Recyclable, Magnetic Ionic Liquid bmim$FeCl_4$ catalyzed Multicomponent, Solvent-free, Green Synthesis of quinazolines

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Electronic Supplementary Information

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1. General Information.

All the starting materials were commercially available (from Sigma Aldrich) and used as received without further purification. Infrared (FTIR) spectra were measured on Varian-3100 FT IR spectrophotometer using KBr plate, and wavelengths ($\tilde{\upsilon}$) are reported in cm^{-1}. ^{1}H and ^{13}C NMR spectra were recorded on JEOL AL-300 FT NMR spectrometer. Chemical shifts (δ) are given in parts per million (ppm) using the residue solvent peaks as reference relative to TMS. '*J*' values are given in Hz. Mass spectra were recorded at 70 eV ionizing voltage on a JEOL SX-102 spectrometer. Thin layer chromatographies (TLC) were performed using silica gel 60 F-254 precoated plates. Crystal data was collected on an OXFORD DIFFRACTION X CALIBER EoS diffractometer using graphite monochromatized Mo Ka radiation at 298 K. The structures were solved by direct methods and refined by full matrix least squares on F2 using SHELX-97. The non-hydrogen atoms were refined with anisotropic thermal parameters. All the hydrogen atoms were geometrically fixed and allowed to

refine using a riding model. The refinement converged to a final R1 and wR2. Drawings were made using ORTEP-III and Mercury.

2. Typical experimental procedure.

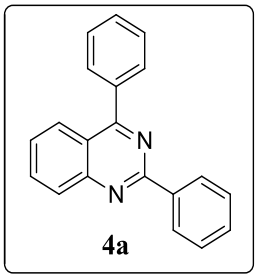
(a) Preparation of magnetic ionic liquid (bmim$FeCl_4$)

Butylmethylimidazoliumchloride (bmim[Cl]) (5.00g, 28.6 mmol) and $FeCl_3$, $6H_2O$ (7.74 g, 28.6 mmol) were taken in a round bottom flask and stirred for 10 minutes at room temperature. Immediately an endothermic reaction was occurred and bmim$FeCl_4$ was remained as a lower layer. After successful removal of the upper aqueous layer, bmim[$FeCl_4$] was collected from the lower layer. The ionic liquid (bmim[$FeCl_4$]) was dried under stirring for 3 day at 70 ˚C and 0.1 mm Hg to yield 8.85 g (~ 92%) of bmim$FeCl_4$ as brown oil. The ionic liquid was characterised via Raman spectroscopy and proved to be identical with authentic material reported in literature.[1]

(b) General procedure for synthesis of quinazoline derivatives and catalyst recycling

2-aminobenzophenone **1** (1 mmol), an aromatic aldehyde **2** (1 mmol), ammonium acetate (2.5 mmol) and bmim**[**$FeCl_4$**]** (0.05 mmol) were taken in a round bottom flask and was heated in an oil bath at 40 ^{0}C for the stipulated period of time till the completion of the reaction (monitored by TLC). After completion of the reaction, diethyl ether (3x20 ml) was added and the ethereal layer was decanted. The remaining residue is mainly pure catalyst (bmim**[**$FeCl_4$**]**). The recovered catalyst is dried in high vacuum and is subjected to another reaction as a catalyst, found to be as effective as the fresh one. Combined organic layer was evaporated and first washed several times with distilled water (3x20 ml) and after that ethanol (3x20 ml). The pure quinazoline derivatives are obtained.

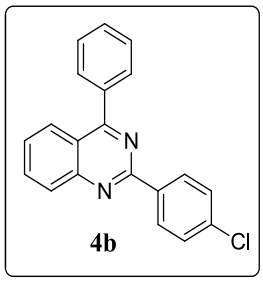
3. Characterization data of the isolated products (4a-4l)



4a

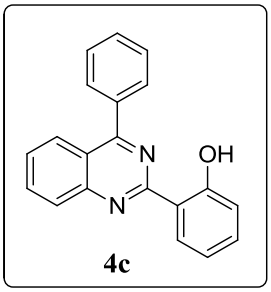
2, 4-Diphenyl-quinazoline (4a)

White solid; mp: 117.2 ˚C (lit.,[2a] 116-117 ˚C); IR (KBr, cm^{-1}): 1612, 1562, 1539, 1341, 872, 769, 702; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 8.68 (d, *J* = 5.7 Hz, 2H), 8.14 (t, *J* = 7.95 Hz, 2H), 7.91-7.87 (m, 3H), 7.60-7.51 (m, 7H). ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 168.3, 160.2, 151.9, 138.1, 137.6, 133.5, 130.4, 130.1, 129.9, 129.1, 128.6, 128.5, 126.9, 121.6; ESI-MS: 283 (M+1); 282 (M); $C_{20}H_{14}N_2$.



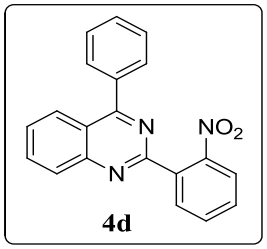
2-(4-Chloro-phenyl)-4-phenylquinazoline (4b)

Yellow solid; mp: 188.3 °C (lit.,[2b] 191-193 °C); IR (KBr; cm^{-1}): 1564, 1538, 1338, 850, 765, 703; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 8.68 (d, *J* = 8.1 Hz, 2H), 8.15 (t, *J* = 9.6 Hz, 2H), 7.96-7.87 (m, 3H), 7.65-7.51 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 168.4, 159.1, 151.8, 137.4, 136.7, 136.6, 133.7, 130.1, 130.0, 129.0, 128.7, 128.5, 127.2, 127.0, 121.6; ESI-MS: 317.4 (M+1); $C_{20}H_{13}N_2Cl$.



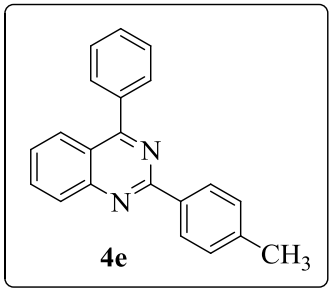
2-(4-Phenyl-quinazolin-2-yl)-phenol (4c)

Yellow solid; mp: 167.2-169.3 °C (lit.,[2c] 169-171 °C); IR (KBr, cm^{-1}): 3100, 1593, 1539, 1344, 830, 753, 700; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 13.90 (s, 1H), 8.73 (d, *J* = 6.6 Hz, 1H), 8.167-8.065 (dd, J_1 = 8.4 Hz, J_2 = 22.2 Hz, 2H), 7.95-7.86 (m, 3H), 7.64-7.56 (m, 4H), 7.41 (t, *J* = 6.75 Hz, 1H), 7.08 - 6.96 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 168.3, 160.9, 160.8, 149.5, 136.9, 134.3, 133.0, 130.3, 130.1, 129.8, 128.6, 127.6, 127.3, 127.2, 121.1, 119.3, 118.9, 117.7; ESI-MS: 299.1 (M+1); $C_{20}H_{14}N_2O$.



2-(2-Nitro-phenyl)-4-phenyl-quinazoline (4d)

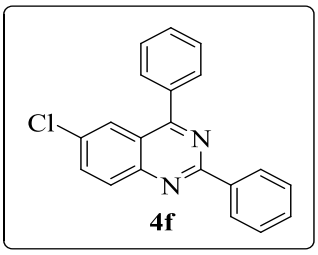
Brown solid; mp: 129.6 °C; IR (KBr, cm^{-1}): 1614, 1564, 1533, 1340, 850, 777, 701; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 8.22-8.14 (m, 3H), 7.97-7.57 (m, 10H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 168.6, 158.7, 151.3, 150.1, 136.8, 134.1, 133.5, 132.2, 131.8, 130.2, 130.1, 128.9, 128.6, 128.1, 127.2, 124.1, 121.5; ESI-MS: 328.2 (M+1); $C_{20}H_{13}N_3O_2$.



2-(4-Methylphenyl)-4-phenylquinazoline (4e)

White solid; m.p.,165.2 °C (lit.,[2b] 166-168 ºC); IR (KBr, cm^{-1}): 1604, 1560, 1534, 1336, 1075, 772, 699; ^{1}H NMR (300 MHz, $CDCl_3$): δ(ppm) 8.58 (d, *J* = 8.1 Hz, 2H), 8.12 (t, *J* = 7.65, 2H), 7.88-7.85 (m, 3H), 7.60-7.50 (m, 4H), 7.32 (d, *J* = 7.8 Hz, 2H), 2.44 (s, 3 H); ^{13}C NMR (75 MHz, CDCl3): δ (ppm) 168.3, 160.4, 152.1, 140.8, 137.9, 135.6, 133.5, 130.3, 129.9, 129.4, 129.2, 128.8, 128.6,127.1, 126.8, 121.7, 21.6; ESI-MS: 297.2 (M+1); $C_{21}H_{16}N_2$.

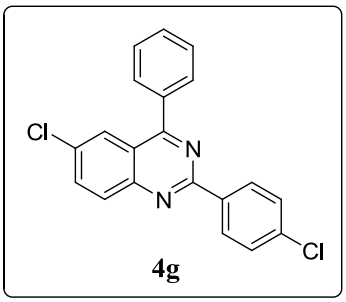
6-chloro-2, 4-diphenyl-quinazoline (4f)



4f

White solid; mp: 193.5-194.5 °C (lit.,[2d] 194 °C); IR (KBr, cm^{-1}): 1559, 1537, 1247, 845, 760; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 8.66 (d, *J* = 4.8 Hz, 2H), 8.11-8.09 (m, 2H), 7.86-7.80 (m, 3H), 7.61 (t, *J* = 2.85 Hz, 3H), 7.54-7.50 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 167.5, 160.4, 150.4, 137.7, 137.0, 134.4, 132.5,130.8, 130.7, 130.2, 130.0, 128.7, 128.6, 128.5, 125.7, 122.1, 120.3; ESI-MS: 317.4 (M+1); $C_{20}H_{13}N_2Cl$.

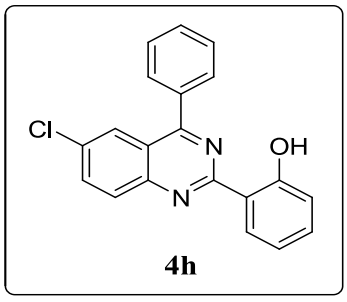
6-chloro-2(4-chloro-phenyl)-4-phenyl-quinazoline (4g)



4g

White solid; mp 192.5 °C (lit.,[2e] 187.0 °C); IR (KBr, cm^{-1}): 1534, 1387, 1084, 703; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 8.60 (d, *J* = 8.4 Hz, 2H), 8.06 (d, *J* = 8.4 Hz, 2H), 7.85-7.80 (m, 3H), 7.61-7.59 (m, 3H), 7.47 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 167.6, 159.4, 150.3, 136.9, 136.2, 134.6, 132.8, 130.7, 130.3, 129.9, 128.7, 125.8, 122.1; ESI-MS: 351.3 (M); 353.3 (M+2); $C_{20}H_{12}N_2Cl_2$.

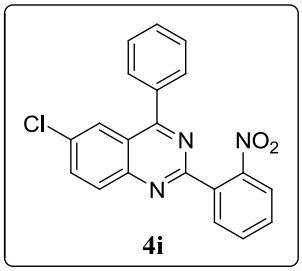
2-(6-chloro-4-phenyl-quinazolin-2-yl)-phenol (4h)



4h

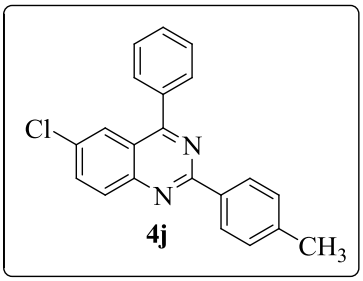
Yellow solid; mp: 197.1 °C (lit.,[2f] 197.0 °C); IR (KBr, cm^{-1}): 3055, 1591, 1538, 1245, 841, 754; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 13.56 (s, 1H), 8.70 (d, *J* = 7.8 Hz, 1H), 8.10 (s, 1H), 8.02 (d, *J* = 8.7 Hz, 1H), 7.85 (d, *J* = 6.9 Hz, 3H), 7.64 (d, *J* = 2.4 Hz, 3H), 7.42 (t, *J* = 7.65 Hz, 1H), 7.06 (d, *J* = 8.1 Hz, 1H), 6.99 (t, *J* = 7.5 Hz, 1H); ^{13}C NMR (300 MHz, $CDCl_3$): δ (ppm) 167.6, 161.1, 160.9, 148.2, 136.3, 135.3, 133.3, 132.9, 130.7, 130.0, 129.9, 129.4, 128.9, 126.1, 121.3, 119.1, 117.8; ESI-MS: 334.1$(M+1)^+$; $C_{20}H_{13}ClN_2O$.

6-chloro-2(2-nitro-phenyl)-4-phenyl-quinazoline (4i)



4i

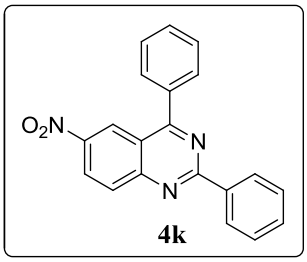
Light yellow solid; mp: 135.0 °C (lit.,[2f] 128.0 °C); IR (KBr, cm^{-1}): 3425, 1541, 1382, 778, 696; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 8.19 (t, *J* = 9.45 Hz, 2H), 8.10 (d, *J* = 9 Hz, 1H), 7.88 (t, *J* = 5.7 Hz, 2H), 7.79-7.70 (m, 3H), 7.63-7.60 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 167.6, 159.0, 150.1, 136.3, 134.9, 133.8, 133.3, 132.1, 131.7, 130.7, 130.5, 130.2, 130.0, 128.8, 125.9, 124.1, 122.1; ESI-MS: 362.2 (M+1); $C_{20}H_{12}ClN_3O_2$.



4j

6-chloro-4-phenyl-2-(p-tolyl)-quinazoline (4j)

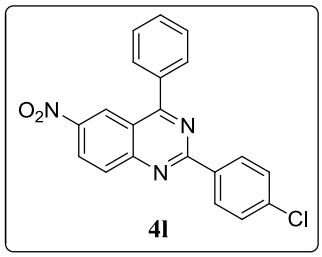
White solid; mp: 212.2 ˚C (lit.,[29]1216-218); IR (KBr, cm^{-1}): 2930, 1610, 1562, 1537, 1335, 1077, 775, 701; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 8.55 (d, *J* = 9Hz, 2H), 8.06 (q, *J* = 2.8, 2H), 7.85-7.77 (m, 3H), 7.60 (t, *J* = 2.7 Hz, 3H), 7.32 (d, *J* = 8.1 Hz, 2H), 2.44 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ(ppm) 167.4, 160.6, 150.5, 141.1, 137.2, 135.8, 134.4, 132.3, 130.2, 129.4, 128.7, 128.6, 125.8, 122.1, 21.6; ESI-MS: 331.9 (M+1); $C_{21}H_{15}ClN_2$.



4k

6-Nitro-2, 4-diphenyl-quinazoline (4k)

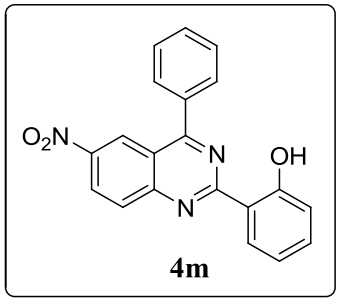
Light yellow solid; mp: 212.1 ˚C (lit.[2e], 214-217 ˚C); IR (KBr, cm^{-1}): 1620, 1538, 1395, 1091, 703; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 9.05 (d, *J* = 1.8 Hz, 1H), 8.74-8.73 (m, 2H), 8.66-8.63 (m, 1H), 8.31 (d, *J* = 7.5 Hz, 1H), 7.90 (t, *J* = 3.3 Hz, 2H), 7.67-7.65 (m, 3H), 7.57-7.54 (m, 3H); ^{13}C NMR (300 MHz, $CDCl_3$): δ (ppm) 162.9, 154.5, 145.5, 137.1, 136.4, 131.8, 131.0, 129.3, 129.1, 128.8, 127.1, 124.3, 120.5; ESI-MS: 388.2 (M+1); $C_{20}H_{13}N_3O_2$.



4l

6-Nitro-2-(2-nitro-phenyl)-4-phenyl-quinazoline (4l)

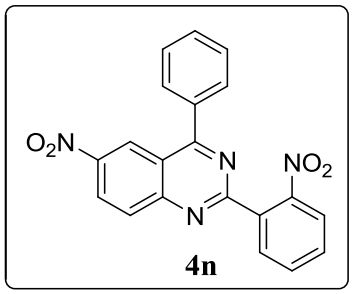
Yellow solid; mp: 230.1 ˚C (lit., [2e] 228-232 ^{0}C); IR (KBr, cm^{-1}): 1538, 1344, 1094, 694; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 9.04 (d, *J* = 2.4 Hz, 1H); 8.69-8.62 (m, 3H), 8.23 (d, *J* = 9.3 Hz, 1H), 7.88 (t, *J* = 3.75 Hz, 2H), 7.66 (t, *J* = 2.1 Hz, 3H), 7.50 (d, *J* = 8.7 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 161.9, 154.4, 145.6, 138.2, 136.2, 135.6, 131.1, 131.0, 130.6, 130.3, 129.2, 129.0, 127.2, 124.3, 120.6; ESI-MS: 362.2 (M+1); $C_{20}H_{12}ClN_3O_2$.



4m

2-(6-Nitro-4-phenyl-quinazolin-2-yl)-phenol (4m)

Yellow solid; mp: 157.2 ˚C; IR (KBr, cm^{-1}): 3132, 1536, 1343, 1092, 702; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 13.36 (s, 1H), 9.06 (s, 1H), 8.75-8.65 (m, 2H), 8.17 (d, *J* = 9.3 Hz, 1H), 7.88 (t, *J* = 7.2 Hz, 2H), 7.69-7.62 (m, 3H), 7.53-7.44 (m, 1H), 7.09-6.98 (m, 2H); ESI-MS: 344.2 (M+1); $C_{20}H_{13}ClN_3O_3$.



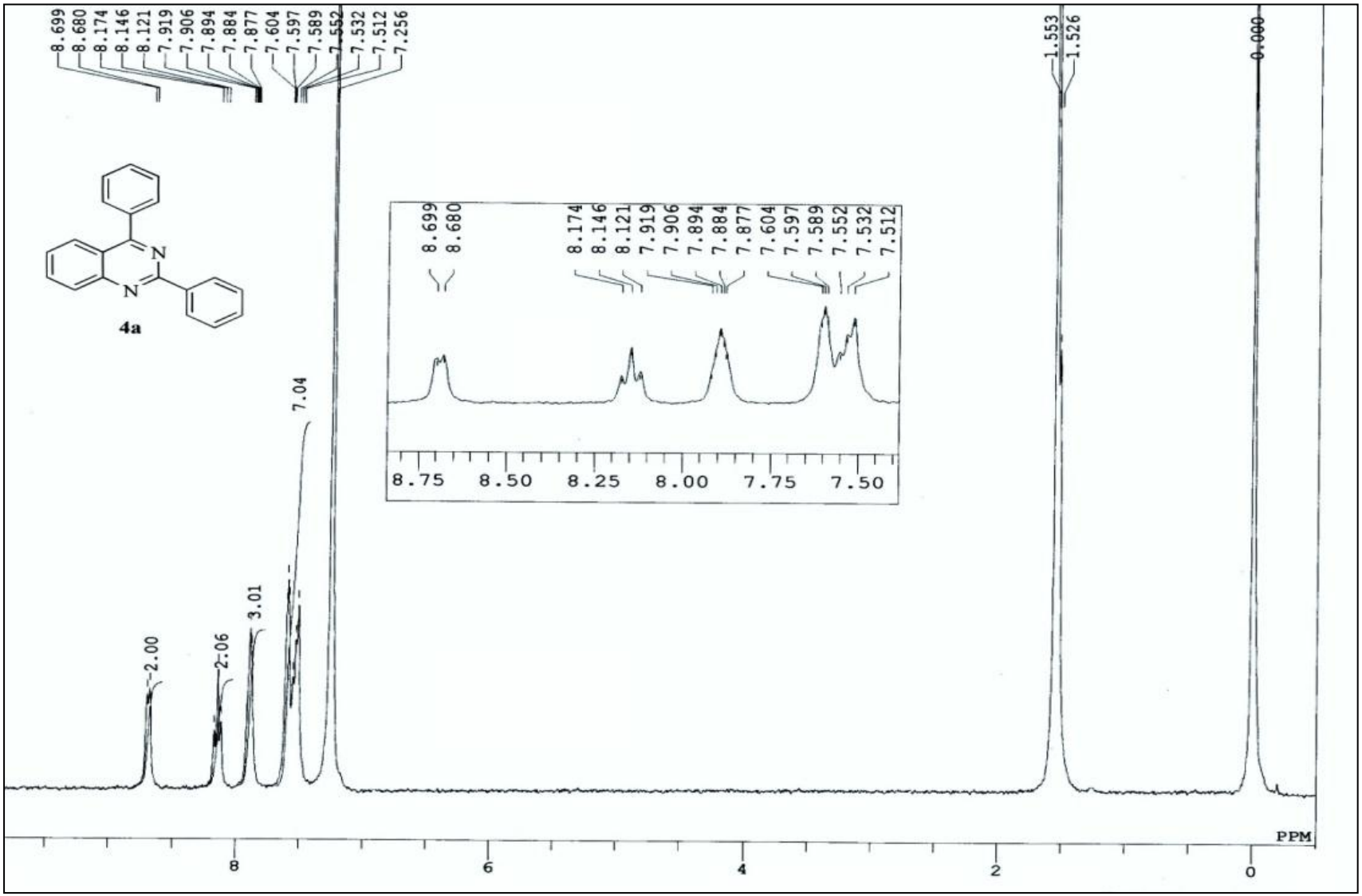
4n

6-Nitro-2-(2-nitro-phenyl)-4-phenyl-quinazoline (4n)

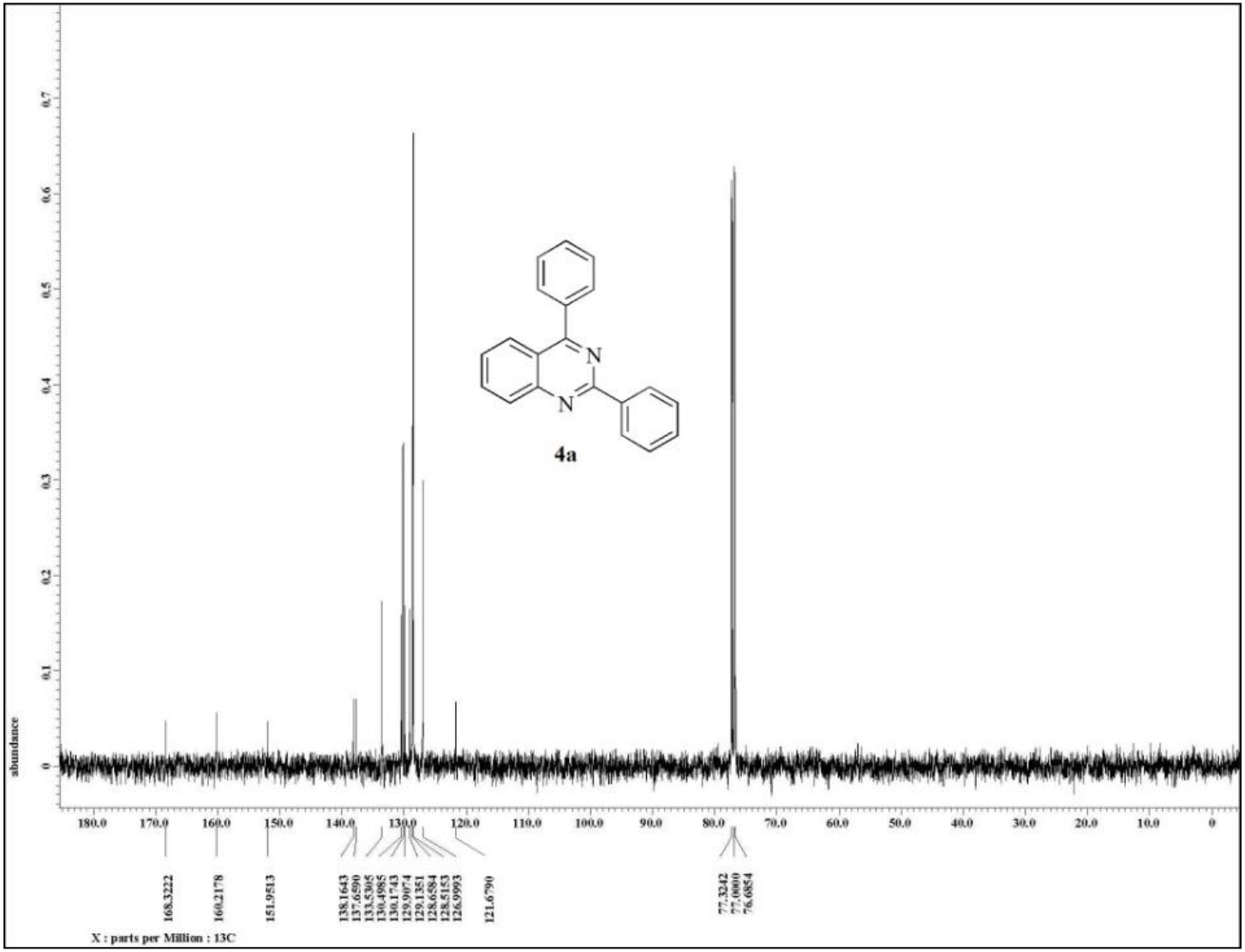
Brown solid; mp., 168.7 °C; IR (KBr, cm^{-1}): 1616, 1535, 1342, 1085, 698; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 9.12 (s, 1H), 8.70 (d, *J* = 9.15 Hz, 2H), 8.27 (t, *J* = 7.33 Hz, 2H), 7.93-7.66 (m, 8H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 170.5, 161.5, 153.9, 150.2, 146.1, 135.5, 132.7, 132.3, 131.8, 131.2, 131.1, 130.9, 130.3, 129.1, 128.5, 127.3, 124.2, 120.4; ESI-MS: 373.2 (M+1); 374.2 (M+2); $C_{20}H_{12}N_4O_4$.

4. ^{1}H and ^{13}C NMR Spectra of Isolatated Products:

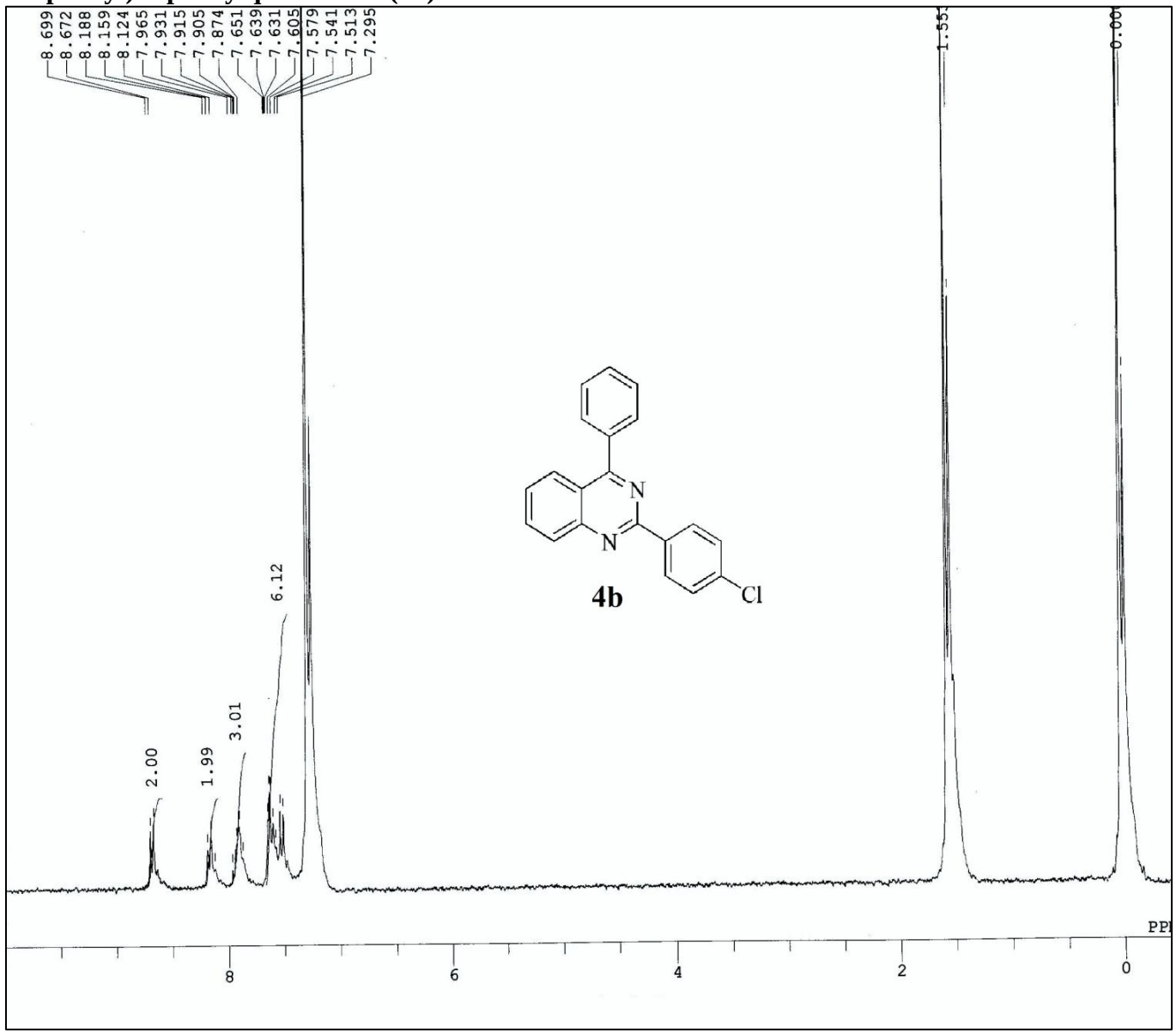
^{1}H-NMR of 2, 4-Diphenyl-quinazoline (4a)



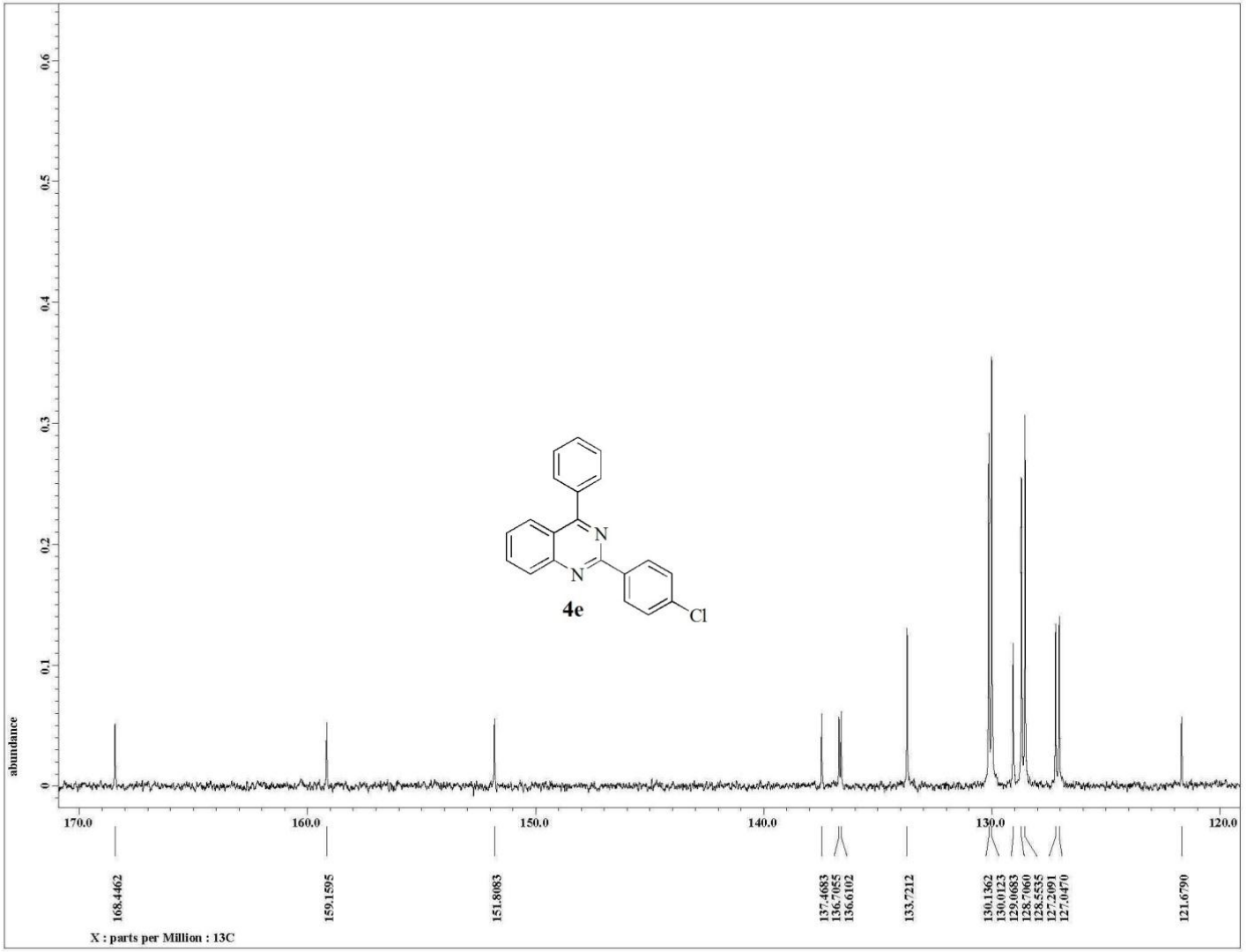
^{13}C-NMR of 2, 4-Diphenyl-quinazoline (4a)



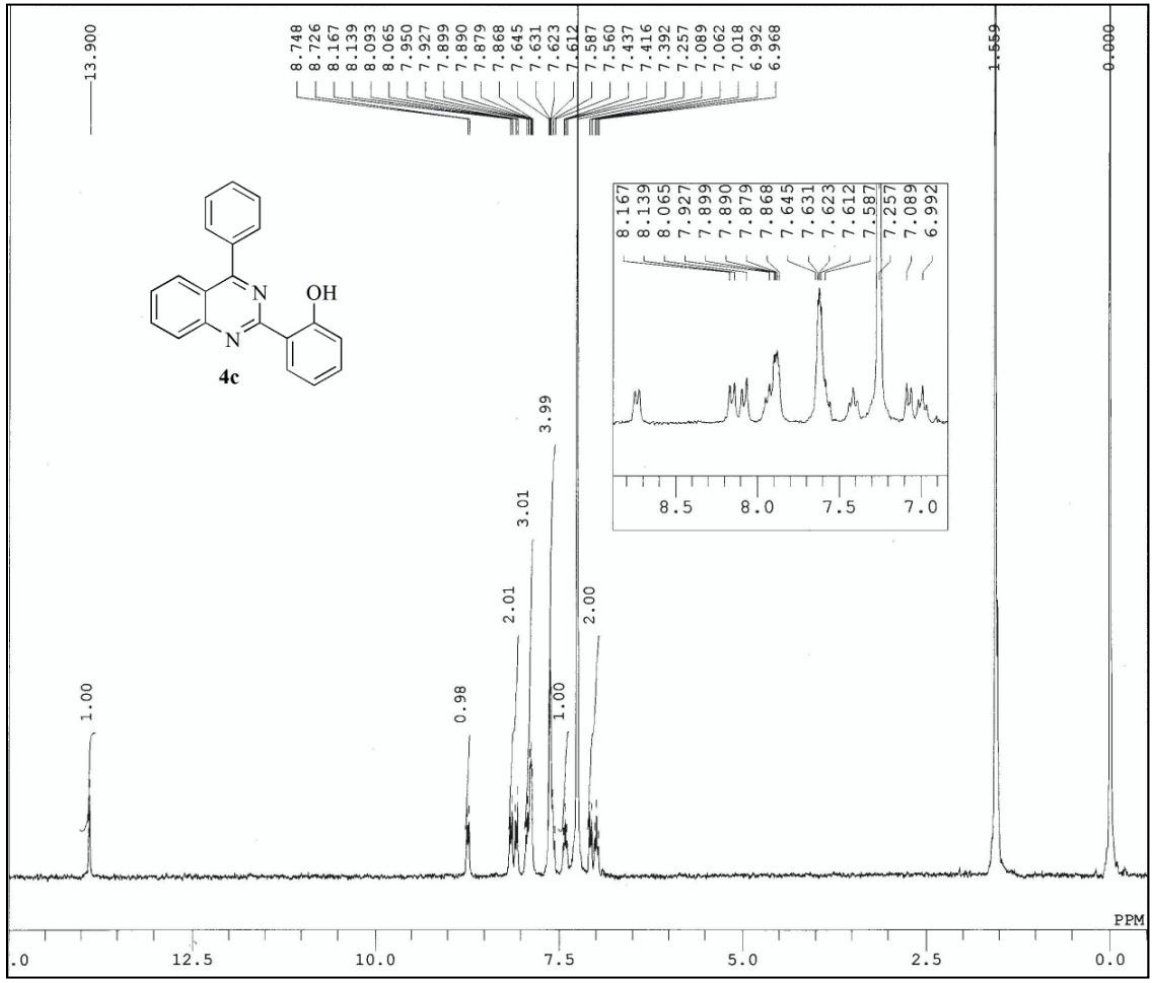
^{1}H-NMR of 2-(4-Chloro-phenyl)-4-phenylquinazoline (4b)



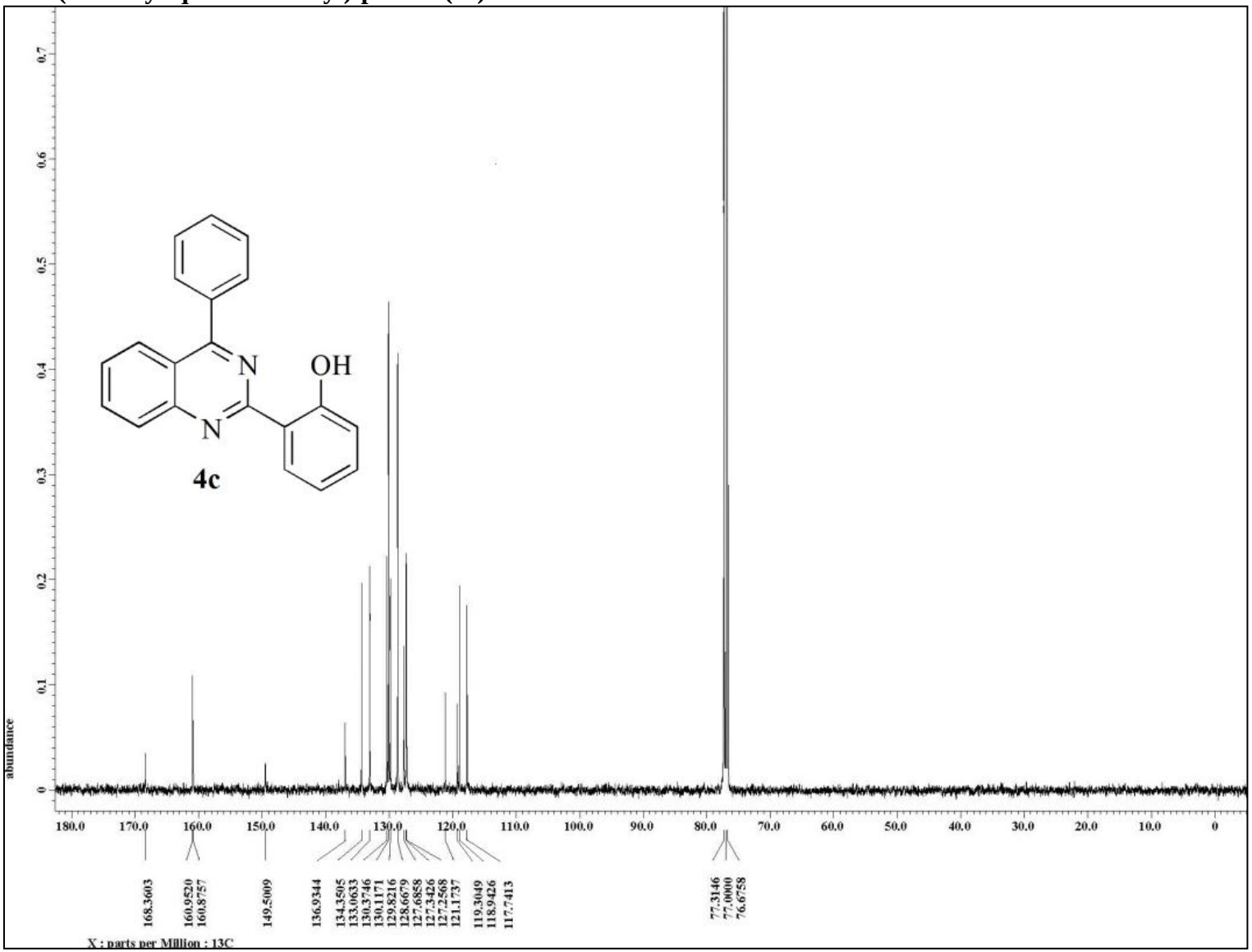
^{13}C-NMR of 2-(4-Chloro-phenyl)-4-phenylquinazoline (4b)



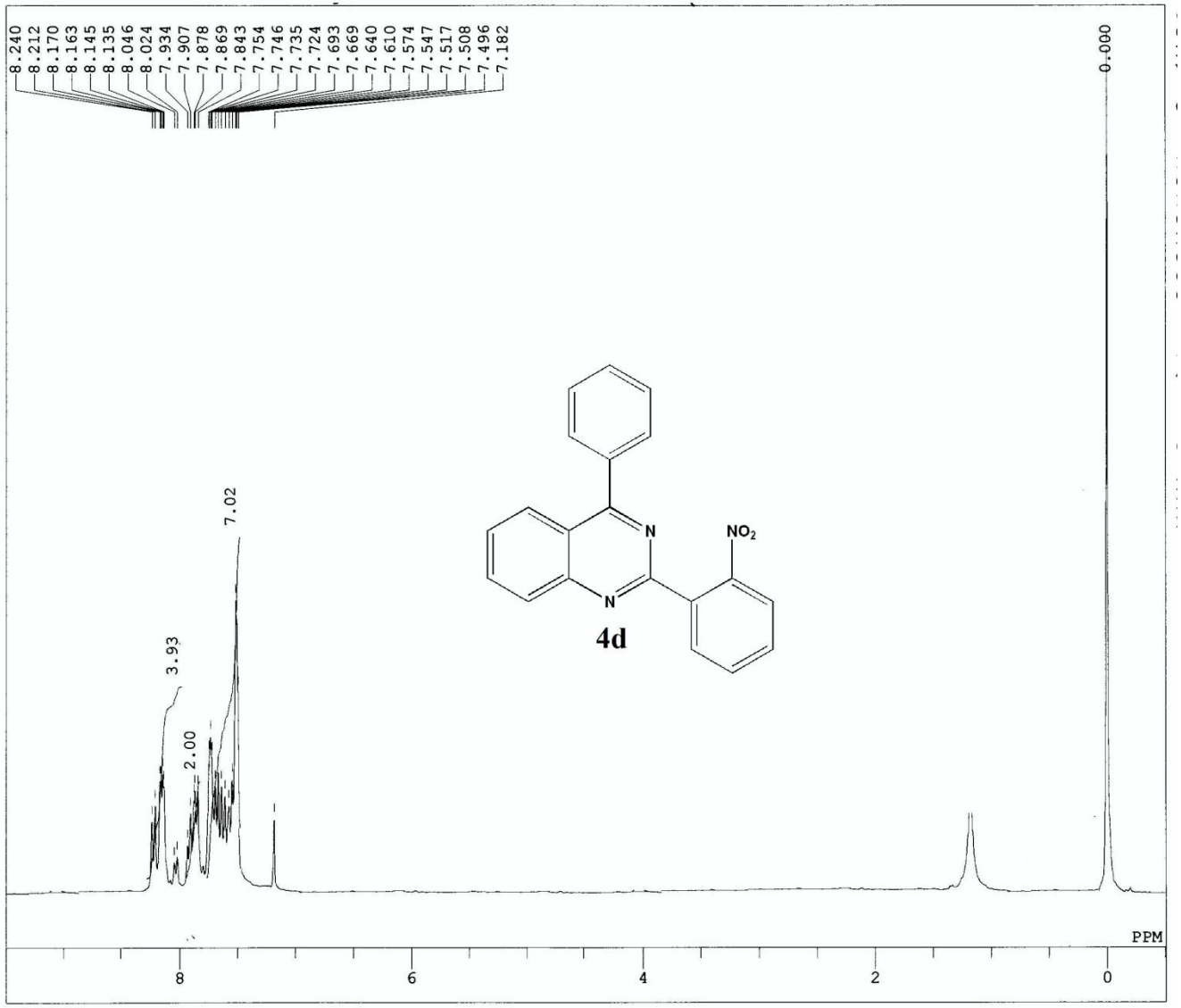
^{1}H-NMR of 2-(4-Phenyl-quinazolin-2-yl)-phenol (4c)



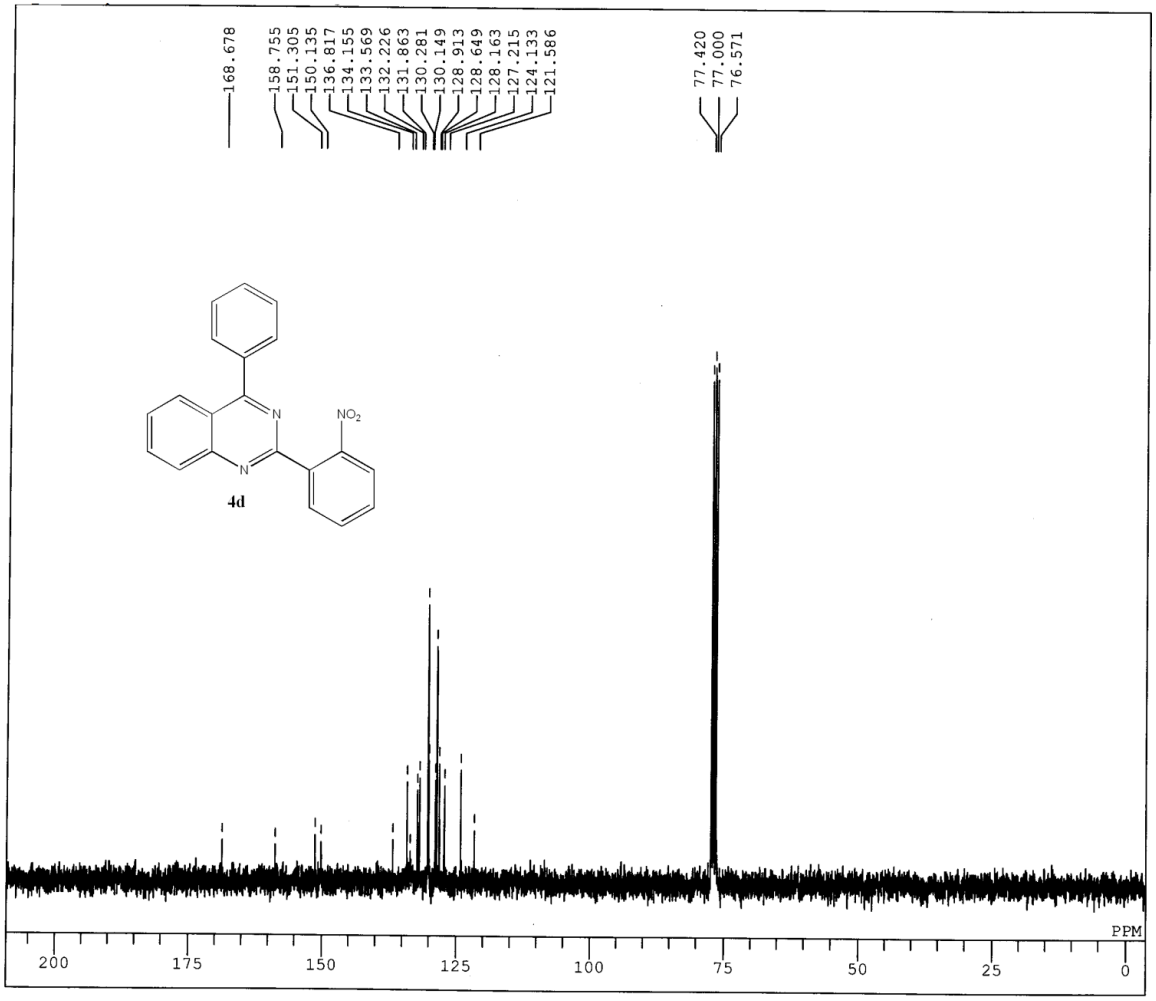
^{13}C-NMR of 2-(4-Phenyl-quinazolin-2-yl)-phenol (4c)



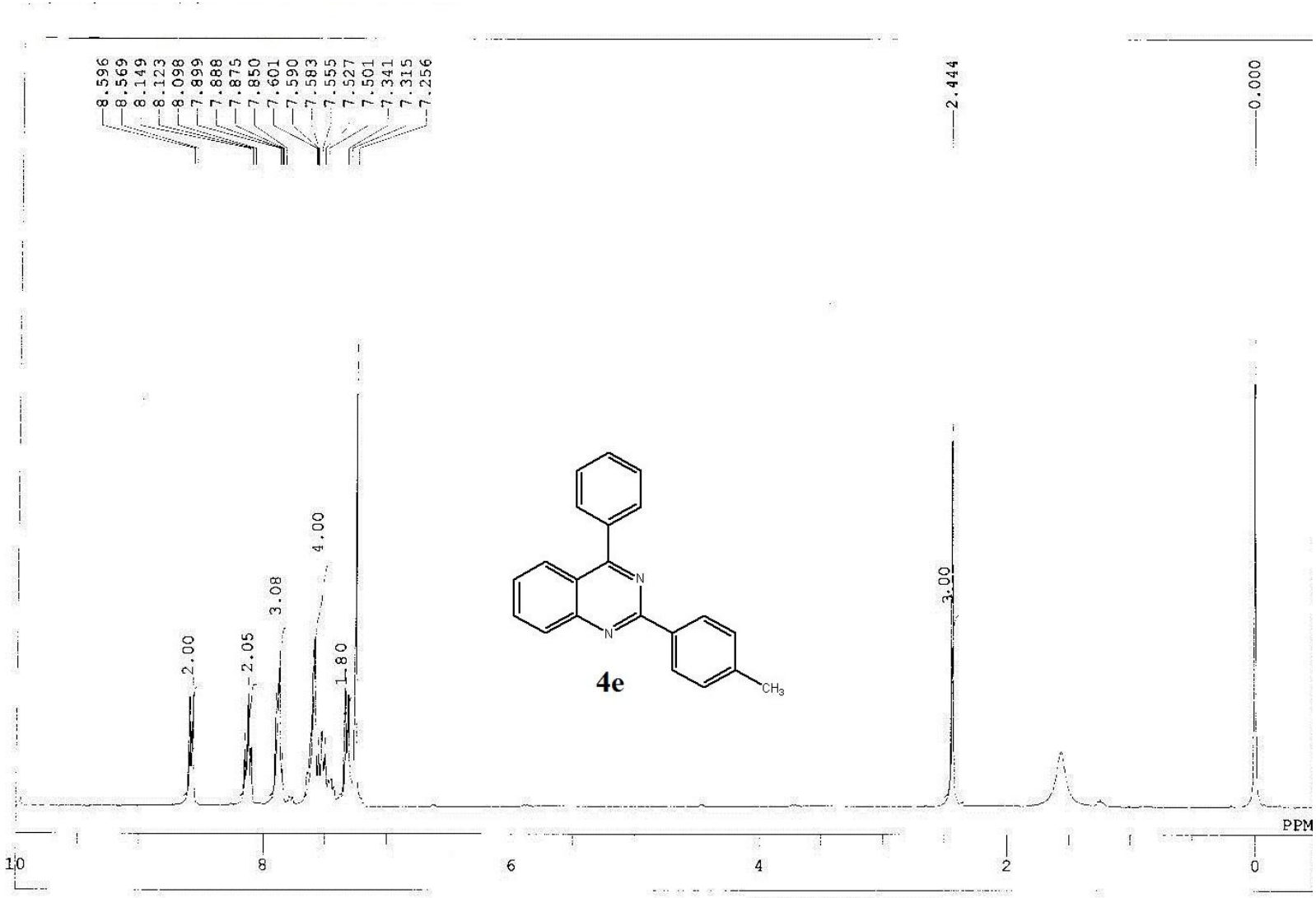
^{1}H-NMR of 2-(2-Nitro-phenyl)-4-phenyl-quinazoline (4d)



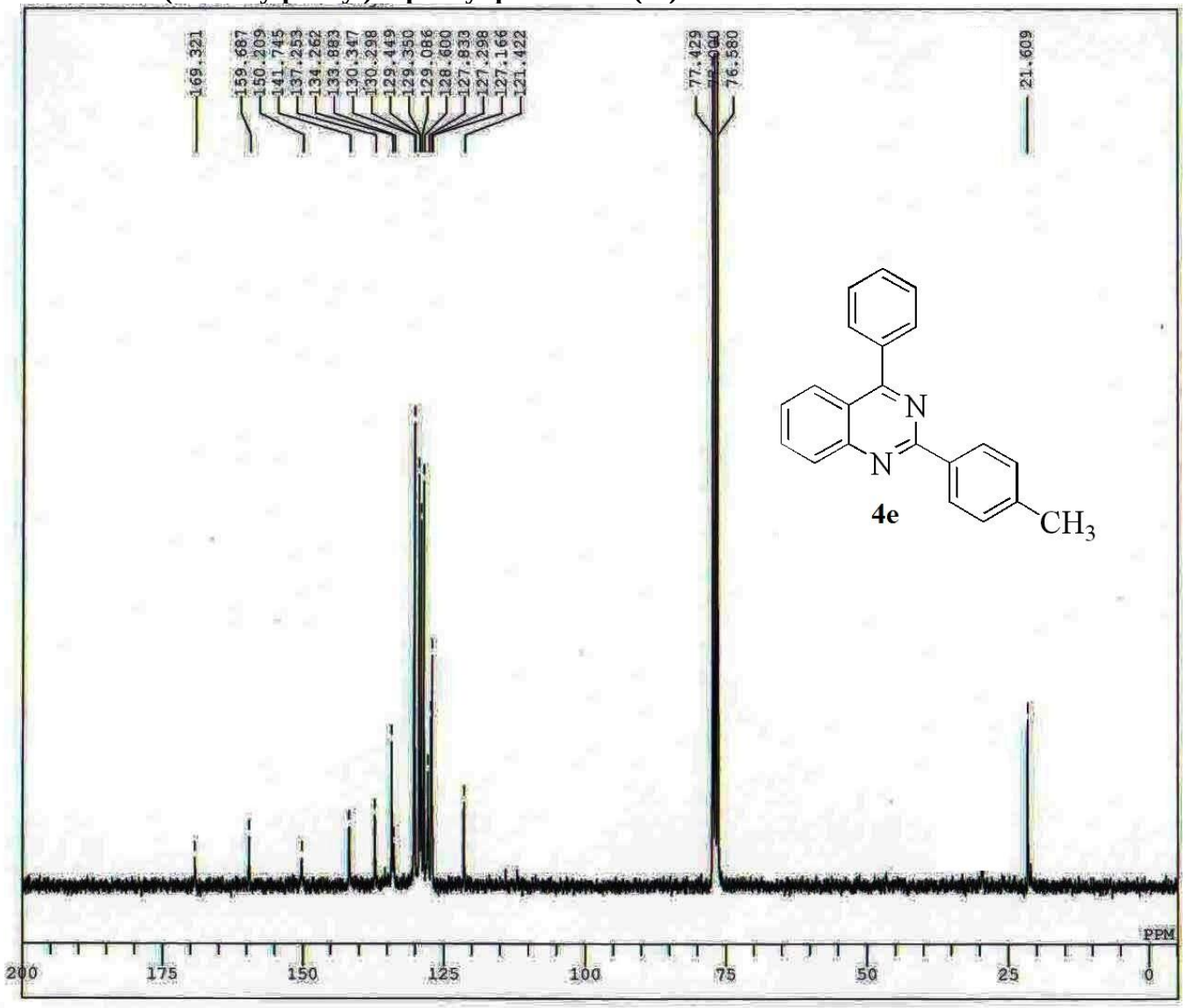
^{13}C-NMR of 2-(2-Nitro-phenyl)-4-phenyl-quinazoline (4d)



^{1}H-NMR of 2-(4-Methylphenyl)-4-phenylquinazoline (4e)



^{13}C-NMR of 2-(4-Methylphenyl)-4-phenylquinazoline (4e)



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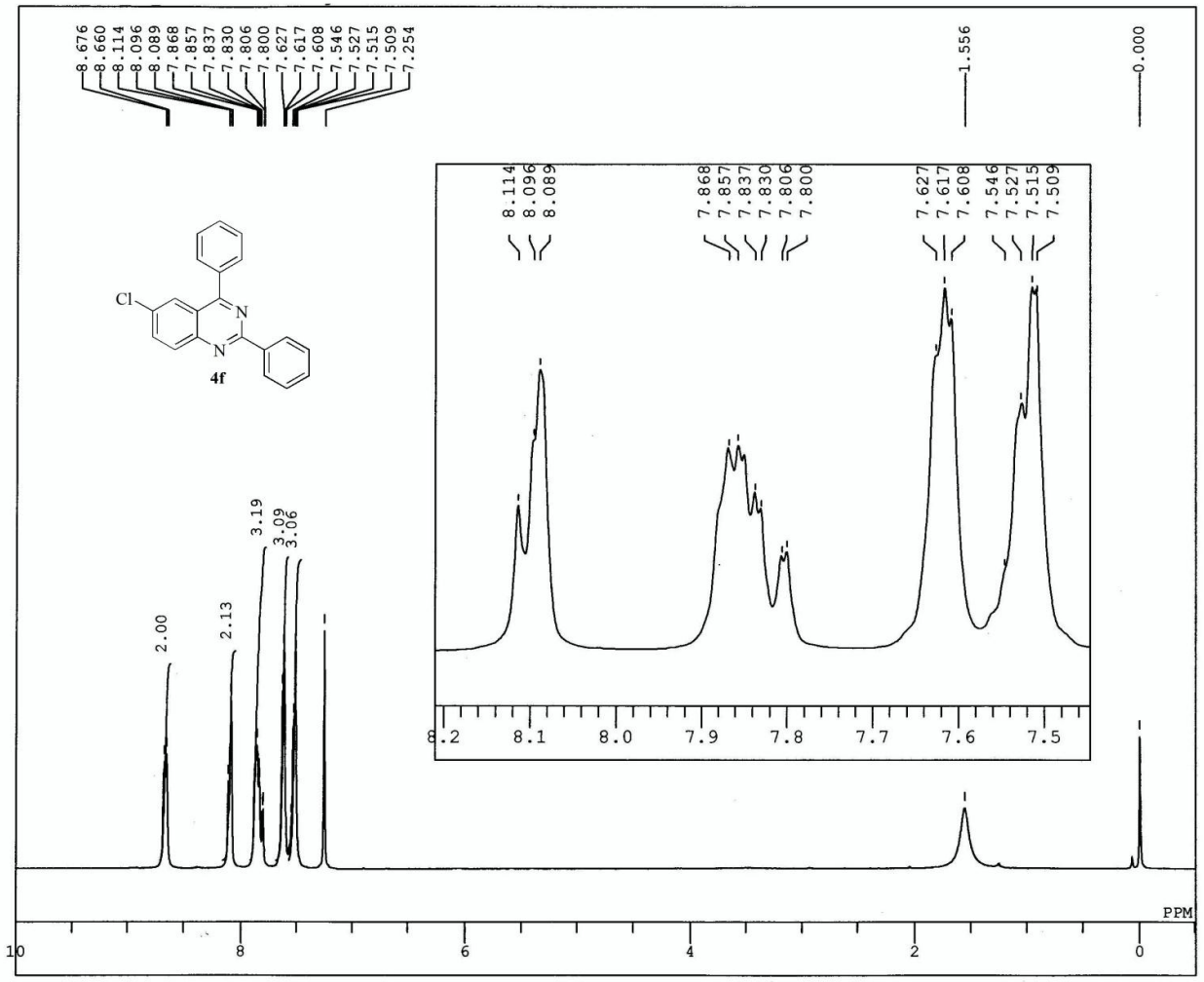

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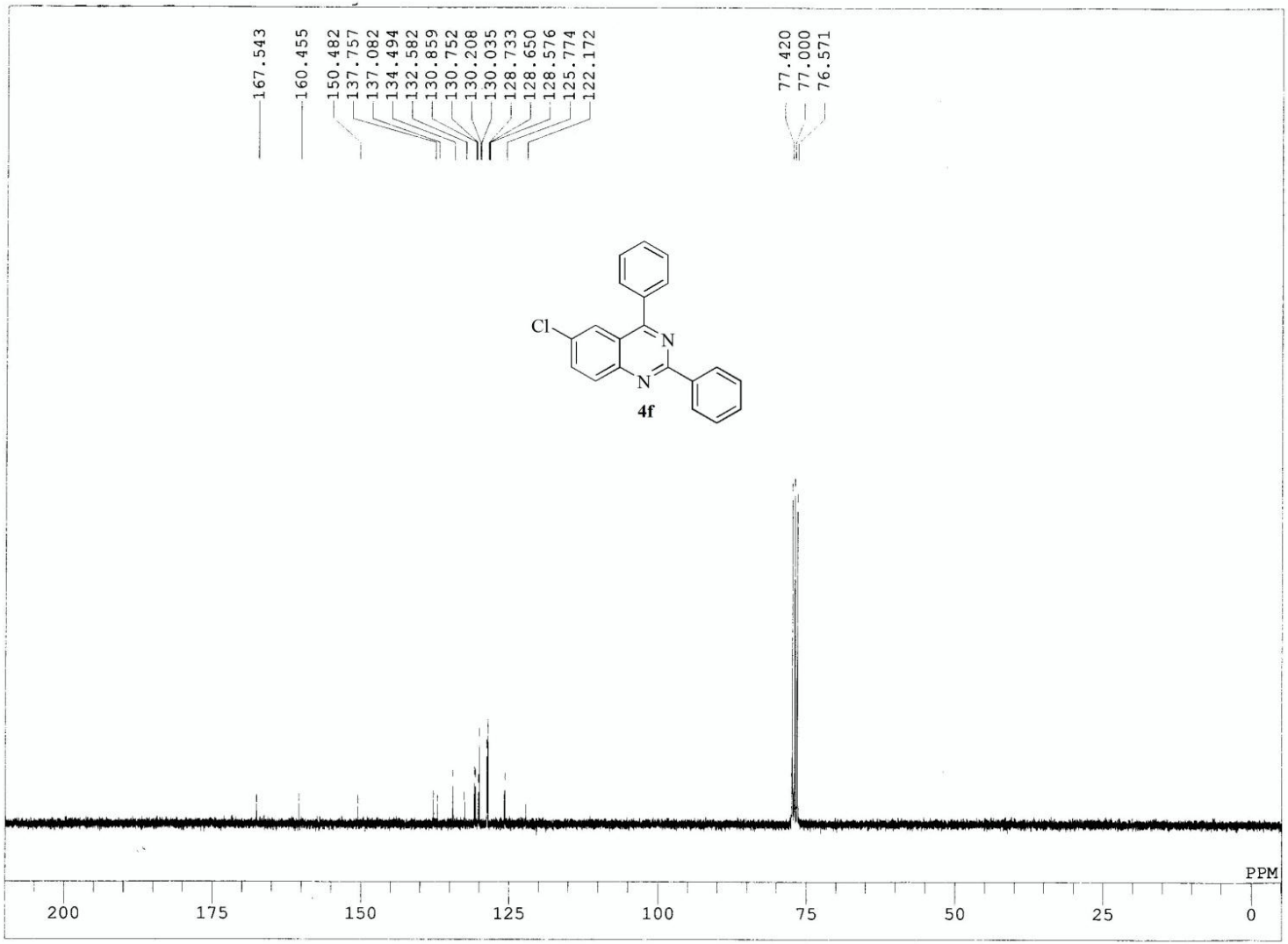
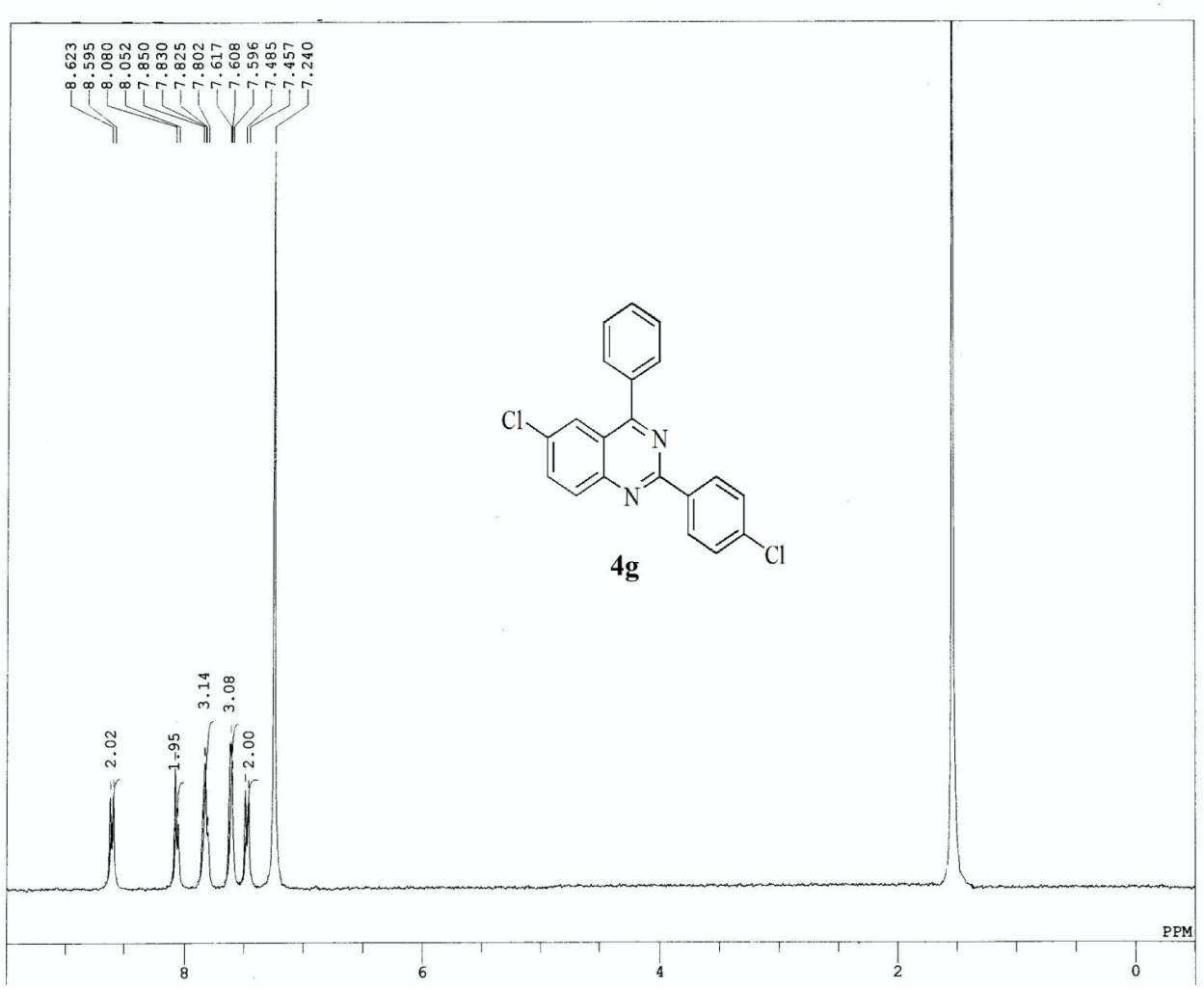


^{1}H-NMR of 6-chloro-2(4-chloro-phenyl)-4-phenyl-quinazoline (4g)



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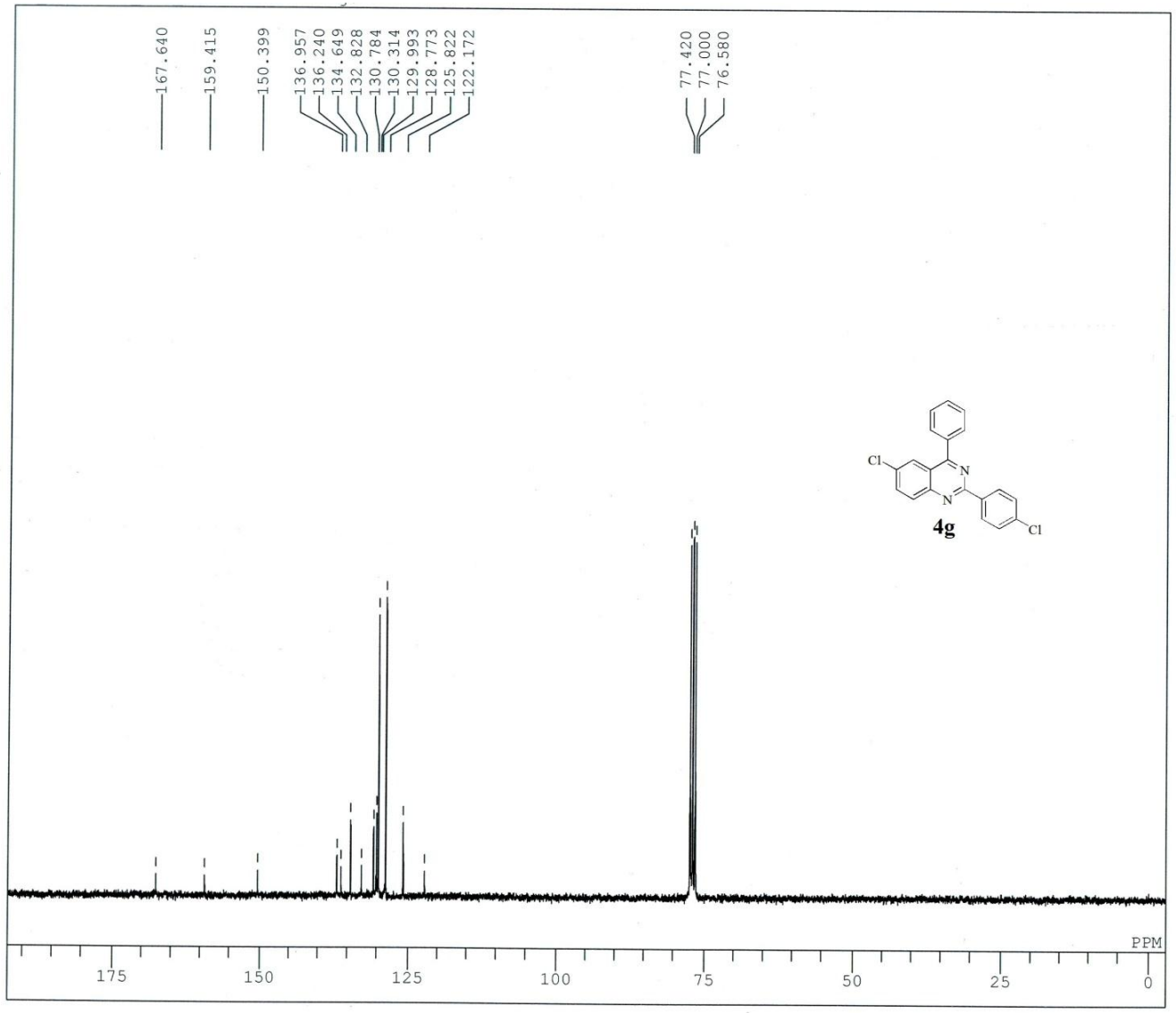

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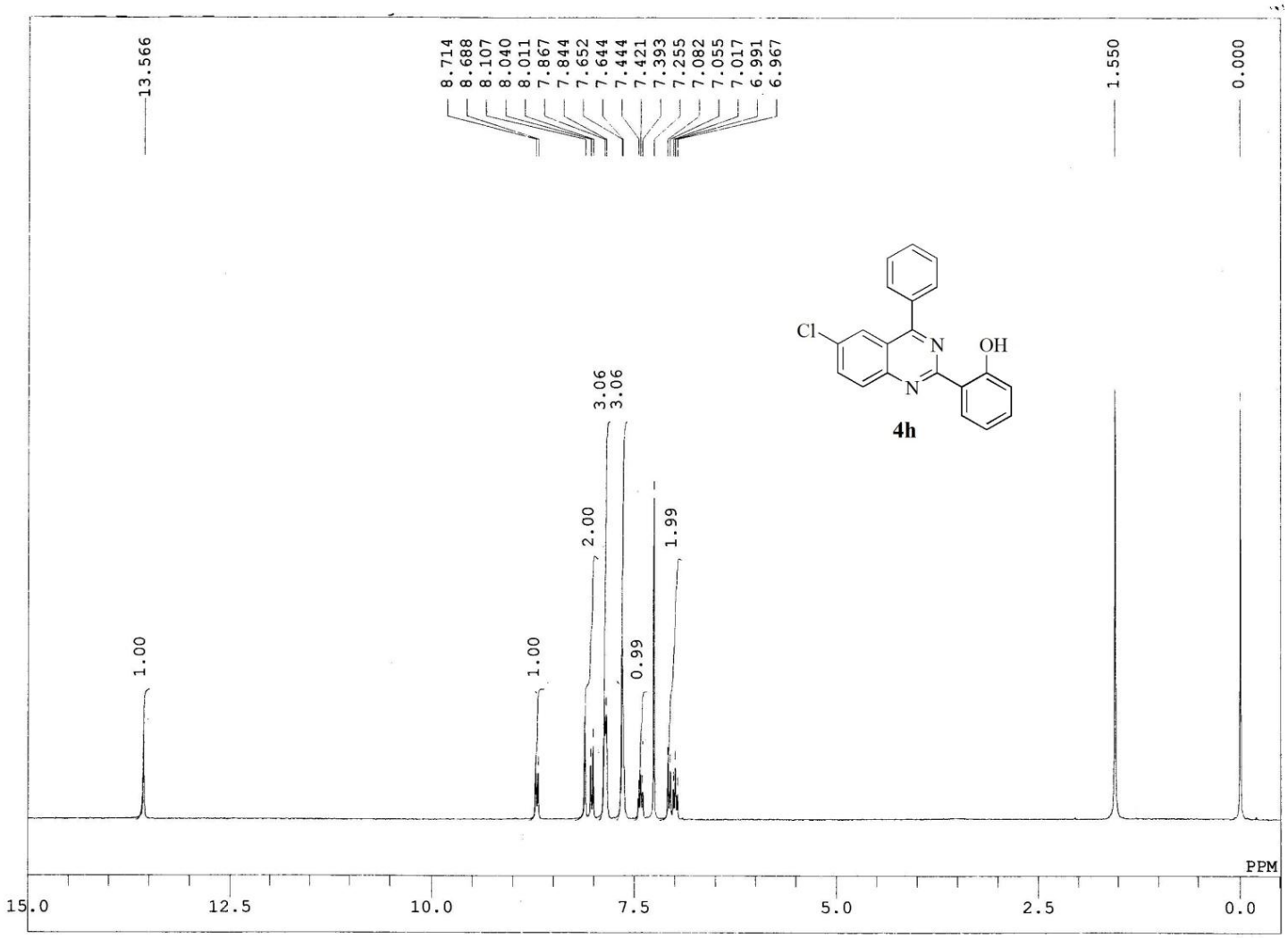

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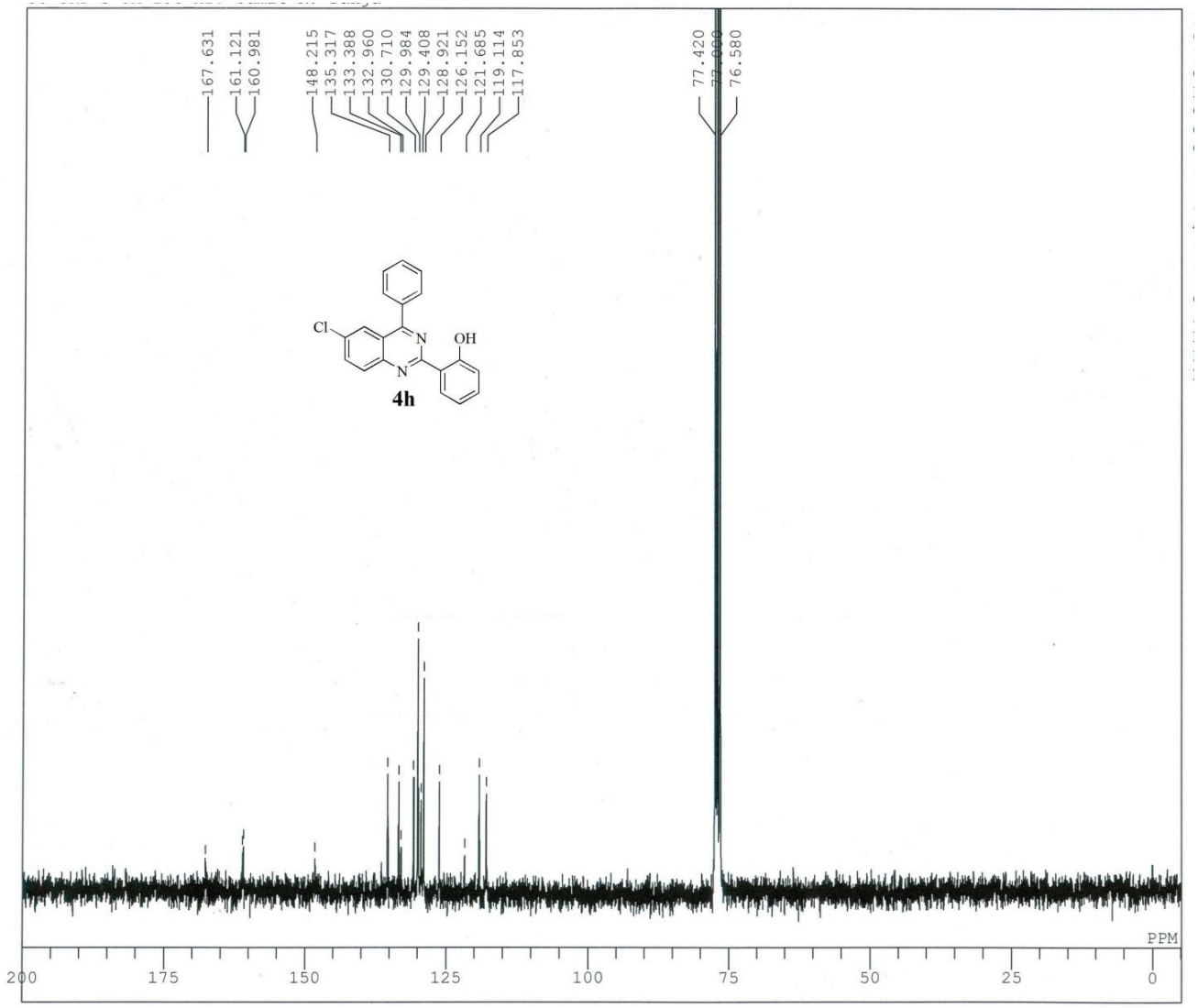
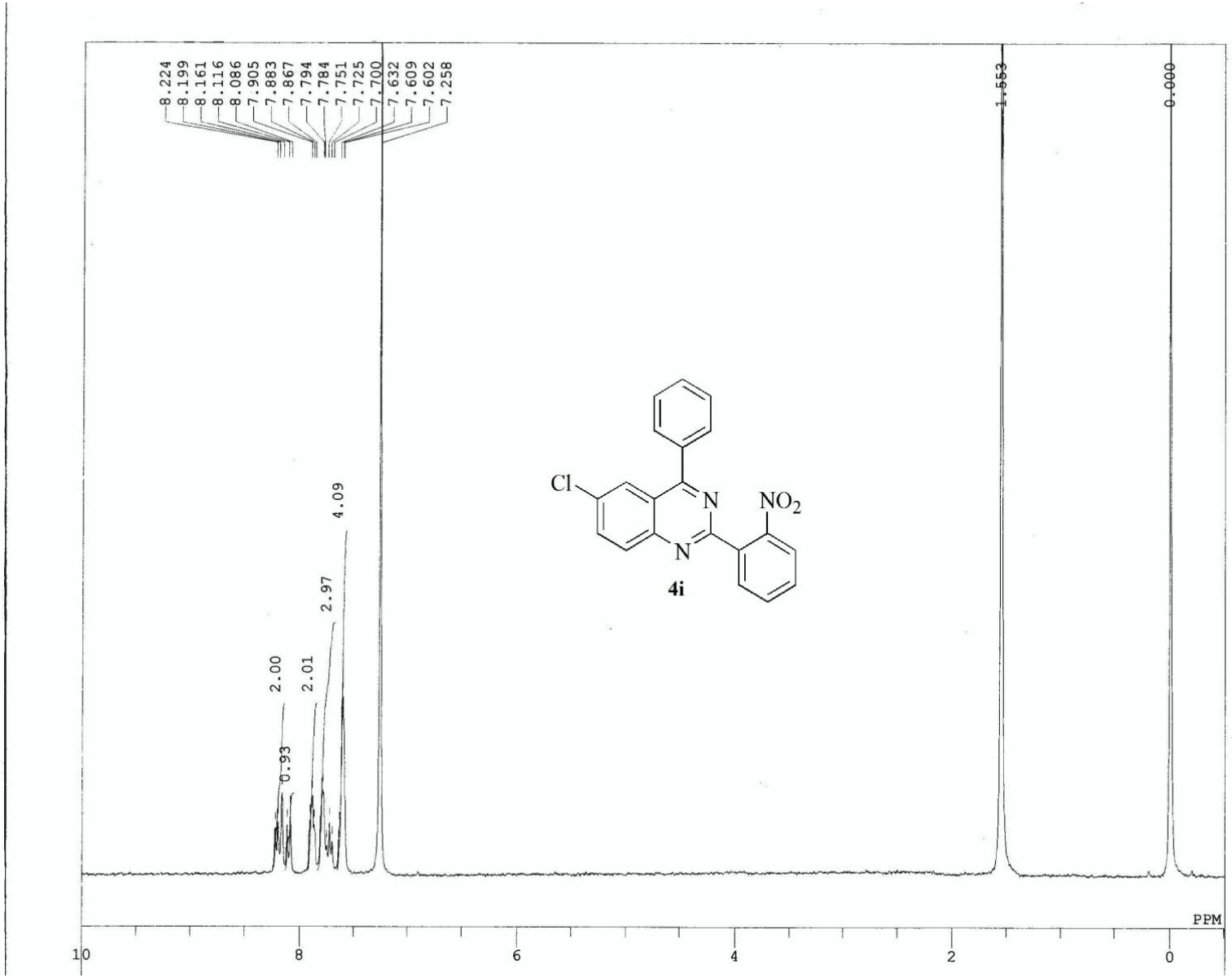


^{1}H-NMR of 6-chloro-2(2-nitro-phenyl)-4-phenyl-quinazoline (4i)



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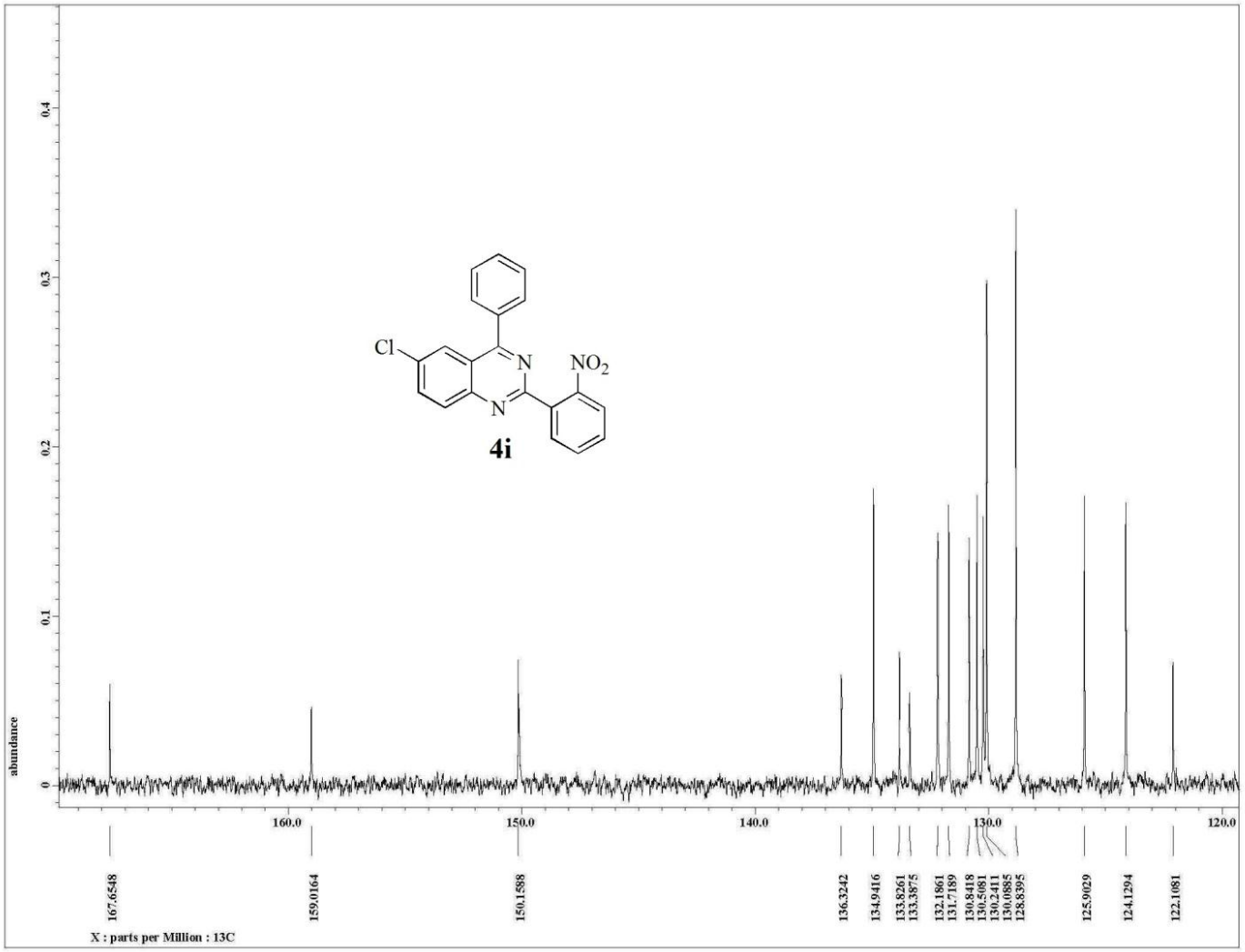
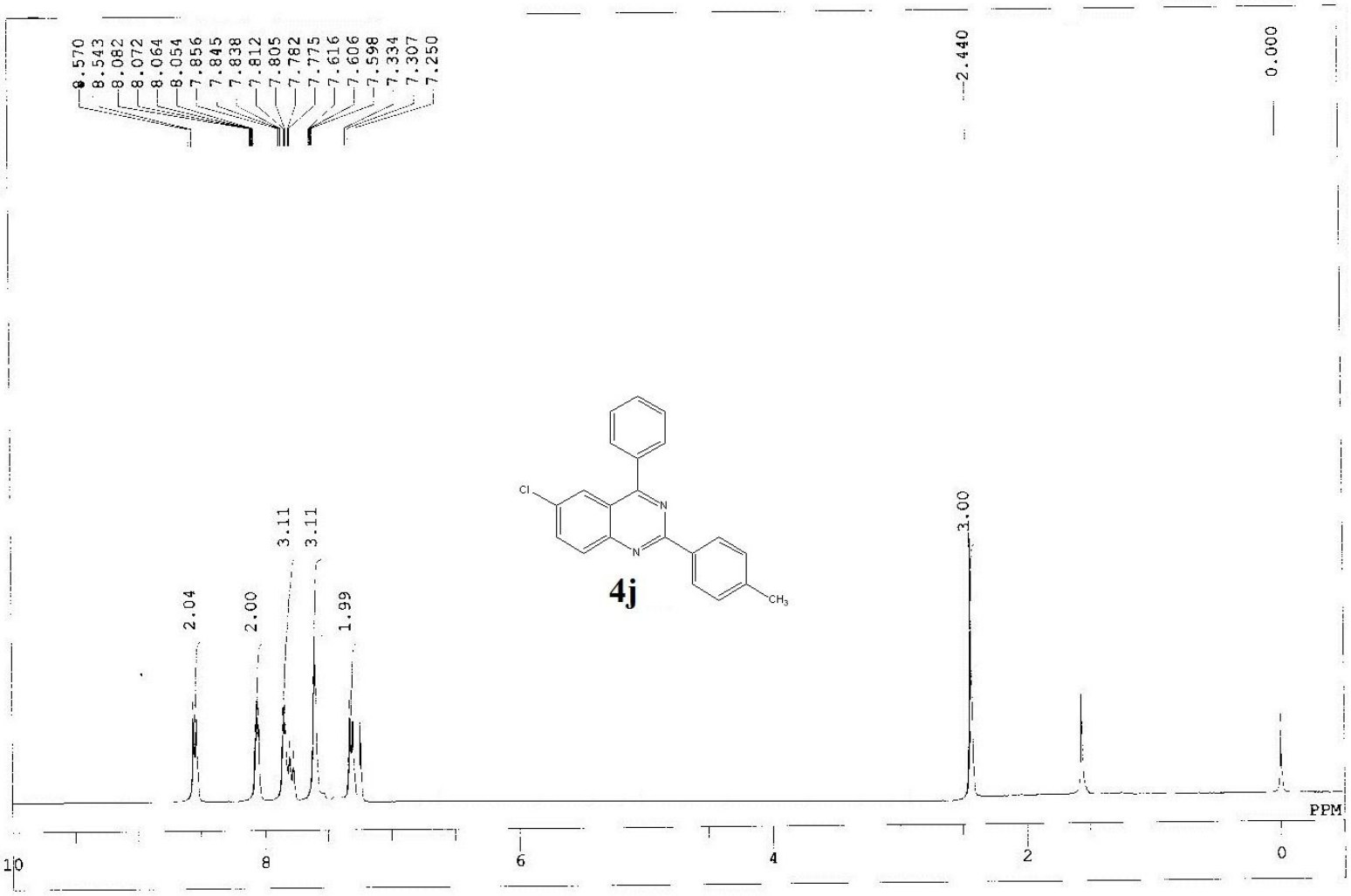


^{1}H-NMR of 6-chloro-4-phenyl-2-(p-tolyl)-quinazoline (4j)



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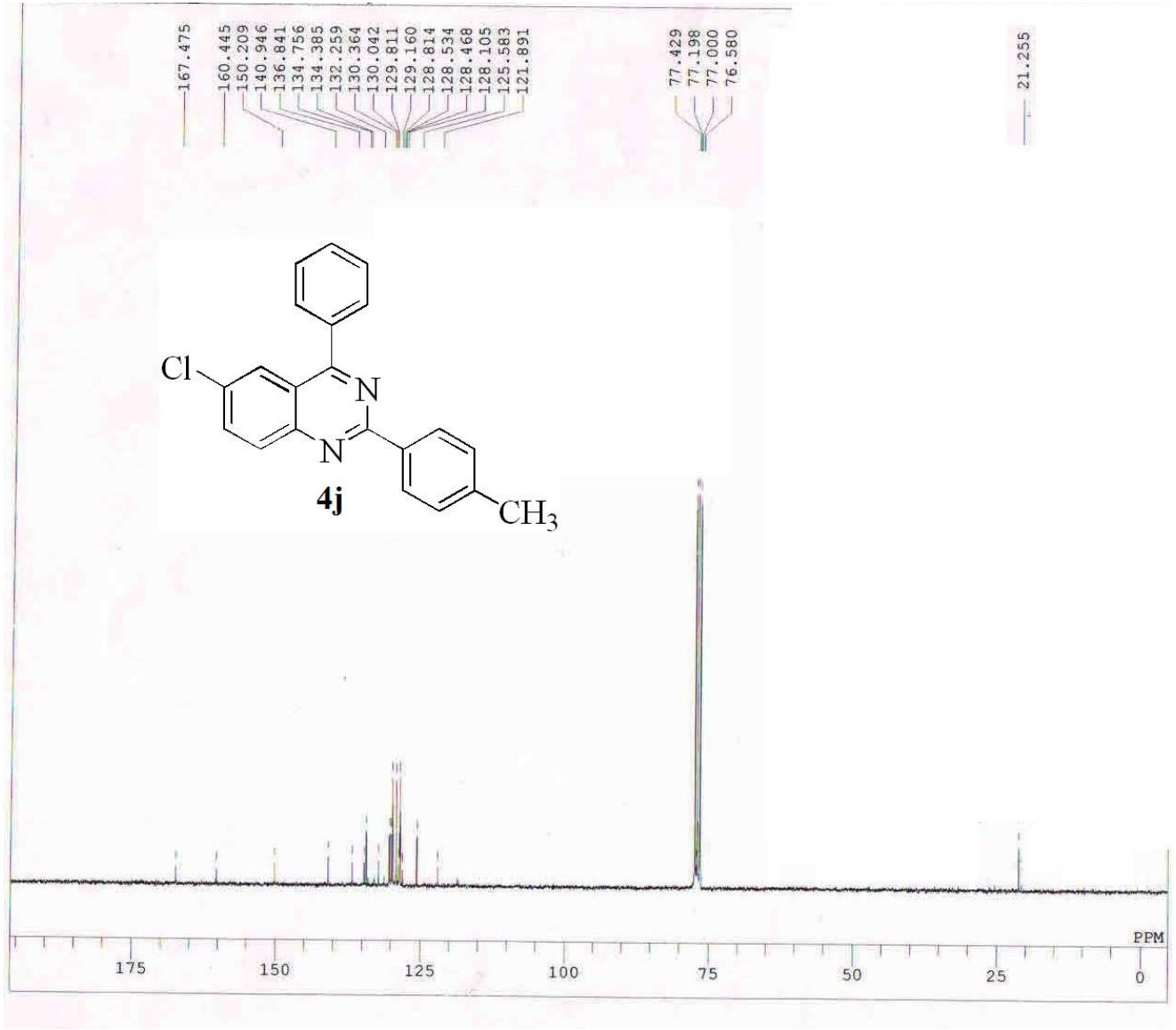

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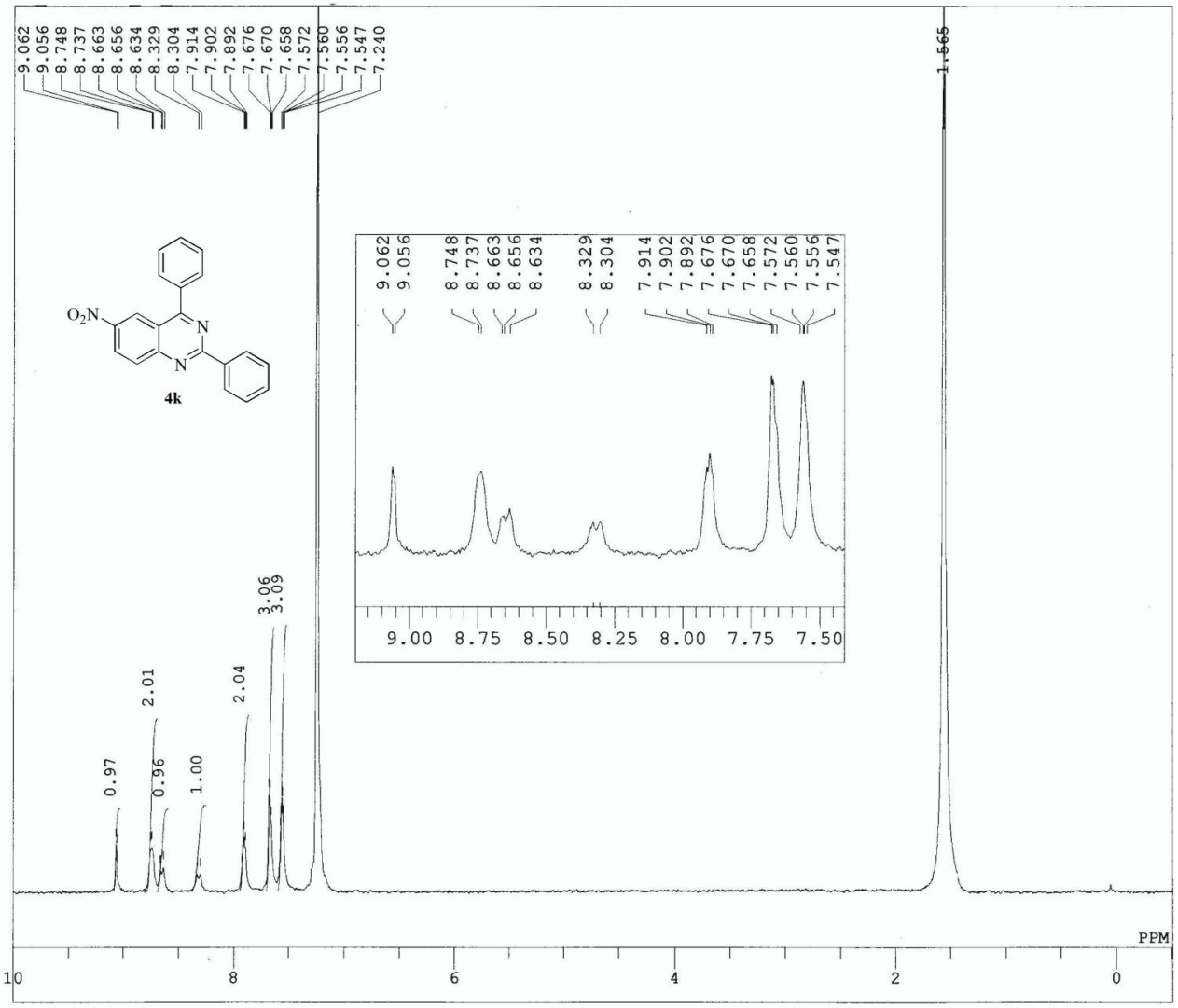

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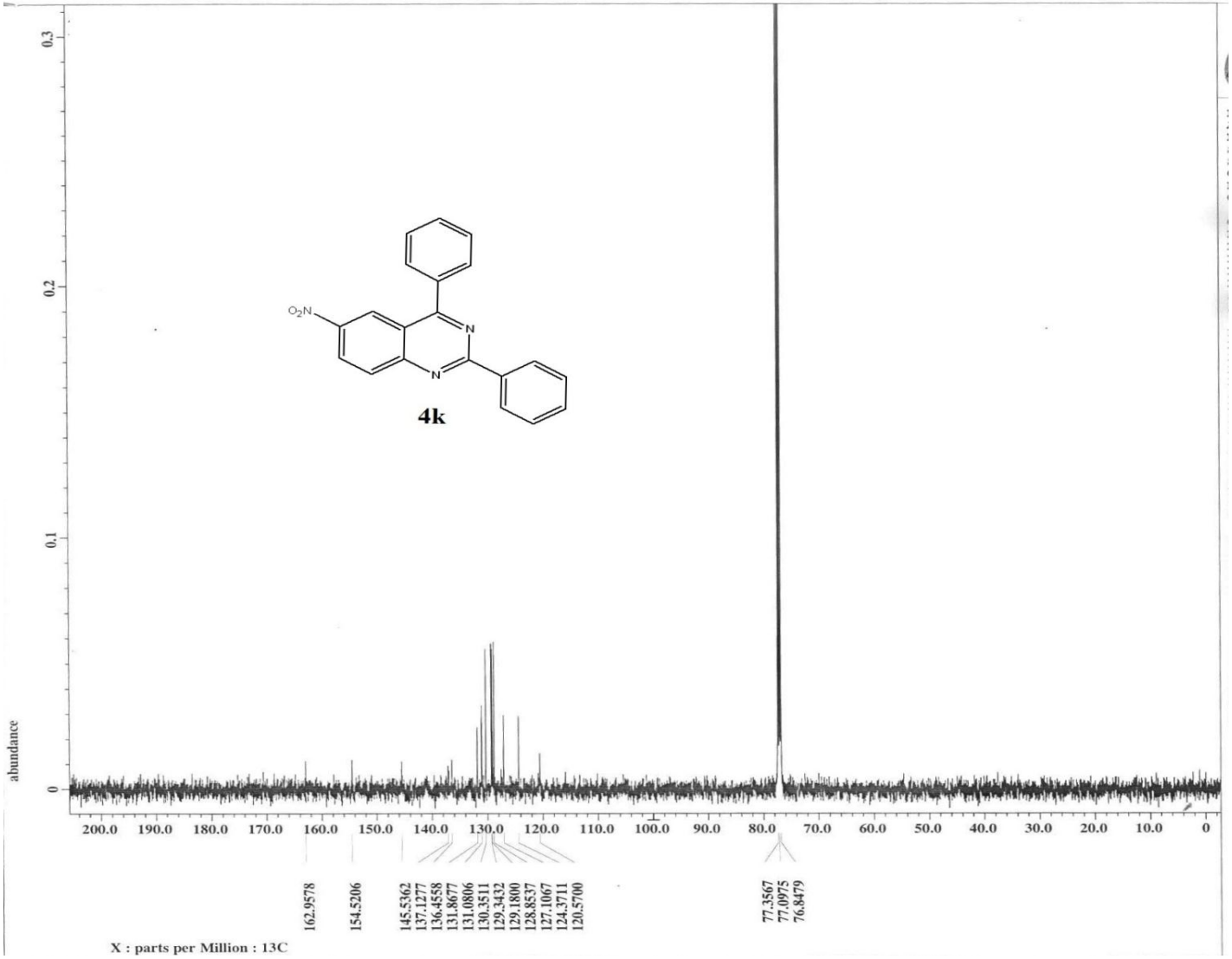
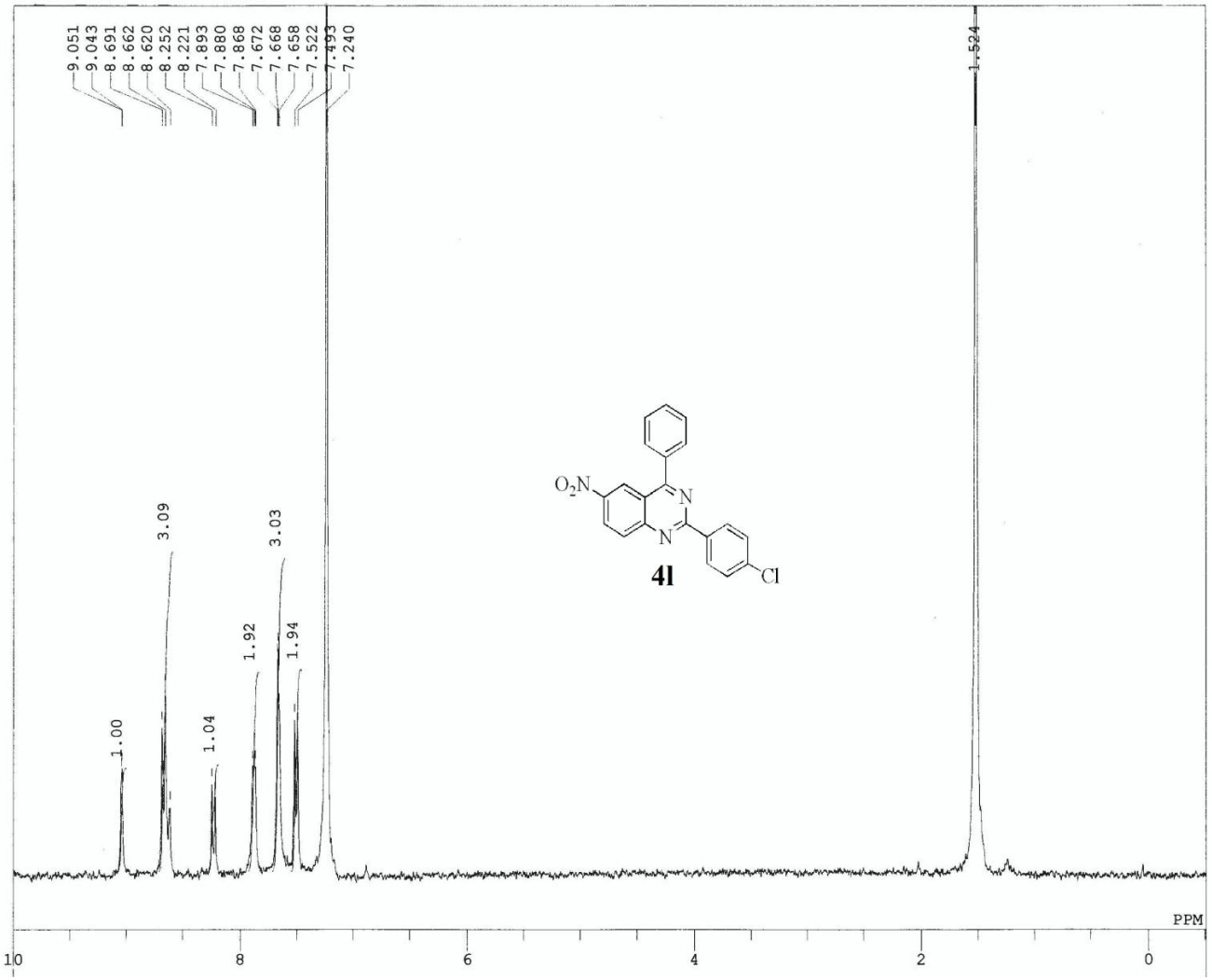


^{1}H-NMR of 6-Nitro-2-(2-nitro-phenyl)-4-phenyl-quinazoline (4l)



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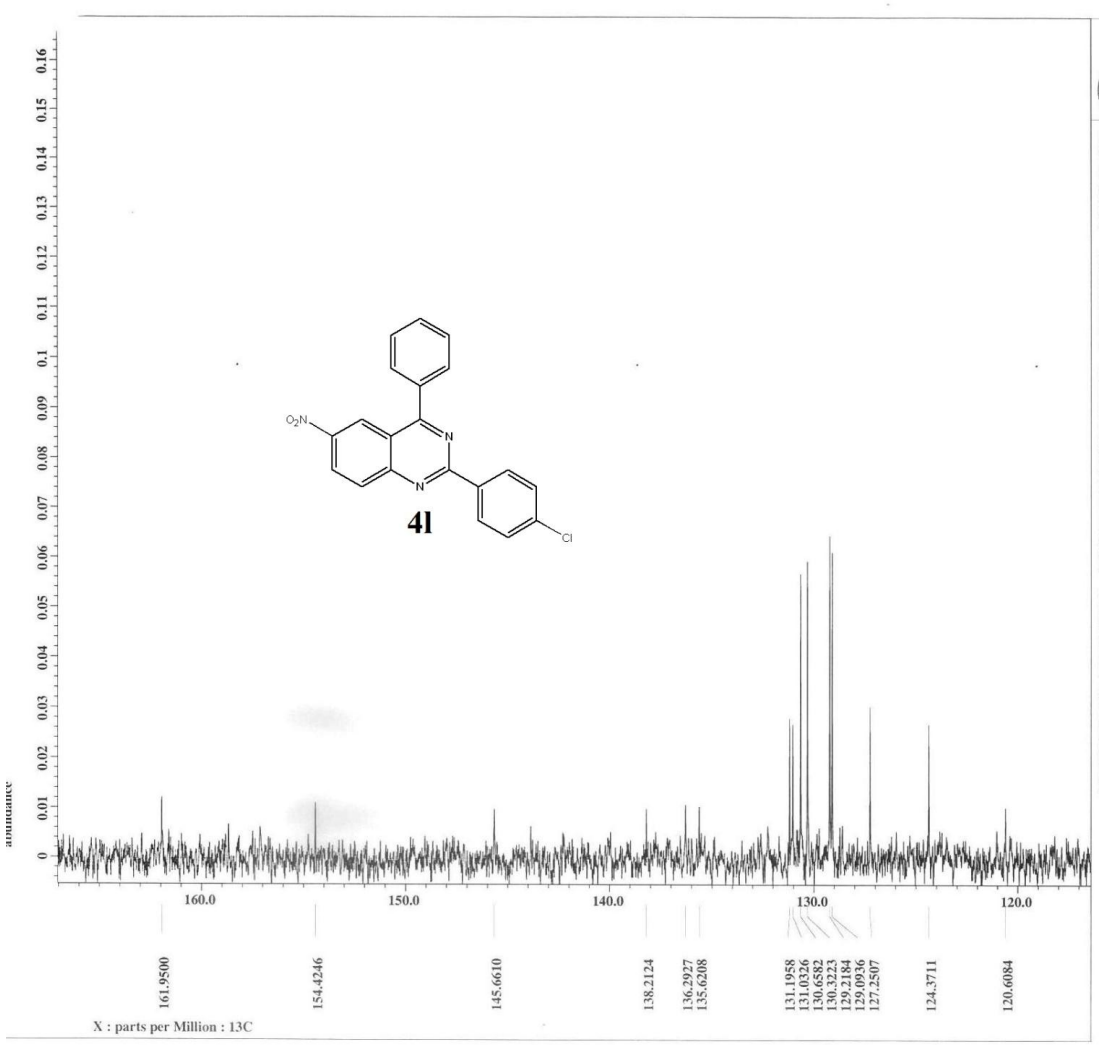
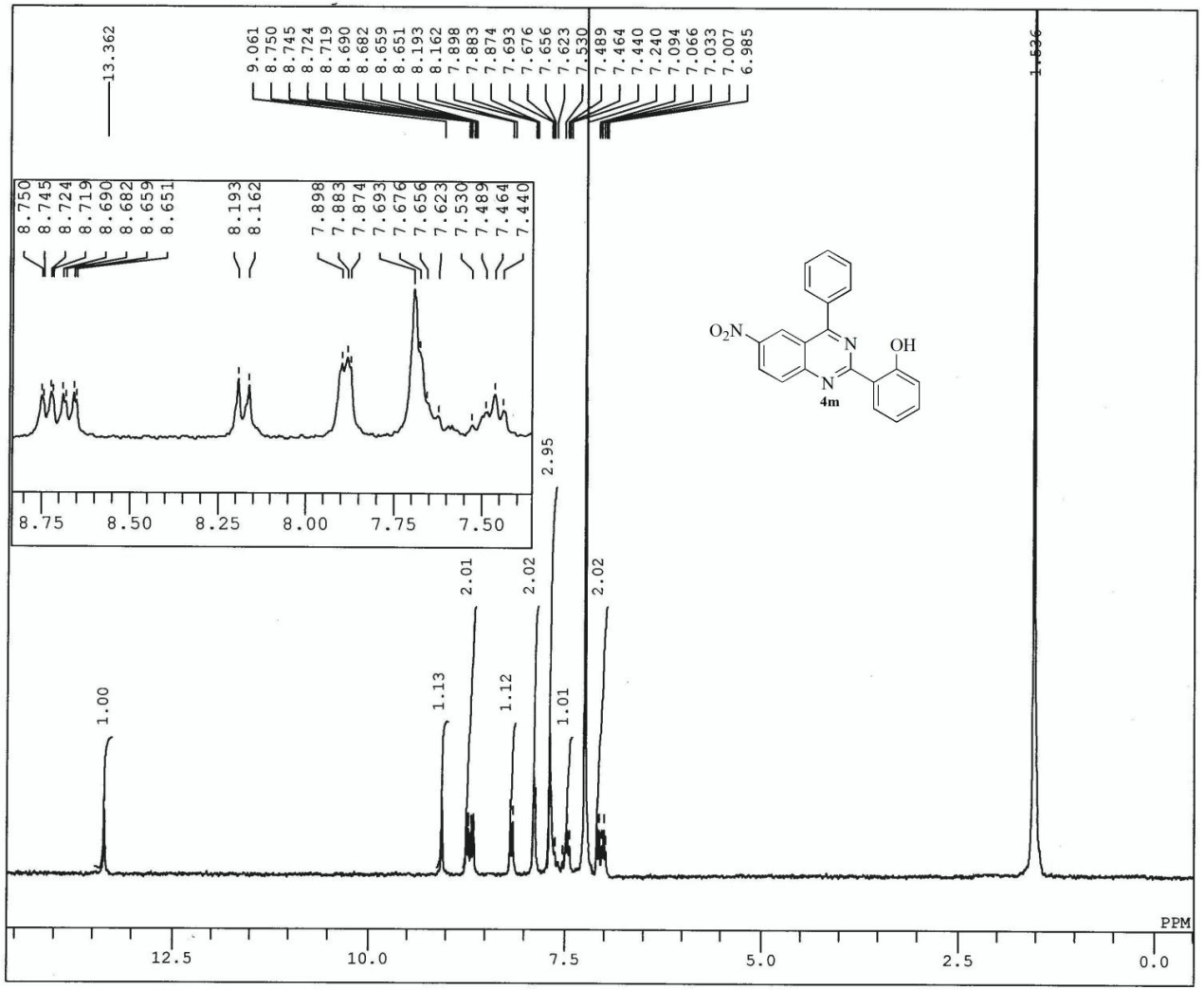


^{1}H-NMR of 2-(6-Nitro-4-phenyl-quinazolin-2-yl)-phenol (4m)



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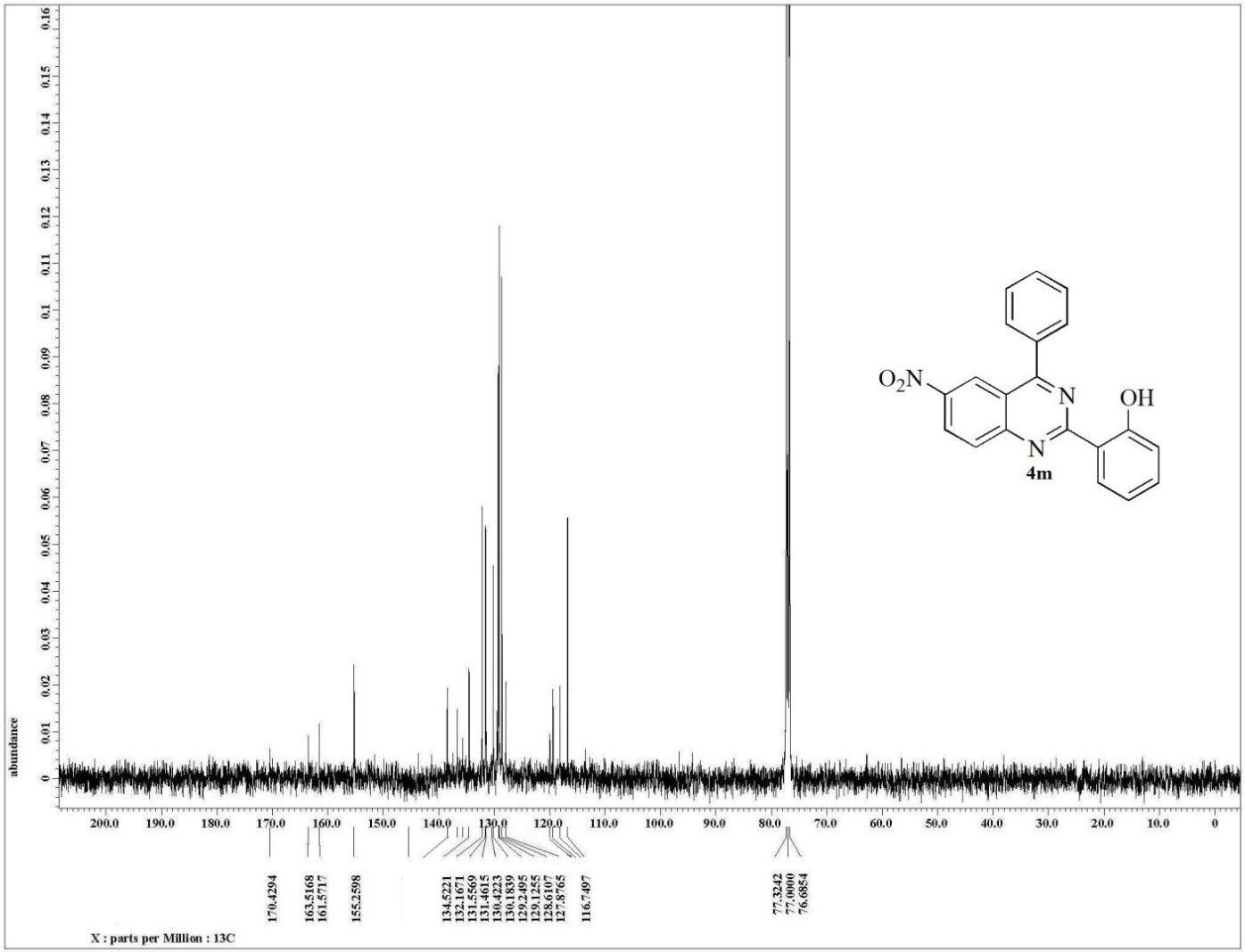

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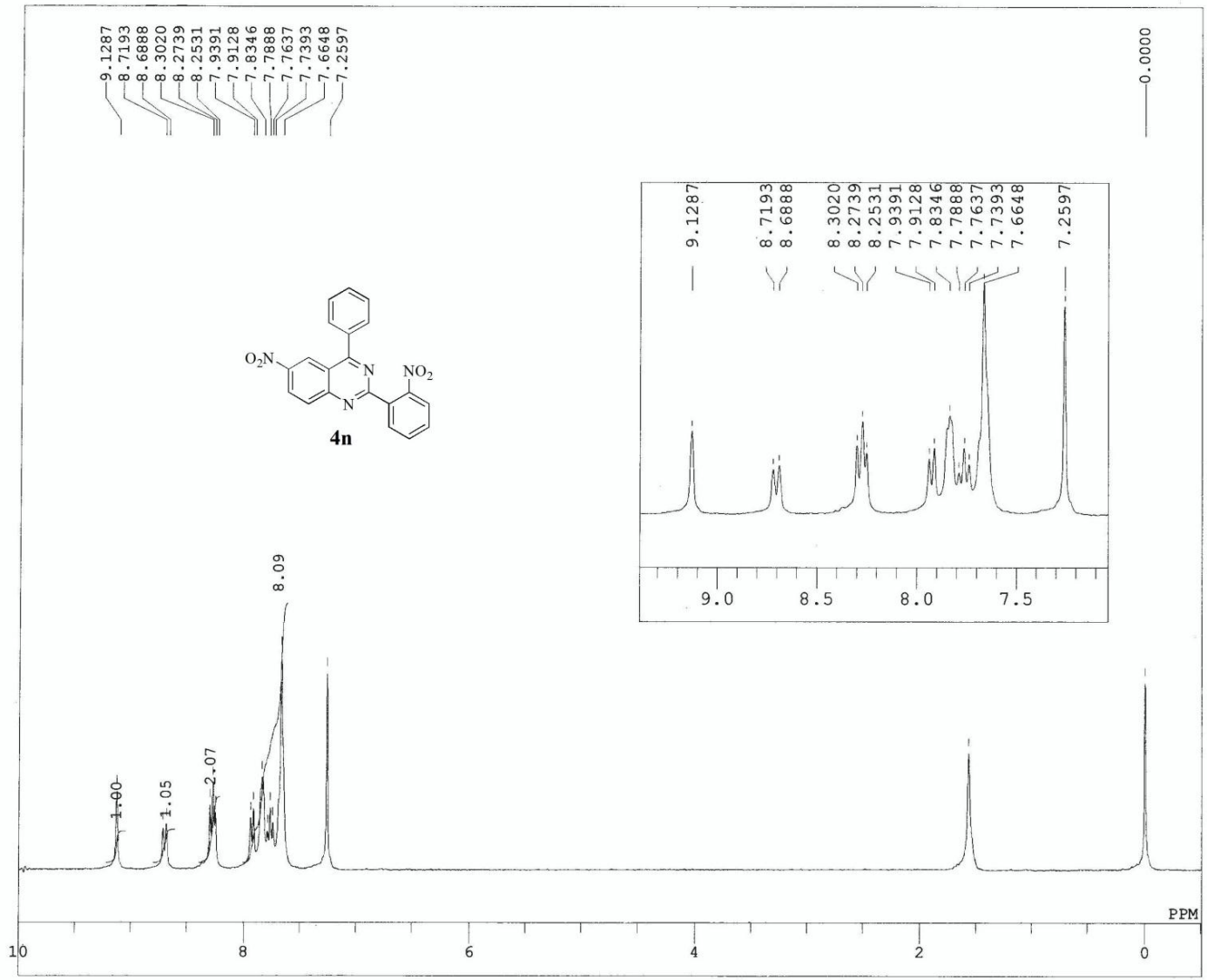

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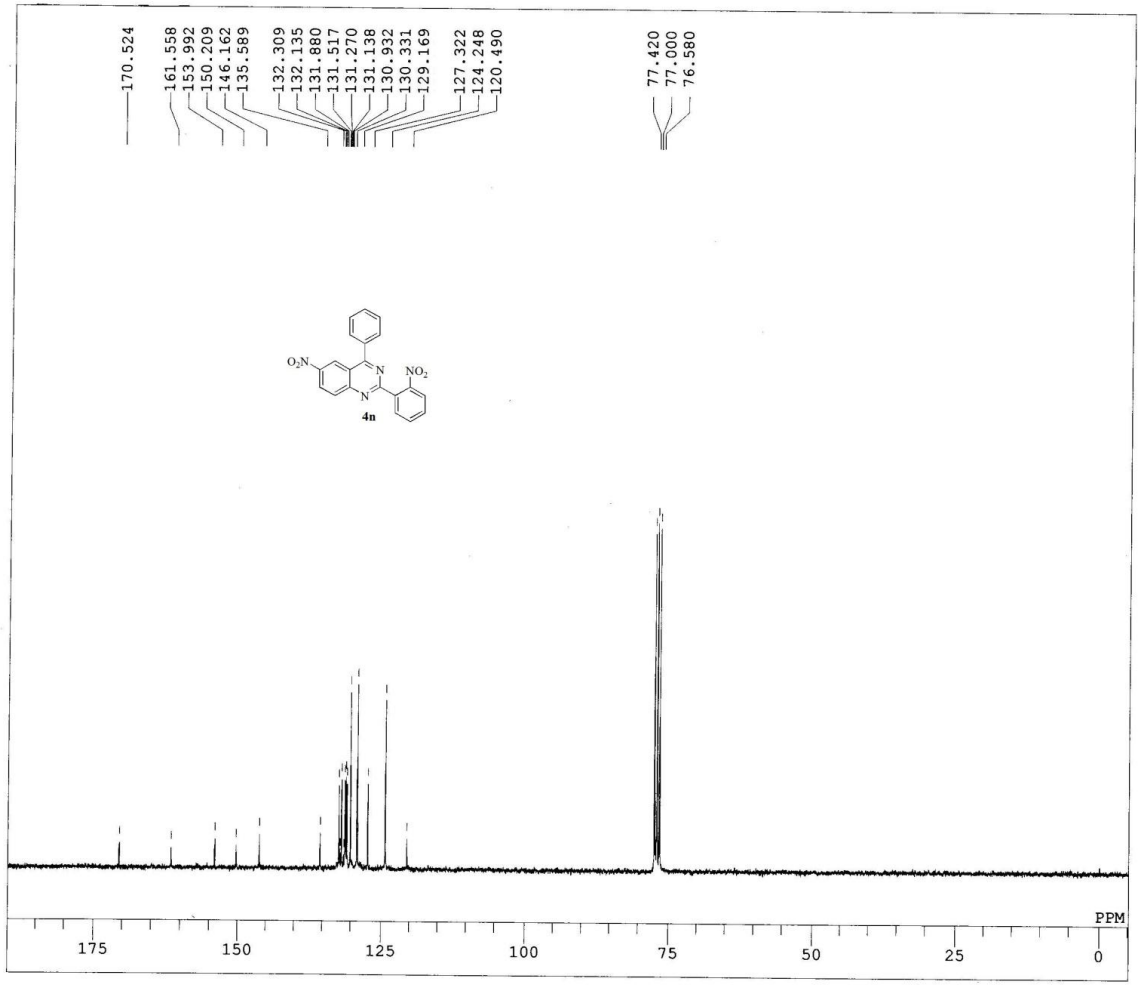

5. UV-Visible spectra of Quinazoline derivatives in acetonitrile solvent (4a-4n, except 4e, and 4j)

Here we are representing the UV-Visible spectra of the synthesized quinazoline derivative in acetonitrile solvent and observing the different substituent affect on electronic spectra of quinazoline derivatives. The Molar extinction coefficient at selected peak maxima in acetonitrile are tabulated **(Table 1).**

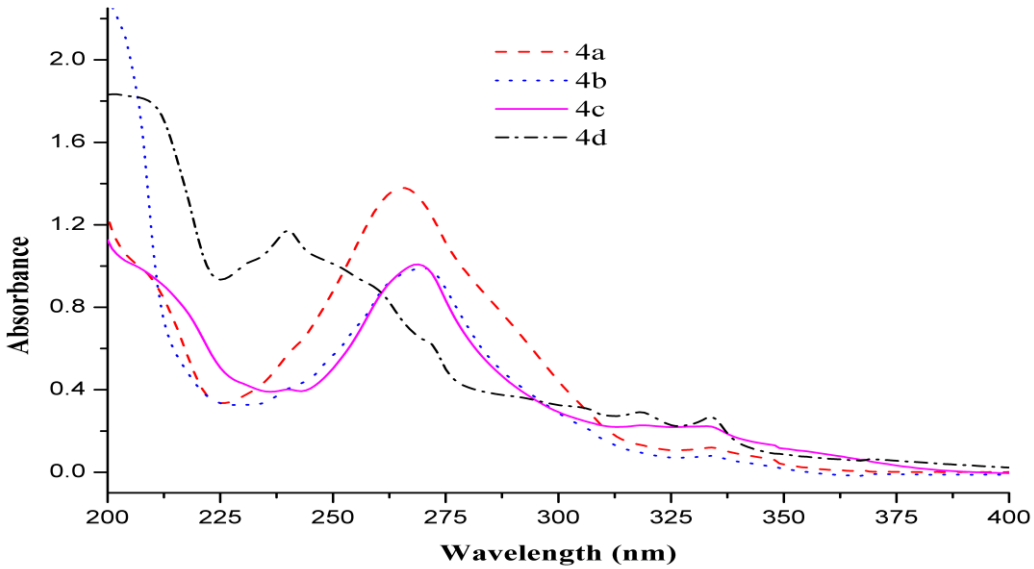

Figure 1 UV-Visible spectra of quinazoline derivatives in acetonitrile (concentrations of **4a**, **4b**, **4c**, and **4d** are 16.6, 14.7, 12.6, and 36.6 μmolar respectively).

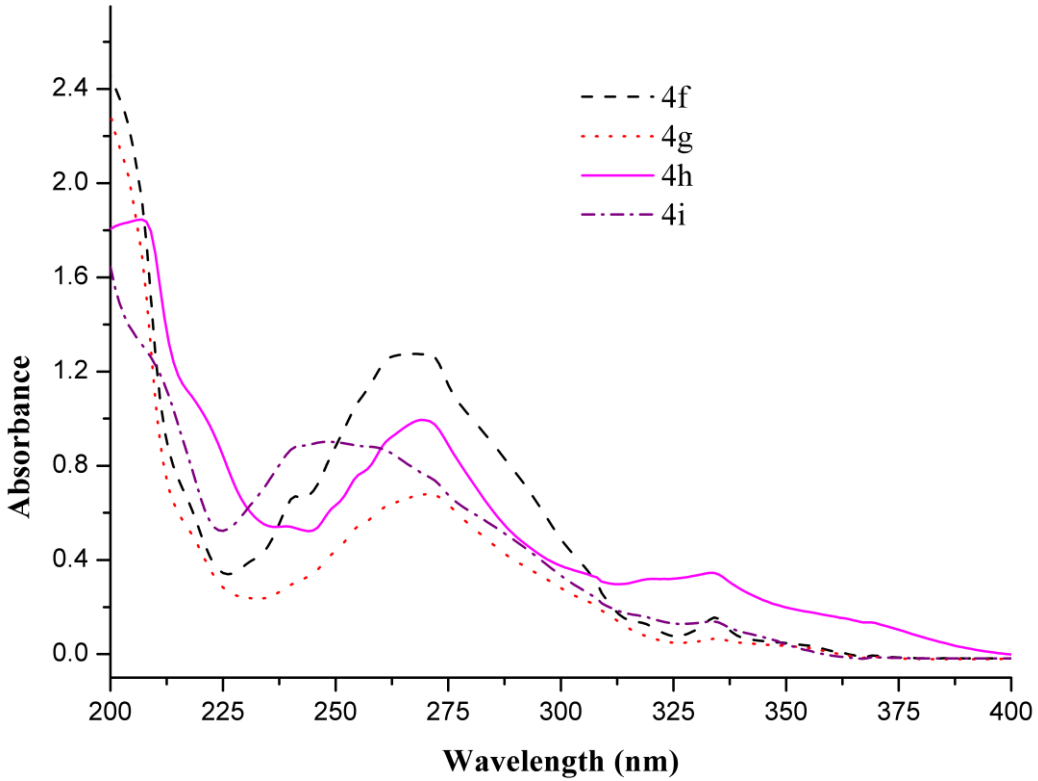

Figure 2 UV-Visible spectra of quinazoline derivatives in acetonitrile (concentrations of **4f**, **4g**, **4h**, and **4i** are 14.7, 15.1, 28.0, and 20.7 μmolar respectively).

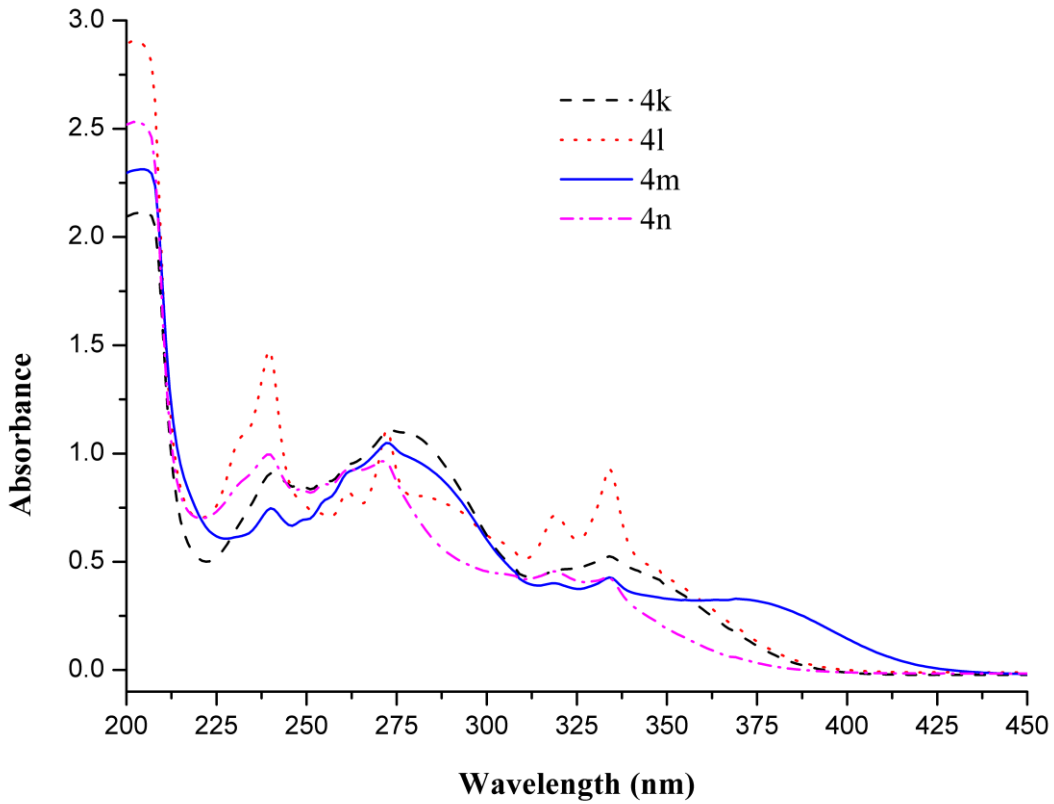

Figure 3: UV-Visible spectra of quinazoline derivatives in acetonitrile (concentrations of **4k**, **4l**, **4m**, and **4n** are 28.5, 25.6, 29.1, and 32.2 μmolar respectively).

Table 1: Molar extinction coefficient at selected peak maxima in acetonitrile

Entry	λ_{max} / nm (ε / $Lmol^{-1}$ cm^{-1})	λ_{max} / nm (ε / $Lmol^{-1}$ cm^{-1}))	λ_{max} / nm (ε / $Lmol^{-1}$ cm^{-1}))
4a	265 ($8.301X10^4$)	334 ($7.222x10^3$)	-
4b	270 ($6.703x10^4$)	334 ($5.281x10^3$)	-
4c	269 ($8.001x10^4$)	334 ($2.345x10^4$)	-
4d	240 ($3.200x10^4$)	334 ($7.341x10^3$)	320 ($7.889x10^3$)
4f	268 ($8.637X10^4$)	334 ($1.053x10^4$)	352 ($2.936x10^3$)
4g	271 ($4.472x10^4$)	334 ($4.295x10^3$)	350 ($2.218x10^3$)
4h	269 ($3.546x10^4$)	334 ($1.231x10^4$)	-
4i	248 ($4.343x10^4$)	334 ($6.498x10^3$)	-
4k	273 ($3.860X10^4$)	334 ($1.841x10^4$)	241 ($3.190x10^4$)
4l	272 ($8.135x10^4$) 240 ($5.761x10^4$)	334 ($3.321x10^4$)	376 ($2.449x10^4$)
4m	273 ($3.597x10^4$)	334 ($1.470x10^4$)	369 ($1.130x10^4$)
4n	272 ($2.990x10^4$) 240 ($3.091x10^4$)	334 ($1.326x10^4$)	320 ($1.414x10^4$)

6. Single Crystal XRD measurement

Crystal data was collected on an OXFORD DIFFRACTION X CALIBER EoS diffractometer using graphite monochromatized Mo Ka radiation at 298 K. The structures were solved by direct methods and refined by full matrix least squares on F2 using SHELX-97.[3a] The non-hydrogen atoms were refined with anisotropic thermal parameters. All the hydrogen atoms were geometrically fixed and allowed to refine using a riding model. The refinement converged to a final R1 and wR2. Drawings were made using ORTEP-III[3b] and Mercury.[3c]. The crystal structure has been deposited in CCDC and can be accessed freely.

Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. **CCDC No. 871913 for 6-Nitro-2-(2-nitro-phenyl)-4-phenyl-quinazoline (4n)**, and …..intermediate C **2-(6-chloro-4-phenyl-1,2-dihydroquinolin-2-yl)phenol** respectively. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (Fax: +44(0)-1223-336033 or e-mail: deposit@ccdc.cam.ac.uk).

Single crystals of $C_{20}H_{13}N_4O_4$ (4l) was recrystallised from chloroform, mounted in normal atomosphere of the diffractometer.

a. Crystal structure determination of 6-Nitro-2-(2-nitro-phenyl)-4-phenyl-quinazoline (4n) and intermediate C 2-(6-chloro-4-phenyl-1,2-dihydroquinolin-2-yl)phenol compounds.

Compound name	**6-Nitro-2-(2-nitro-phenyl)-4-phenyl-quinazoline (4n)**	**2-(6-chloro-4-phenyl-1,2-dihydroquinolin-2-yl)phenol**
Chemical Formula	$C_{20}H_{12}N_4O_4$	$C_{20}H_{15}ClN_2O$
Molecular Weight (M)	372.33	334.79
Symmetry Cell Setting	orthorhombic	orthorhombic
Space Group Name: Hall	*P 21/n*	P 2ac 2ab
Cell Length	*a* = 10.7619(5) Å, *b* = 7.9318(4) Å, *c* = 19.9964(10) Å	*a* = 7.8795(7) Å, *b* = 10.8790(8) Å, *c* = 19.733(2) Å
Cell Angle	α =90, β = 96.129 *γ*= 90	α =90, β = 90 *γ*= 90

Cell Volume (U)	1697.17(14) Å^3	1691.5(3) Å^3
Cell Formula units (Z)	4	4
Cell Measurement Temperature	298 K	298 K
Cell Measurement Reflections used	4539	1253
*R*int	0.052	0.0202
wR2 (F_2)	0.1273	0.1309

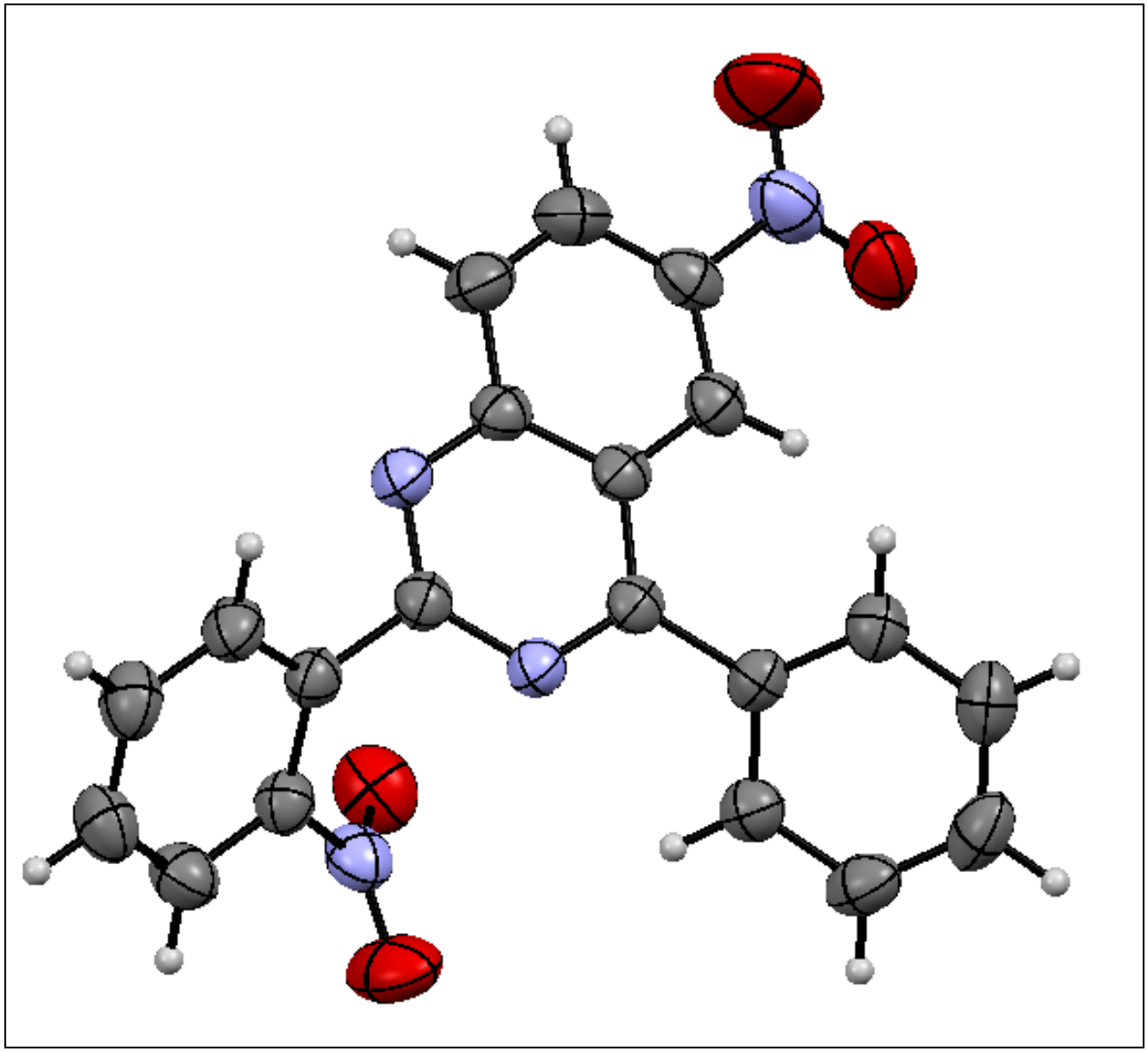

Fig 4: ORTEP diagram of 6-Nitro-2-(2-nitro-phenyl)-4-phenyl-quinazoline (4n)

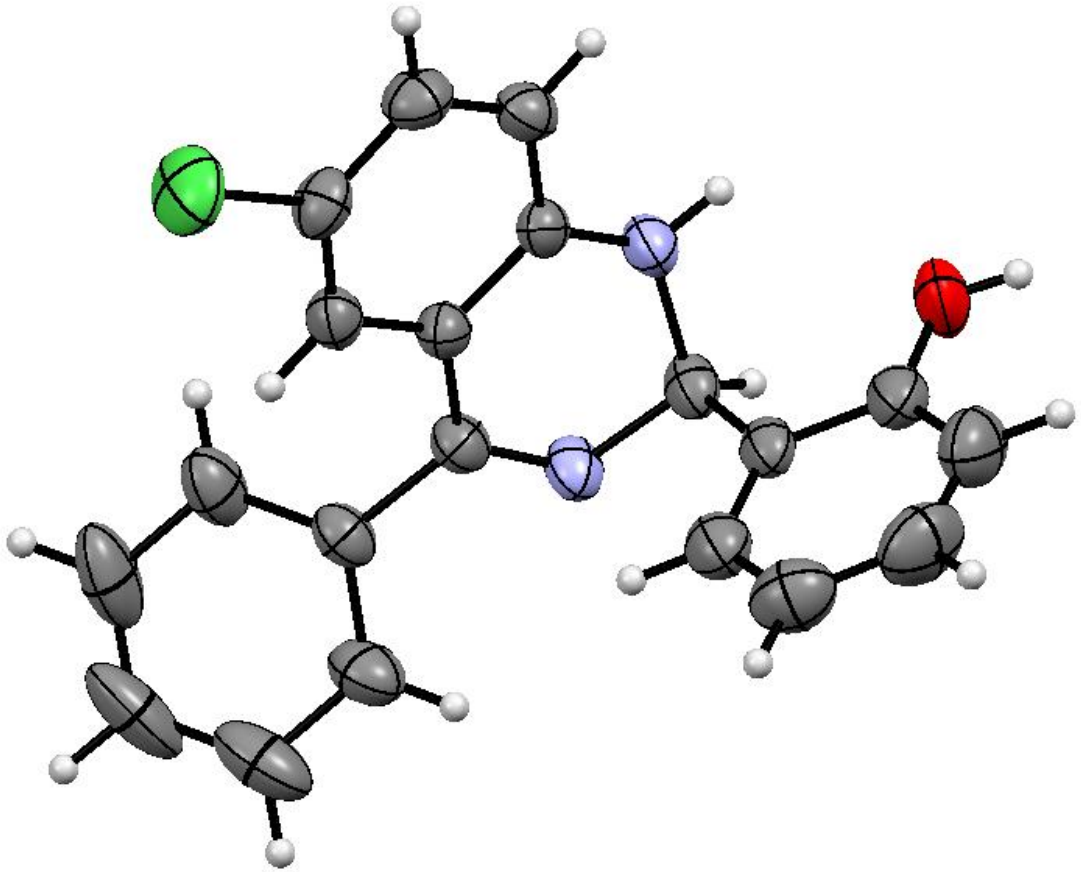

Fig 5: ORTEP diagram of intermediate C 2-(6-chloro-4-phenyl-1,2-dihydroquinolin-2-yl)phenol

7. References and notes

[1] (a) S. Hayashi and H. Hamaguchi, *Chem. Lett.* 2004**, 33**, 1590; (b) M. S. Sitze, E. R. Schreiter, E. V. Patterson and R. G. Freeman, *Inorg. Chem.* 2001**, 40**, 2298.

[2] (a) C. Huang, Y. Fu, H. Fu, Y. Jiang and Y. Zhao, *Chem. Commum*. 2008, **47**, 6333; (b) J. Zhang, C. Yu, S. Wang, C. Wan and Z. Wang, *Chem. Commum*. 2010, **46**, 5244; (c) R. Tachikawa, K. Wachi and A. Terada, *Chem. Pharm. Bull.* 1982, **30**, 559; (d) J. Bergman, A. Brynolf, B. Elman and E. Vuorinen, *Tetrahedron* 1986, **42**, 3697; (e) K. Karnakar, J. Shankar, S. Narayana Murthy, K. Ramesh, Y. V. D. Nageswar, *Synlett.* 2011, **8**, 1089; (f) M. Dabiri, P. Salehi and M. Bahramnejad, *Synth. Commun.* 2010, **40**, 3214; (g) Z.-H. Zhang, X-N. Zhang, L.-P. Mo, Y.-X. Li and F.-P. Ma, *Green Chem.* 2012, **13**, 718.

[3] (a) Sheldrick, G. M. Acta Cryst. **2008**, 64A, 112; (b) Burnett M. N.; Johnson, C. K. Report ORNL-6895. Oak Ridge National Laboratory, Oak Ridge, Tennessee, 1996; (c) Bruno, I. J.; Cole, J. C.; Edgington, P. R.; Kessler, M. K.; Macrae, C. F.; McCabe, P.; Pearson J.; Taylor, R. Acta Cryst. **2002**, B58, 389.