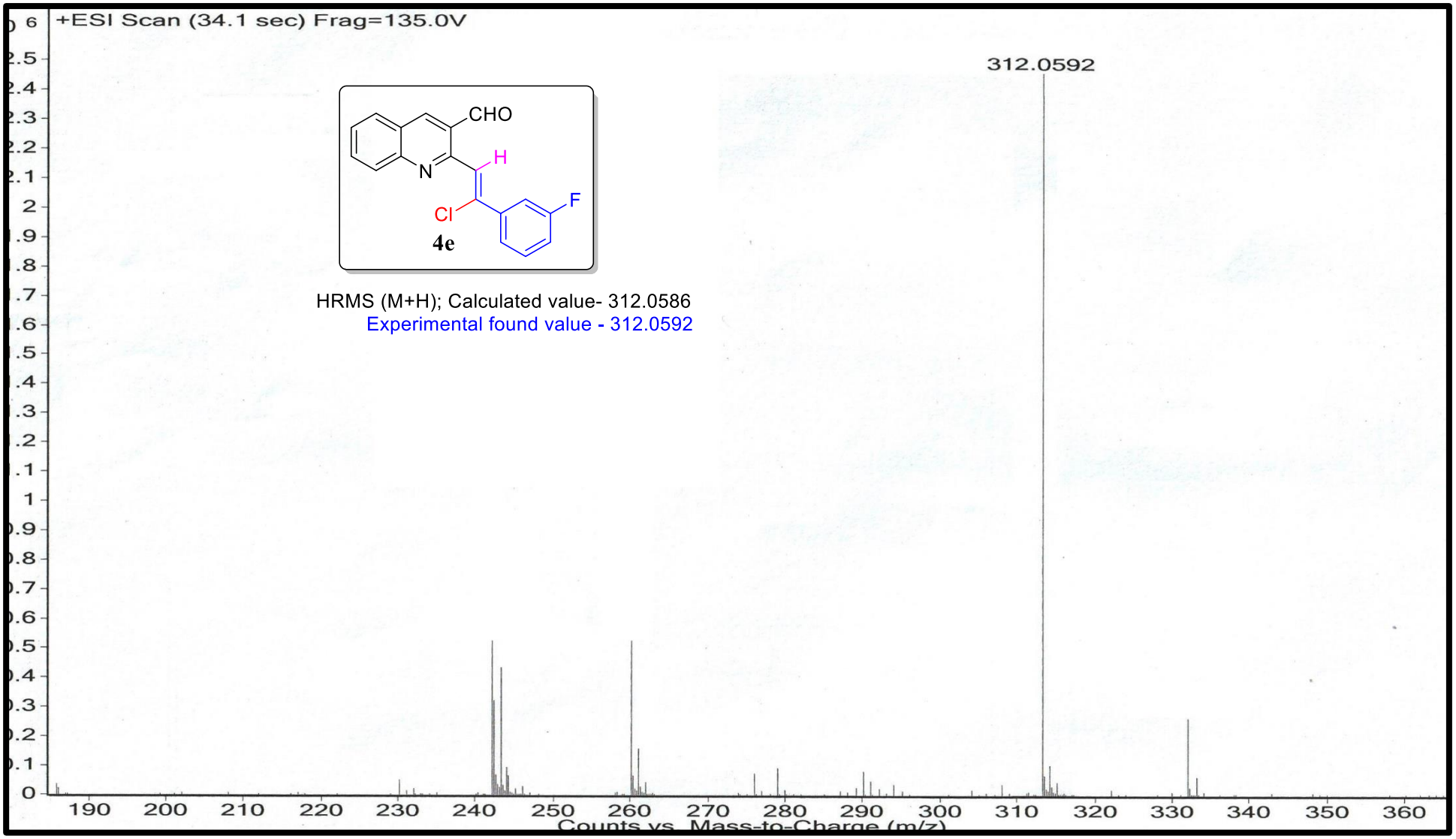
HRMS (M+H); Calculated value- 308.0837
Experimental found value - 308.0839

HRMS spectrum of 2-[2-Chloro-2-(4-methoxy-phenyl)vinyl]quinoline-3-carbaldehyde (4d)

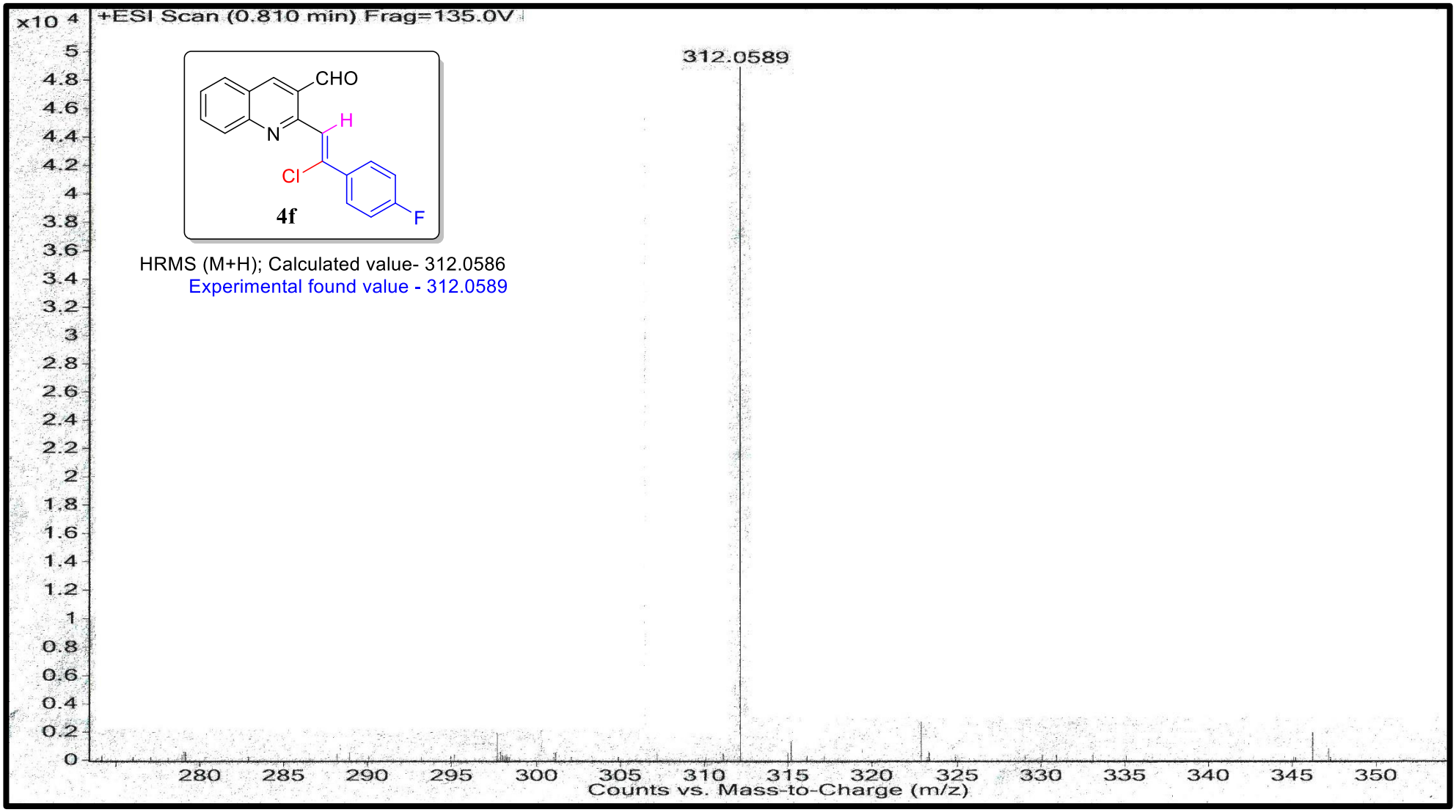


HRMS (M+H); Calculated value- 324.0786
Experimental found value - 324.0788

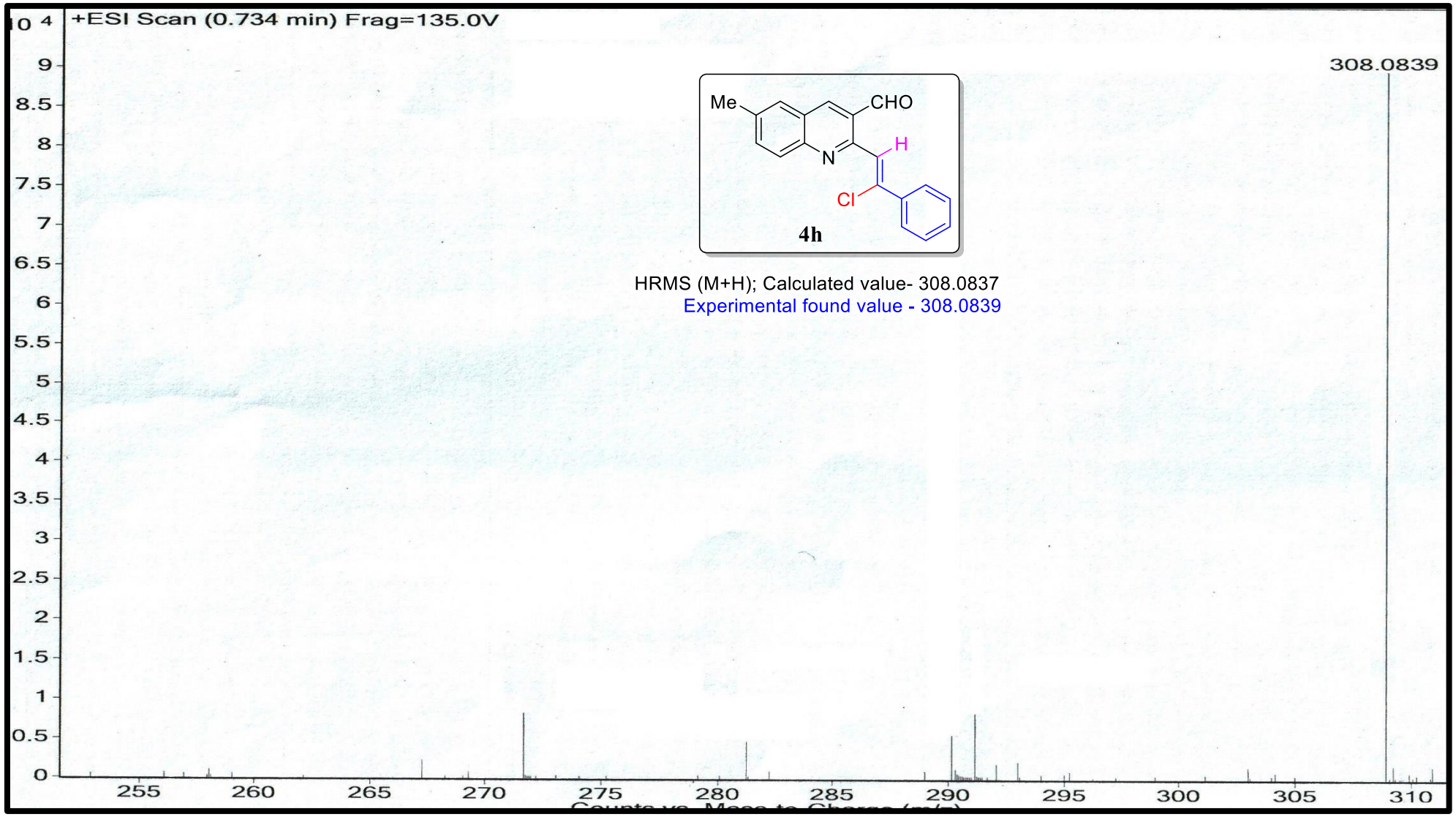
HRMS spectrum of 2-(2-chloro-2-(3-fluorophenyl)vinyl)quinoline-3-carbaldehyde (4e)



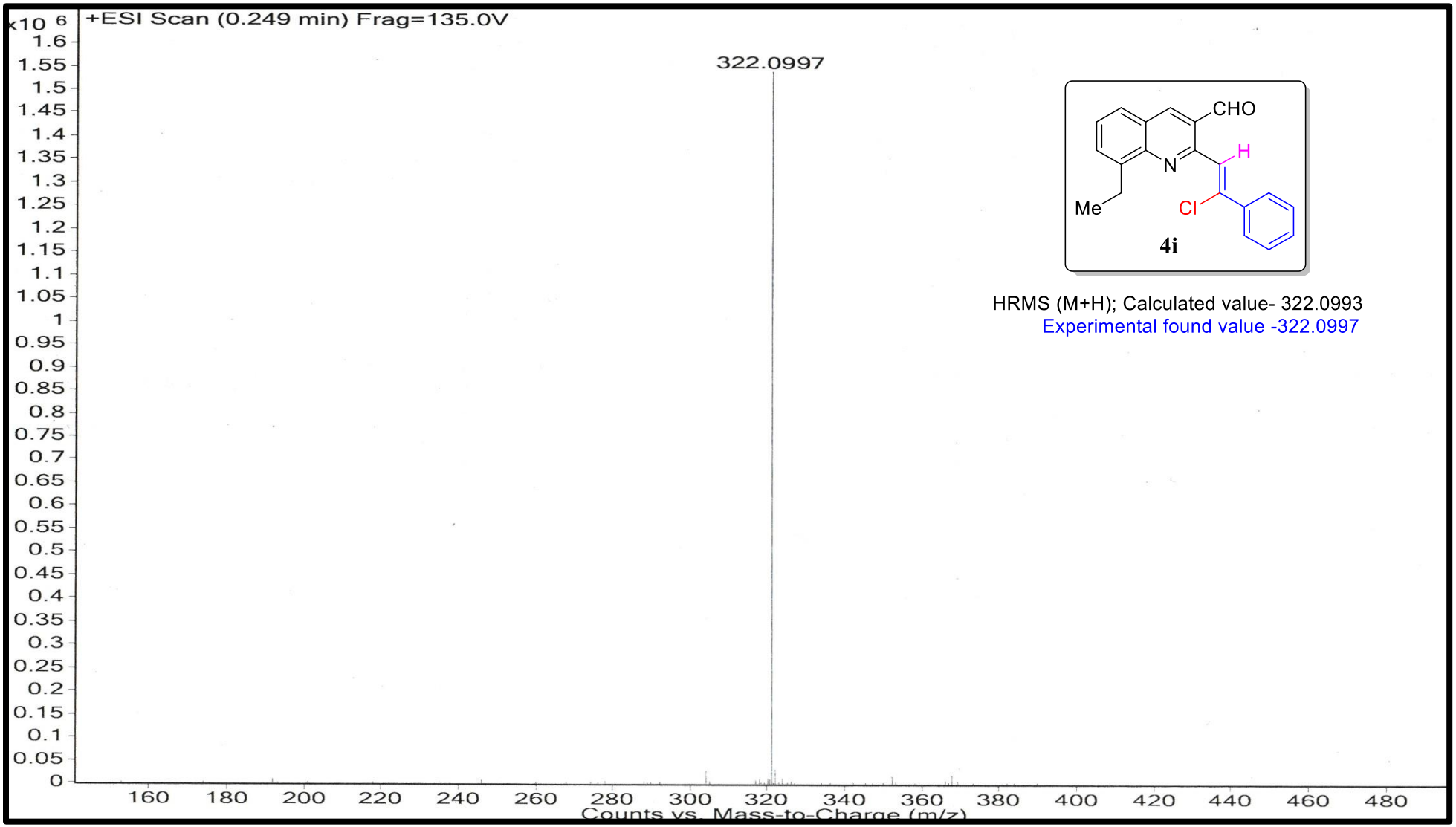
HRMS spectrum of 2-[2-Chloro-2-(4-fluoro-phenyl)vinyl]quinoline-3-carbaldehyde (4f)



HRMS spectrum of 2-(2-Chloro-2-phenylvinyl)-7-methyl-quinoline-3-carbaldehyde (4h)

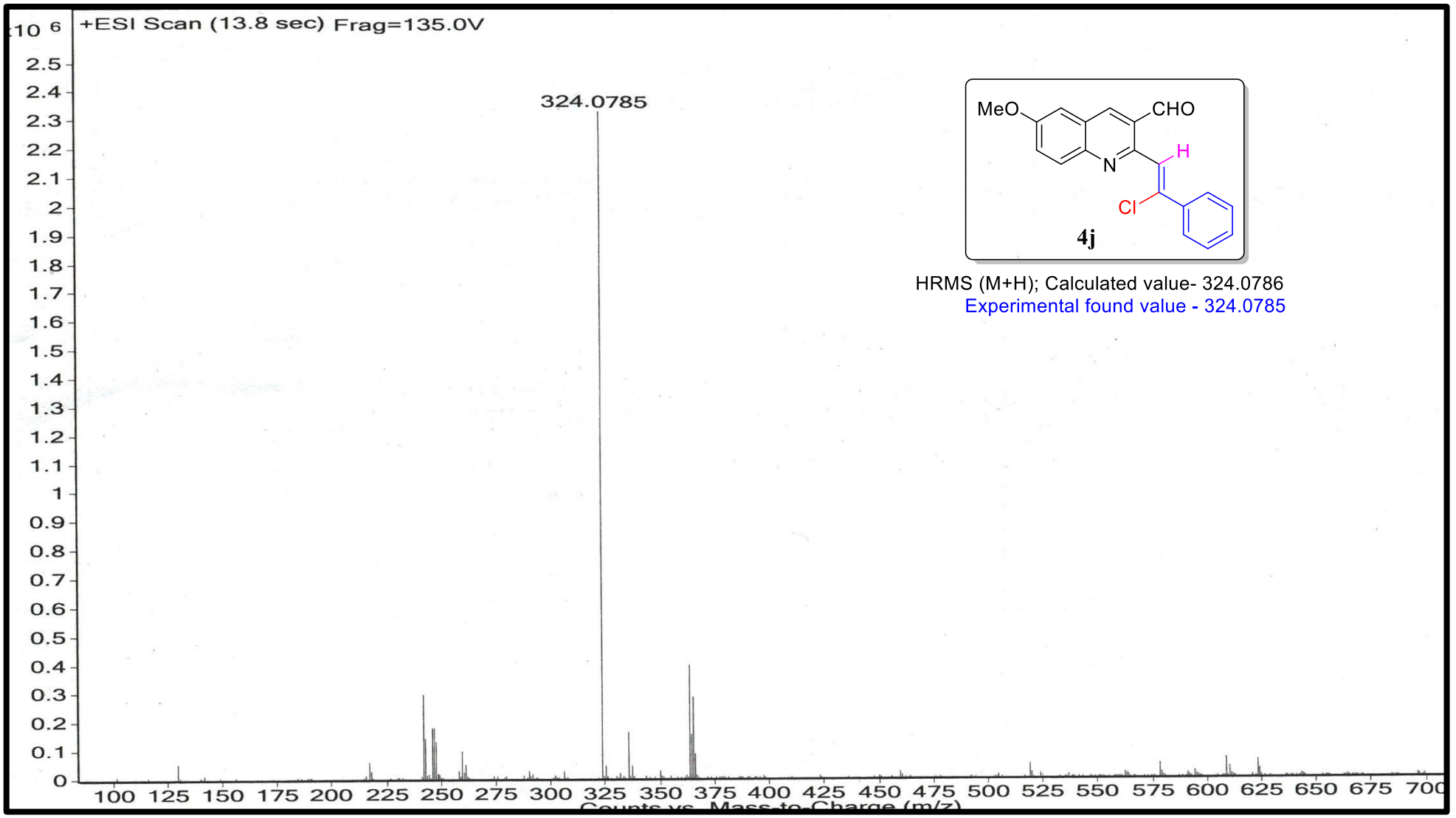


HRMS spectrum of 2-(2-Chloro-2-phenylvinyl)-8-ethyl-quinoline-3-carbaldehyde (4i)



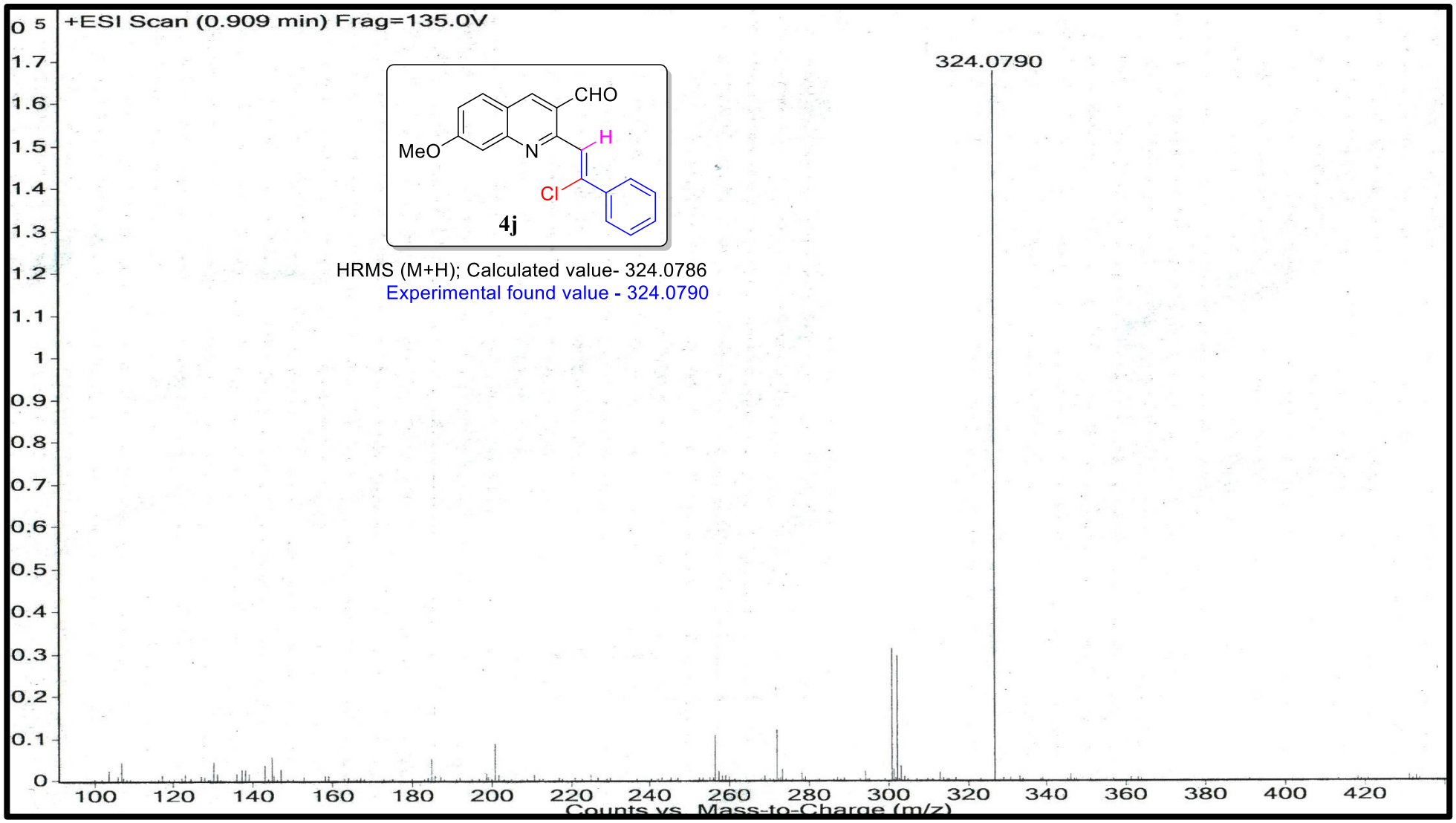
HRMS (M+H); Calculated value- 322.0993
Experimental found value -322.0997

HRMS spectrum of 2-(2-Chloro-2-phenylvinyl)-6-methoxy-quinoline-3-carbaldehyde (4j).

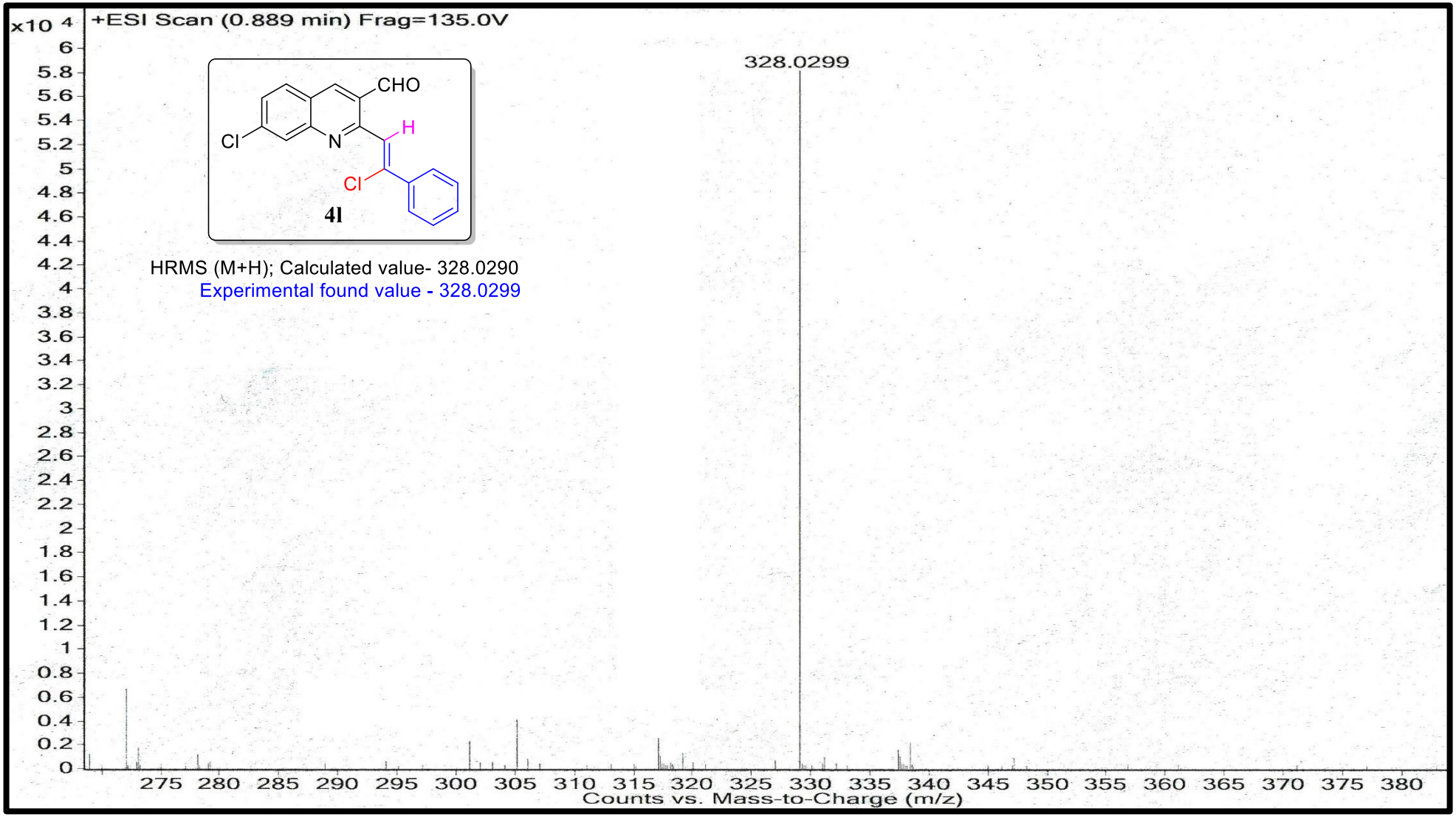


HRMS (M+H); Calculated value- 324.0786
Experimental found value - 324.0785

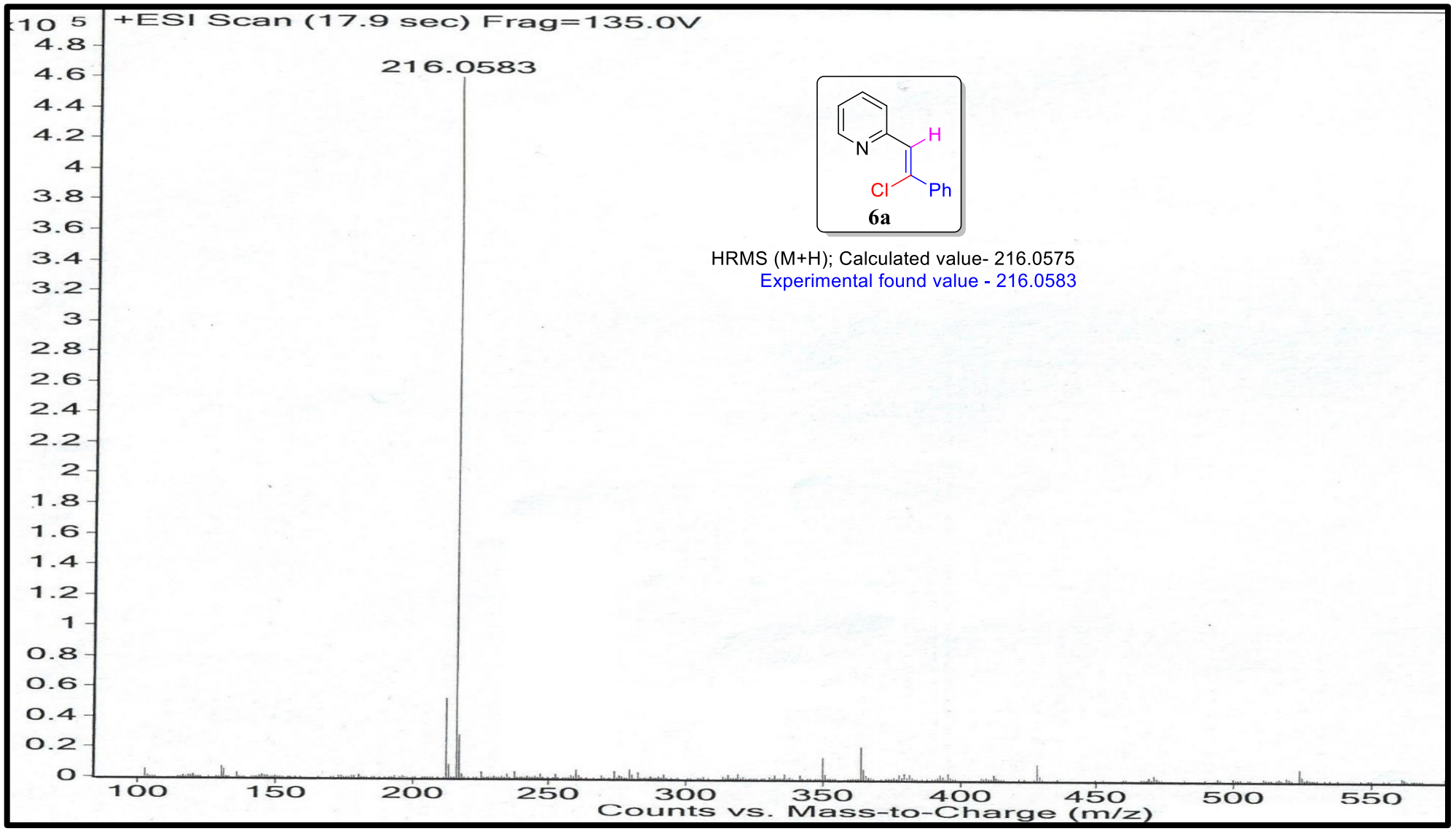
HRMS spectrum of 2-(2-Chloro-2-phenylvinyl)-7-methoxy-quinoline-3-carbaldehyde (4k)



HRMS spectrum of 7-Chloro-2-(2-chloro-2-phenylvinyl)-quinoline-3-carbaldehyde (4l)

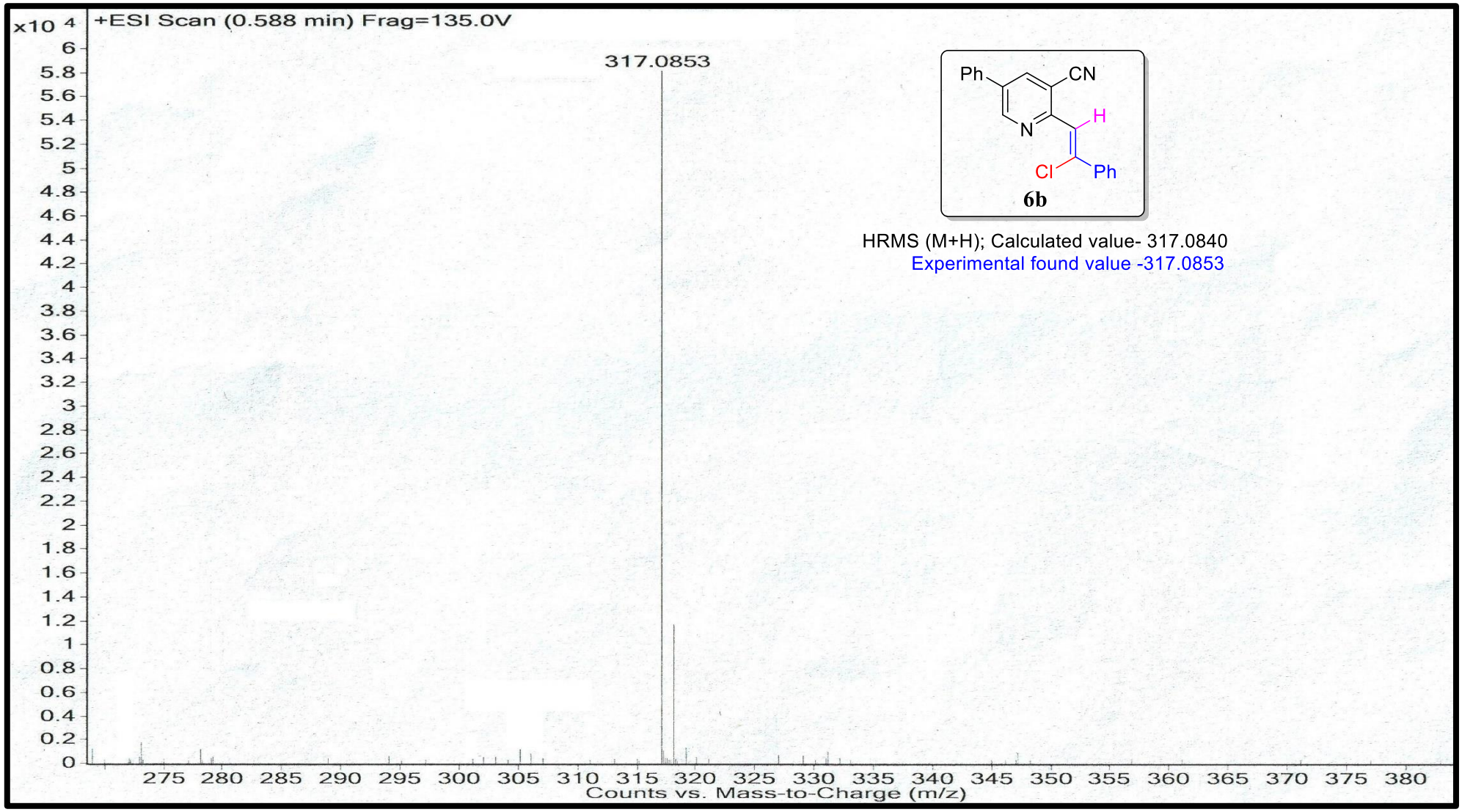


HRMS spectrum of 2-(2-chloro-2-phenylvinyl)pyridine (6a)

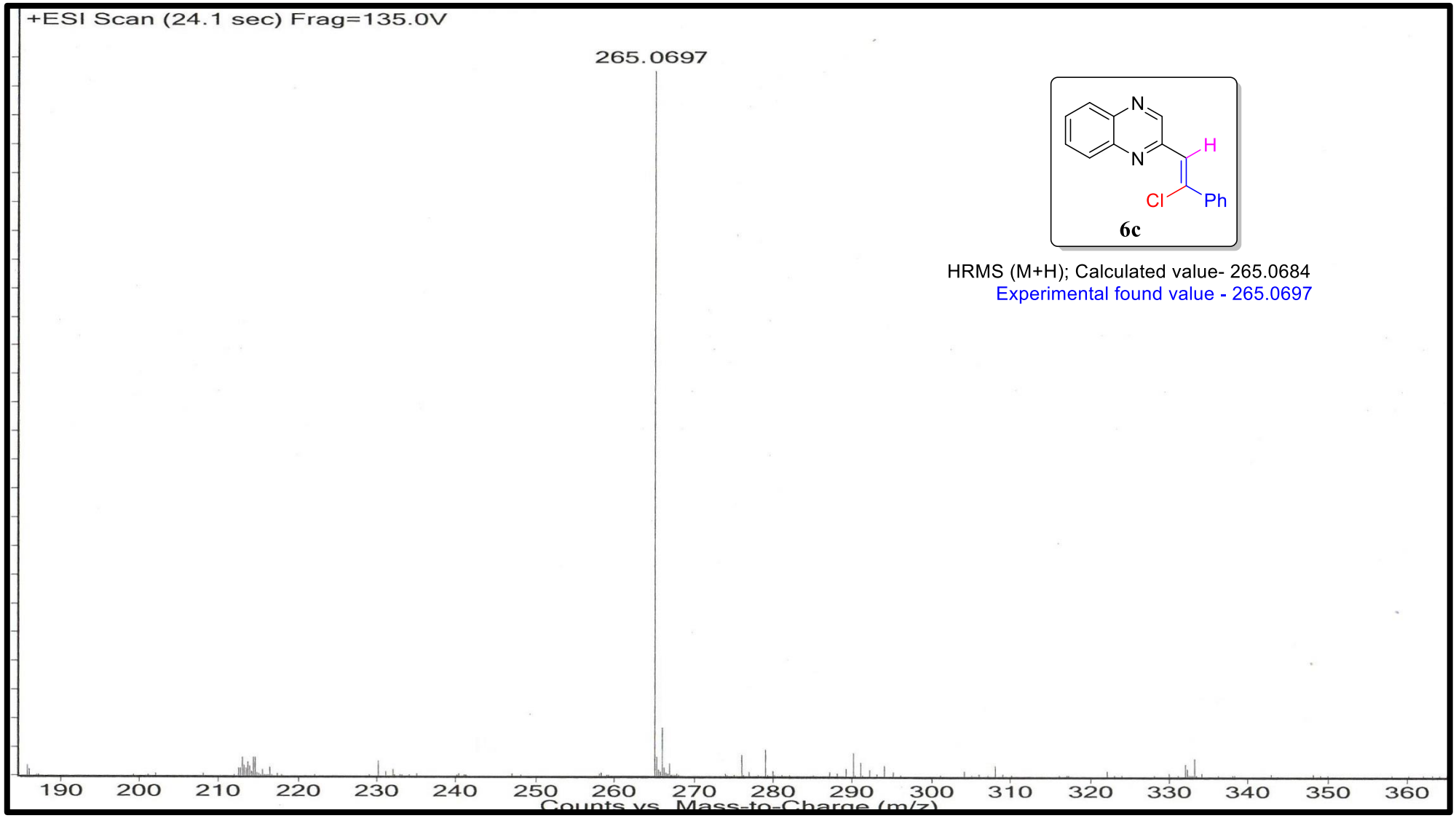


HRMS (M+H); Calculated value- 216.0575
Experimental found value - 216.0583

HRMS spectrum of 2-(2-chloro-2-phenylvinyl)-5-phenylnicotinonitrile (6b)

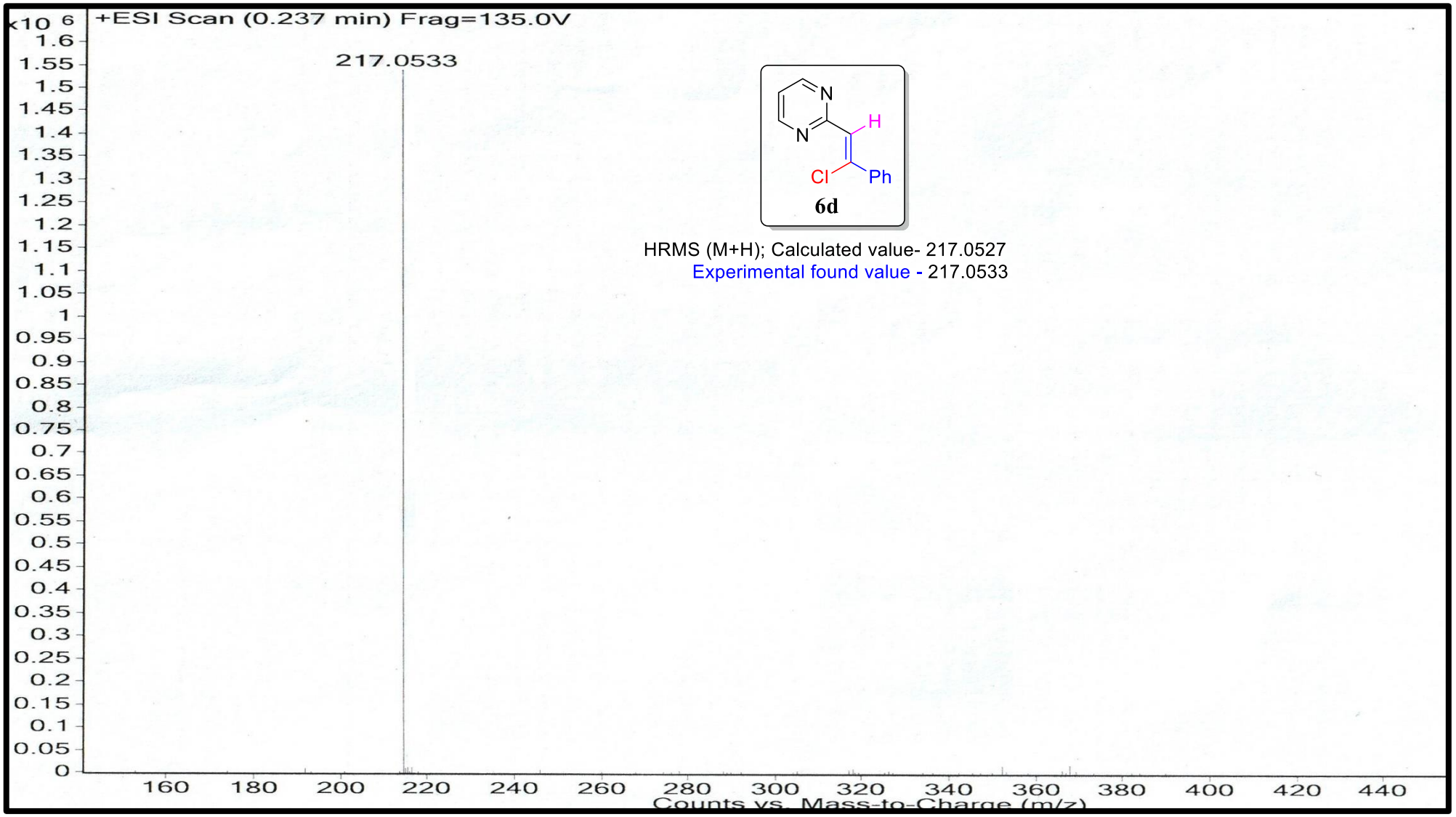


HRMS spectrum of 2-(2-chloro-2-phenylvinyl)quinoxaline (6c)



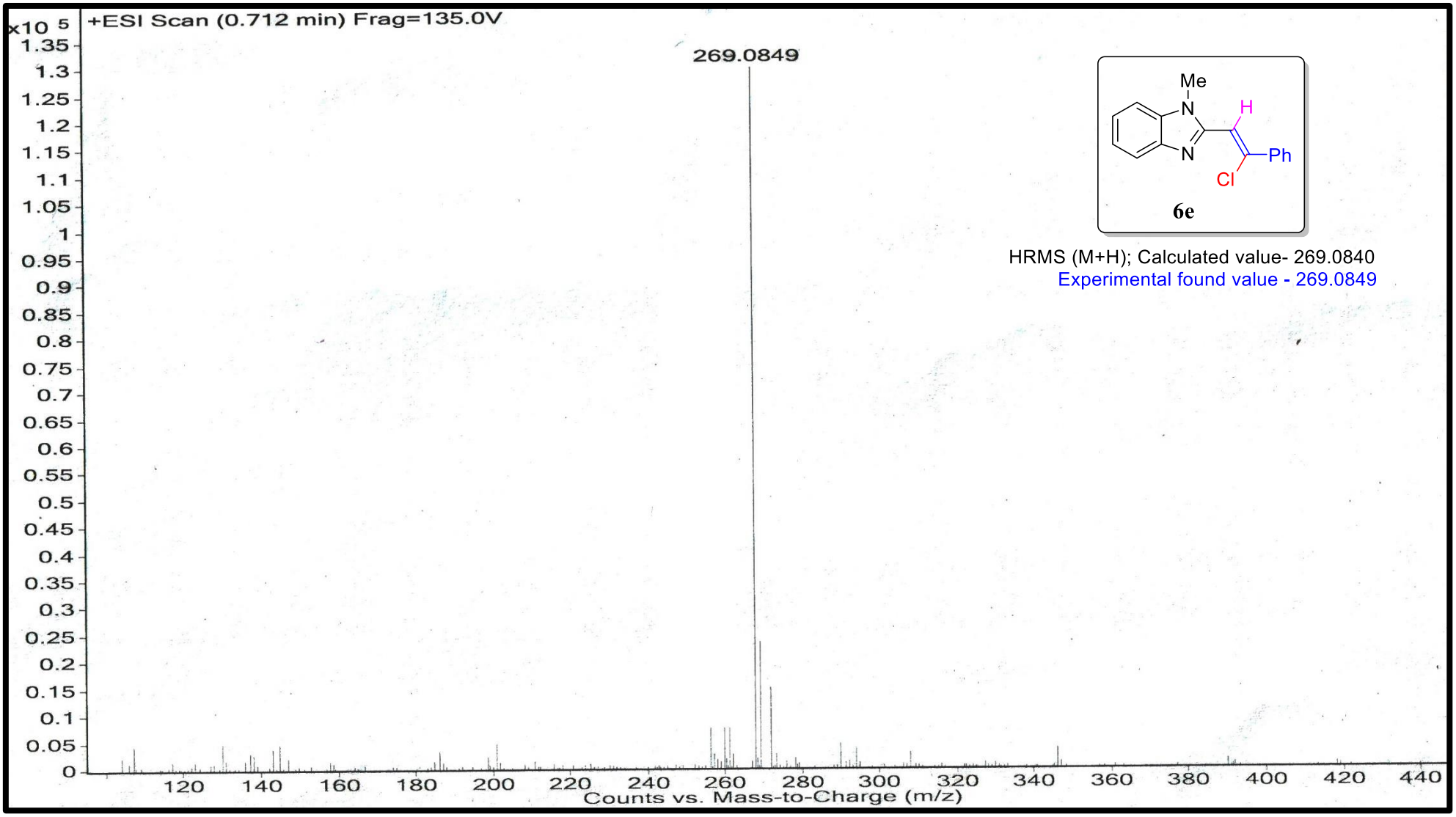
HRMS (M+H); Calculated value- 265.0684
Experimental found value - 265.0697

HRMS spectrum of 2-(2-chloro-2-phenylvinyl)pyrimidine (6d)

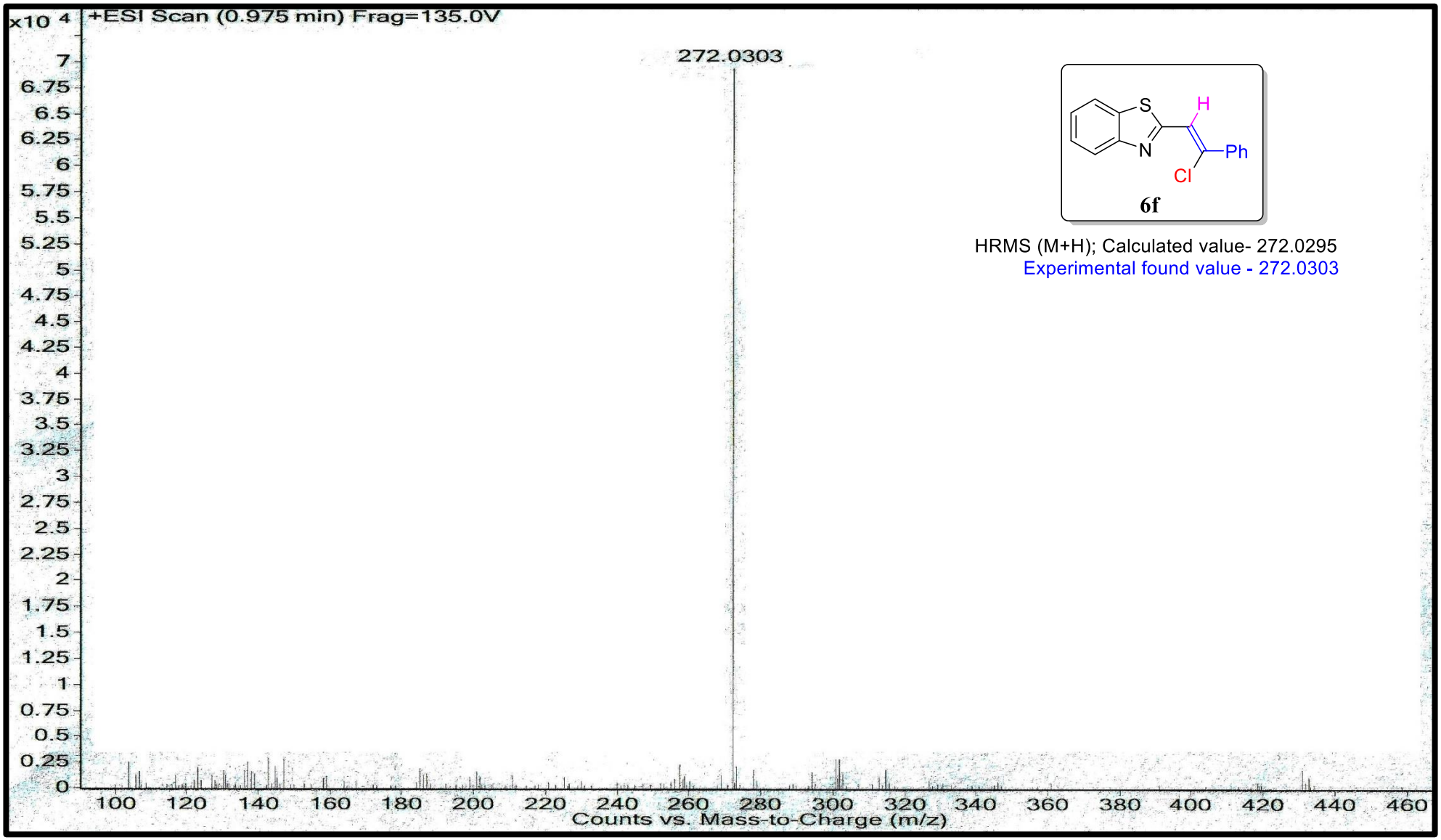


HRMS (M+H); Calculated value- 217.0527
Experimental found value - 217.0533

HRMS spectrum of 2-(2-chloro-2-phenylvinyl)-1-methyl-1H-benzo[d]imidazole (6e)

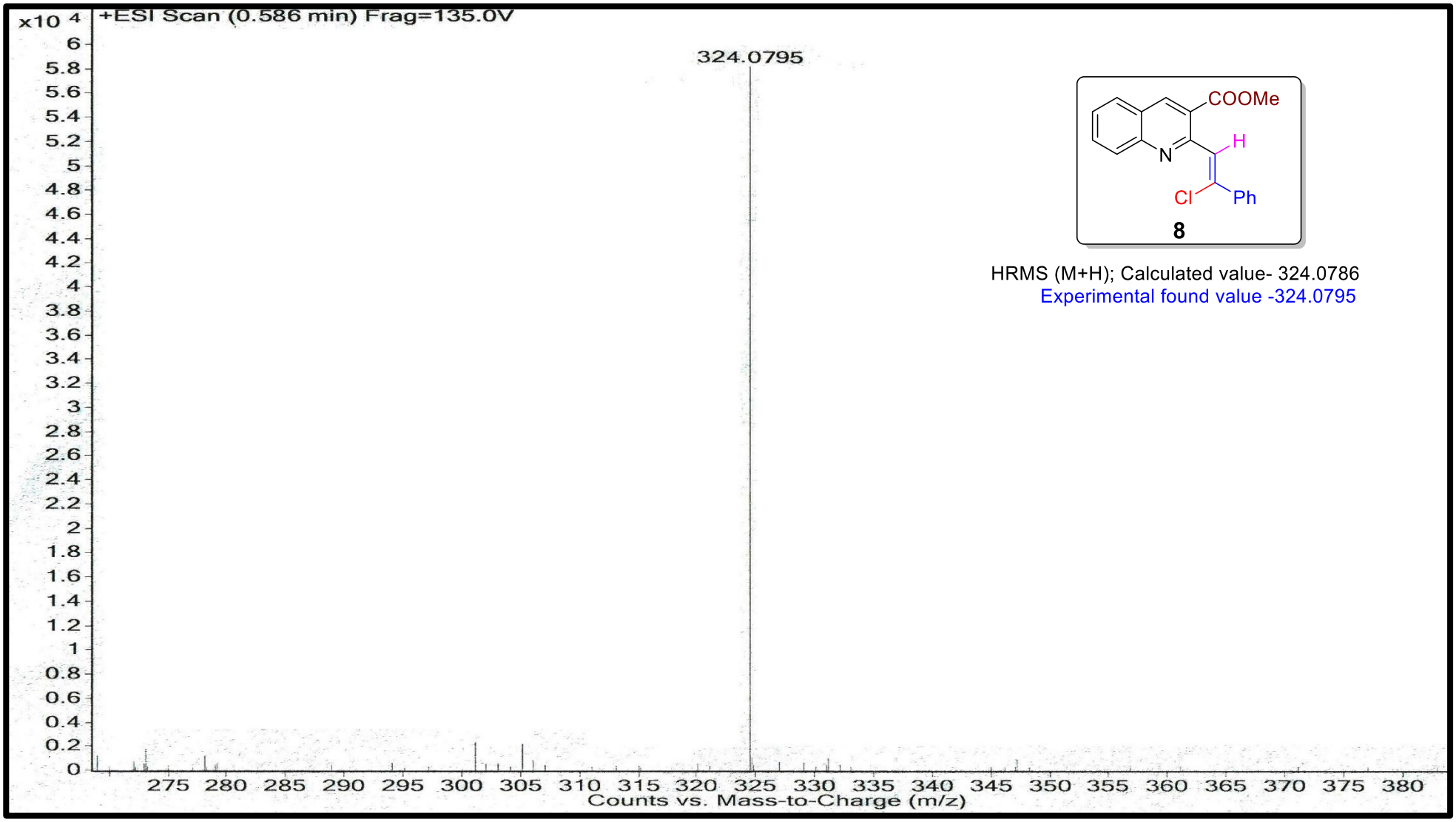


HRMS spectrum of 2-(2-chloro-2-phenylvinyl)benzo[d]thiazole (6f)



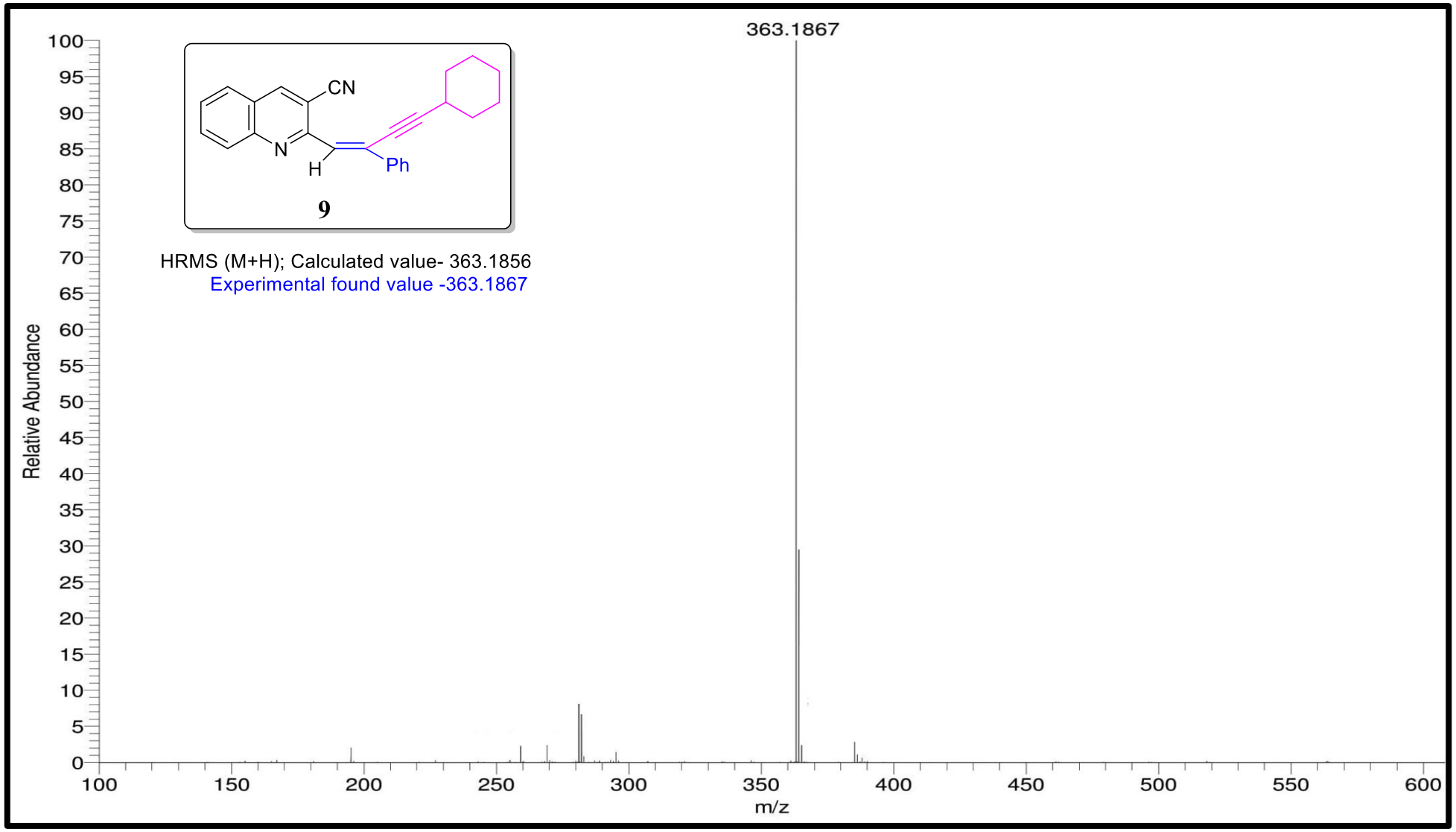
HRMS (M+H); Calculated value- 272.0295
Experimental found value - 272.0303

HRMS spectrum of 2-(2-Chloro-2-phenylvinyl)-quinoline-3-carboxylic acid methyl ester (8)

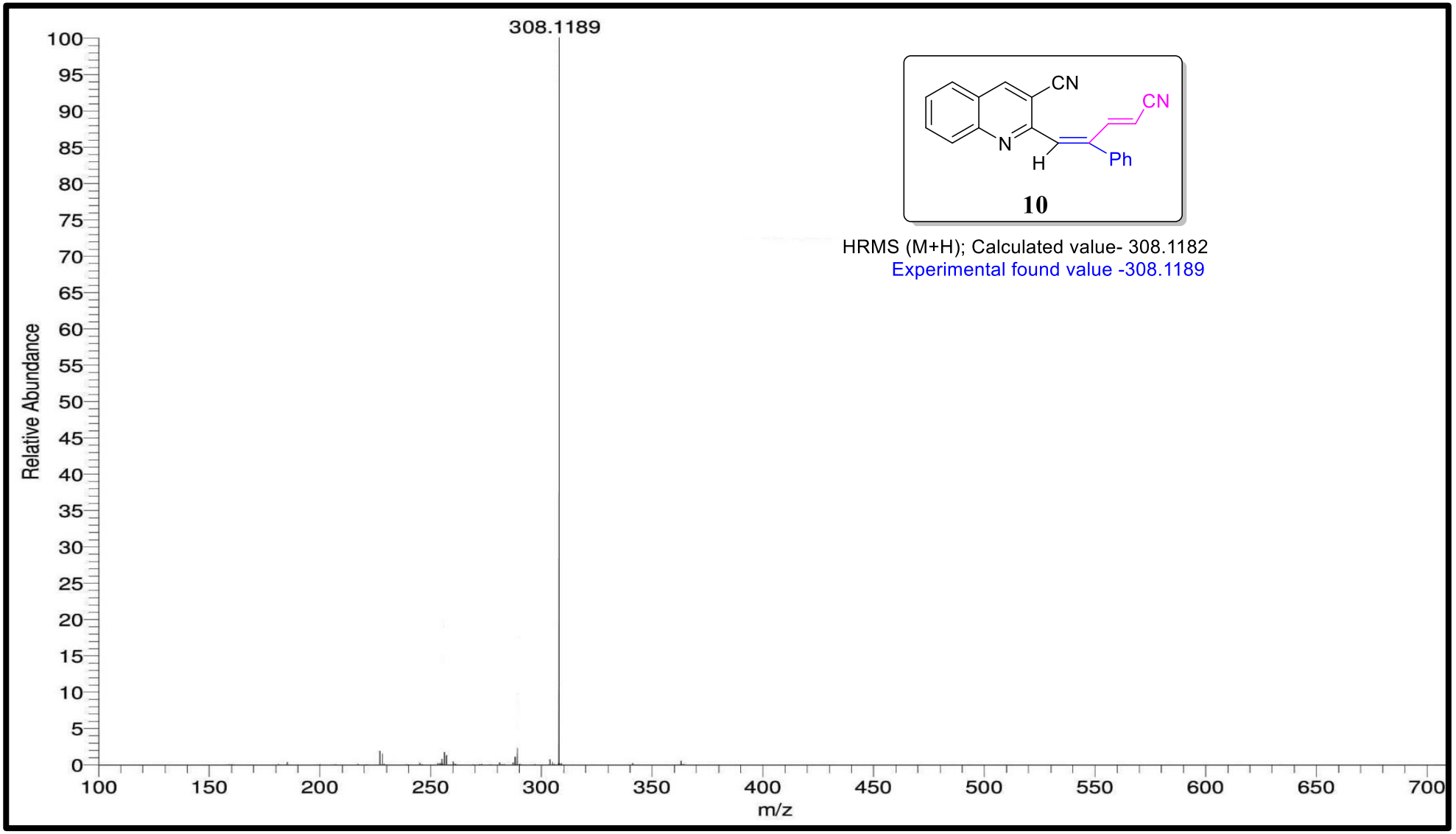


HRMS (M+H); Calculated value- 324.0786
Experimental found value -324.0795

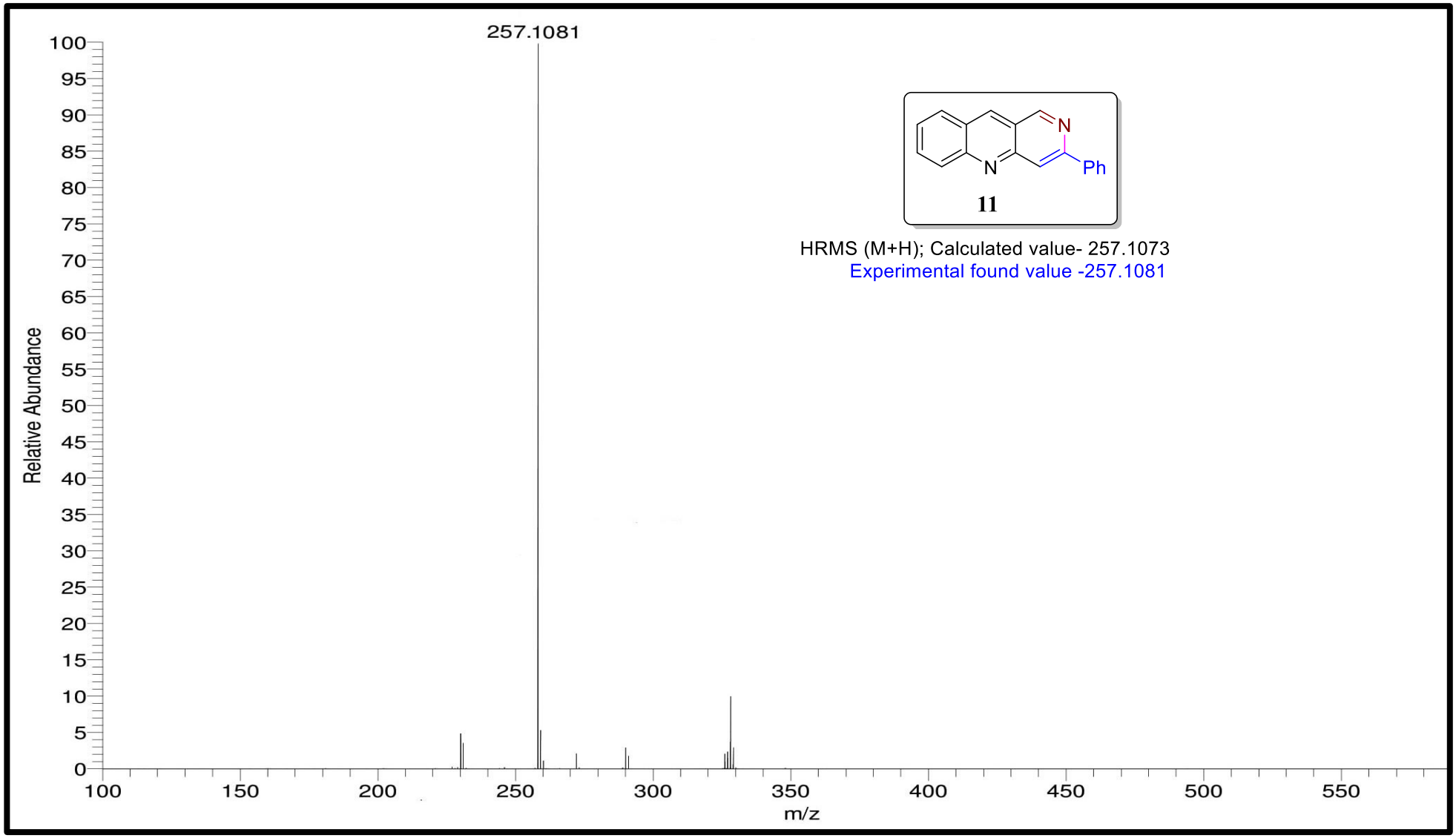
HRMS spectrum of 2-(4-cyclohexyl-2-phenyl-but-1-en-3-ynyl)-quinoline-3-carbonitrile (9)



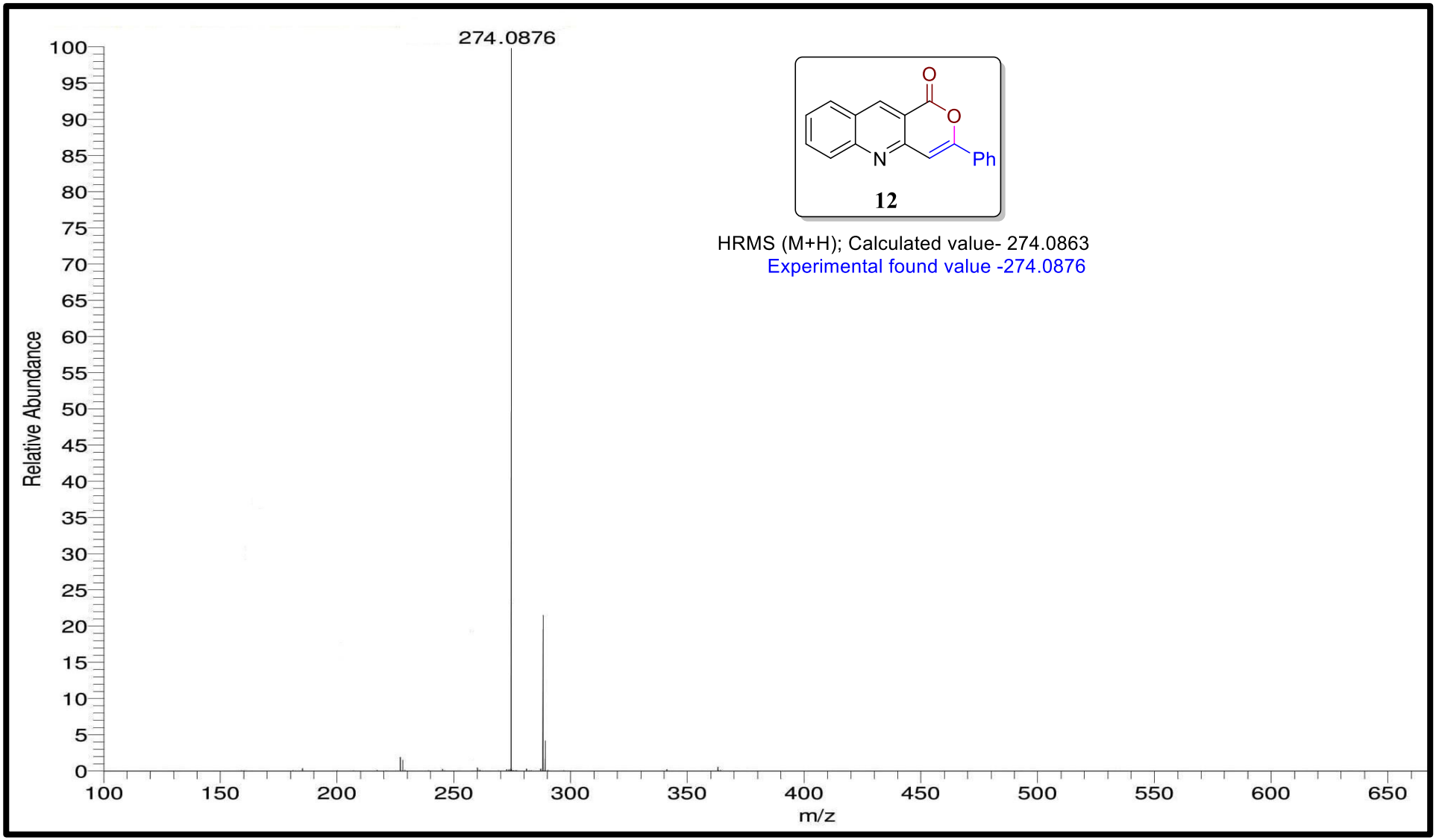
HRMS spectrum of 2-(4-cyano-2-phenyl-buta-1,3-dienyl)-quinoline-3-carbonitrile (10)



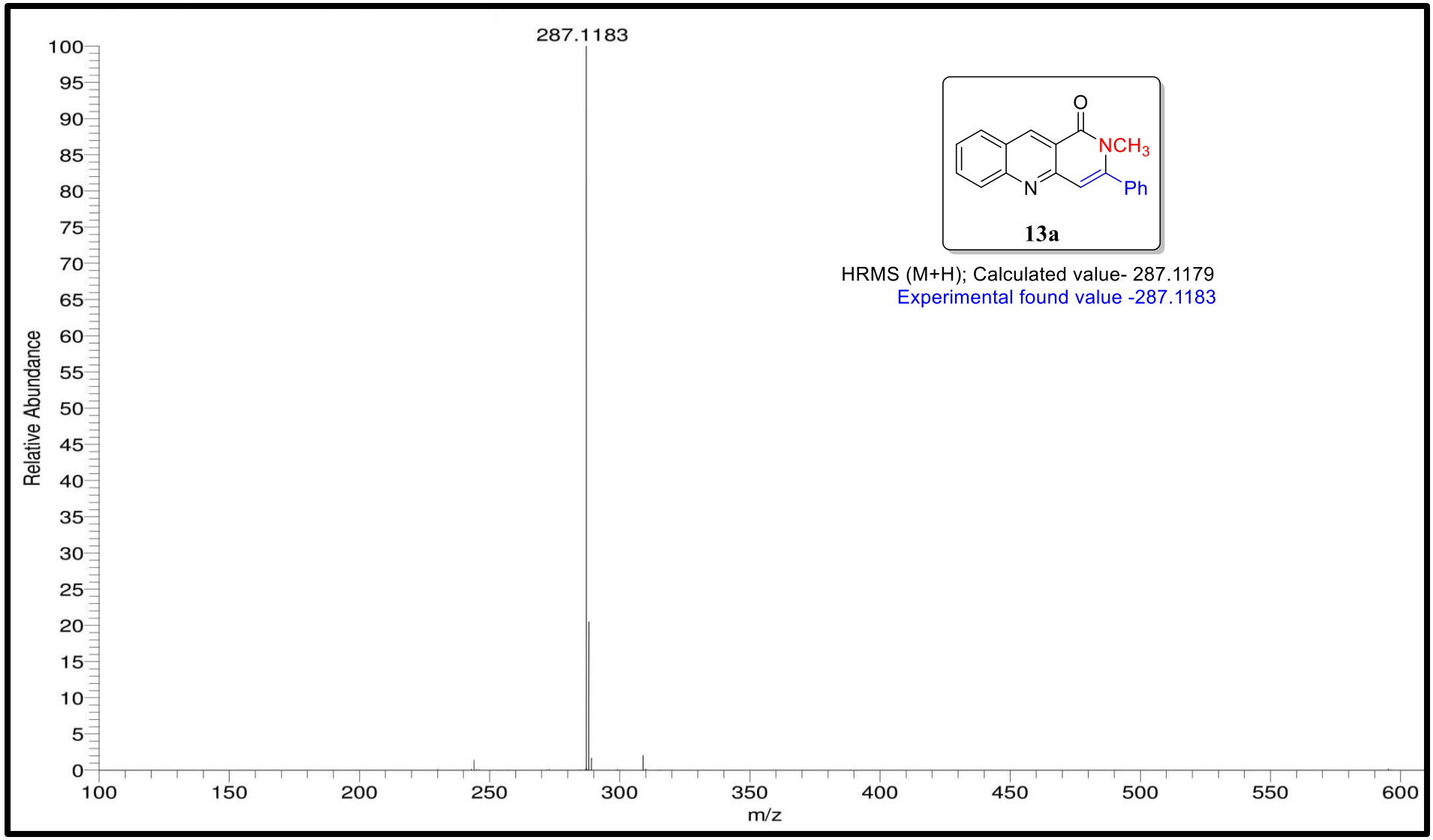
HRMS spectrum of 3-phenylbenzo[b][1,6]naphthyridine (11)



HRMS spectrum of 3-phenyl-1H-pyrano[4,3-b]quinolin-1-one (12)

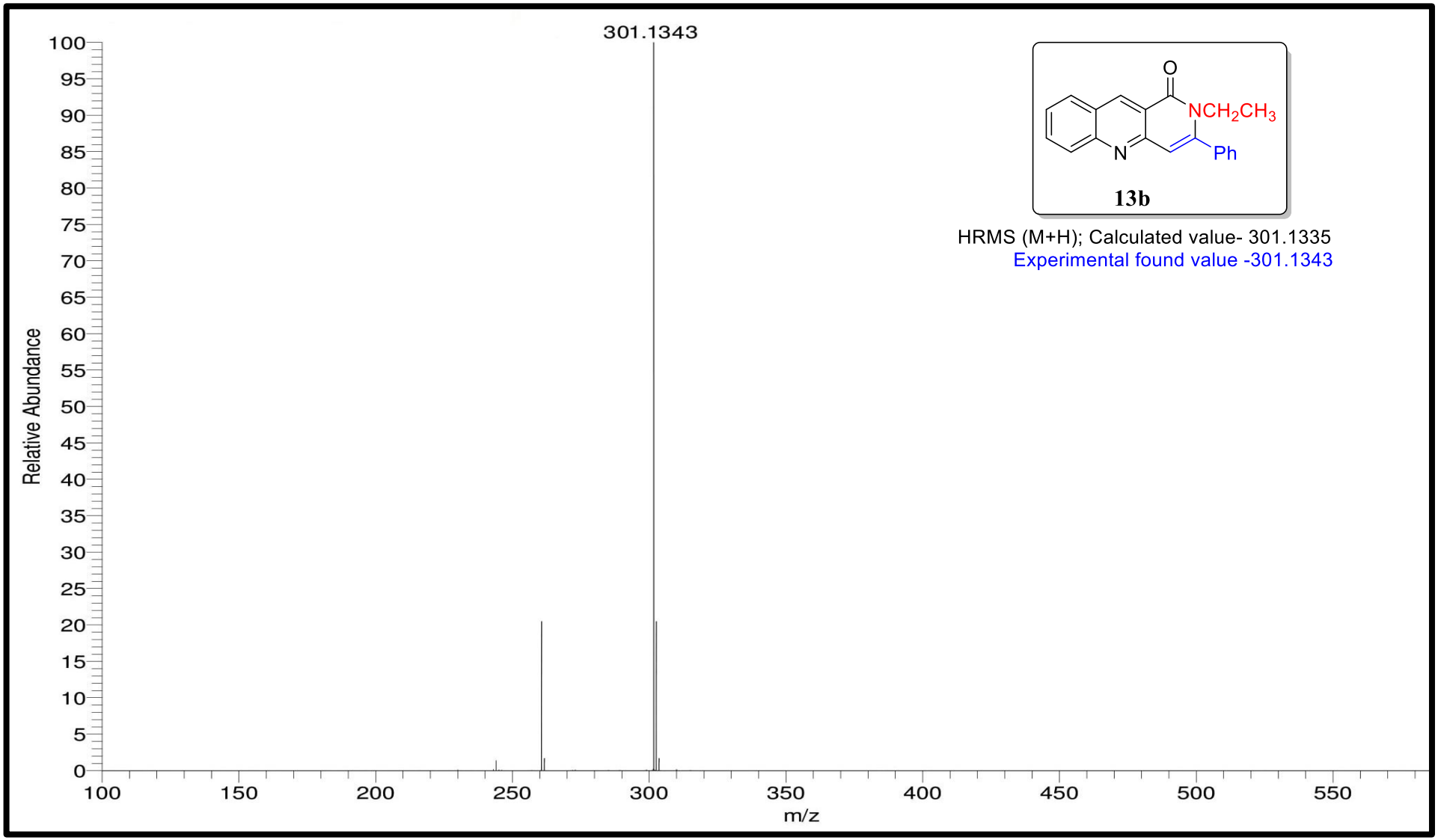


HRMS spectrum of N-methyl-3-phenyl-2H-benzo[b][1,6]naphthyridin-1-one (13a)



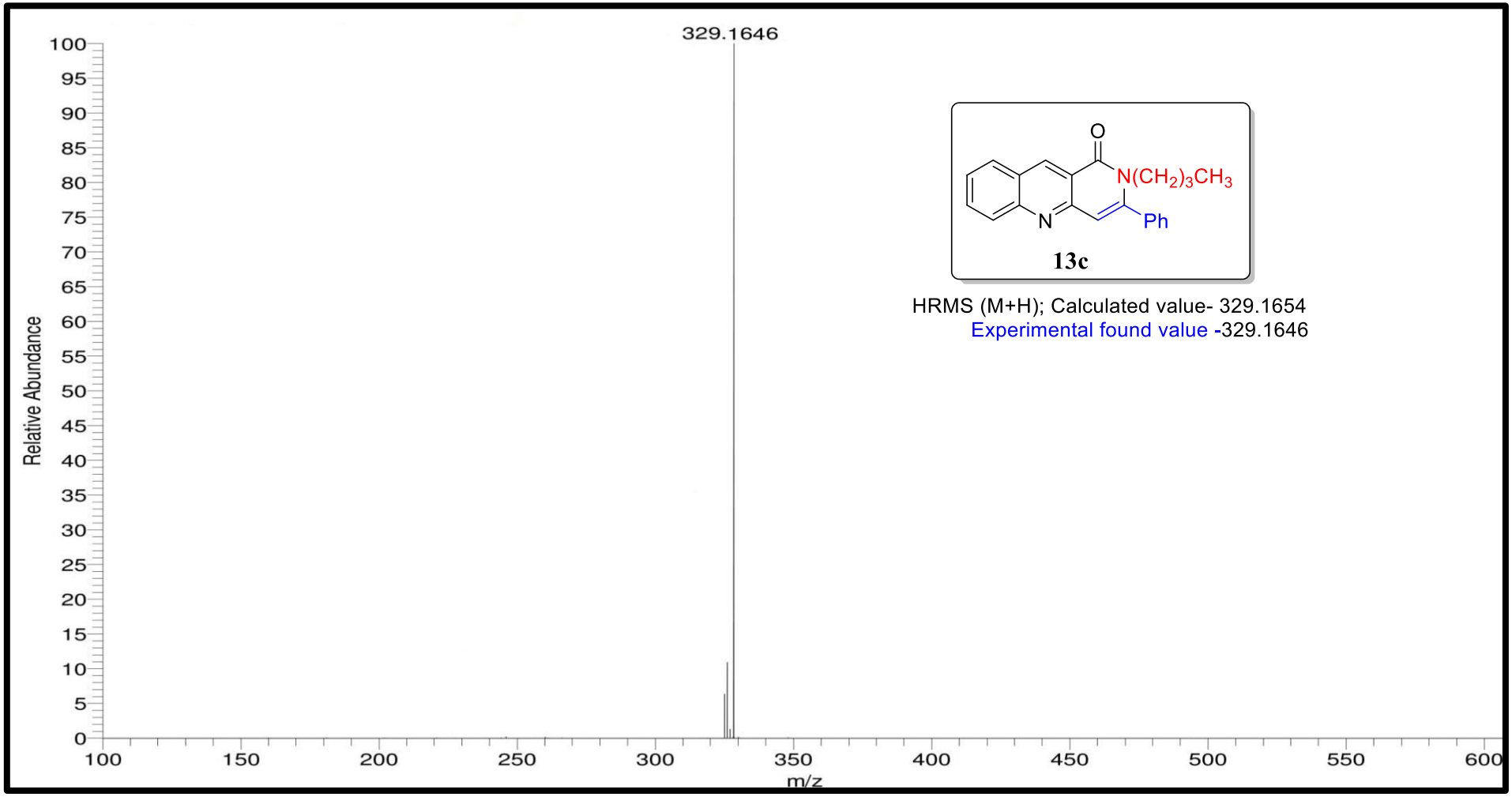
HRMS (M+H); Calculated value- 287.1179
Experimental found value -287.1183

HRMS spectrum of N-Ethyl-3-phenylbenzo[b][1,6]naphthyridin-1(2H)-one (13b)



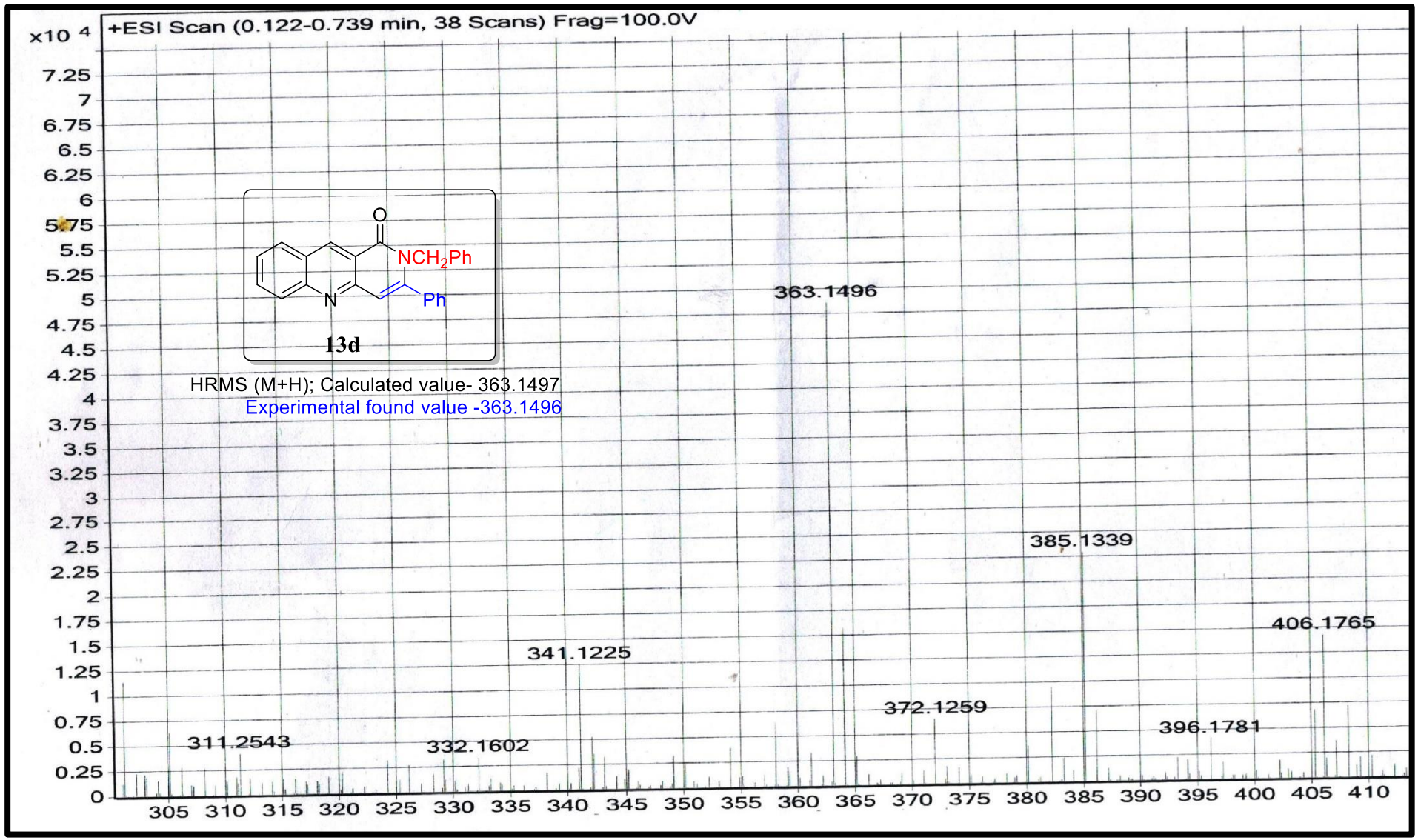
HRMS (M+H); Calculated value- 301.1335
Experimental found value -301.1343

HRMS spectrum of N-Butyl-3-phenylbenzo[b][1,6]naphthyridin-1(2H)-one (13c)

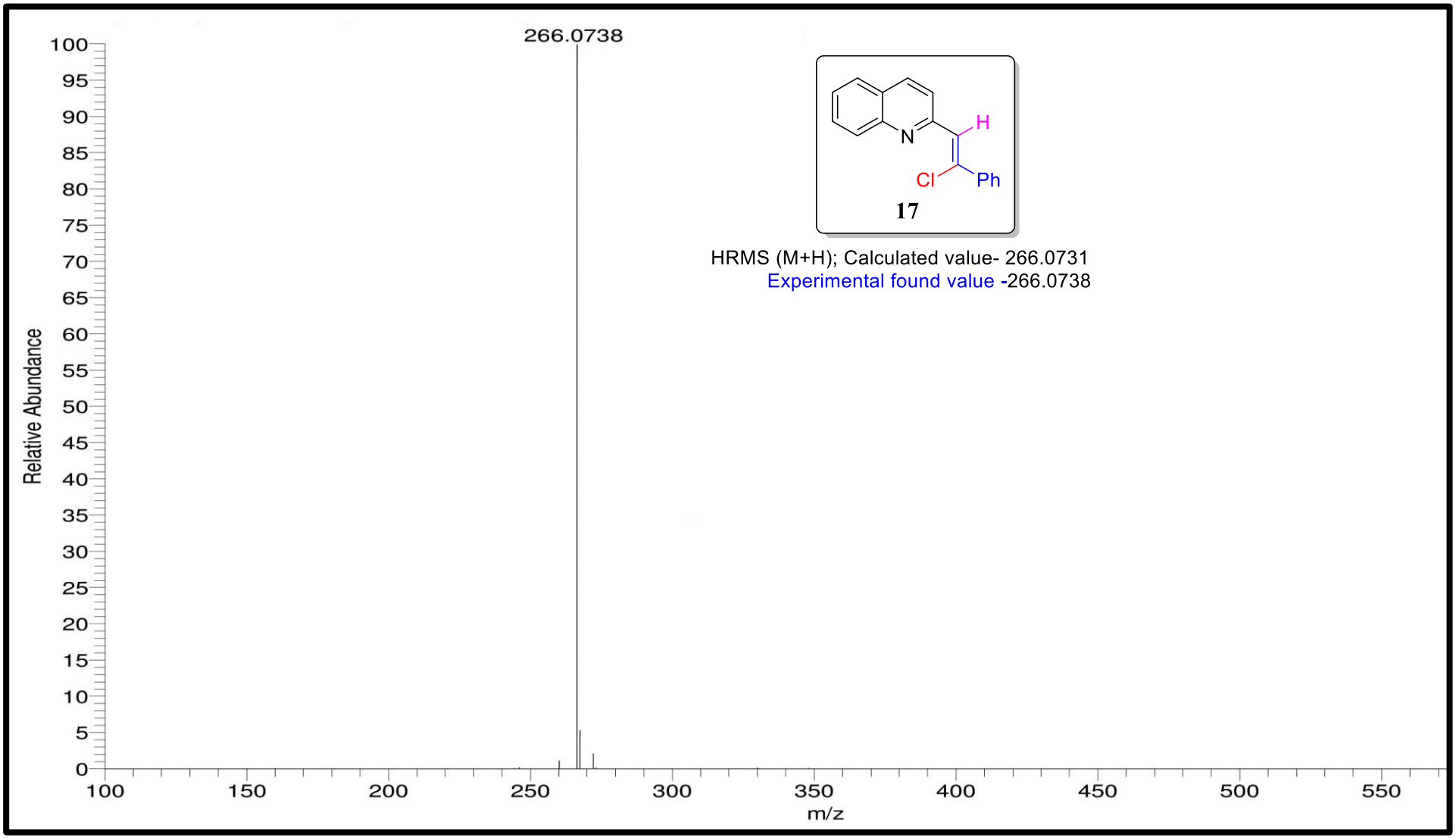


HRMS (M+H); Calculated value- 329.1654
Experimental found value -329.1646

HRMS spectrum of N-Benzyl-3-phenyl-2H-benzo[b][1,6]naphthyridin-1-one (13d)



HRMS spectrum of 2-(2-chloro-2-phenylvinyl)quinoline (17)



HRMS (M+H); Calculated value- 266.0731
Experimental found value -266.0738