Supporting Information

I_2-Catalyzed Oxidative Synthesis of *N*,4-Disubstituted Quinazolines and Quinazoline Oxides

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General information and Reagents:

The glassware to be used in reactions was thoroughly washed and dried in an oven and the experiments were carried out with required precautions. Chemicals and all solvents were obtained from commercial suppliers and used without further purification. ^{1}H-NMR was measured on Bruker Avance-300, Varian Unity-400 MHz and Avance New-500 MHz and ^{13}C-NMR was measured with Varian Unity-400 MHz (100 MHz) and with Avance New-500 MHz (125 MHz), as specified and referred as the internal standard to TMS (tetramethylsilane). Chemical shifts (δ) are given in ppm and J values are given in Hz. High Resolution Mass Spectra (HRMS) were performed on a high resolution magnetic sector mass spectrometer. TLC analysis was performed on Merck silica gel 60 F_{254} plates. Column chromatography was performed on silica gel (100-200 mesh) from Merck. Melting points were measured using melting point apparatus and were uncorrected. Evaporation of solvents was performed at reduced pressure, using a rotary vacuum evaporator.

Typical procedure for the synthesis of intermediate A:

The mixture of phenyl isothiocyanate (**1a**) (1.0 mmol, 135mg) and 2-aminobenzophenone (**2a**) (1.0 mmol, 197mg) in DMSO (3 mL) was stirred magnetically at 50 ^{o}C. After completion of the reaction as monitored by TLC, the reaction mixture was treated with brain solution and extracted with EtOAc. The organic and aqueous layers were then separated and the aqueous layer was extracted with ethyl acetate twice. The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to get crude. The crude was purified by silica gel column chromatography using EtOAc : hexane as eluents to afford corresponding product **A.**

Typical procedure for the synthesis of intermediate A to 3a:

The intermediate A (1.0 mmol 332 mg) and ammonium acetate (6 equiv) and iodine (0.5 equiv) mixture was stirred magnetically at 50 ^{o}C temperature After completion of the reaction as monitored by TLC, the reaction mixture was quenched with a saturated aqueous solution of $Na_2S_2O_3$. The organic and aqueous layers were then separated and the aqueous layer was extracted with ethyl acetate twice. The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to get crude. The crude was purified by silica gel column chromatography using EtOAc : hexane as eluents to afford corresponding product **3a.**

3a yield 96% (285 mg).

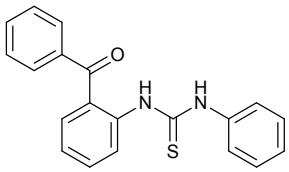
Typical procedure for the synthesis of *N*,4- Disubstituted Quinazolines (3a-3q):

The mixture of isothiocyanate (**1**) (1.0 mmol), *2*-aminobenzophenone (**2**) (1.0 mmol) in DMSO (3 mL) was stirred magnetically at 50 ^{o}C temperature, after 1 to 1.5 h addition of ammonium acetate (6 equiv) and iodine (0.5 equiv) After completion of the reaction as monitored by TLC, the reaction mixture was quenched with a saturated aqueous solution of $Na_2S_2O_3$. The organic and aqueous layers were then separated and the aqueous layer was extracted with ethyl acetate twice. The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to get crude. The crude was purified by silica gel column chromatography using EtOAc : hexane as eluents to afford corresponding product **3a-3q.**

Typical procedure for the synthesis of *N*,4- Disubstituted Quinazolines 3-oxide (5a-5h):

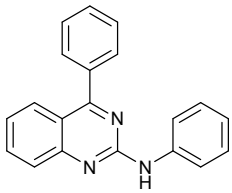
The mixture of phenyl isothiocyanate (**1**) (1.0 mmol) and (2-aminophenyl)(phenyl)methanone oxime (**4**) (1.0 mmol) and I_2 (0.5 equiv) in DMSO (3 mL) was stirred magnetically at room temperature. After completion of the reaction as monitored by TLC, the reaction mixture was quenched with a saturated aqueous solution of $Na_2S_2O_3$. The organic and aqueous layers were then separated and the aqueous layer was extracted with ethyl acetate twice. The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to get crude. The crude was purified by silica gel column chromatography using EtOAc : hexane as eluents to afford corresponding product of **5a-5h**.

1-(2-Benzoylphenyl)-3-phenylthiourea (**A**)



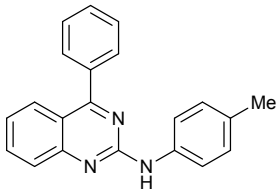
Yield 98% (325 mg); wight solid; Mp 185-187 °C; eluent; hexane/ethyl acetate 85:15; ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.36 (s, 1H), 7.72 (s, 1H), 7.36 (d, *J* = 8.1 Hz, 1H), 7.31-7.23 (m, 2H), 7.23-7.14 (m, 6H), 7.09 (dd, *J* = 10.6, 4.2 Hz, 1H), 6.98-6.90 (m, 2H), 6.89-6.84 (m, 1H), 6.31 (d, *J* = 8.1 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 179.6, 149.9, 146.2, 138.3, 137.0, 135.9, 134.2, 133.1, 132.8, 132.6, 132.1, 131.9, 131.6, 131.1, 127.9, 119.0, 92.6; HRMS (ESI-TOF) m/z: [M + H] $^{+}$ calcd for $C_{20}H_{17}N_2OS$, 333.1062; found, 333.1058.

***N*-4-Diphenylquinazolin-2-amine** (**3a**)



Yield 95% (282 mg); yellow solid; Mp 120-123 °C; eluent; hexane/ethyl acetate 96:4; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.90-7.81 (m, 4H), 7.71-7.75 (m, 3H), 7.58-7.54 (m, 3H), 7.43 (s, 1H), 7.37 (t, *J* = 7.9 Hz, 2H), 7.29-7.24 (m, 1H), 7.05 (t, *J* = 7.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.0, 156.1, 152.7, 139.9, 137.2, 133.9, 129.9, 129.6, 128.9, 128.6, 127.4, 126.9, 123.6, 122.3, 119.1, 118.7; HRMS (ESI-TOF) m/z: [M + H] $^{+}$ calcd for $C_{20}H_{16}N_3$, 298.1344; found, 298.1348.

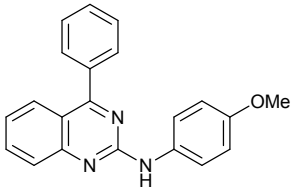
4-Phenyl-*N*-(p-tolyl)quinazolin-2-amine (**3b**)



Yield 94% (292 mg); yellow solid; Mp 137-140 °C; eluent; hexane/ethyl acetate 96:4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.2 Hz, 1H), 7.80 (d, *J* = 8.4 Hz, 1H), 7.74-7.68 (m, 5H), 7.57-7.51 (m, 3H), 7.39 (s, 1H), 7.23 (t, *J* = 7.5 Hz, 1H), 7.16 (d, *J* = 8.2 Hz, 2H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.0, 156.3, 152.9, 137.3, 137.2, 133.8, 131.8, 129.8, 129.6, 129.4,

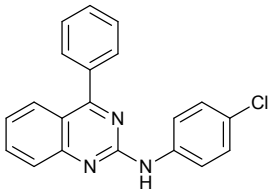
128.6, 127.3, 126.9, 123.4, 119.0, 20.9; HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{21}H_{18}N_3$, 312.1501; found, 312.1499.

***N*-(4-methoxyphenyl)-4-phenylquinazolin-2-amine (3c)**



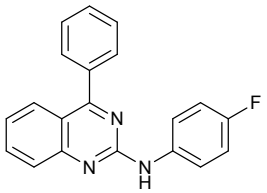
Yield 95% (310 mg); Yellow solid: Mp 128-129 °C; eluent; hexane/ethyl acetate 94:6; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.2 Hz, 1H), 7.80-7.65 (m, 6H), 7.60-7.51 (m, 3H), 7.35 (s, 1H), 7.24-7.20 (m, 1H), 6.92 (d, *J* = 8.9 Hz, 2H), 3.81 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.0, 156.4, 155.2, 152.9, 137.2, 133.8, 133.1, 129.8, 129.6, 128.5, 127.4, 126.8, 123.2, 120.7, 119.0, 114.2, 55.6; HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{21}H_{18}N_3O$, 328.1450; found, 328.1466.

***N*-(4-chlorophenyl)-4-phenylquinazolin-2-amine (3d)**



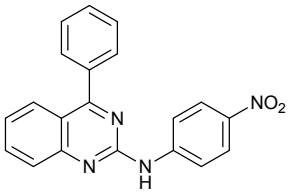
Yield 94% (310 mg); yellow solid; Mp 175-176 °C; eluent; hexane/ethyl acetate 95:5; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (dd, *J* = 8.3, 0.8 Hz, 1H), 7.84-7.70 (m, 6H), 7.58-7.53 (m, 3H), 7.50 (s, 1H), 7.33-7.25 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 170.1, 155.9, 152.6, 138.5, 137.0, 134.0, 130.0, 129.6, 128.8, 128.6, 127.4, 126.9, 126.9, 123.8, 119.9, 119.2; HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{20}H_{15}ClN_3$, 332.0955; found, 332.0952.

***N*-(4-fluorophenyl)-4-phenylquinazolin-2-amine (3d)**



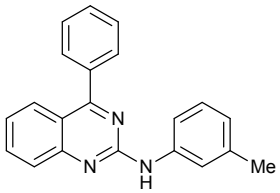
Yield 94% (311 mg); yellow solid; Mp 158-160 °C; eluent; hexane/ethyl acetate 95:5; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.1 Hz, 1H), 7.81-7.74 (m, 6H), 7.57 (s, 3H), 7.39 (s, 1H), 7.29-7.26 (m, 1H), 7.07 (t, *J* = 8.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.2, 159.5, 157.1, 156.1, 152.6, 137.1, 135.9, 134.0, 129.9, 129.5, 128.6, 127.4, 126.8, 123.6, 120.4, 120.3, 119.1, 115.6, 115.4; HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{20}H_{15}FN_3$, 316.1250, found, 316.1258.

***N*-(4-nitrophenyl)-4-phenylquinazolin-2-amine (3f)**



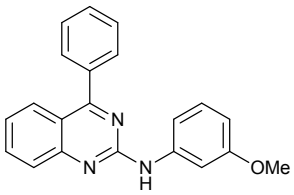
Yield 92% (314 mg); yellow solid; Mp 213-215 °C; eluent; hexane/ethyl acetate 90:10; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.29-8.22 (m, 2H), 8.05-8.00 (m, 2H), 7.98 (dd, *J* = 8.3, 0.7 Hz, 1H), 7.92 (d, *J* = 8.3 Hz, 1H), 7.87-7.81 (m, 2H), 7.78-7.74 (m, 2H), 7.62-7.57 (m, 3H), 7.41-7.38 (m,1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.4, 155.1, 152.2, 145.9, 141.7, 136.7, 134.4, 130.3, 129.6, 128.7, 127.5, 127.2, 125.3, 124.9, 119.7, 117.5; HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{20}H_{15}N_4O_2$, 343.1195, found, 343.1196.

4-Phenyl-*N*-(m-tolyl)quinazolin-2-amine (3g)



Yield 94% (292 mg); yellow solid; Mp 136-138 °C; eluent; hexane/ethyl acetate 96:4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.2 Hz, 1H), 7.83 (d, *J* = 8.4 Hz, 1H), 7.74 (dt, *J* = 9.3, 5.4 Hz, 4H), 7.61 (s, 1H), 7.59-7.54 (m, 3H), 7.40 (d, *J* = 3.0 Hz, 1H), 7.26 (dd, *J* = 10.5, 4.9 Hz, 2H), 6.88 (d, *J* = 7.5 Hz, 1H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.0, 156.2, 152.8, 139.7, 138.7, 137.2, 133.9, 129.9, 129.6, 128.8, 128.6, 127.3, 126.9, 123.5, 123.2, 119.4, 119.1, 116.0, 21.7; HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{21}H_{18}N_3$, 312.1501, found, 312.1497.

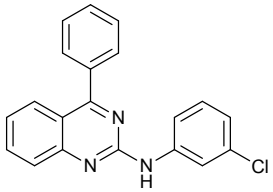
***N*-(3-methoxyphenyl)-4-phenylquinazolin-2-amine (3h)**



Yield 93% (304 mg); yellow solid; Mp 135-138 °C; eluent; hexane/ethyl acetate 92:8; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.2 Hz, 1H), 7.85-7.79 (m, 2H), 7.74 (dd, *J* = 8.6, 6.1 Hz, 3H), 7.61-7.52 (m, 3H), 7.43 (s, 1H), 7.31-7.21 (m, 3H), 6.62 (d, *J* = 7.3 Hz, 1H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.0, 160.2, 156.1, 152.7, 141.1, 137.1, 133.9, 129.9, 129.6, 128.6,

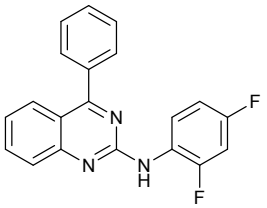
127.3, 126.9, 123.7, 119.1, 111.1, 107.8, 104.6, 55.3; HRMS (ESI-TOF) m/z: $[M + H]^+$calcd for $C_{21}H_{18}N_3O$, 328.1450, found, 328.1462.

***N*-(3-chlorophenyl)-4-phenylquinazolin-2-amine (3i)**



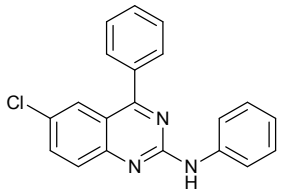
Yield 93% (307 mg); yellow solid; Mp 187-190 °C; eluent; hexane/ethyl acetate 94:6; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.92 (d, J = 8.2 Hz, 1H), 7.87 (d, J = 8.4 Hz, 1H), 7.80-7.73 (m, 3H), 7.62-7.54 (m, 5H), 7.29 (dt, J = 16.1, 6.9 Hz, 2H), 7.01 (d, J = 7.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.2, 155.7, 152.5, 141.1, 137.0, 130.0, 129.8, 129.6, 128.6, 127.4, 127.0, 124.0, 122.1, 119.3, 118.5, 116.6; HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{20}H_{15}ClN_3$, 332.0955; found, 332.0954.

***N*-(2,4-difluorophenyl)-4-phenylquinazolin-2-amine (3j)**



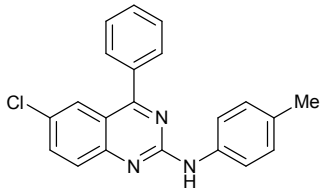
Yield 92% (304 mg); yellow solid; Mp 146-149 °C; eluent; hexane/ethyl acetate 95:5; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.87 (td, J = 9.2, 6.2 Hz, 1H), 7.91 (d, J = 8.3 Hz, 1H), 7.82 (d, J = 8.3 Hz, 1H), 7.75 (t, J = 6.6 Hz, 3H), 7.61-7.53 (m, 3H), 7.47 (s, 1H), 7.30 (t, J = 7.5 Hz, 1H), 7.01-6.83 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.2, 158.4, 158.3, 156.0, 155.8, 153.4, 153.3, 152.5, 151.0, 150.8, 137.0, 134.0, 130.0, 129.6, 128.6, 127.4, 126.9, 124.8, 124.8, 123.9, 121.0, 120.9, 119.3, 110.8, 110.6, 103.6, 103.3, 103.1; HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{20}H_{14}F_2N_3$, 334.1156; found, 334.1153.

6-Chloro-*N*,4-diphenylquinazolin-2-amine (3k)



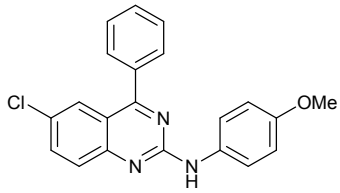
Yield 95% (314 mg); yellow solid; Mp 135-137 °C; eluent; hexane/ethyl acetate 94:6; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (dd, *J* = 7.1, 5.1 Hz, 3H), 7.79-7.70 (m, 3H), 7.66 (dd, *J* = 9.0, 2.3 Hz, 1H), 7.61-7.56 (m, 3H), 7.39 (dd, *J* = 18.3, 10.8 Hz, 3H), 7.07 (t, *J* = 7.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.2, 156.2, 151.3, 139.5, 136.6, 134.6, 130.2, 129.4, 129.0, 128.8, 128.5, 126.1, 122.6, 119.6, 118.8; HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{20}H_{15}ClN_3$, 332.0955; found, 332.0947.

6-Chloro-4-phenyl-*N*-(p-tolyl)quinazolin-2-amine (3l)



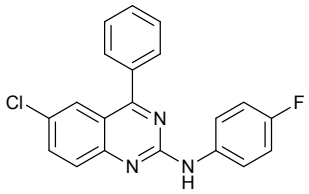
Yield 95% (327 mg); yellow solid; Mp 163-165 °C; eluent; hexane/ethyl acetate 95:5; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 2.2 Hz, 1H), 7.75-7.67 (m, 5H), 7.64 (dd, *J* = 9.0, 2.3 Hz, 1H), 7.60-7.55 (m, 3H), 7.36 (s, 1H), 7.17 (d, *J* = 8.2 Hz, 2H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.2, 156.4, 151.4, 136.9, 136.6, 134.5, 132.2, 130.1, 129.4, 128.7, 128.6, 128.5, 126.1, 119.5, 119.1, 20.8; HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{21}H_{17}ClN_3$, 346.1111; found, 346.115.

6-Chloro-*N*-(4-methoxyphenyl)-4-phenylquinazolin-2-amine (3m)



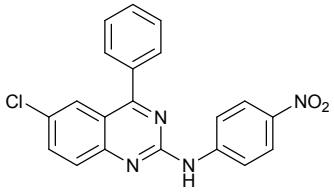
Yield 94% (339 mg); yellow solid; Mp 147-148 °C; eluent, hexane/ethyl acetate 92:8; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 2.2 Hz, 1H), 7.72-7.69 (m, 5H), 7.63 (dd, *J* = 9.0, 2.3 Hz, 1H), 7.58 (dd, *J* = 3.9, 2.4 Hz, 3H), 7.34 (s, 1H), 6.95-6.91 (m, 2H), 3.82 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.3, 156.5, 155.5, 151.4, 136.6, 134.6, 132.7, 130.1, 129.4, 128.7, 128.4, 128.3, 126.1, 120.9, 119.4, 114.2, 55.6 ; HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{21}H_{17}ClN_3O$, 362.1060; found, 362.1052.

6-Chloro-*N*-(4-fluorophenyl)-4-phenylquinazolin-2-amine (3n)



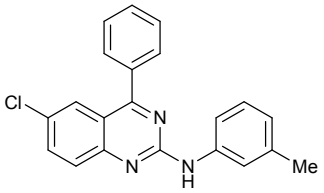
Yield 94% (328 mg); yellow solid; Mp 185-188 °C; eluent; hexane/ethyl acetate 94:6; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (d, *J* = 1.8 Hz, 1H), 7.79-7.65 (m, 6H), 7.60-7.58 (m, 3H), 7.40 (s, 1H), 7.07 (t, *J* = 8.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.4, 159.7, 157.3, 156.2, 151.2, 136.5, 135.6, 134.7, 130.2, 129.4, 128.9, 128.8, 128.4, 126.1, 120.5, 119.6, 115.6, 115.4; HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{20}H_{14}ClFN_3$, 350.0860; found, 350.0852.

6-Chloro-*N*-(4-nitrophenyl)-4-phenylquinazolin-2-amine (**3o**)



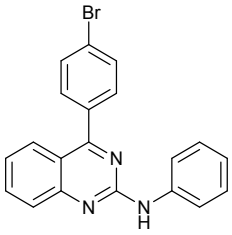
Yield 91% (342 mg); yellow solid; Mp 258-260 °C; eluent; hexane/ethyl acetate 90:10; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.28 (d, *J* = 9.1 Hz, 2H), 8.02 (d, *J* = 9.2 Hz, 2H), 7.94 (d, *J* = 2.1 Hz, 1H), 7.88 (d, *J* = 8.9 Hz, 2H), 7.78-7.74 (m, 3H), 7.62 (dd, *J* = 5.0, 1.7 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 169.8, 165.1, 155.2, 145.5, 142.0, 136.1, 135.2, 130.6, 130.3, 129.5, 128.9, 128.6, 126.2, 125.3, 120.1, 117.7; HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{20}H_{14}ClN_4$,O 377.0805; found, 377.0810.

6-Chloro-4-phenyl-*N*-(m-tolyl)quinazolin-2-amine (**3p**)



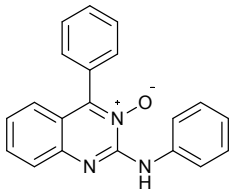
Yield 92% (317 mg); yellow solid; Mp 101-103 °C; eluent; hexane/ethyl acetate 94:6; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 2.3 Hz, 1H), 7.78-7.64 (m, 5H), 7.58 (dd, *J* = 3.7, 2.7 Hz, 4H), 7.37 (s, 1H), 7.26 (t, *J* = 3.9 Hz, 1H), 6.89 (d, *J* = 7.5 Hz, 1H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.2, 156.3, 151.4, 139.4, 138.8, 136.6, 134.6, 130.2, 129.4, 128.8, 128.8, 128.6, 126.1, 123.5, 119.5, 116.12, 21.7; HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{21}H_{17}ClN_3$, 346.1111; found, 346.1109.

4-(4-Bromophenyl)-*N*-phenylquinazolin-2-amine (**3q**)



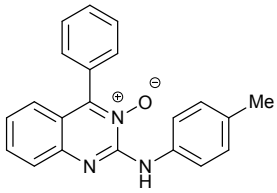
Yield 87% (325 mg); yellow solid; Mp 146-148 °C; eluent; hexane/ethyl acetate 94:6; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.1 Hz, 4H), 7.75-7.57 (m, 6H), 7.35 (t, *J* = 7.7 Hz, 2H), 7.25 (dd, *J* = 13.2, 5.4 Hz, 1H), 7.05 (t, *J* = 7.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.9, 156.0, 152.6, 139.7, 136.0, 134.1, 131.8, 131.2, 128.9, 126.9, 126.9, 124.6, 123.8, 122.5, 118.9, 118.8; HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{20}H_{15}BrN_3$, 376.0449; found, 376.0450.

4-Phenyl-2-(phenylamino)quinazoline 3-oxide (**5a**)



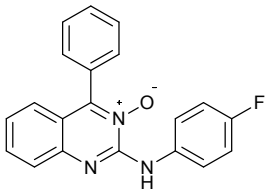
Yield 98% (306 mg); yellow solid; Mp 168-170 °C; eluent; hexane/ethyl acetate 87:13; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.92 (s, 1H), 7.93 (d, *J* = 7.8 Hz, 2H), 7.82 (d, *J* = 8.3 Hz, 1H), 7.67-7.57 (m, 6H), 7.43 (t, *J* = 7.9 Hz, 2H), 7.36 (d, *J* = 8.2 Hz, 1H), 7.30-7.23 (m, 1H), 7.15 (t, *J* = 7.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.3, 147.2, 141.9, 137.7, 131.8, 130.2, 129.7, 129.2, 129.1, 128.7, 126.2, 125.7, 124.9, 123.8, 119.6, 119.4; HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{20}H_{16}N_3O$, 314.1293; found, 341.1290.

4-Phenyl-2-(p-tolylamino)quinazoline 3-oxide (**5b**)



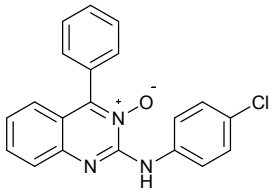
Yield 96% (313 mg); yellow solid; Mp 204-206 °C; eluent; hexane/ethyl acetate 88:12; ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.82 (s, 1H), 7.80 (d, *J* = 8.3 Hz, 3H), 7.63 (d, *J* = 13.0 Hz, 6H), 7.35 (d, *J* = 8.2 Hz, 1H), 7.25 (t, *J* = 8.1 Hz, 3H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.3, 147.3, 142.0, 135.1, 133.5, 131.7, 130.2, 129.7, 129.6, 129.3, 128.7, 126.2, 125.7, 124.7, 119.8, 119.3, 20.9; HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{21}H_{18}N_3O$, 328.1450; found, 328.1455.

2-((4-Fluorophenyl)amino)-4-phenylquinazoline 3-oxide (**5c**)



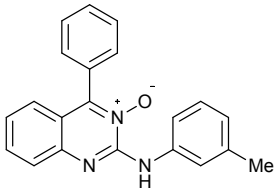
Yield 97% (321 mg); yellow solid; Mp 197-199 °C; eluent; hexane/ethyl acetate 89:11; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.87 (s, 1H), 7.91 – 7.85 (m, 2H), 7.80 (d, *J* = 8.3 Hz, 1H), 7.68-7.58 (m, 6H), 7.37 (dd, *J* = 8.4, 0.9 Hz, 1H), 7.30-7.26 (m, 1H), 7.16-7.09 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.4, 157.9, 149.4, 147.3, 141.8, 133.7, 131.8, 130.3, 129.7, 129.2, 128.7, 126.1, 125.7, 125.0, 121.3, 121.3, 119.4, 115.9, 115.6; HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{20}H_{15}FN_3O$, 332.1199; found, 332.1196.

2-((4-Chlorophenyl)amino)-4-phenylquinazoline 3-oxide (**5d**)



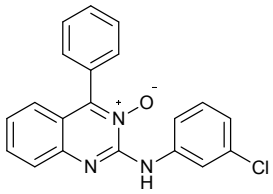
Yield 96% (333 mg); yellow solid; Mp 220-222 °C; eluent; hexane/ethyl acetate 88:12; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.94 (s, 1H), 7.92-7.86 (m, 2H), 7.82 (d, *J* = 8.3 Hz, 1H), 7.69-7.59 (m, 6H), 7.40-7.37 (m,3H), 7.32-7.28 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.4, 147.0, 141.7, 136.3, 131.9, 130.3, 129.7, 129.1, 128.7, 128.7, 126.2, 125.7, 125.2, 120.8, 119.5; HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{20}H_{15}ClN_3O$, 348.0904; found, 348.0909.

4-Phenyl-2-(m-tolylamino)quinazoline 3-oxi*de* (**5e**)



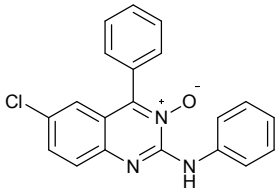
Yield 94% (307 mg); yellow solid; Mp 177-180 °C; eluent; hexane/ethyl acetate 88:12; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.85 (s, 1H), 7.80 (t, *J* = 8.7 Hz, 2H), 7.67-7.58 (m, 7H), 7.36-7.24 (m, 3H), 6.97 (d, *J* = 7.5 Hz, 1H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.2, 147.3, 141.9, 139.0, 137.6, 131.7, 130.2, 129.7, 129.3, 129.0, 128.7, 126.2, 125.7, 124.9, 124.7, 120.3, 119.3, 116.8, 21.7; HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{21}H_{18}N_3O$, 328.1450; found, 328.1455.

2-((3-Chlorophenyl)amino)-4-phenylquinazoline 3-oxide (**5f**)



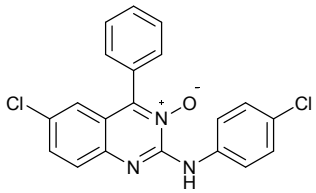
Yield 95% (329 mg); yellow solid; Mp 208-210 °C; eluent; hexane/ethyl acetate 90:10; ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.97 (s, 1H), 8.18 (s, 1H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.71-7.57 (m, 7H), 7.41-7.27 (m, 3H), 7.12 (d, *J* = 8.0 Hz, 1H).^{13}C NMR (100 MHz, $CDCl_3$) δ 149.5, 146.9, 141.6, 138.9, 134.8, 131.9, 130.3, 130.0, 129.7, 129.1, 128.7, 126.4, 125.7, 125.3, 123.7, 119.5, 119.3, 117.6; HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{20}H_{15}ClN_3O$, 348.0904; found, 348.0908.

***6*-Chloro-4-phenyl-2-(phenylamino)quinazoline 3-oxide (5g)**



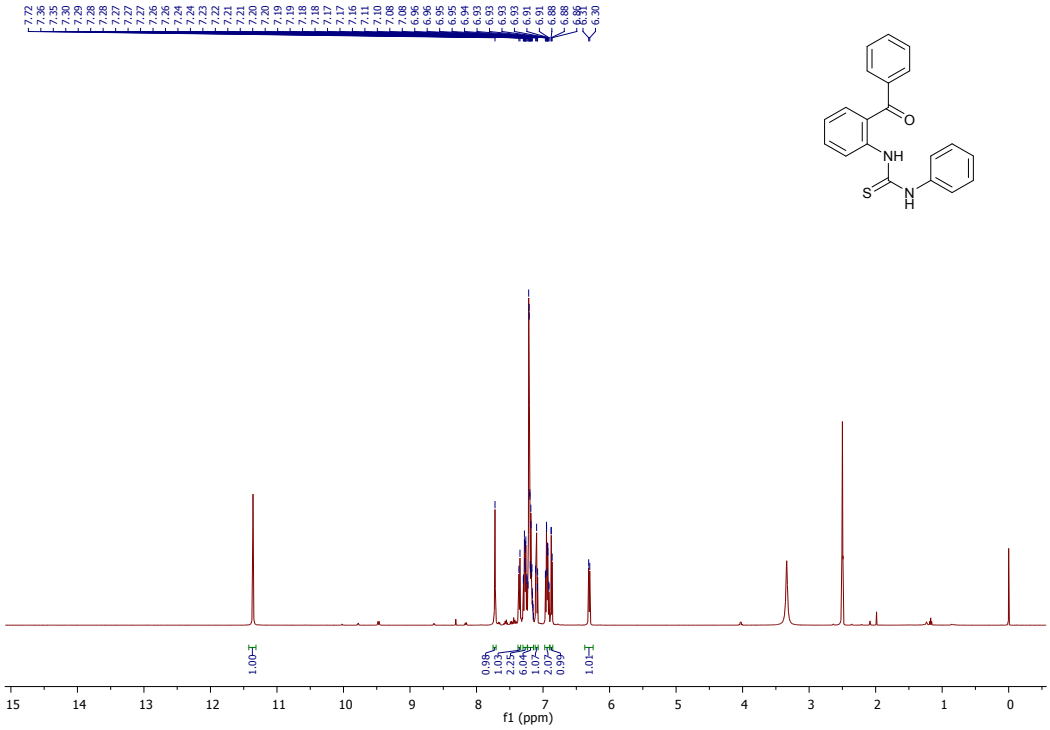
Yield 96% (333 mg); yellow solid; Mp 192-196 °C; eluent; hexane/ethyl acetate 90:10; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.87 (s, 1H), 7.90 (dd, *J* = 8.5, 0.9 Hz, 2H), 7.75 (d, *J* = 8.9 Hz, 1H), 7.67-7.54 (m, 6H), 7.44 (dd, *J* = 10.8, 5.2 Hz, 2H), 7.32 (d, *J* = 2.2 Hz, 1H), 7.17 (t, *J* = 7.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.3, 147.3, 140.2, 137.3, 132.3, 130.5, 130.4, 129.6, 129.1, 128.9, 128.7, 127.8, 124.2, 124.1, 120.1, 119.7; HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{20}H_{15}ClN_3O$, 348.0904; found, 348.0926.

6-Chloro-2-((4-chlorophenyl)amino)-4-phenylquinazoline 3-oxide (5h)

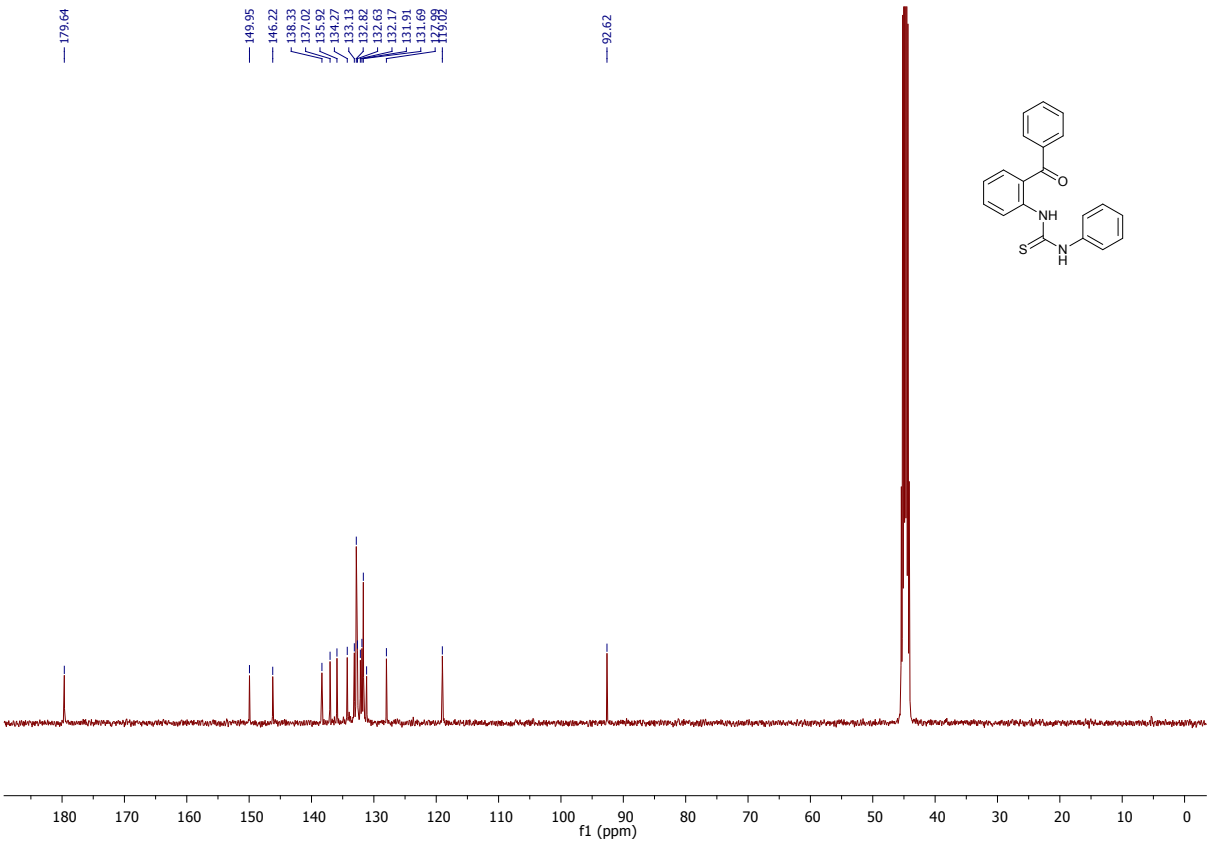


Yield 94% (358 mg); yellow solid; Mp 237-240 °C; eluent, hexane/ ethyl acetate 91:9; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.89 (s, 1H), 7.88-7.83 (m, 2H), 7.78-7.74 (m, 1H), 7.68-7.56 (m, 6H), 7.42-7.37 (m, 2H), 7.33 (d, *J* = 2.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.5, 147.1, 140.0, 136.0, 132.4, 130.7, 130.6, 129.6, 129.2, 129.0, 128.5, 127.8, 124.2, 120.9, 120.2; HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{20}H_{14}Cl_2N_3O$, 382.0513; found, 382.0526.

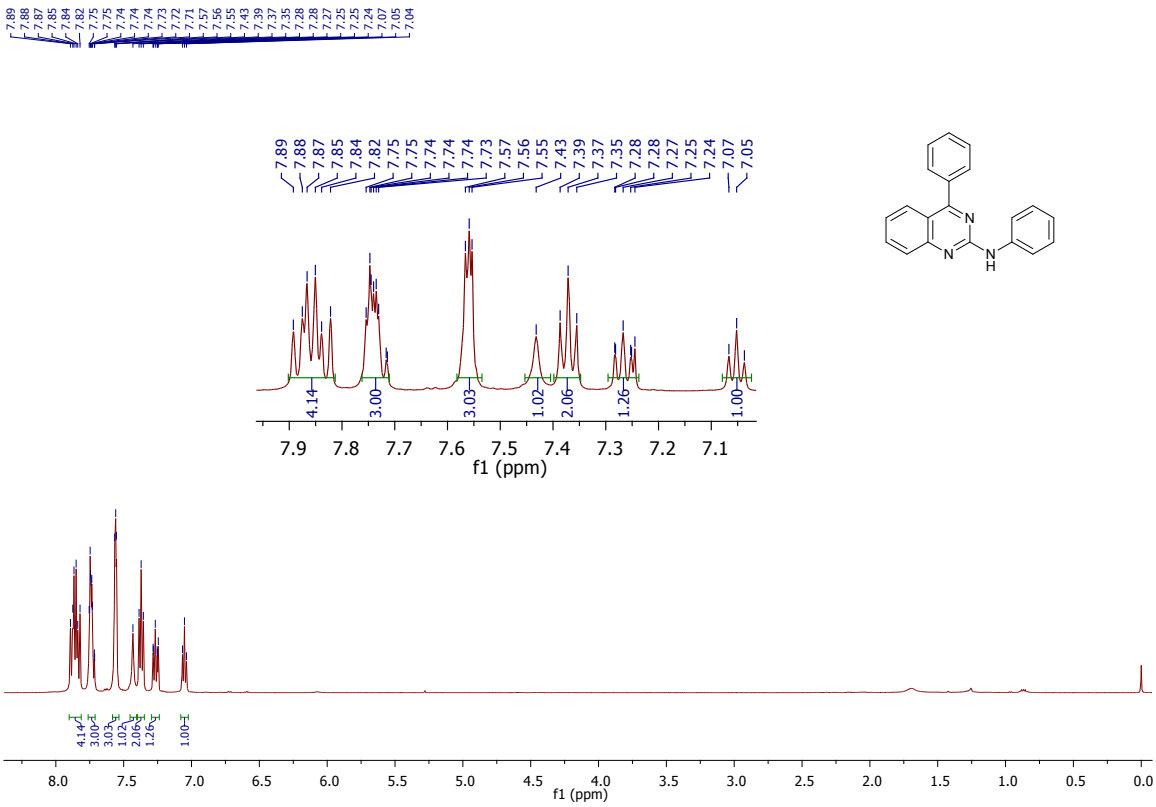
^{1}H NMR spectra of **(A)**



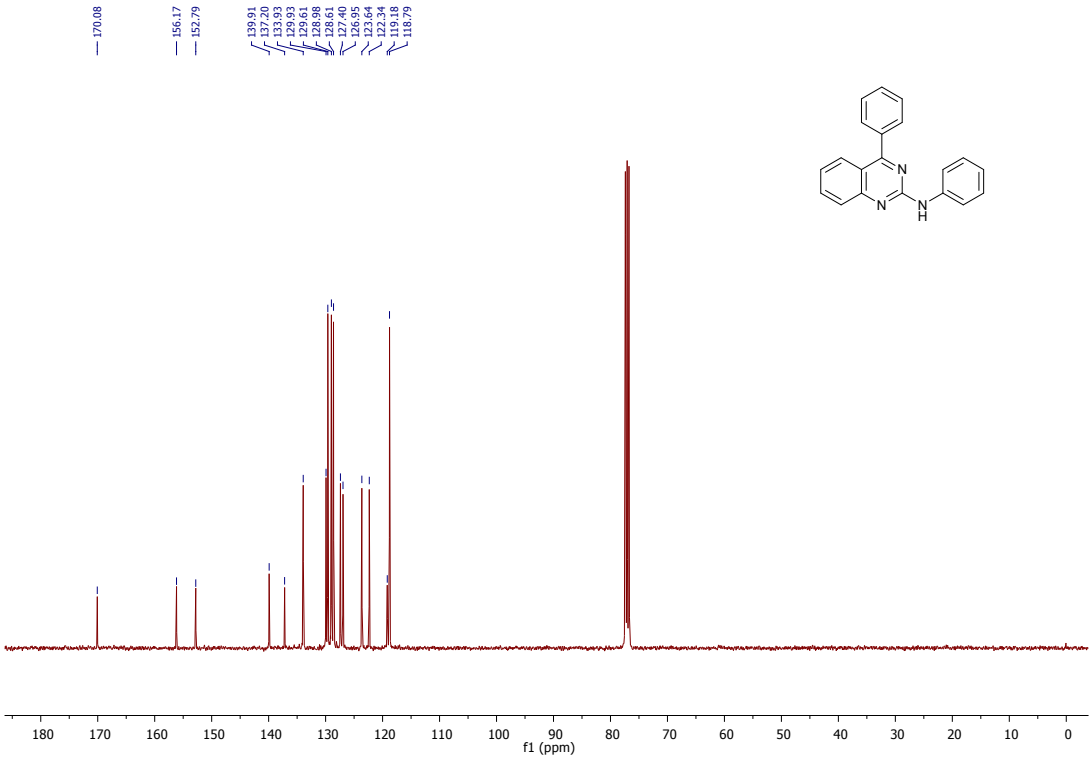
^{13}C NMR spectra of (**A**)



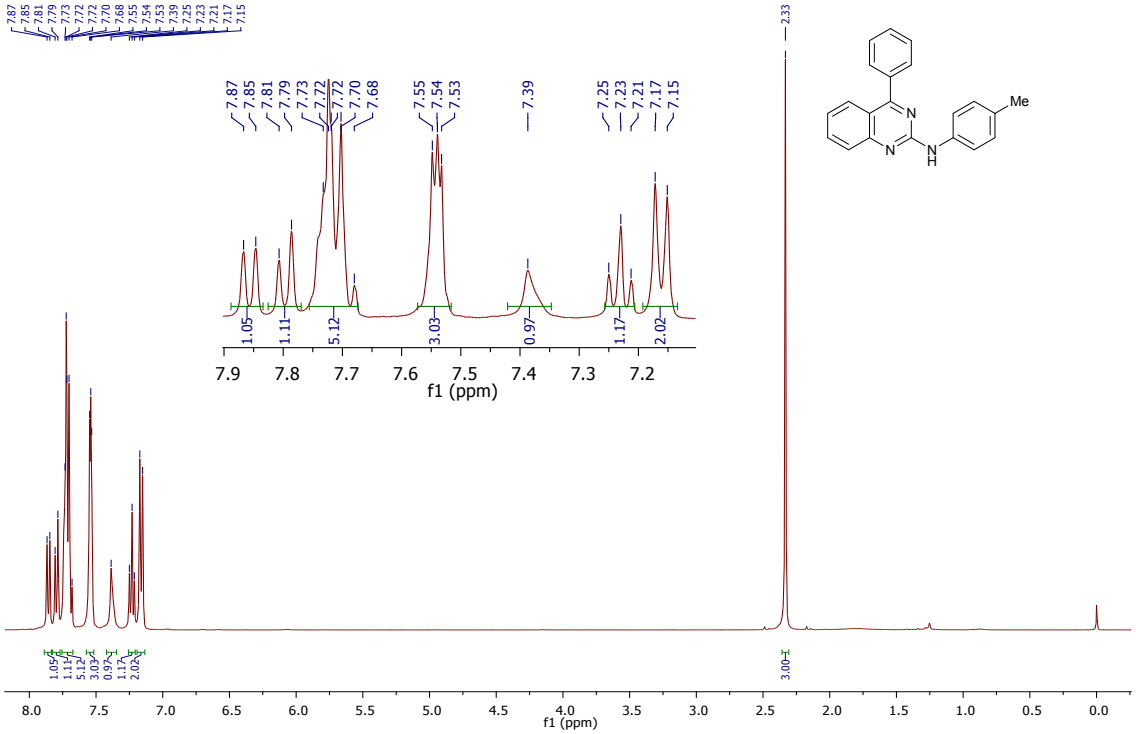
^{1}H NMR spectra of (**3a**)



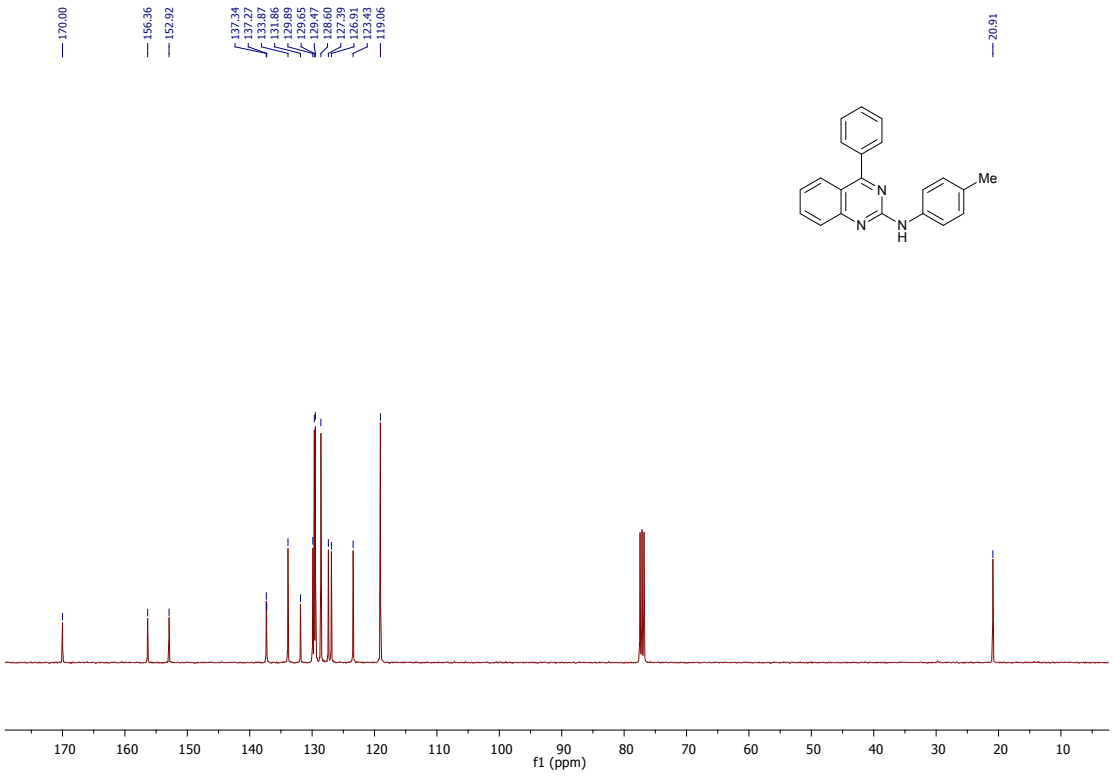
^{13}C NMR spectra of (**3a**)



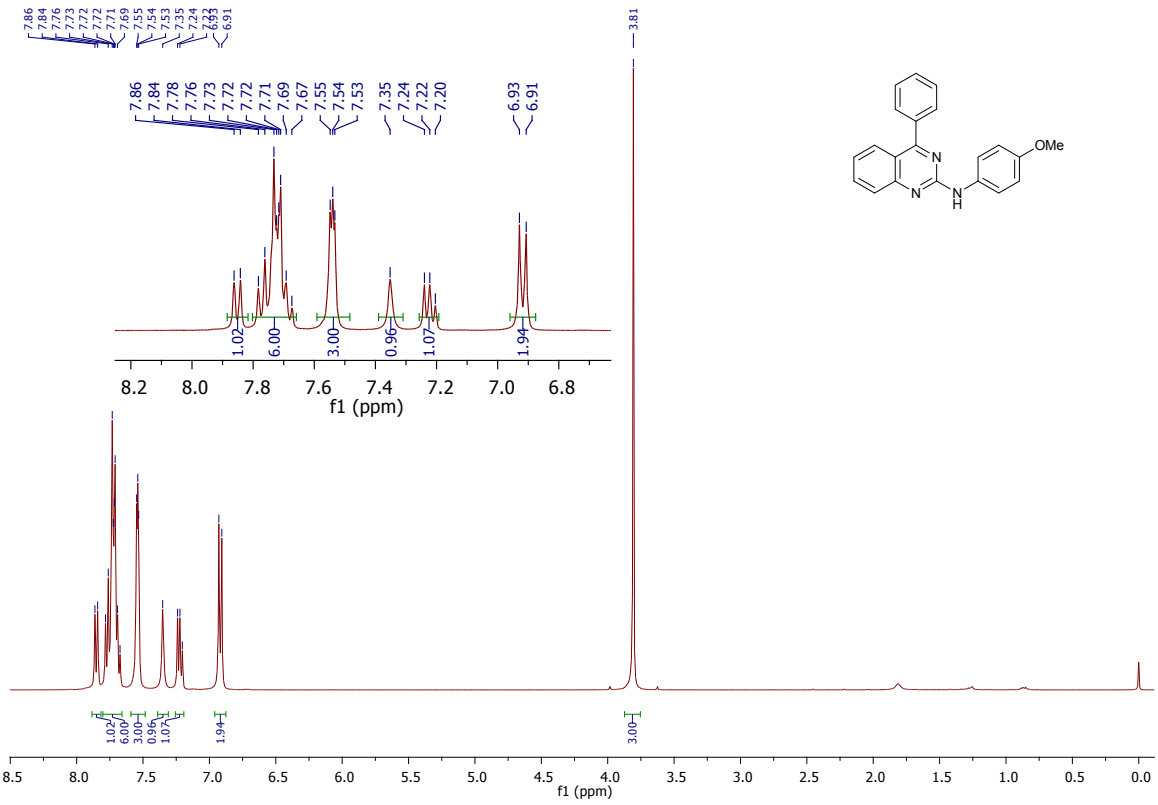
1H NMR spectra of (**3b**)



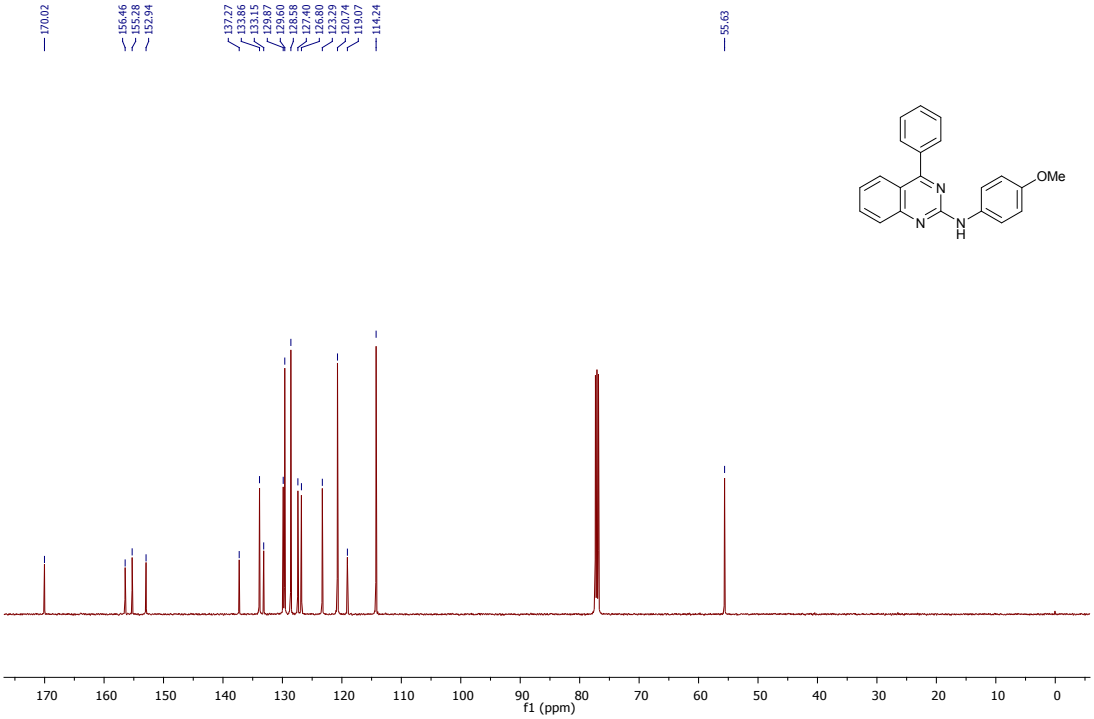
^{13}C NMR spectra of (**3b**)



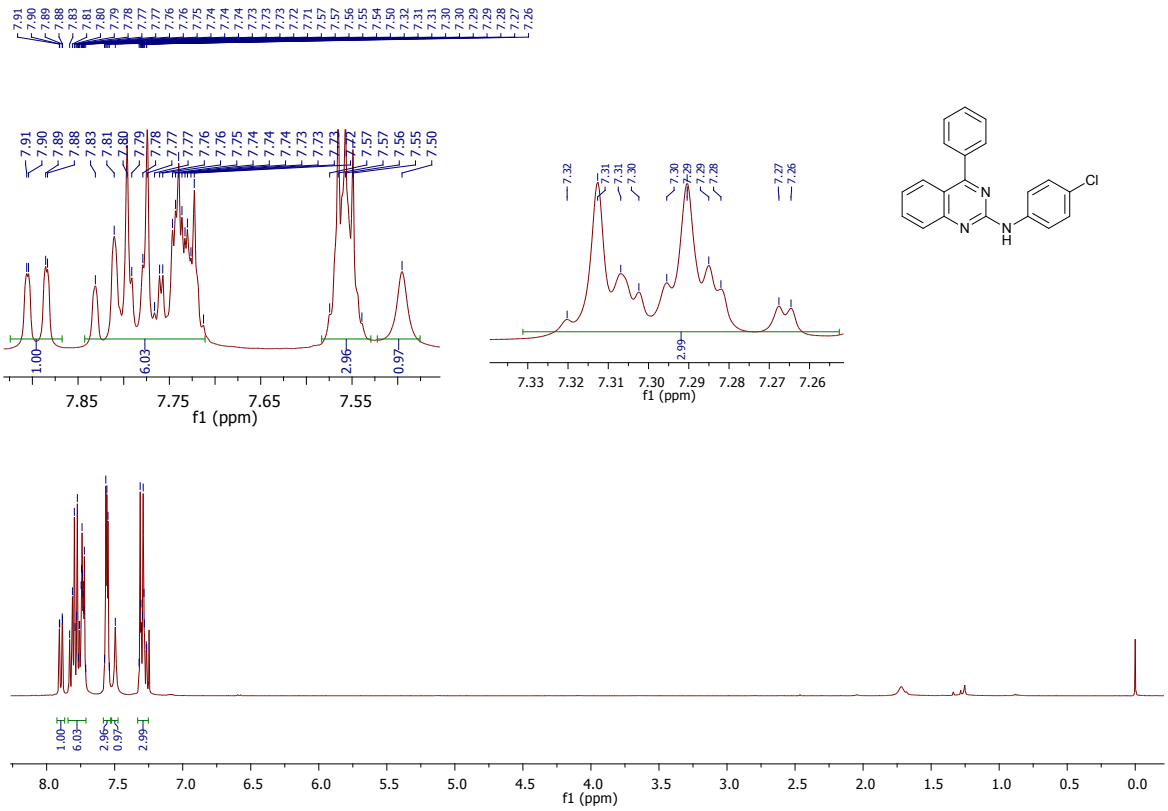
^{1}H NMR of spectra (**3c**)



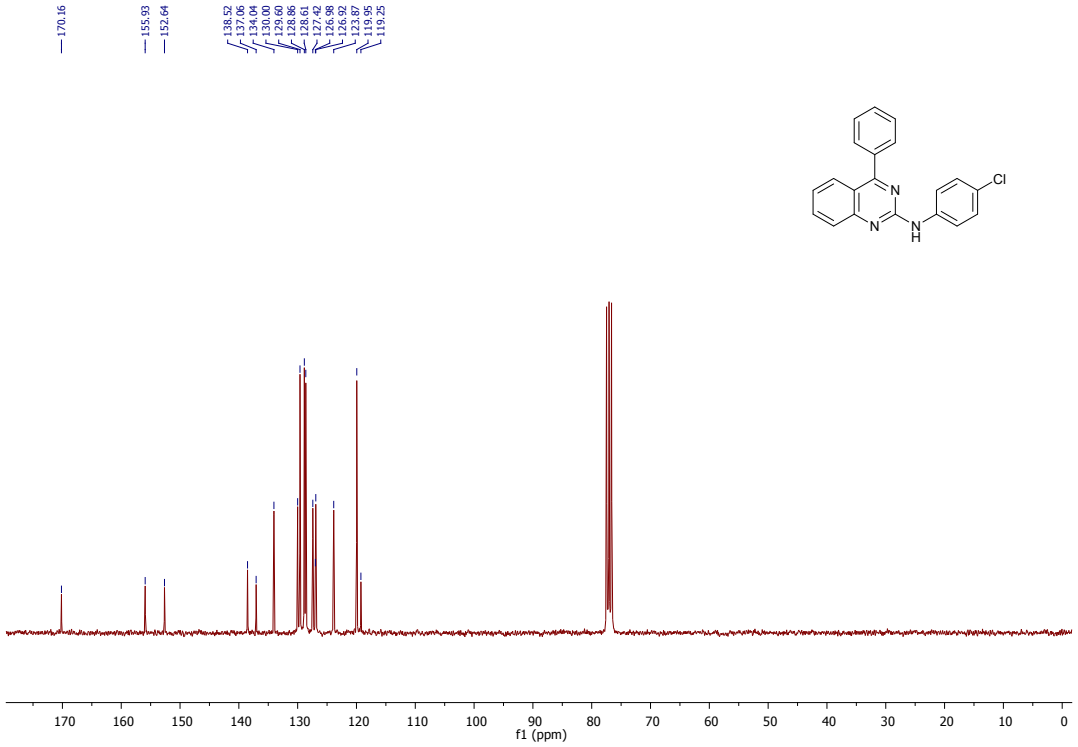
^{13}C NMR of spectra (**3c**)



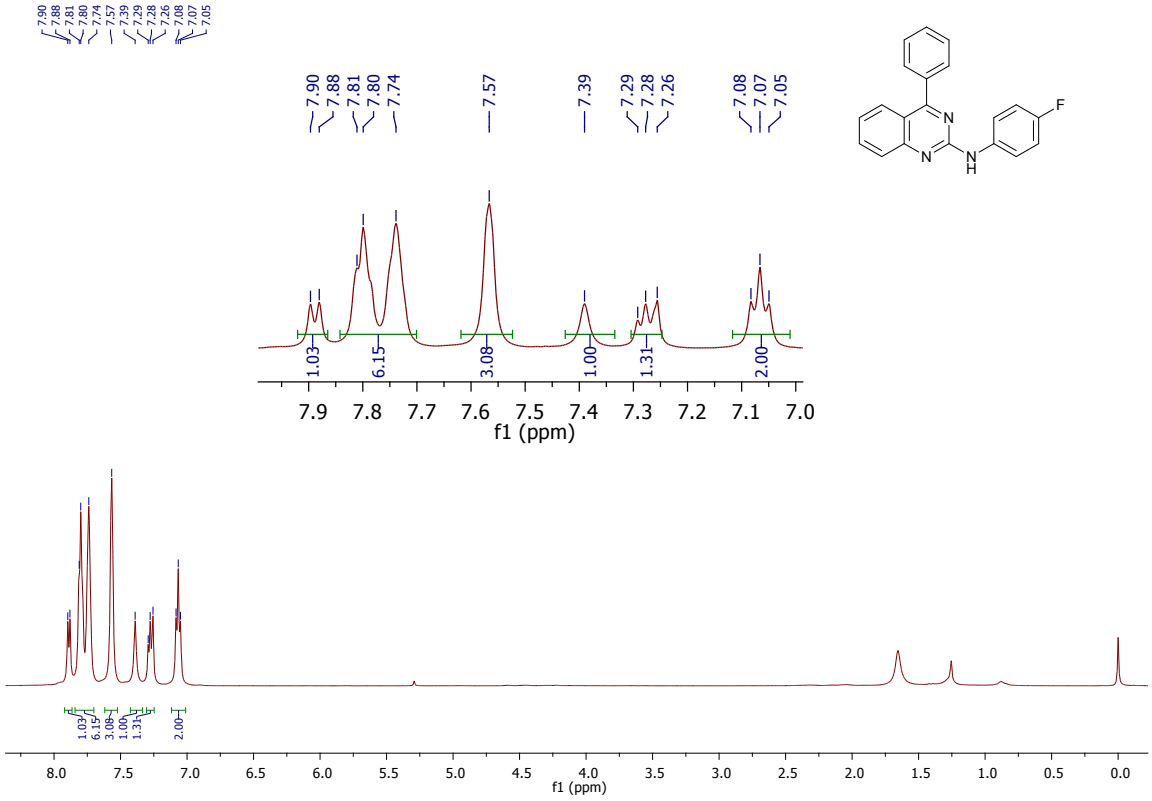
^{1}H NMR of spectra (**3d**)



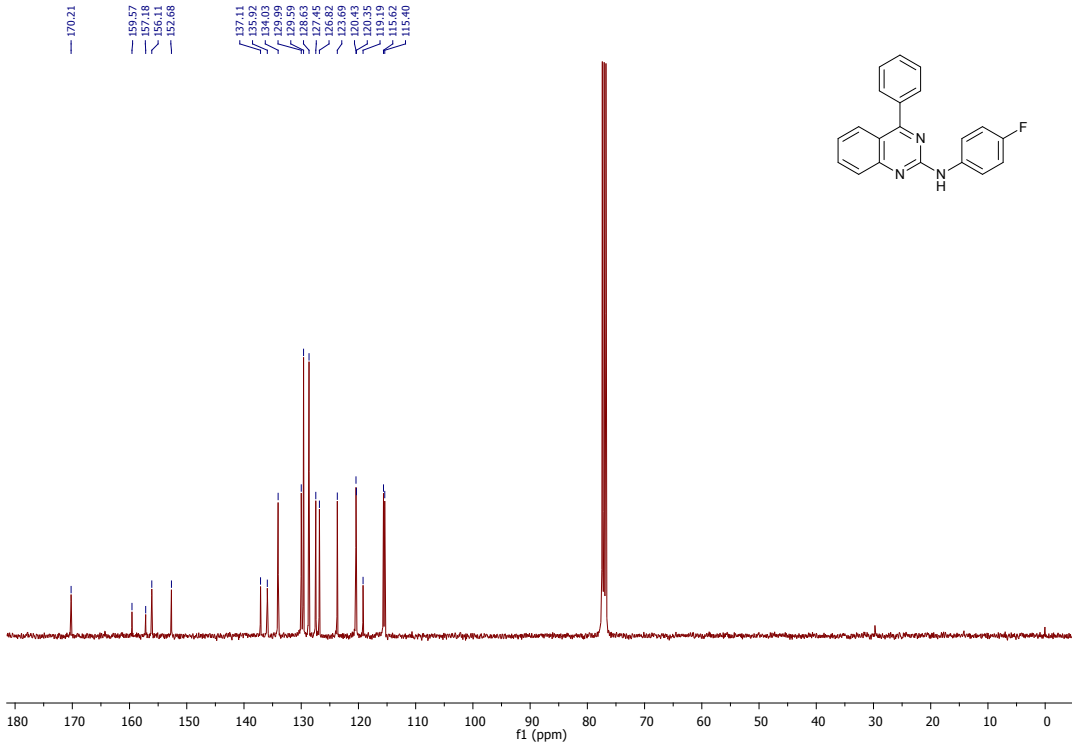
^{13}C NMR of spectra (**3d**)



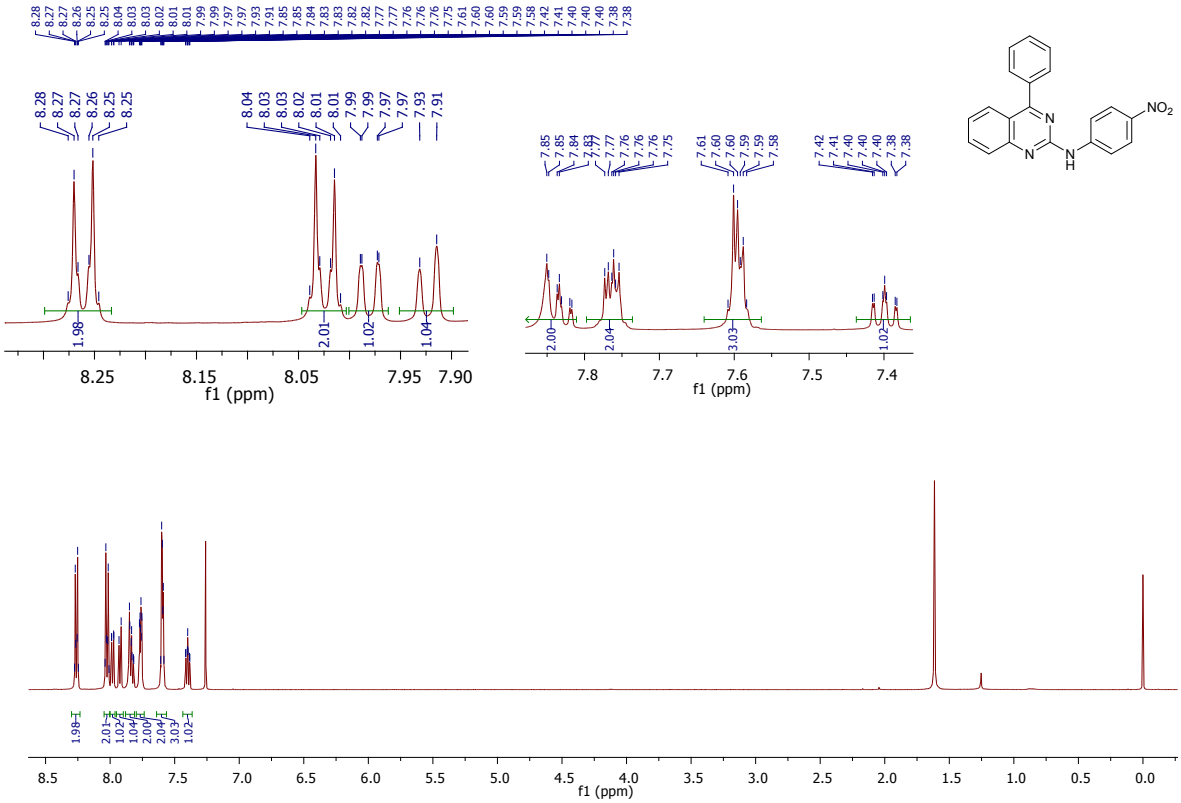
^{1}H NMR of spectra (**3e**)



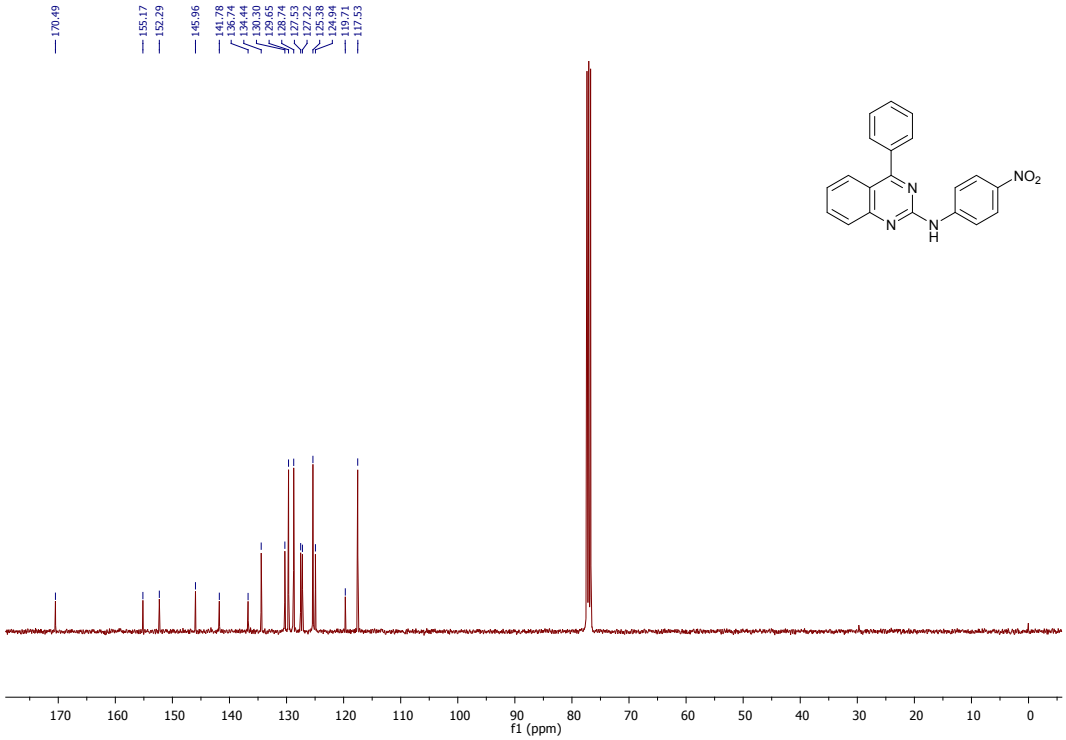
^{13}C NMR spectra of (**3e**)



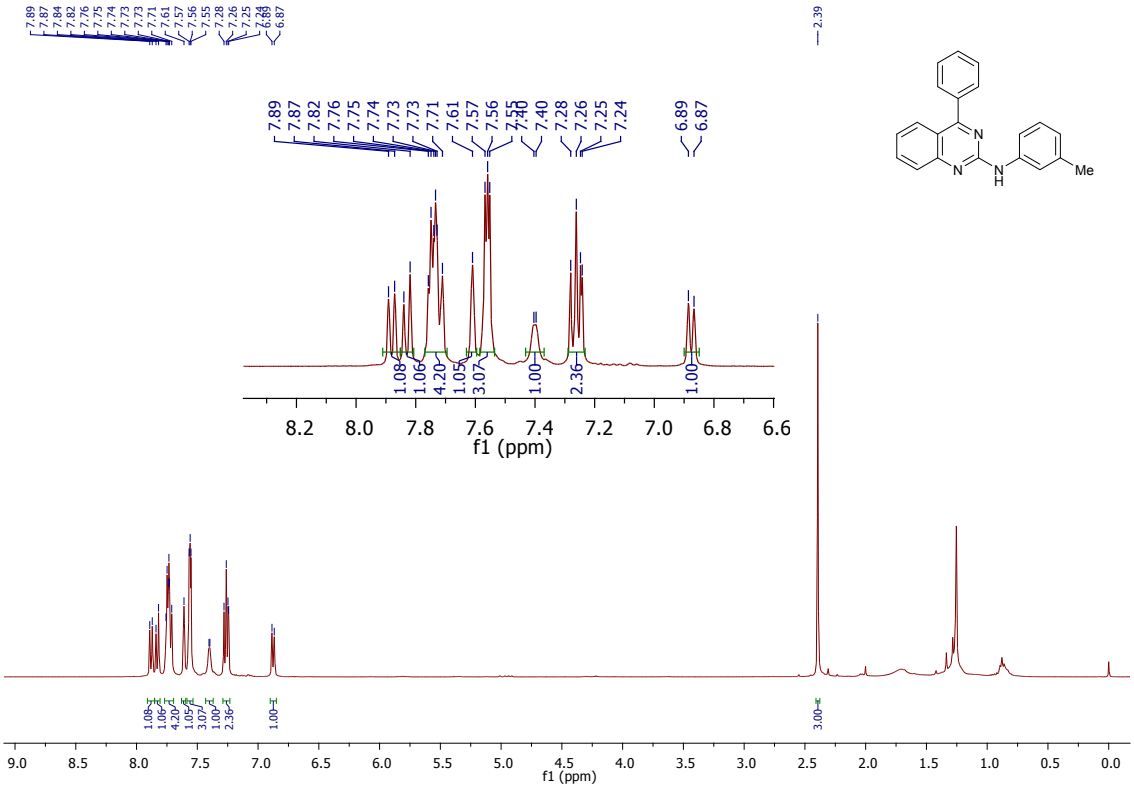
^{1}H NMR of spectra (**3f**)



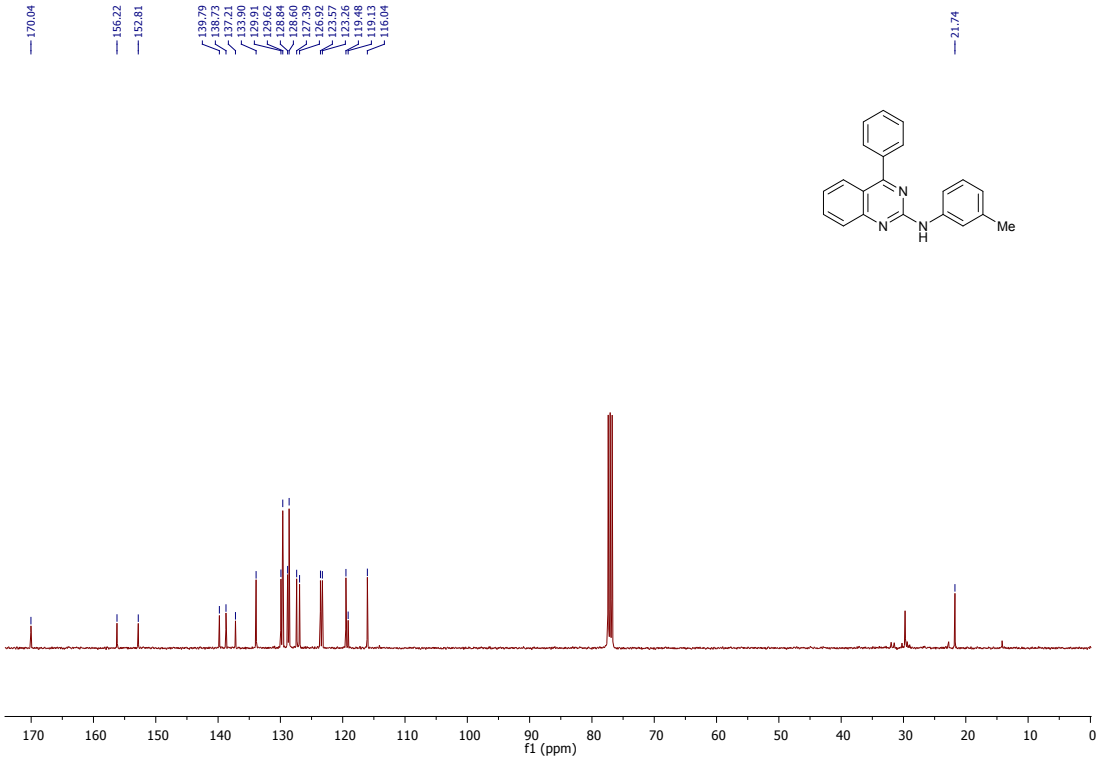
^{13}C NMR of spectra (**3f**)



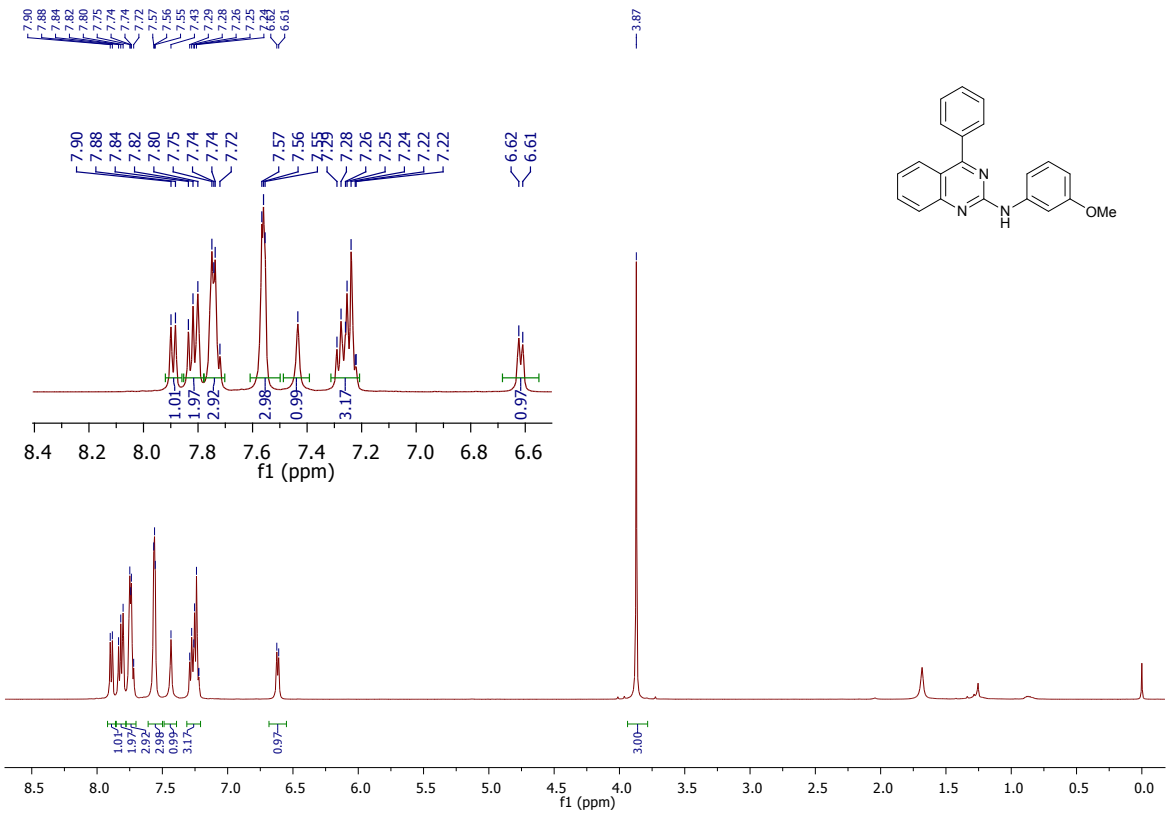
^{1}H NMR of spectra (**3g**)



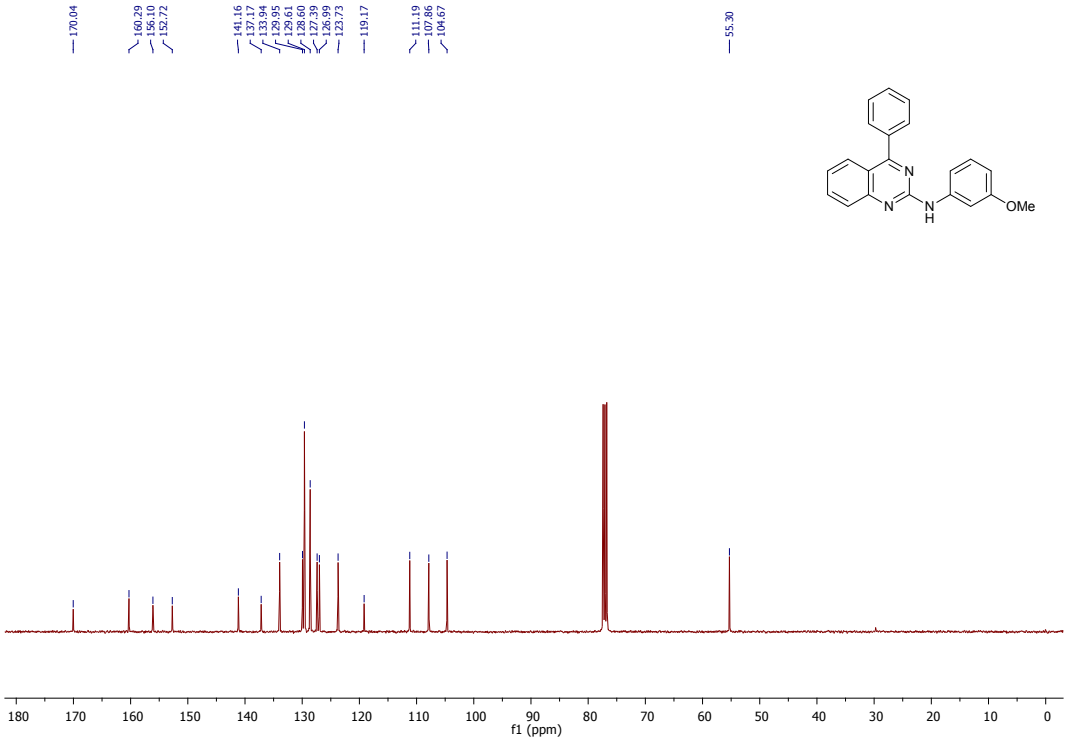
^{13}C NMR of spectra (**3g**)



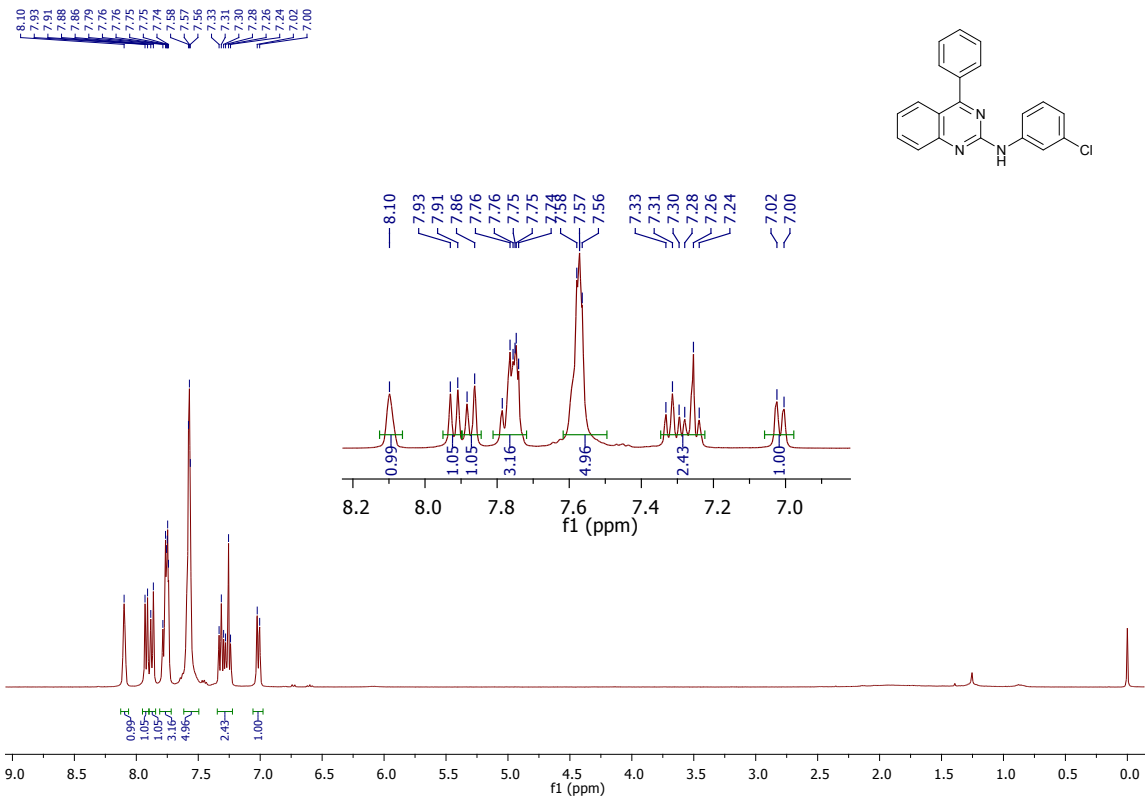
^{1}H NMR spectra of (**3h**)



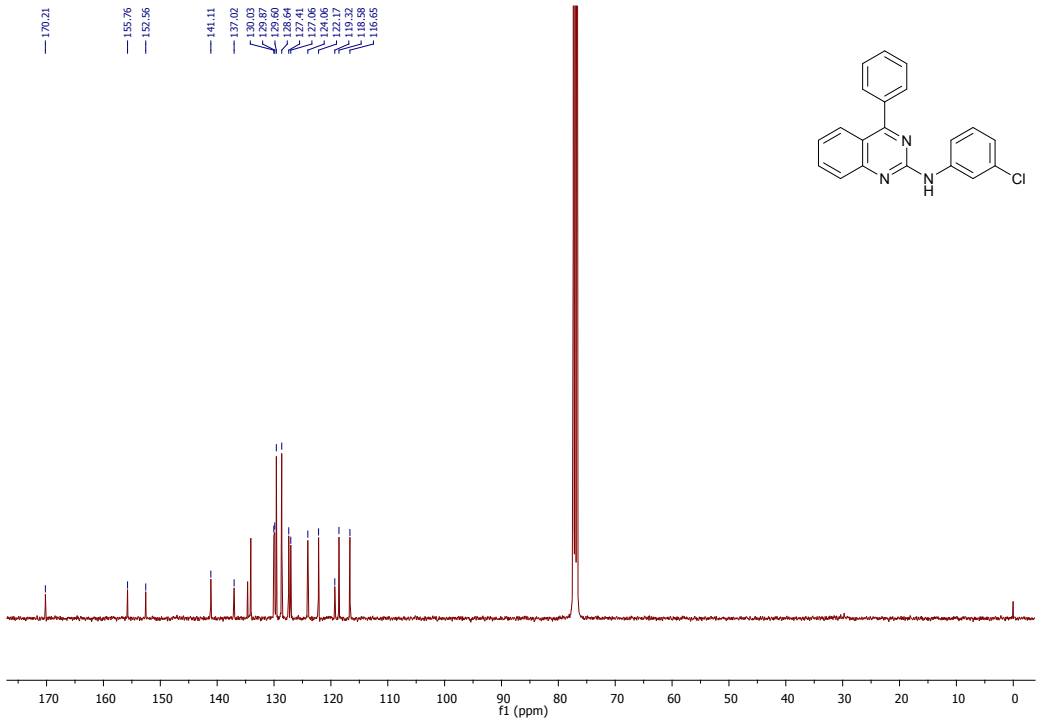
^{13}C NMR of spectra (**3h**)



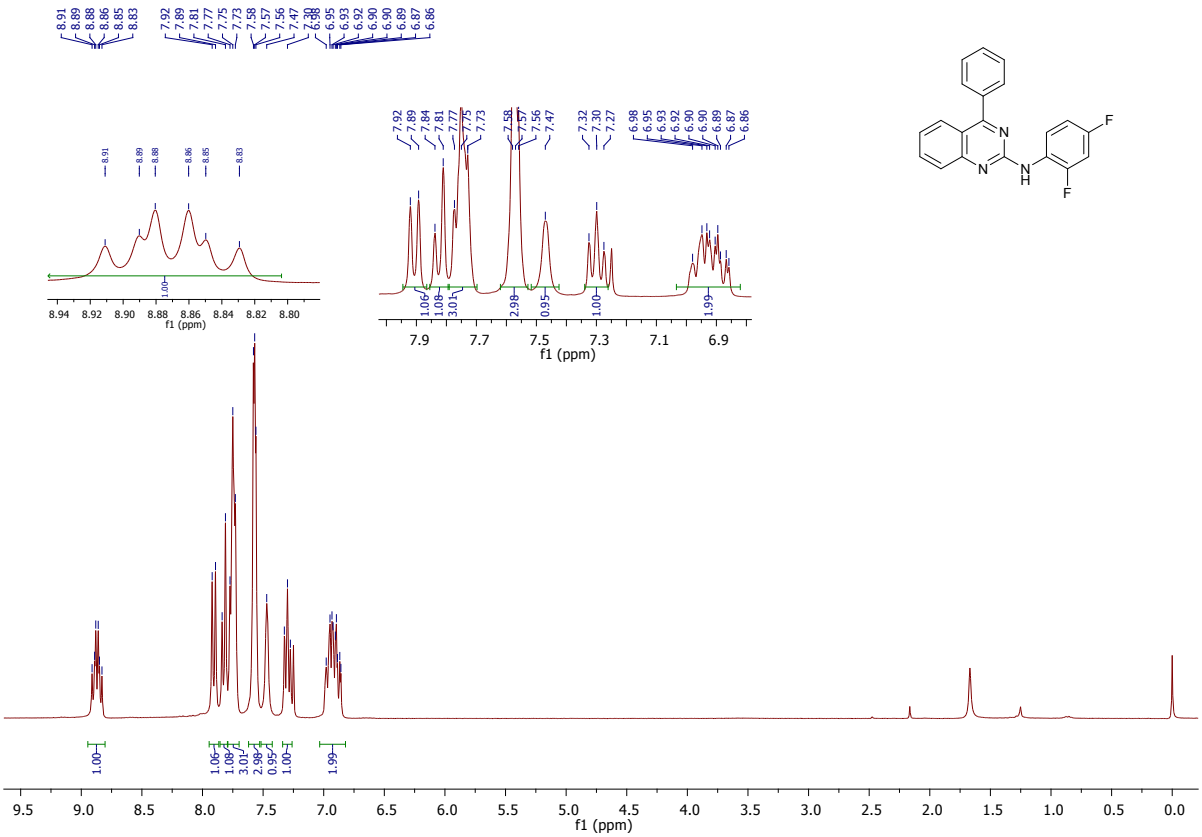
^{1}H NMR spectra of (**3i**)



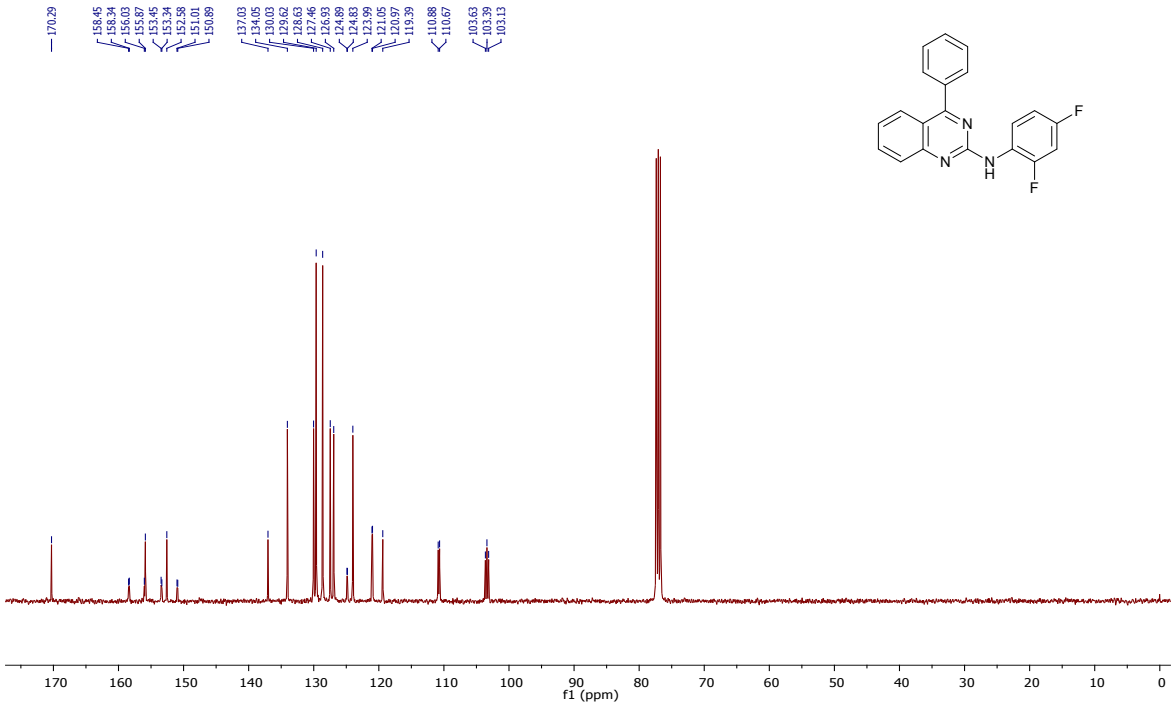
^{13}C NMR of spectra (**3i**)



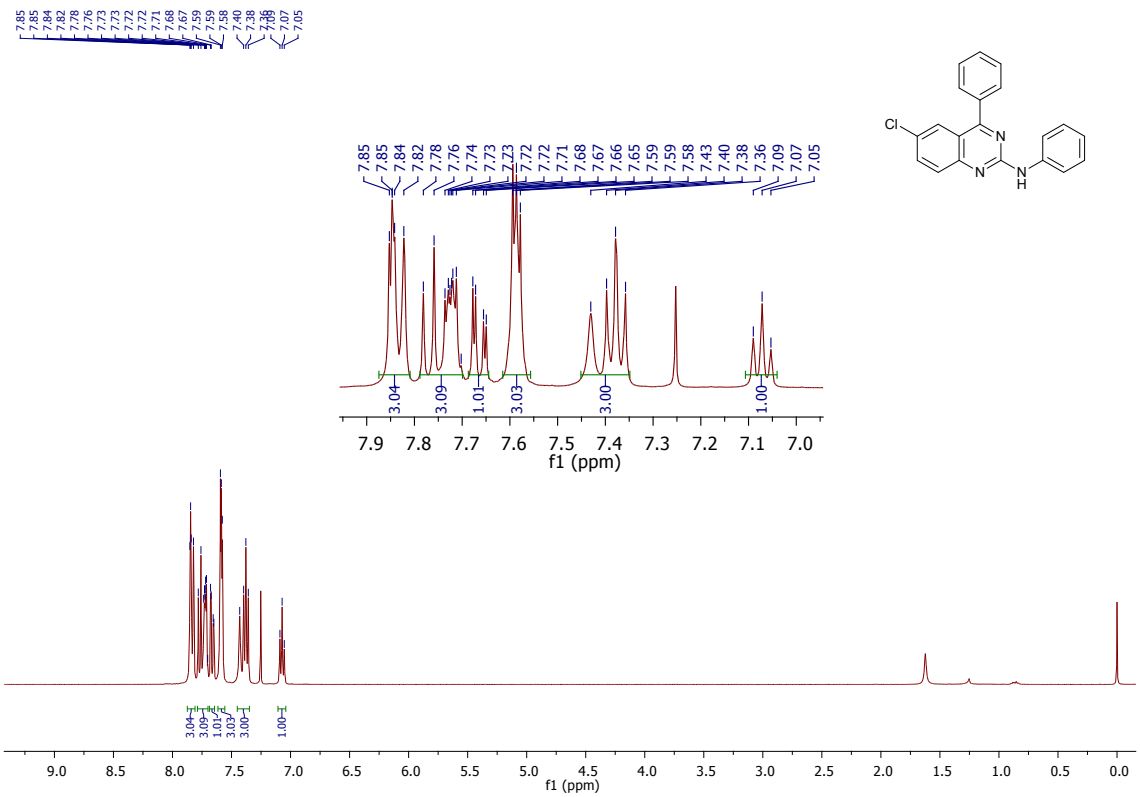
^{1}H NMR spectra of (**3j**)



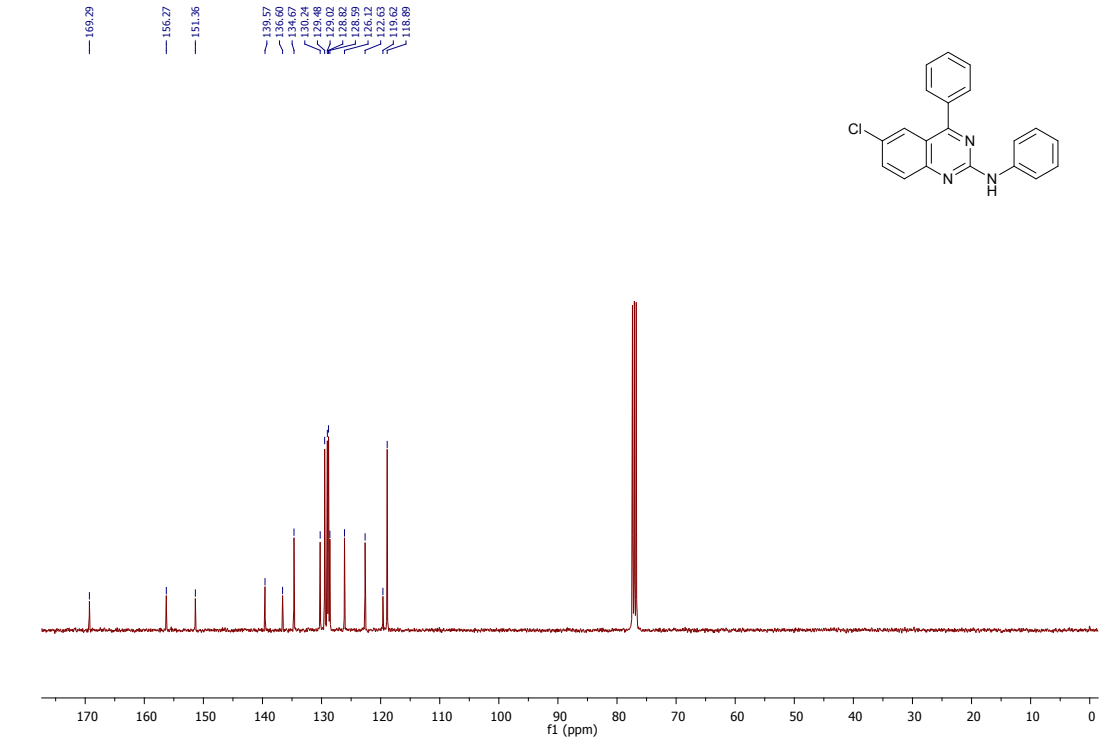
^{13}C NMR spectra of (**3j**)



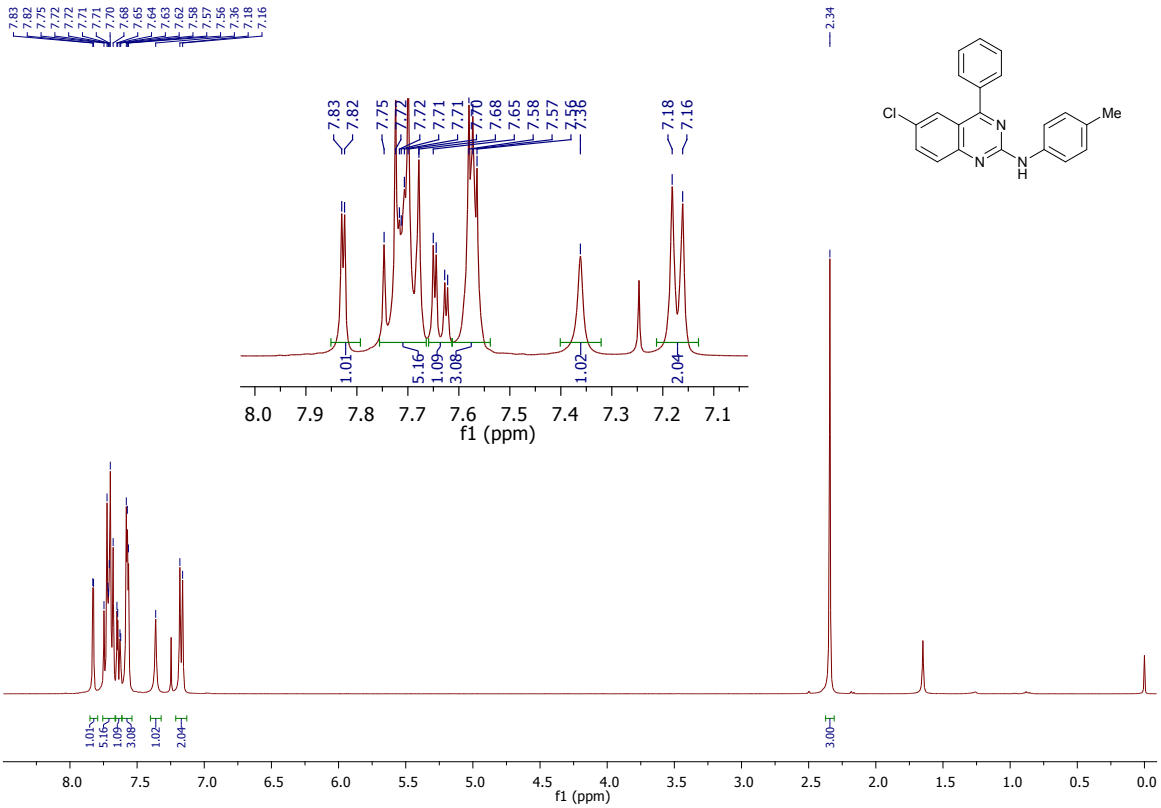
^{1}H NMR of spectra(**3k**)



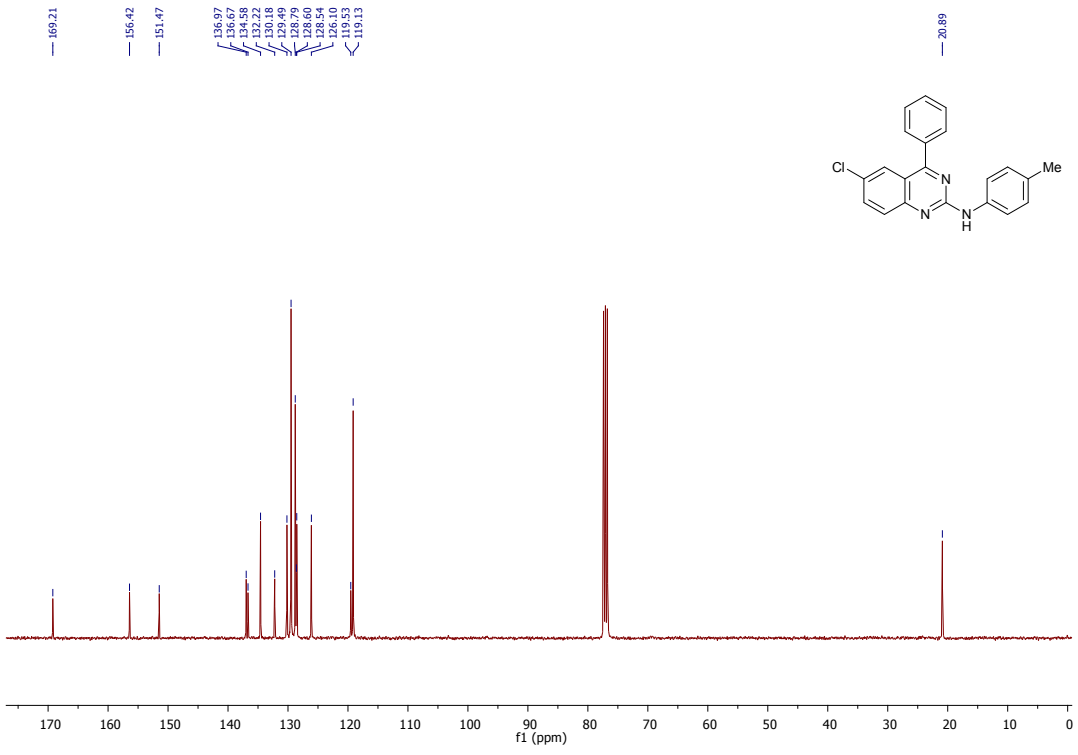
^{13}C NMR of spectra (**3k**)



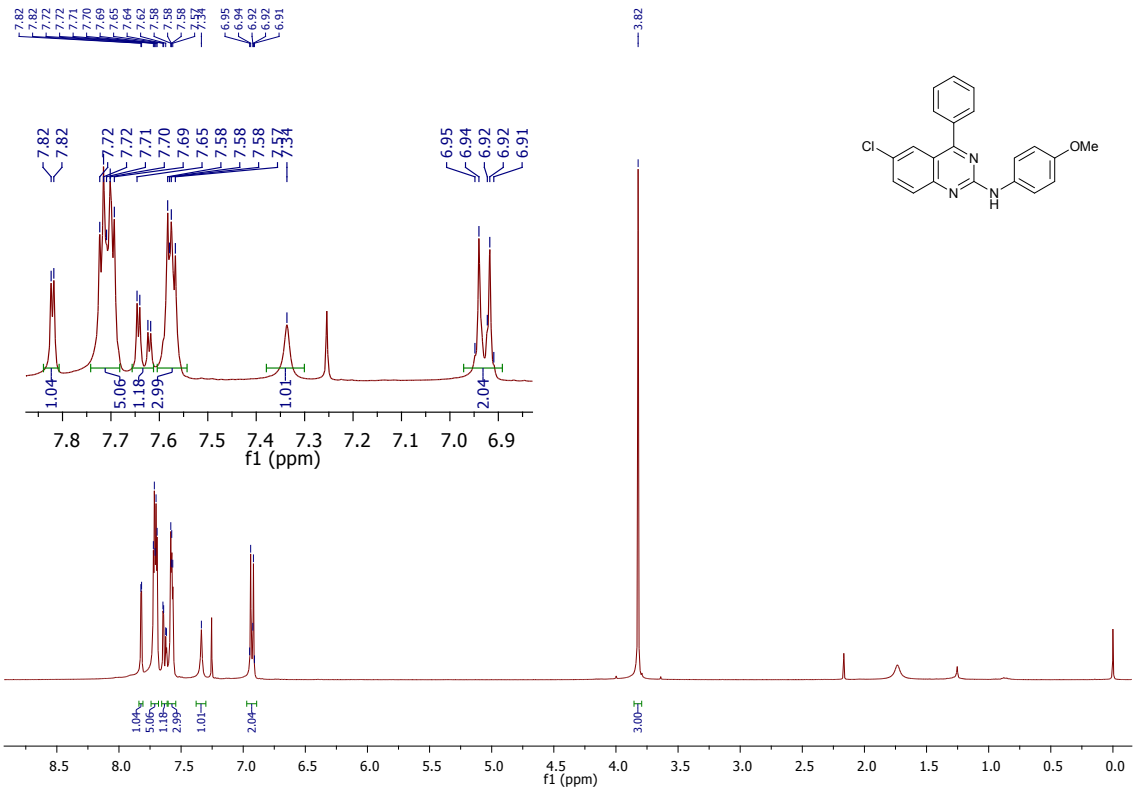
^{1}H NMR spectra of (**3l**)



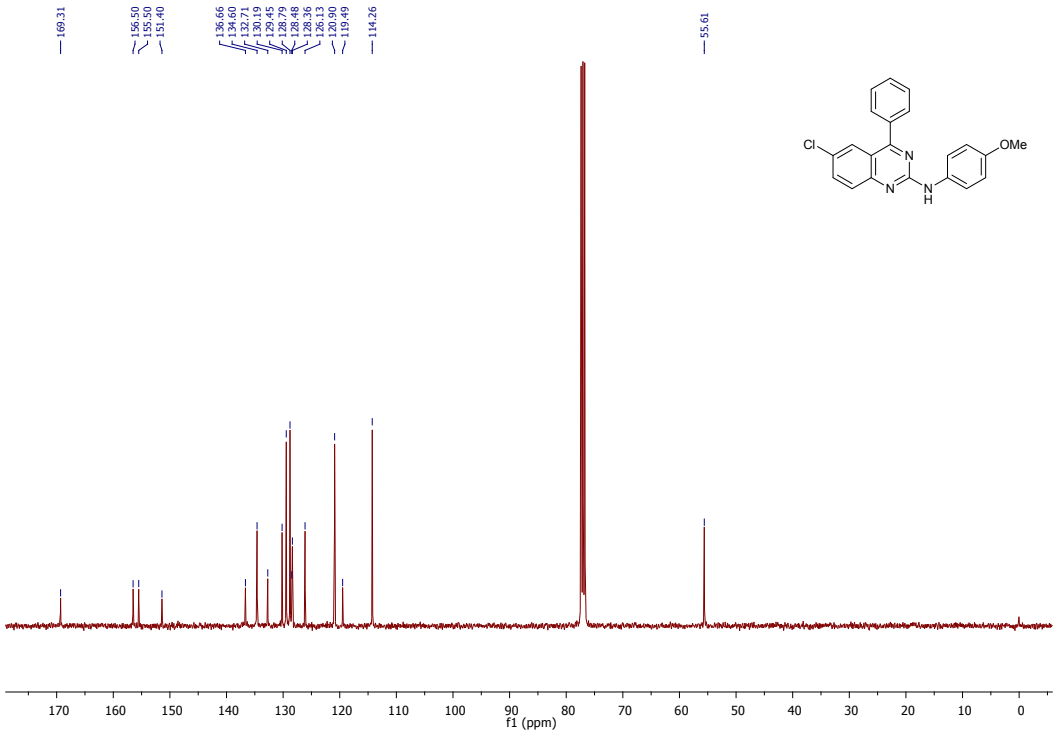
^{13}C NMR of spectra (**3l**)



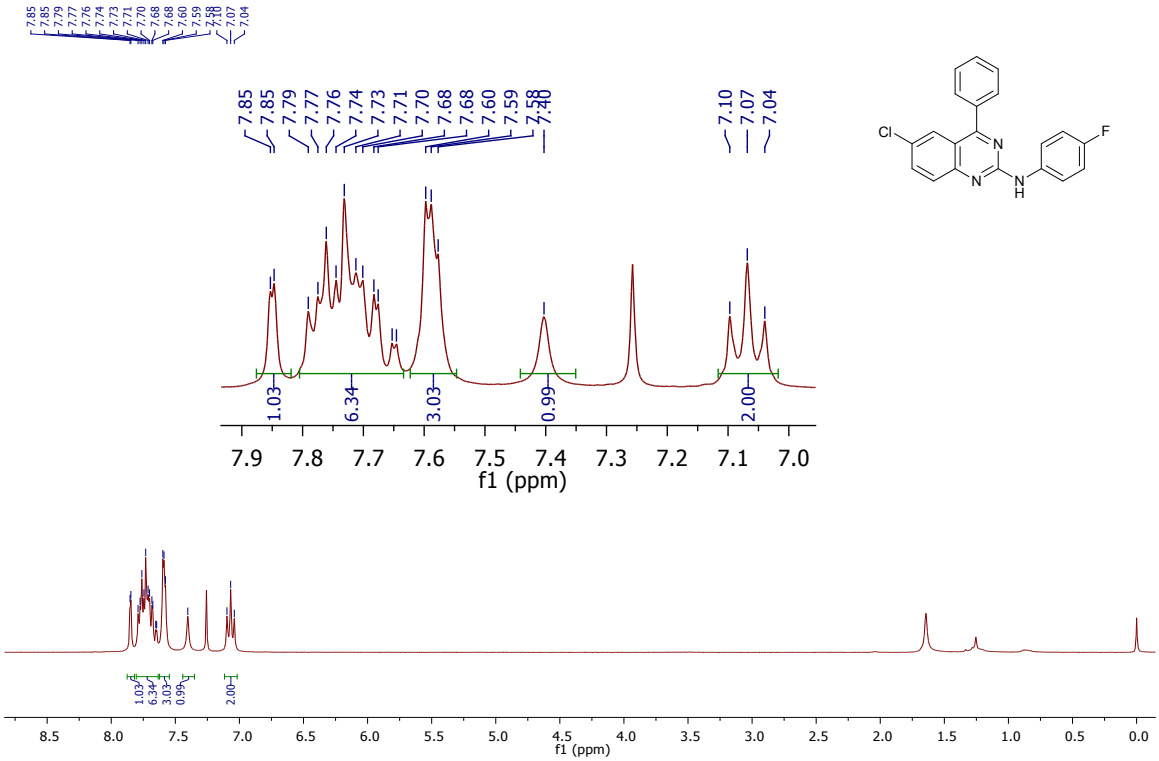
^{1}H NMR of spectra (**3m**)



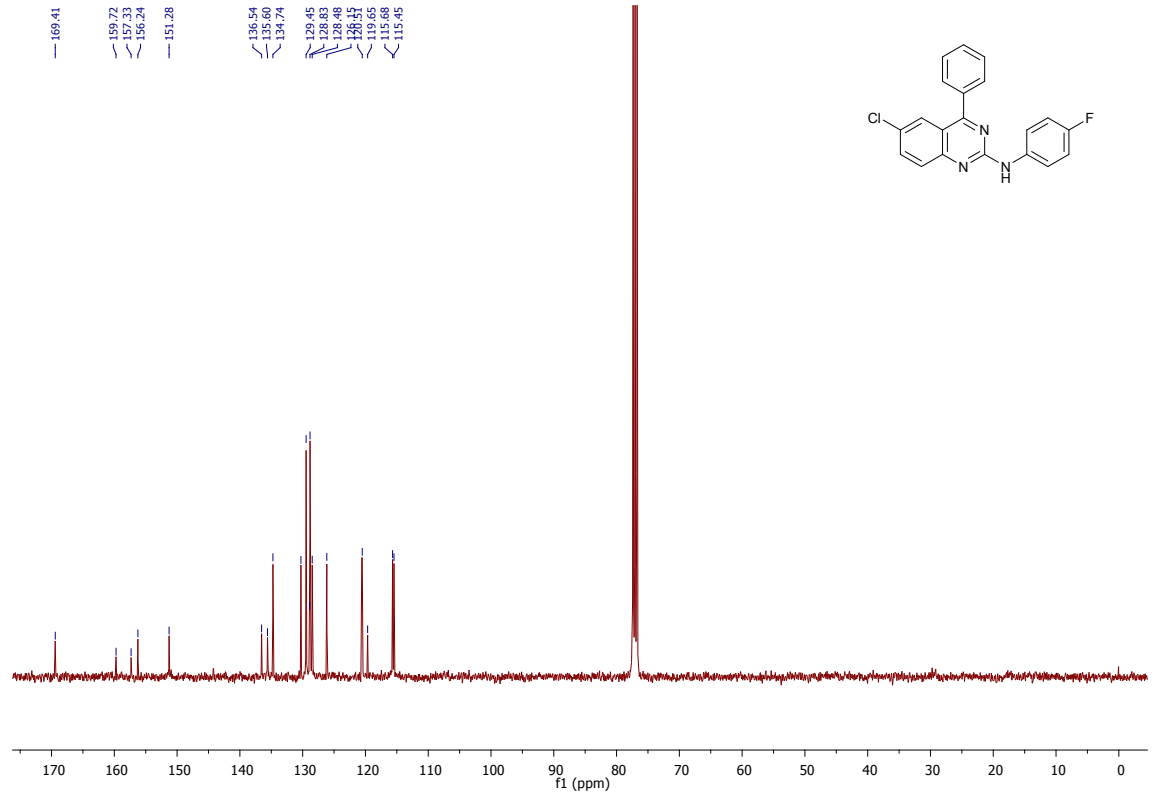
^{13}C NMR of spectra (**3m**)



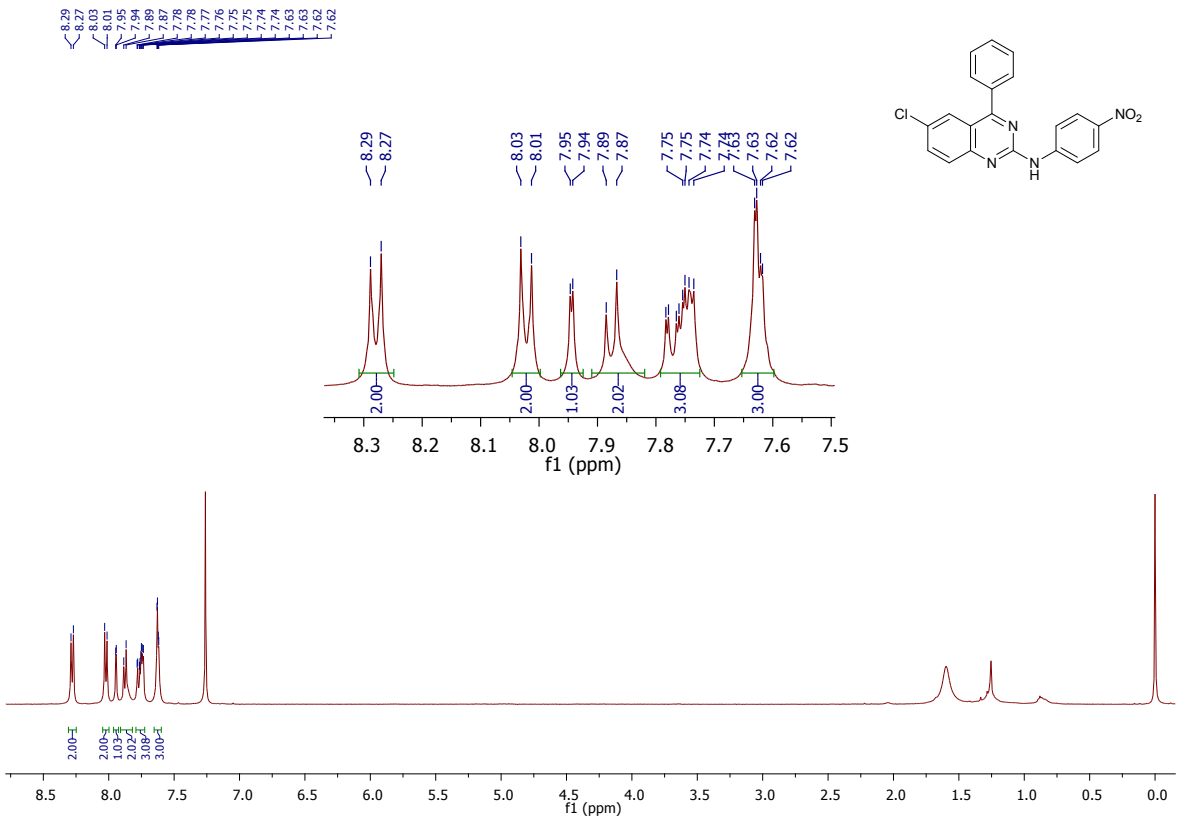
^{1}H NMR of spectra (**3n**)



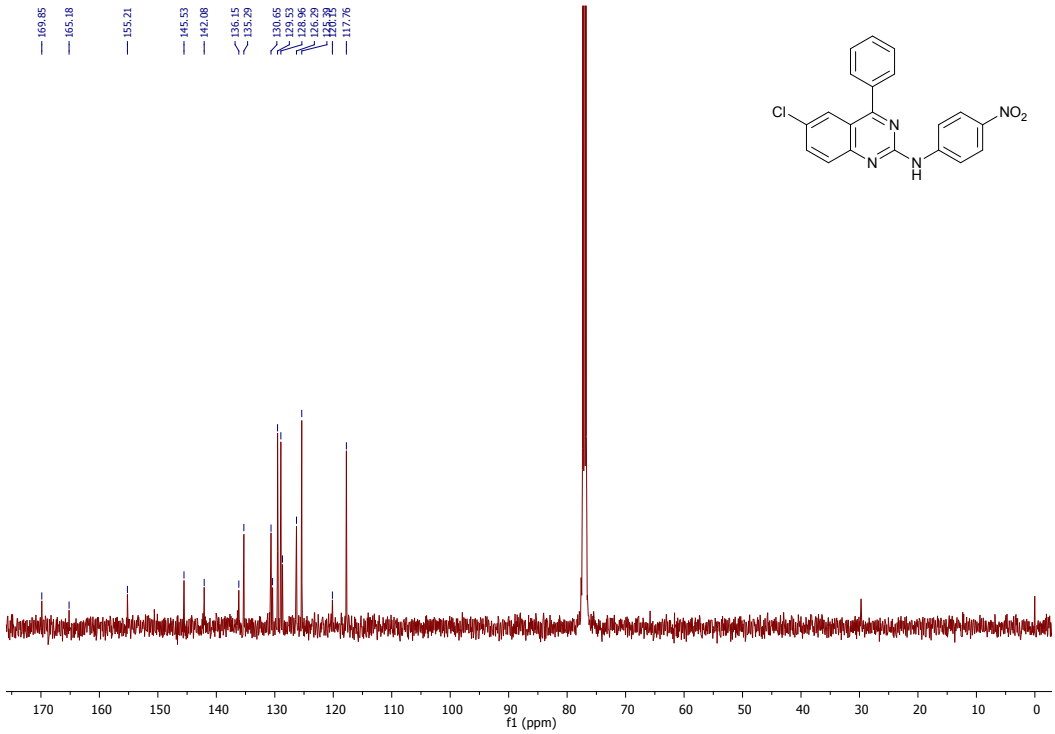
^{13}C NMR of spectra (**3n**)



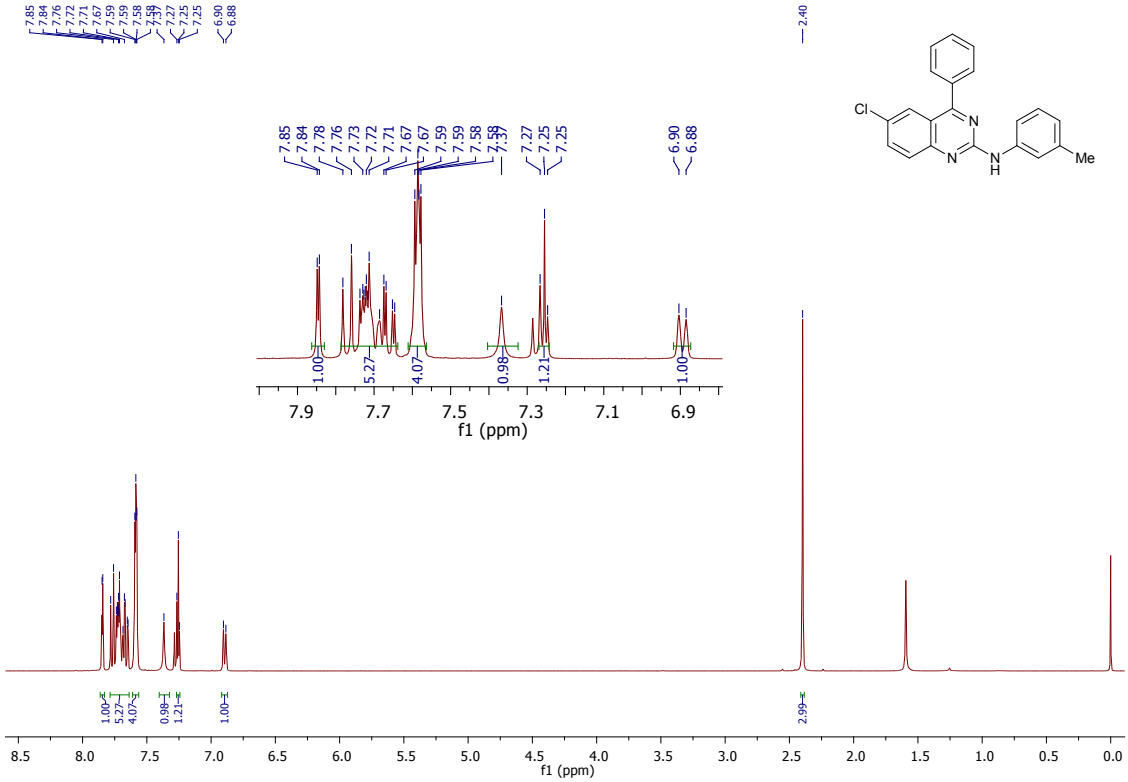
^{1}H NMR of spectra (**3o**)



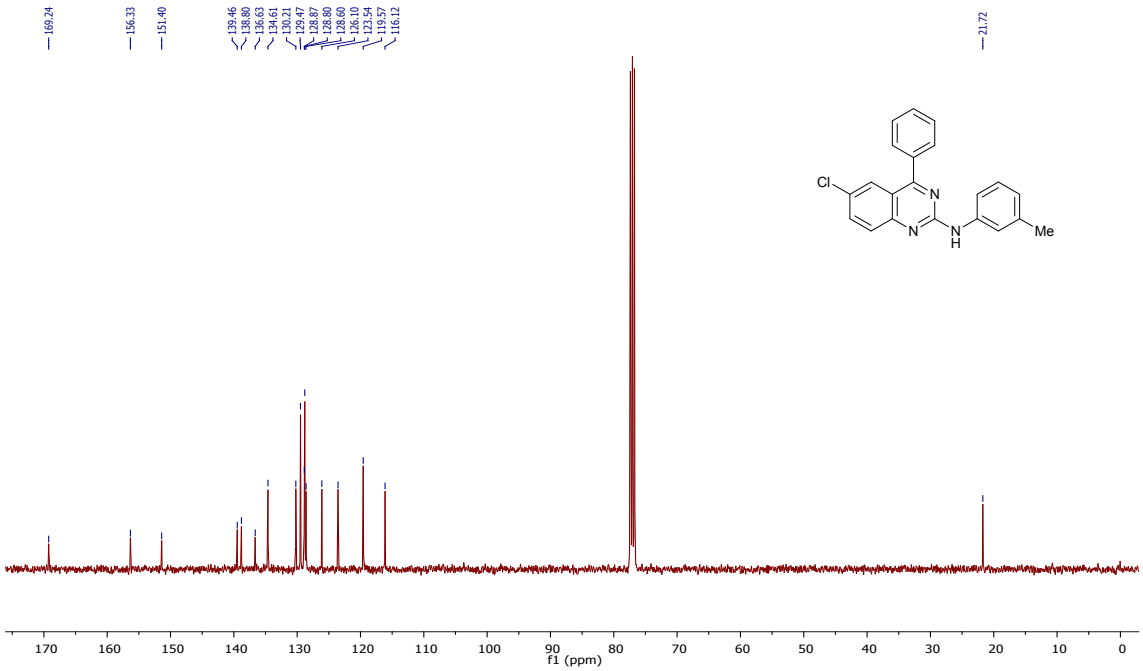
^{13}C NMR spectra of (**3o**)



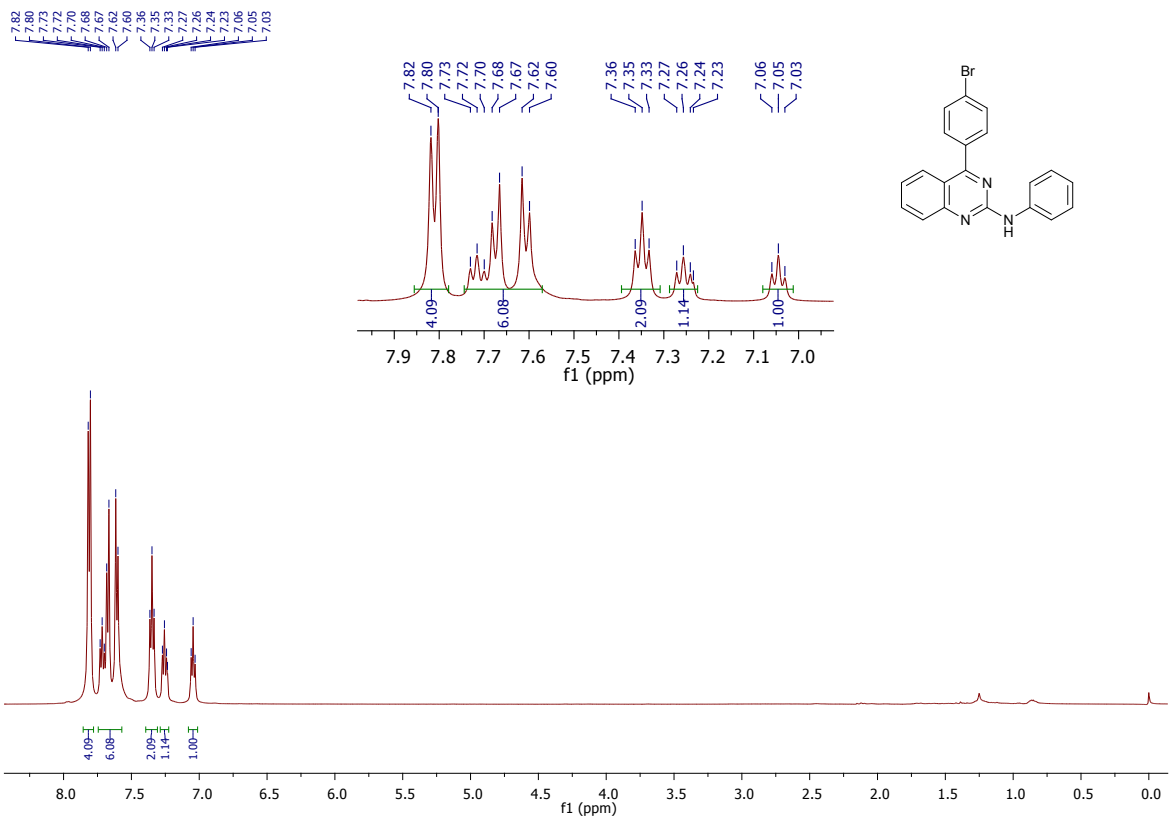
^{1}H NMR of spectra (**3p**)



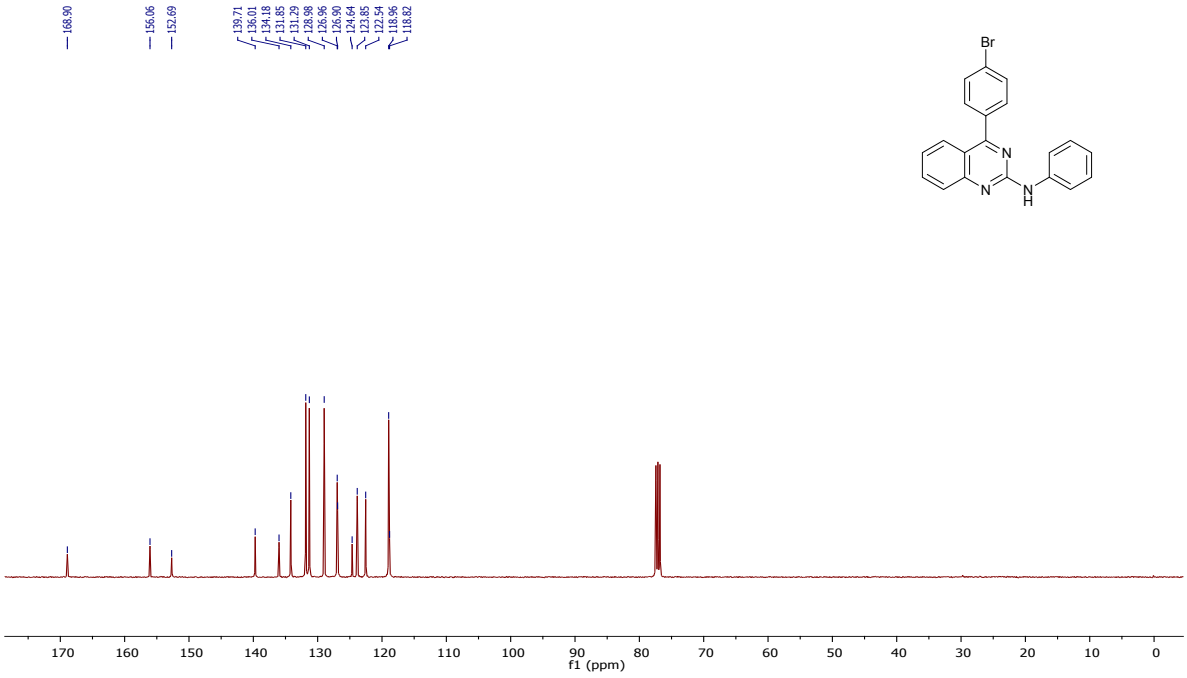
^{13}C NMR of spectra (**3p**)



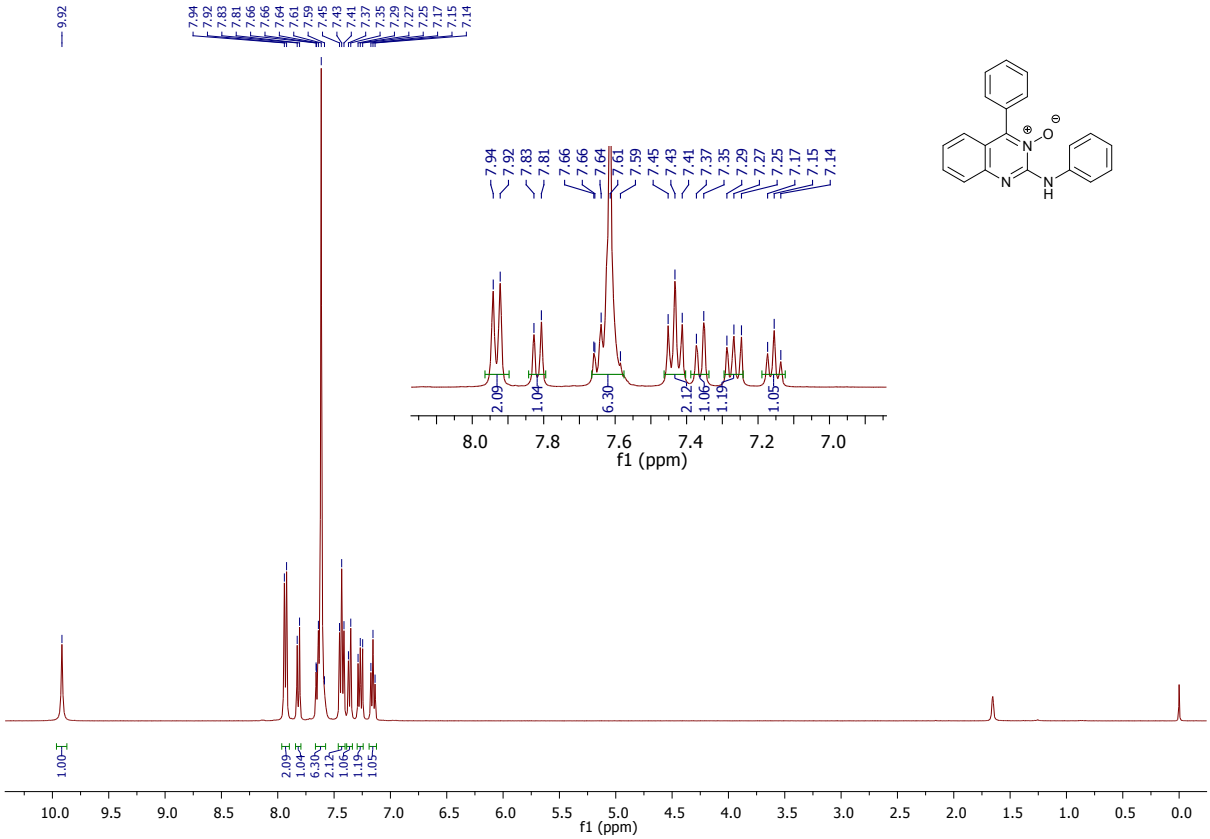
^{1}H NMR of spectra (**3q**)



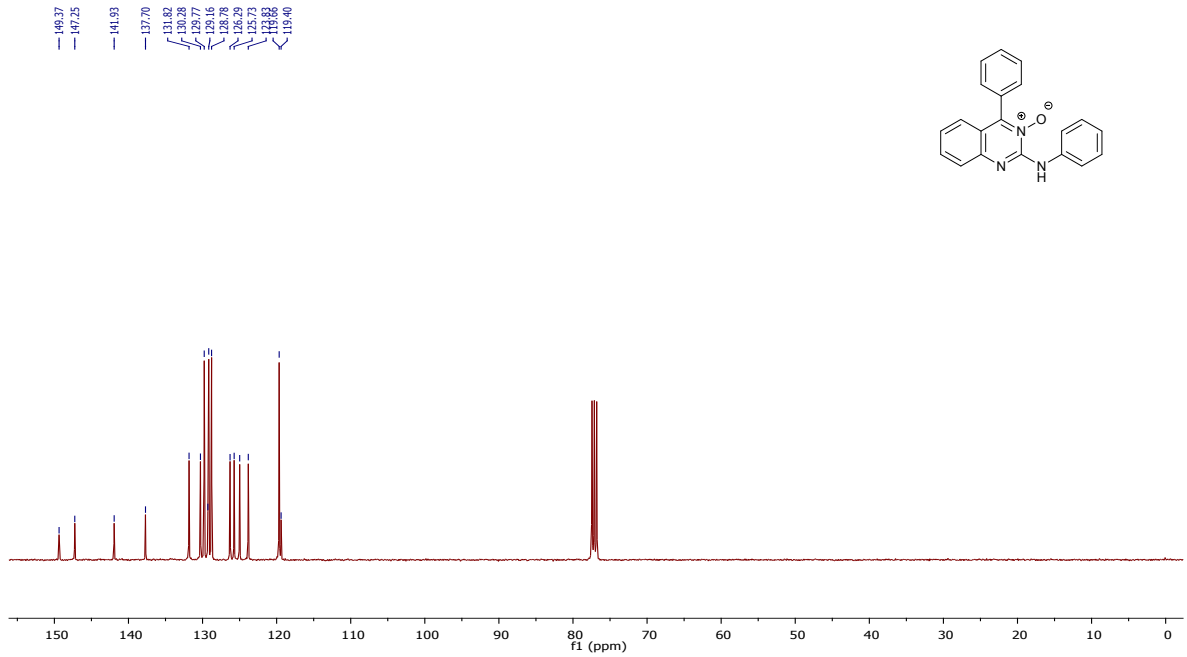
^{13}C NMR of spectra (**3q**)



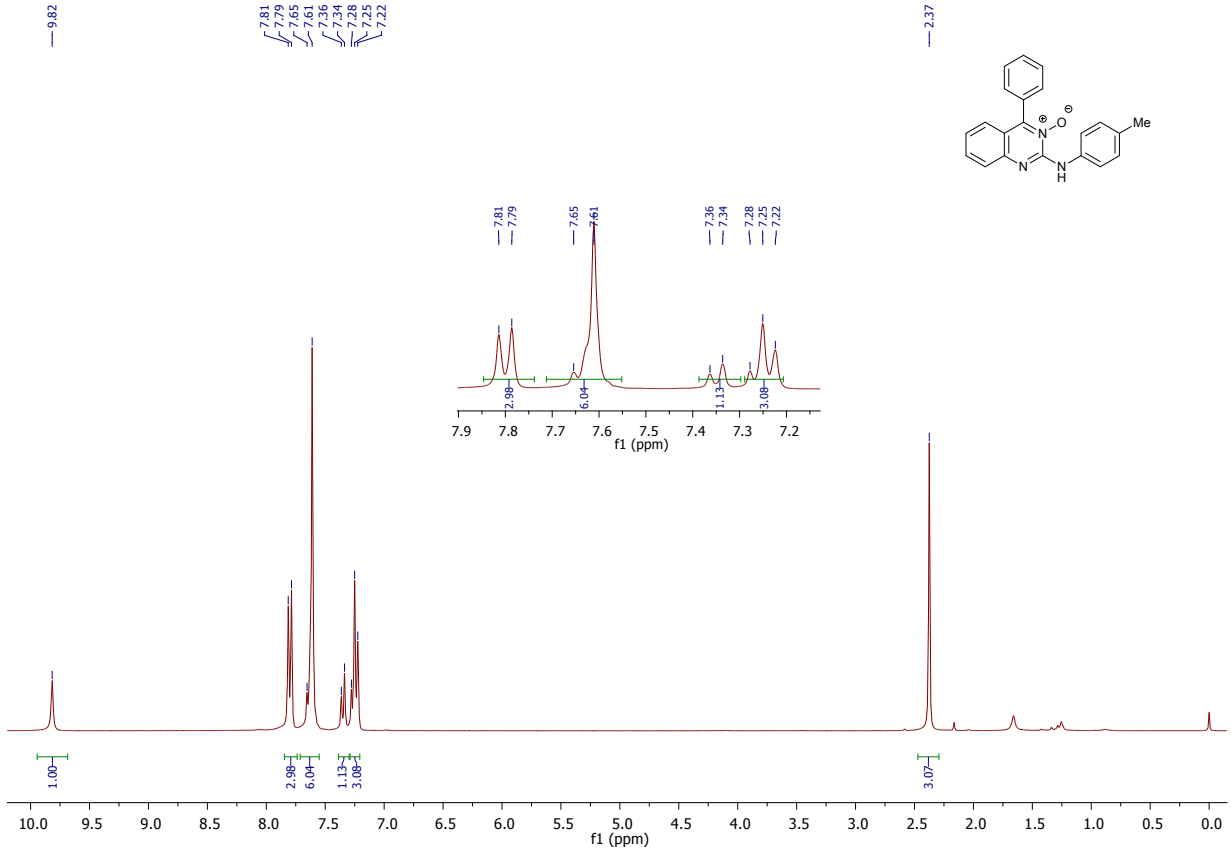
^{1}H NMR of spectra (**5a**)



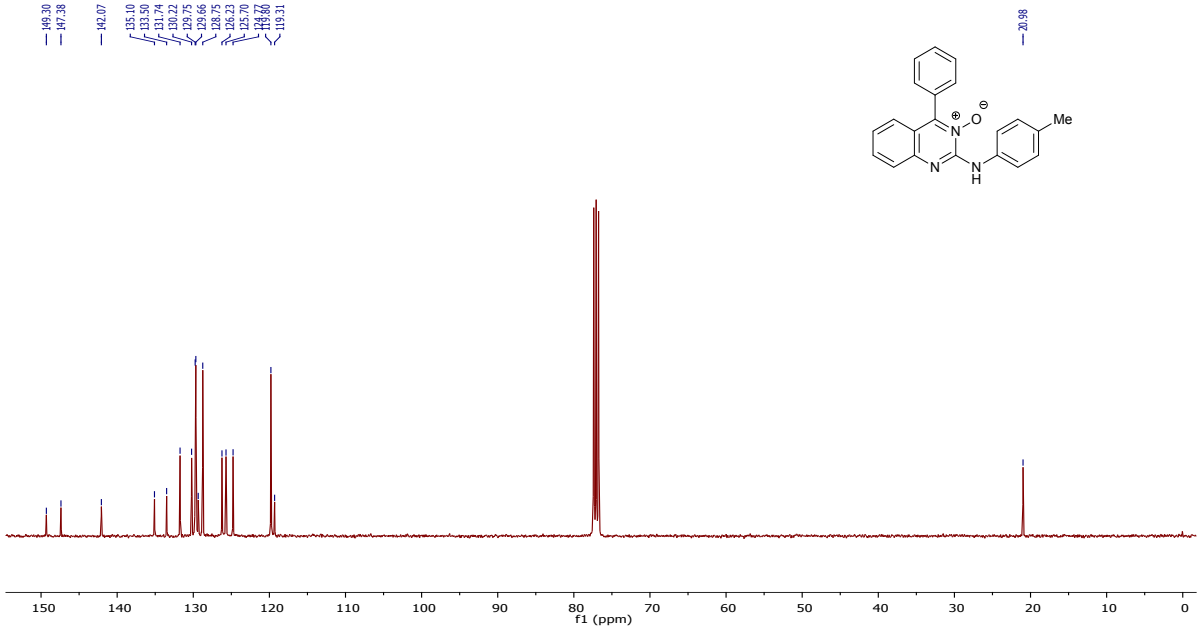
^{13}C NMR of spectra (**5a**)



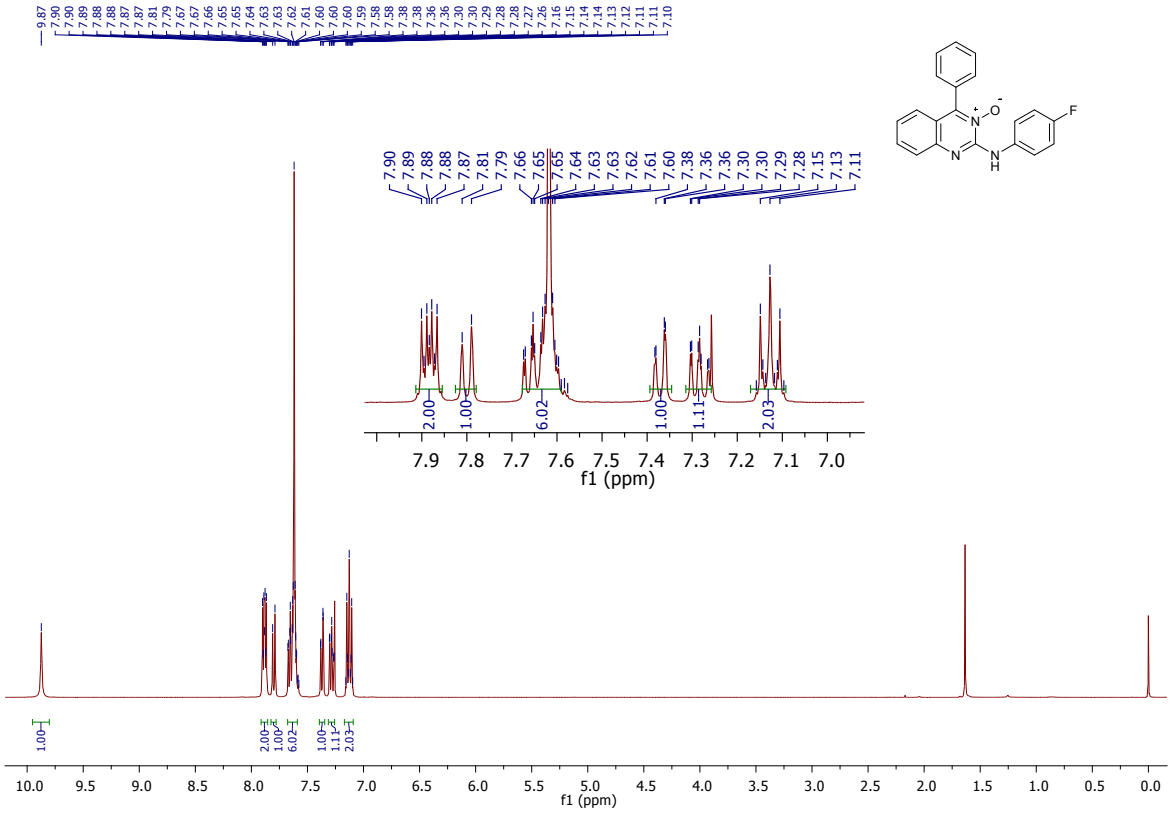
^{1}H NMR of spectra (**5b**)



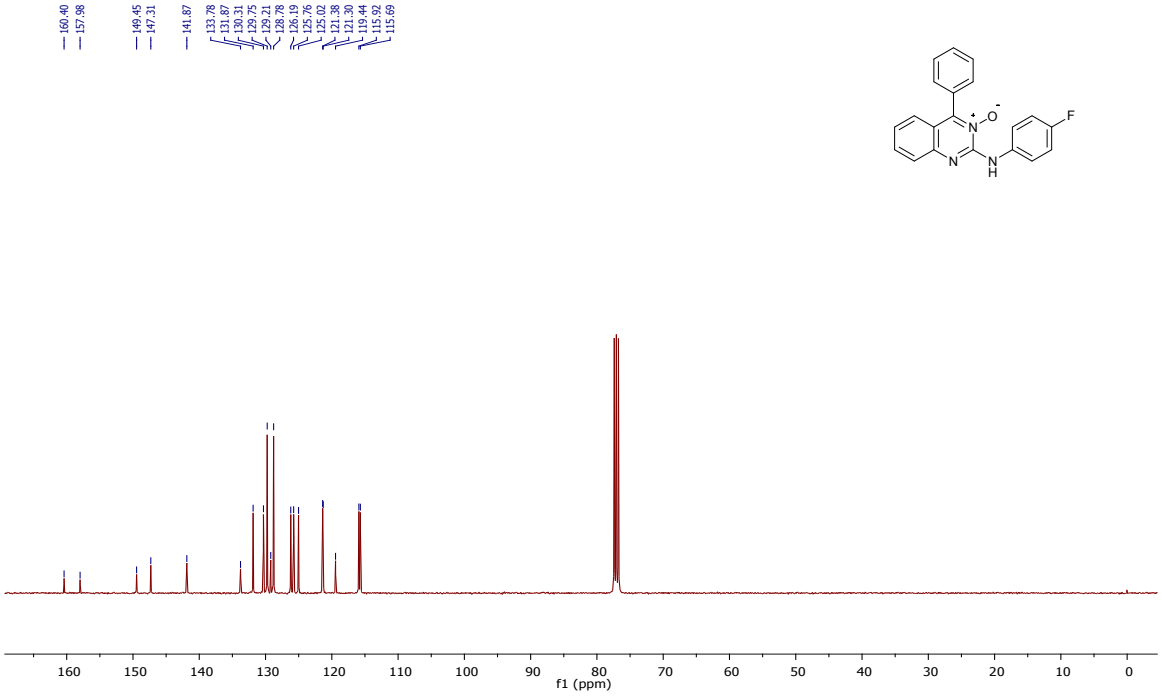
^{13}C NMR of spectra (**5b**)



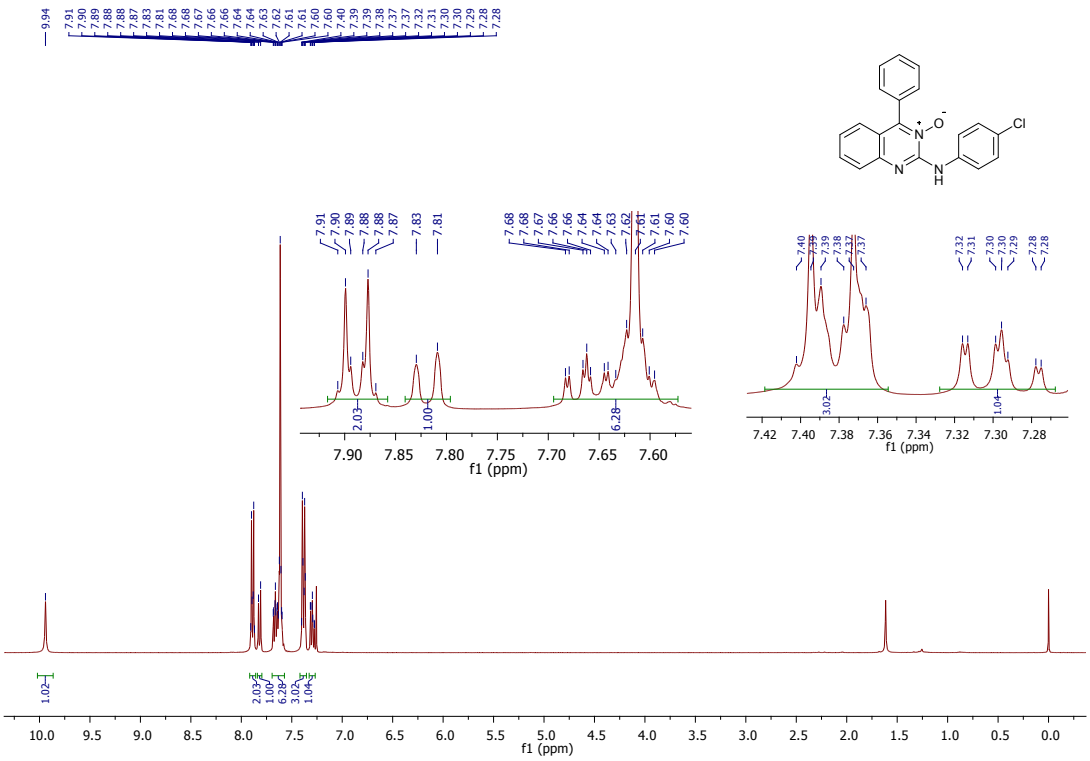
^{1}H NMR of spectra (**5c**)



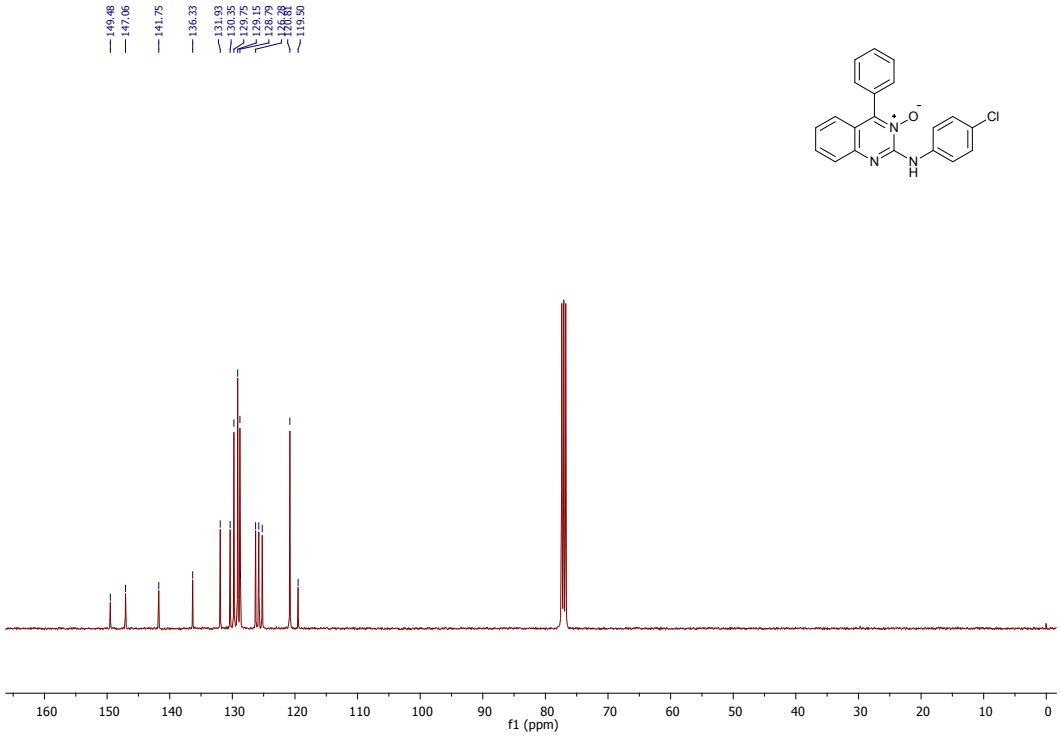
^{13}C NMR of spectra (**5c**)



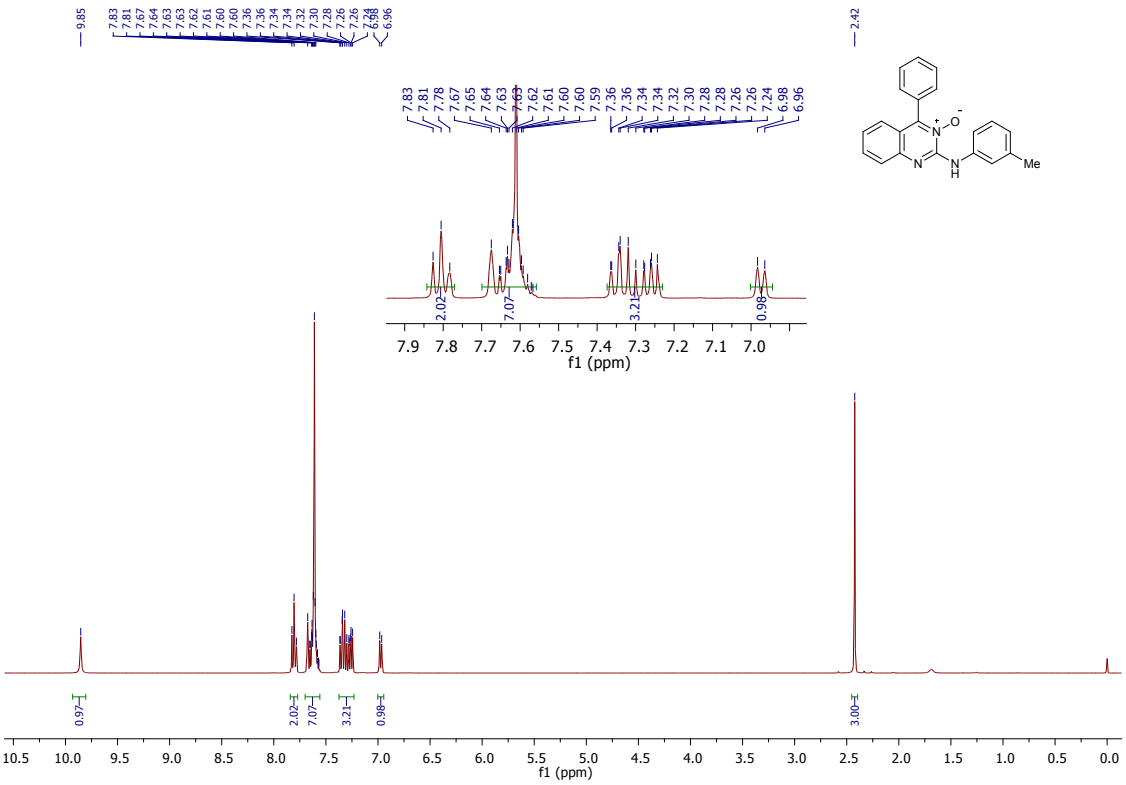
^{1}H NMR of spectra (**5d**)



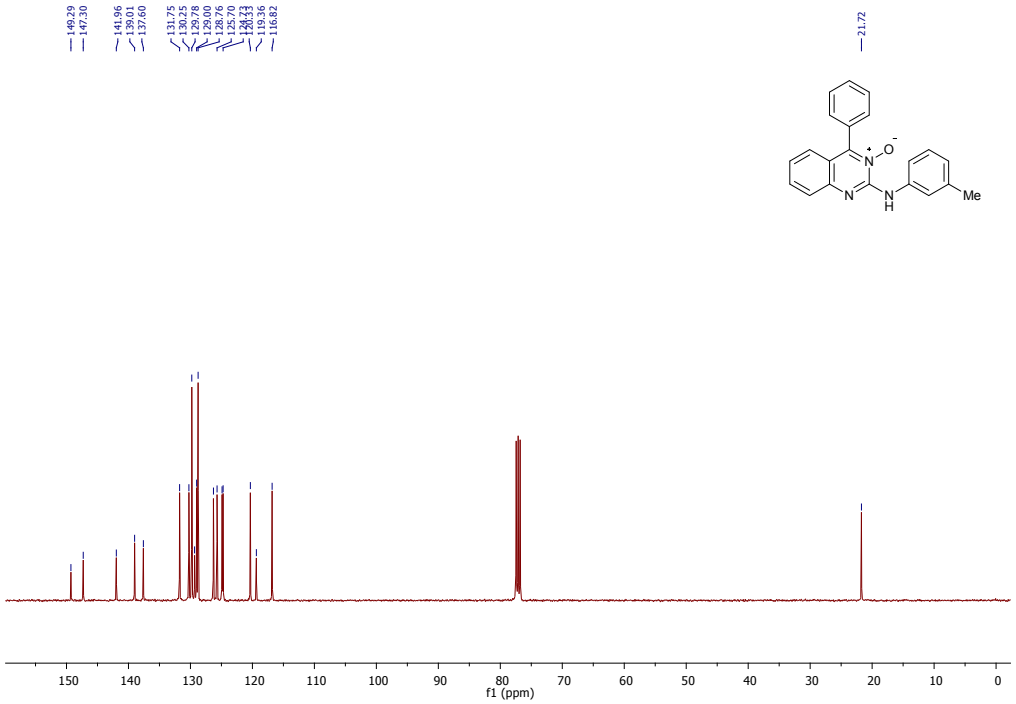
^{13}C NMR of spectra (**5d**)



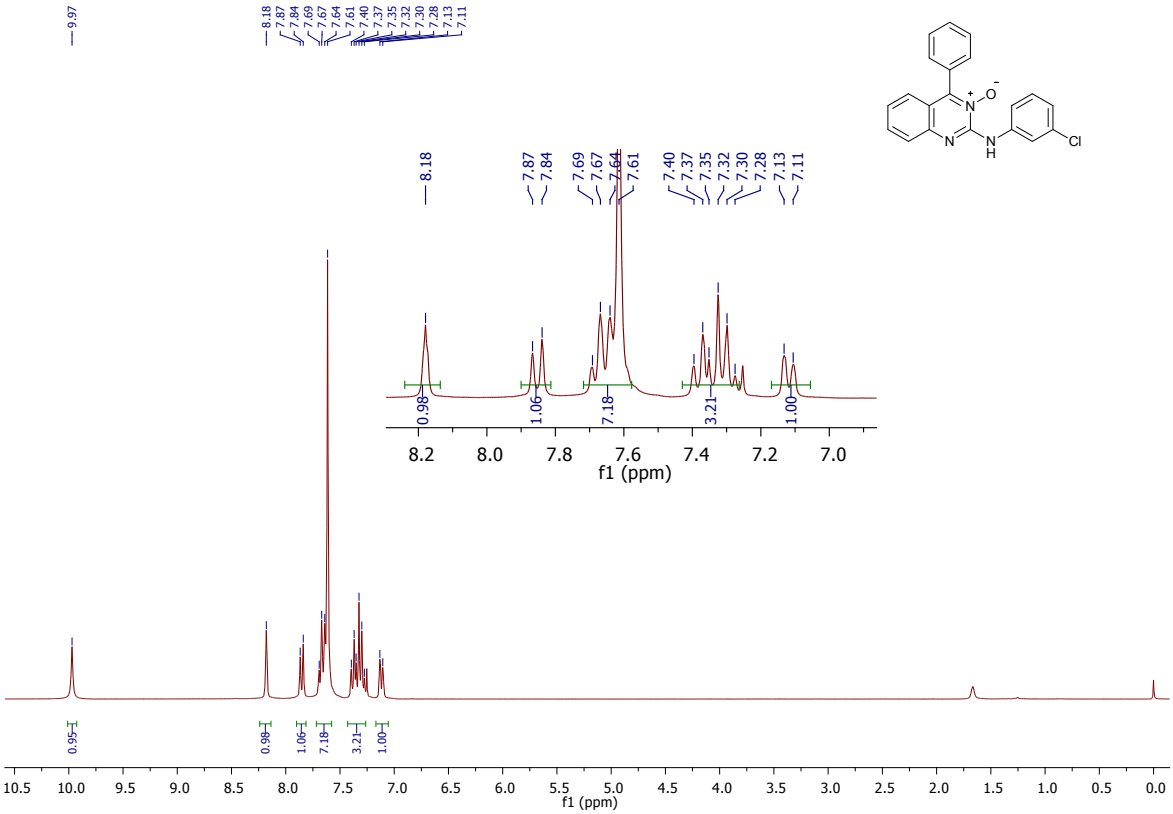
^{1}H NMR of spectra (**5e**)



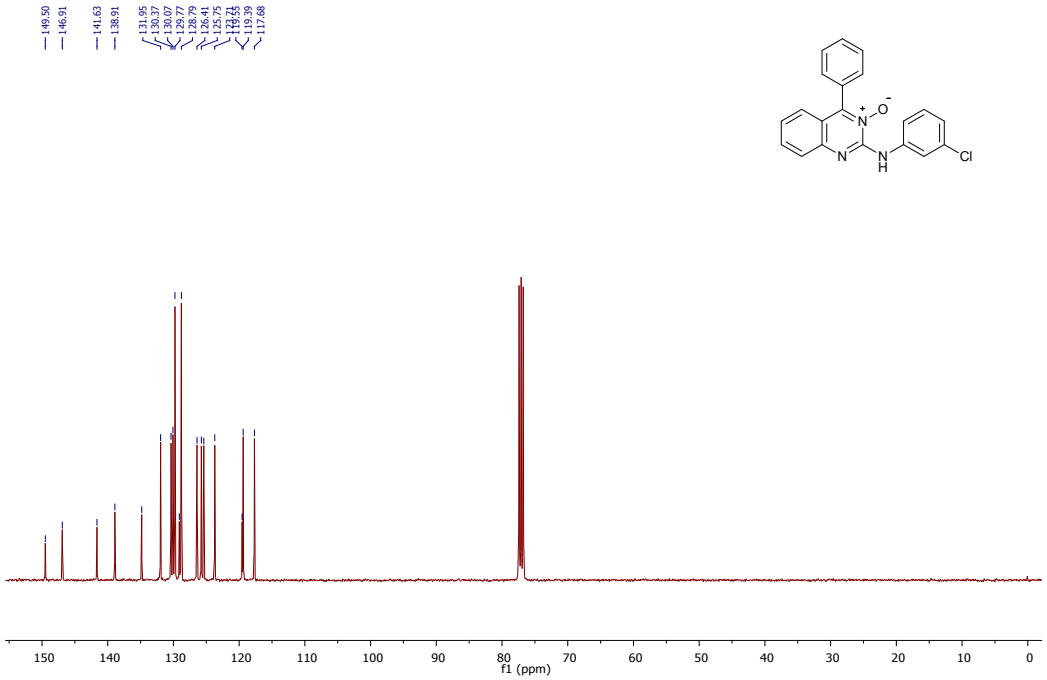
^{13}C NMR of spectra (**5e**)



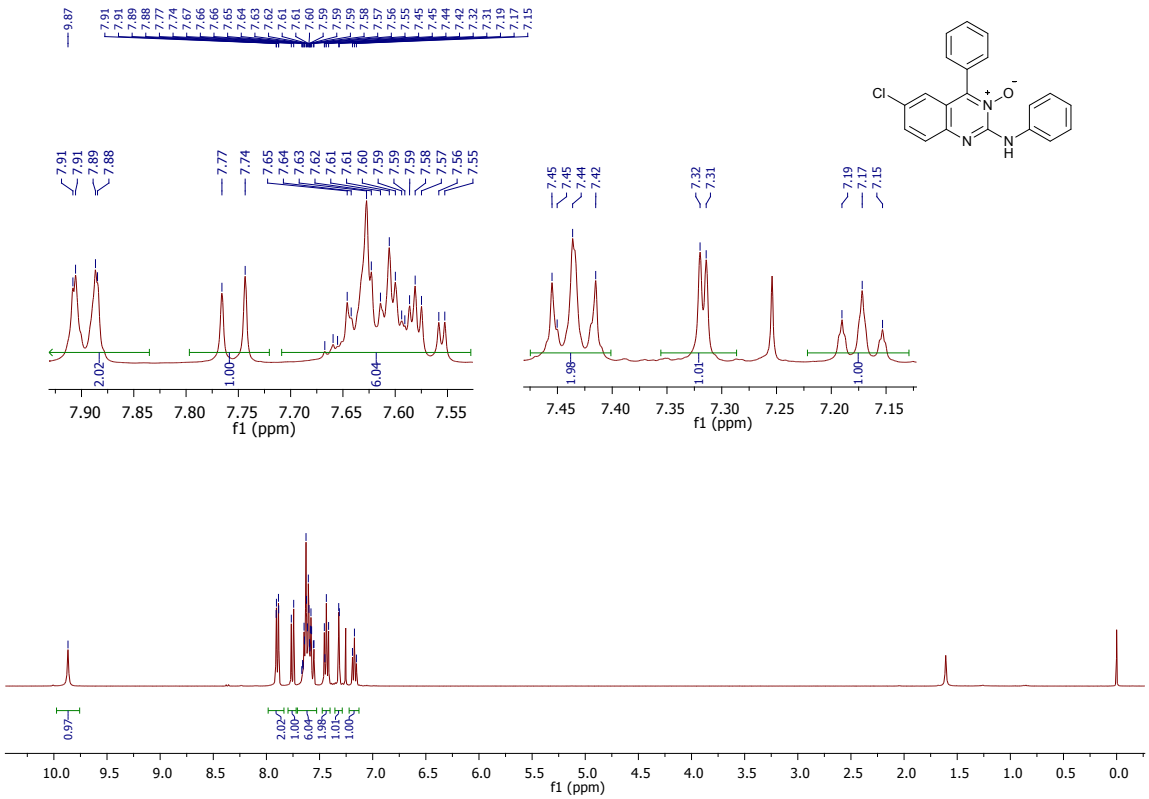
^{1}H NMR of spectra (**5f**)



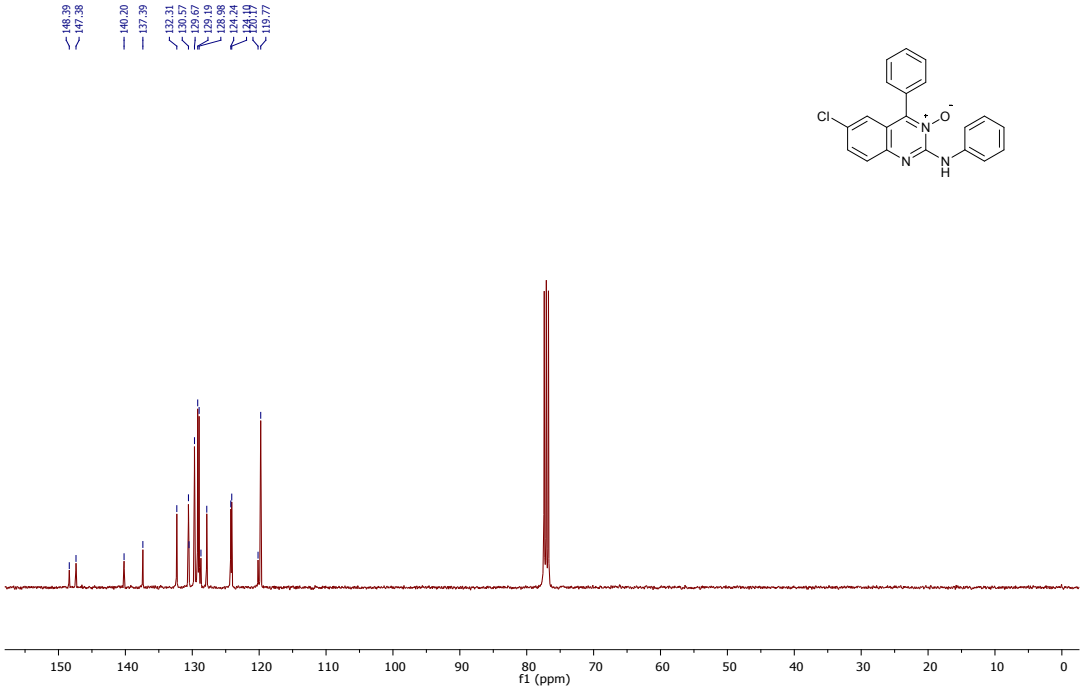
^{13}C NMR of spectra (**5f**)



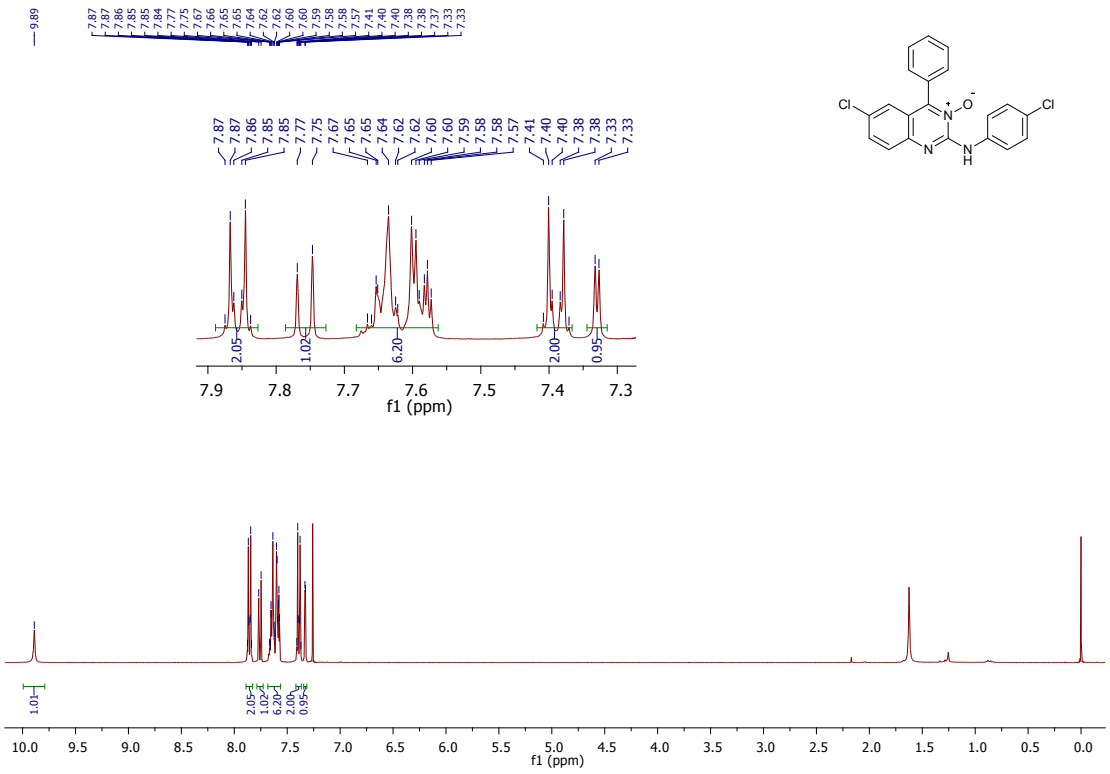
^{1}H NMR of spectra (**5g**)



^{13}C NMR of spectra (**5g**)



^{1}H NMR of spectra (**5h**)



^{13}C NMR of spectra (**5h**)