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Supporting Information

Copper-Catalyzed Three-Component Formal [3 +1+2] Annulations for the Synthesis of 2-Aminopyrimidines from *O*-Acyl Ketoximes

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General information

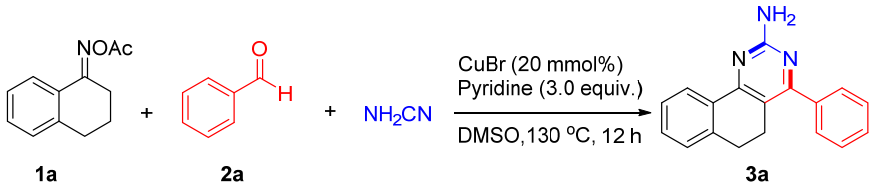
All reactions were carried out under air atmosphere unless otherwise noted. Column chromatography was performed using silica gel (200-300 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker-AV (400 and 100 MHz, respectively) instrument internally referenced to tetramethylsilane (TMS) or chloroform signals. Mass spectra were measured on Agilent 5975 GC-MS instrument (EI). High-resolution mass spectra were recorded at the Institute of Chemistry, Chinese Academy of Sciences. The structures of known compounds were further corroborated by comparing their ^{1}H NMR, ^{13}C NMR data and MS data with those of literature. Ketoxime acetates were synthesized according to the literature[1], and data of known compounds were compared with the reported data. All other reagents were obtained from commercial suppliers and used without further purification.

General procedure for the synthesis of 2-aminopyrimidines

General procedure A: Oxime acetate **1** (0.3 mmol), aldehyde **2** (0.2 mmol), CuBr (6.0 mg, 0.04 mmol, 20 mol %), cyanamide (84.0 mg, 2.0 mmol, 10.0 equiv), pyridine (48 μL, 0.6 mmol, 3.0 equiv), and DMSO (1.0 mL) were added successfully to a 10 mL oven-dried reaction vessel. The sealed reaction vessel was stirred at 130 ºC for 12 h. After cooling to room temperature, the reaction was diluted with ethyl acetate (10 mL) and water (10 mL). The organic layer was separated, and the aqueous layer was extracted with ethyl acetate (10 mL) for three times. The combined organic layer was brine and dried over magnesium sulfate and the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether (PE)/ethyl acetate (EA)) to yield the desired product **3**.

Effect the molecular ratio of substrates on the yield

Table S1

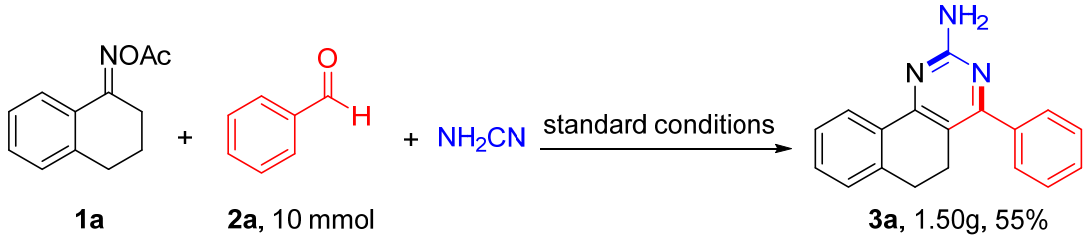


1a **2a** **3a**

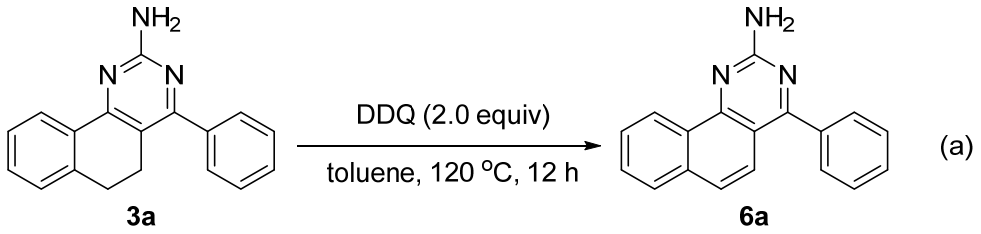
entry	**1a** (x mmol)	**2a** (y mmol)	NH_2CN (z equiv.)	GC yield (%)
1	0.2	0.2	10.0	45
2	0.3	0.2	10.0	64
3	0.4	0.2	10.0	67
4	0.2	0.3	10.0	56
5	0.2	0.4	10.0	63
6	0.3	0.2	9.0	58
7	0.3	0.2	11.0	65

Gram scale and further transformation experiments.

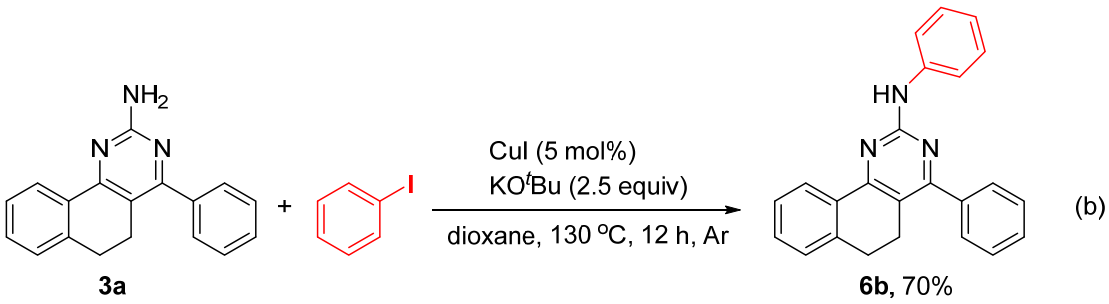
Gram-scale experiment for the synthesis of **3a**: (*E*)-3,4-dihydronaphthalen-1-(2*H*)-one *O*-acetyl oxime (**1a**, 3.05 g, 15 mmol), benzaldehyde (**2a**, 1.03 mL, 10 mmol), CuBr (0.29 g, 2.0 mmol, 20 mol %), cyanamide (4.2 g, 100 mmol, 10.0 equiv), pyridine (2.5 mL, 30.0 mmol, 3.0 equiv), and DMSO (30 mL) were added successfully to a 75 mL ovendried reaction pressure tube. The sealed reaction tube was stirred at 130 ºC for 30 h. After cooling to room temperature, the reaction was diluted with ethyl acetate (100 mL) and water (100 mL). The organic layer was separated, and the aqueous layer was extracted with ethyl acetate (60 mL) for three times. The combined organic layer was brine and dried over magnesium sulfate and the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (PE/EA: 5/1) to yield the desired product **3a** (1.50 g, 55%) as a yellow solid.



further transformation experiments of 3a: (a) To a 10 mL vial equipped with a Teflon septum and a magnetic stir bar was charged **3a** (27.3 mg, 0.1 mmol), DDQ (45.4 mg, 2.0 equiv) and toluene (1.0 mL). Thereafter, the reaction mixture was allowed to stir at 120 ºC (oil bath) for 12 h. After cooling to room temperature, the reaction was diluted with ethyl acetate (20 mL) and the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (PE/EA: 5/1) to yield the desired product **6a** (10.0 mg, 37%).

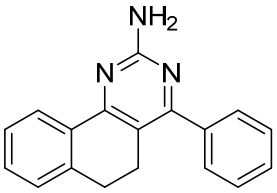


(b) To a 10 mL vial equipped with a Teflon septum and a magnetic stir bar was charged **3a** (27.3 mg, 0.1 mmol), iodobenzene (17 μL, 1.5 equiv), CuI (1.0 mg, 5 mol%), KO^{t}Bu (28 mg, 2.5 equiv), and dioxane (0.6 mL). Thereafter, the reaction mixture was allowed to stir at 130 ºC (oil bath) for 12 h under Ar. The reaction was diluted with ethyl acetate (20 mL) and the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (PE/EA: 10/1) to yield the desired product **6b** (24.4 mg, 70%).


NH2
N
N
3a
+
I
CuI (5 mol%)
KO^{t}Bu (2.5 equiv)
dioxane, 130 °C, 12 h, Ar
HN
N
N
6b, 70%

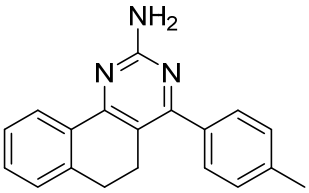
(b)

Characterization data of products



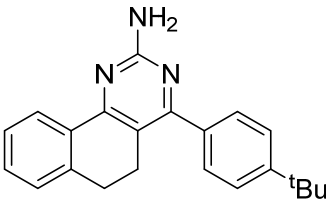
4-Phenyl-5,6-dihydrobenzo[*h*]quinazolin-2-amine (3a)

Following the general procedure A, **3a** was obtained as a yellow solid (32.7 mg, 60% yield), mp 173-175 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39–8.18 (m, 1H), 7.56–7.48 (m, 2H), 7.46–7.37 (m, 3H), 7.35–7.28 (m, 2H), 7.20–7.12 (m, 1H), 5.66 (brs, 2H), 2.83–2.67 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.2, 161.7, 160.9, 139.4, 138.1, 133.0, 130.3, 128.7, 128.4, 128.0, 127.5, 126.8, 125.4, 115.6, 28.1, 23.9. HRMS (ESI) m/z calcd for $C_{18}H_{16}N_3^+$ $(M+H)^+$ 274.1339, found 274.1341.



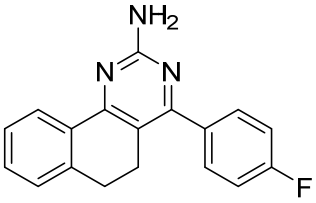
4-(*p*-Tolyl)-5,6-dihydrobenzo[*h*]quinazolin-2-amine (3b)

Following the general procedure A, **3b** was obtained as a yellow solid (33.3 mg, 58% yield), mp: 210-212 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37–8.15 (m, 1H), 7.45 (d, J = 7.8 Hz, 2H), 7.36 (dd, J = 5.6, 3.0 Hz, 2H), 7.27 (d, J = 7.8 Hz, 2H), 7.24–7.18 (m, 1H), 5.34 (brs, 2H), 2.89–2.76 (m, 4H), 2.41 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 161.7, 160.9, 139.5, 138.9, 135.4, 133.2, 130.4, 128.9, 128.5, 127.6, 127.0, 125.5, 115.9, 28.3, 24.1, 21.3. HRMS (ESI) m/z calcd for $C_{19}H_{18}N_3^+$ $(M+H)^+$ 288.1495, found 288.1499.



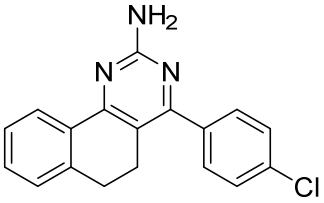
4-(4-(*tert*-Butyl)phenyl)-5,6-dihydrobenzo[*h*]quinazolin-2-amine (3c)

Following the general procedure A, **3c** was obtained as a yellow solid (34.8 mg, 53% yield), mp: 237-239 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33–8.22 (m, 1H), 7.56–7.44 (m, 4H), 7.39–7.31 (m, 2H), 7.23–7.16 (m, 1H), 5.33 (brs, 2H), 2.92–2.75 (m, 4H), 1.35 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.4, 161.7, 160.9, 152.0, 139.4, 135.3, 133.2, 130.4, 128.3, 127.6, 126.9, 125.5, 125.1, 115.9, 34.7, 31.2, 28.3, 24.1. HRMS (ESI) m/z calcd for $C_{22}H_{24}N_3^+$ $(M+H)^+$ 330.1965, found 330.1968.



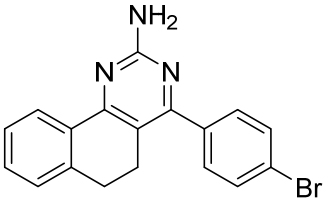
4-(4-Fluorophenyl)-5,6-dihydrobenzo[*h*]quinazolin-2-amine (3d)

Following the general procedure A, **3d** was obtained as a yellow solid (38.4mg, 66% yield), mp: 226-228 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33–8.23 (m, 1H), 7.55 (dd, J = 8.6, 5.5 Hz, 2H), 7.38 (td, J = 6.7, 5.9, 3.8 Hz, 2H), 7.23 (dd, J = 6.3, 2.4 Hz, 1H), 7.16 (t, J = 8.6 Hz, 2H), 5.26 (s, 2H), 2.83 (s, 4H).^{13}C NMR (100 MHz, $CDCl_3$) δ 164.3, 163.1 (d, J = 247.6 Hz), 161.6, 161.2, 139.4, 134.3 (d, J = 3.5 Hz), 133.0, 130.6 (d, J = 8.4 Hz), 130.6, 127.7, 127.0, 125.6, 115.9, 115.3 (d, J = 21.5 Hz), 28.2, 24.1. HRMS (ESI) m/z calcd for $C_{18}H_{15}FN_3^+$ $(M+H)^+$ 292.1245, found 292.1248.



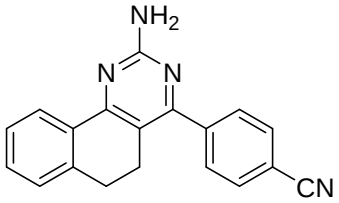
4-(4-Chlorophenyl)-5,6-dihydrobenzo[*h*]quinazolin-2-amine (3e)

Following the general procedure A, **3e** was obtained as a yellow solid (46.1 mg, 75% yield), mp:237-239 ºC; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.17 (dd, J = 7.3, 1.9 Hz, 1H), 7.60 (d, J = 8.5 Hz, 2H), 7.54 (d, J = 8.4 Hz, 2H), 7.39 (td, J = 7.2, 1.7 Hz, 2H), 7.28 (dd, J = 7.2, 1.8 Hz, 1H), 6.58 (brs, 2H), 2.75 (s, 4H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 164.0, 162.6, 160.5, 139.8, 137.5, 134.1, 133.4, 131.1, 130.9, 128.6, 128.3, 127.2, 125.5, 114.6, 28.0, 23.9. HRMS (ESI) m/z calcd for $C_{18}H_{15}ClN_3^+$ $(M+H)^+$ 308.0949, found 308.0953.



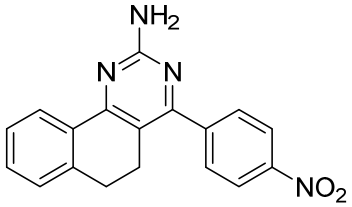
4-(4-Bromophenyl)-5,6-dihydrobenzo[*h*]quinazolin-2-amine (3f)

Following the general procedure A, **3f** was obtained as a yellow solid (56.2 mg, 80% yield), mp: 250-252 ºC; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.16 (dd, J = 7.3, 1.8 Hz, 1H), 7.69–7.63 (m, 2H), 7.56–7.48 (m, 2H), 7.36 (td, J = 7.3, 1.7 Hz, 2H), 7.26 (dd, J = 7.0, 1.8 Hz, 1H), 6.54 (brs, 2H), 2.74 (s, 4H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.1, 162.6, 160.5, 139.9, 137.9, 133.4, 131.5, 131.3, 130.9, 128.3, 127.2, 125.5, 122.8, 114.5, 28.0, 23.9. HRMS (ESI) m/z calcd for $C_{18}H_{15}BrN_3^+$ $(M+H)^+$ 352.0444, found 352.0448.



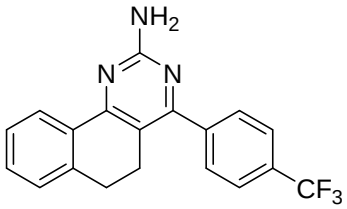
4-(2-Amino-5,6-dihydrobenzo[*h*]quinazolin-4-yl)benzonitrile (3g)

Following the general procedure A, **3g** was obtained as a yellow solid (38.7 mg, 65% yield), mp: 249-251 ºC; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.18 (d, J = 7.3 Hz, 1H), 7.96 (d, J = 7.8 Hz, 2H), 7.76 (d, J = 7.9 Hz, 2H), 7.45–7.33 (m, 2H), 7.28 (d, J = 7.1 Hz, 1H), 6.69 (brs, 2H), 2.92–2.63 (m, 4H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.5, 162.7, 160.7, 143.3, 139.9, 133.2, 132.6, 131.1, 130.1, 128.4, 127.3, 125.5, 119.2, 114.7, 111.9, 27.9, 23.8. HRMS (ESI) m/z calcd for $C_{19}H_{14}N_4Na^+$ $(M+Na)^+$ 321.1111, found 321.1117.



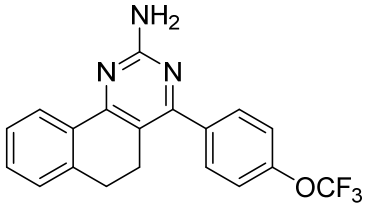
4-(4-Nitrophenyl)-5,6-dihydrobenzo[*h*]quinazolin-2-amine (3h)

Following the general procedure A, **3h** was obtained as a yellow solid (45.8 mg, 72% yield), mp: 228-230 ºC; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.36 – 8.27 (m, 2H), 8.17 (dd, J = 7.3, 1.9 Hz, 1H), 7.90–7.78 (m, 2H), 7.41–7.32 (m, 2H), 7.25 (dd, J = 7.1, 1.8 Hz, 1H), 6.69 (brs, 2H), 2.72 (d, J = 5.1 Hz, 4H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.1, 162.7, 160.8, 147.9, 145.1, 139.9, 133.2, 131.1, 130.6, 128.4, 127.2, 125.5, 123.7, 114.8, 27.9, 23.8. HRMS (ESI) m/z calcd for $C_{18}H_{14}N_4NaO_2^+$ $(M+Na)^+$ 341.1009, found 341.1015.



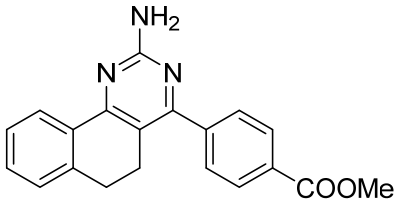
4-(4-(Trifluoromethyl)phenyl)-5,6-dihydrobenzo[*h*]quinazolin-2-amine (3i)

Following the general procedure A, **3i** was obtained as a yellow solid (49.1 mg, 72% yield), mp: 216-218 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35–8.19 (m, 1H), 7.72 (d, J = 8.2 Hz, 2H), 7.66 (d, J = 8.1 Hz, 2H), 7.41–7.30 (m, 2H), 7.22 (dd, J = 6.9, 1.9 Hz, 1H), 5.46 (brs, 2H), 2.80 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.9, 161.7, 161.5, 141.8, 139.4, 132.9, 130.9 (q, J = 32.4 Hz), 130.8, 129.0, 127.7, 127.1, 125.6, 125.2 (q, J =3.7 Hz), 123.9 (q, J =270.6 Hz), 116.0, 28.1, 23.9. HRMS (ESI) m/z calcd for $C_{19}H_{15}F_3N_3^+$ $(M+H)^+$ 342.1213, found 342.1214.



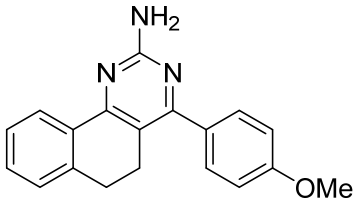
4-(4-(Trifluoromethoxy)phenyl)-5,6-dihydrobenzo[*h*]quinazolin-2-amine (3j)

Following the general procedure A, **3j** was obtained as a yellow solid (49.3 mg, 69% yield), mp: 170-172 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29–8.25 (m, 1H), 7.61–7.57 (m, 2H), 7.40–7.34 (m, 2H), 7.31 (d, J = 7.8 Hz, 2H), 7.22 (dd, J = 6.8, 2.0 Hz, 1H), 5.40 (brs, 2H), 2.82 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.9, 161.7, 161.4, 149.6 (d, J = 2.0 Hz), 139.4, 136.9, 132.9, 130.7, 130.2, 127.7, 127.0, 125.6, 120.6, 120.4 (q, J = 256.0 Hz), 115.9, 28.1, 24.0. HRMS (ESI) m/z calcd for $C_{19}H_{15}F_3N_3O^+$ $(M+H)^+$ 358.1162, found 358.1164.



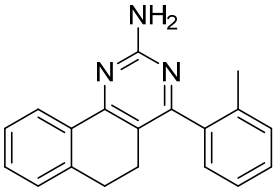
Methyl 4-(2-amino-5,6-dihydrobenzo[*h*]quinazolin-4-yl)benzoate (3k)

Following the general procedure A, **3k** was obtained as a yellow solid (45.0 mg, 68% yield), mp: 218-220 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30–8.24 (m, 1H), 8.19–8.10 (m, 2H), 7.62 (d, J = 8.4 Hz, 2H), 7.42–7.32 (m, 2H), 7.25–7.17 (m, 1H), 5.45 (brs, 2H), 3.95 (s, 3H), 2.81 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 164.2, 161.7, 161.3, 142.6, 139.4, 132.9, 130.7, 130.3, 129.5, 128.7, 127.7, 127.0, 125.6, 115.9, 52.2, 28.1, 23.9. HRMS (ESI) m/z calcd for $C_{20}H_{17}N_3NaO_2^+$ $(M+Na)^+$ 354.1213, found 354.1216.



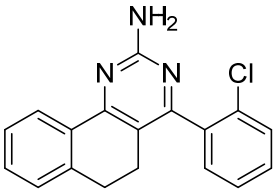
4-(4-Methoxyphenyl)-5,6-dihydrobenzo[*h*]quinazolin-2-amine (3l)

Following the general procedure A, **3l** was obtained as a yellow solid (26.1 mg, 43% yield), mp: 190-192 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31–8.22 (m, 1H), 7.58–7.50 (m, 2H), 7.40–7.32 (m, 2H), 7.24–7.17 (m, 1H), 7.03–6.93 (m, 2H), 5.25 (brs, 2H), 3.86 (s, 3H), 2.93–2.76 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.0, 161.6, 160.9, 160.2, 139.4, 133.3, 130.6, 130.4, 130.1, 127.6, 127.0, 125.5, 115.9, 113.6, 55.3, 28.3, 24.3. HRMS (ESI) m/z calcd for $C_{19}H_{18}N_3NaO^+$ $(M+Na)^+$ 326.1264, found 326.1269.



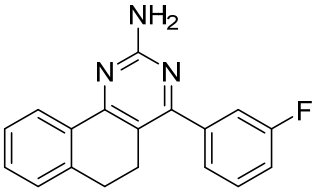
4-(*o*-Tolyl)-5,6-dihydrobenzo[*h*]quinazolin-2-amine (3m)

Following the general procedure A, **3m** was obtained as a brown solid (25.3 mg, 44% yield), mp: 85-87 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38–8.24 (m, 1H), 7.40–7.35 (m, 2H), 7.33–7.25 (m, 3H), 7.24–7.18 (m, 2H), 5.23 (brs, 2H), 2.81 (t, J = 7.3 Hz, 2H), 2.61–2.47 (m, 2H), 2.21 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 161.6, 160.6, 139.7, 137.9, 135.2, 133.0, 130.6, 130.3, 128.5, 127.9, 127.8, 127.0, 125.8, 125.5, 116.8, 28.1, 23.1, 19.4. HRMS (ESI) m/z calcd for $C_{19}H_{17}N_3Na^+$ $(M+Na)^+$ 310.1315, found 310.1317.



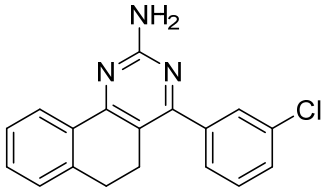
4-(2-Chlorophenyl)-5,6-dihydrobenzo[*h*]quinazolin-2-amine (3n)

Following the general procedure A, **3n** was obtained as a yellow solid (41.8 mg, 68% yield), mp: 143-145 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40–8.20 (m, 1H), 7.48–7.43 (m, 1H), 7.42–7.29 (m, 5H), 7.25–7.17 (m, 1H), 5.41 (brs, 2H), 2.91–2.75 (m, 2H), 2.75–2.63 (m, 1H), 2.53–2.39 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8, 161.6, 160.7, 139.8, 137.3, 132.8, 132.2, 130.7, 129.9, 129.8, 129.5, 127.8, 127.0, 125.5, 117.1, 27.9, 23.0. HRMS (ESI) m/z calcd for $C_{18}H_{14}ClN_3Na^+$ $(M+Na)^+$ 330.0768, found 330.0769.



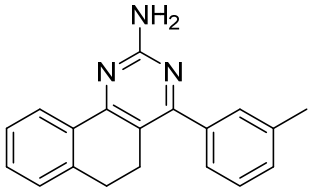
4-(3-Fluorophenyl)-5,6-dihydrobenzo[*h*]quinazolin-2-amine (3o)

Following the general procedure A, **3o** was obtained as a yellow solid (40.7 mg, 70% yield), mp: 157-159 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40–8.21 (m, 1H), 7.47–7.34 (m, 3H), 7.33 (d, J = 7.7 Hz, 1H), 7.28 (d, J = 9.8 Hz, 1H), 7.25–7.19 (m, 1H), 7.16–7.12 (m, 1H), 5.32 (brs, 2H), 2.83 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.0, 162.5 (d, J = 245.2 Hz), 161.5 (d, J = 24.1 Hz), 140.4 (d, J = 7.4 Hz), 139.4, 132.9, 130.7, 129.9 (d, J = 8.1 Hz), 127.7, 127.1, 125.6, 124.3 (d, J = 2.2 Hz), 116.0, 115.9, 115.8 (d, J = 6.4 Hz), 115.6, 28.2, 23.9. HRMS (ESI) m/z calcd for $C_{18}H_{14}FN_3Na^+$ $(M+Na)^+$ 314.1064, found 314.1065.



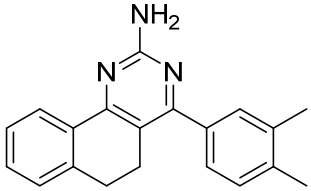
4-(3-Chlorophenyl)-5,6-dihydrobenzo[*h*]quinazolin-2-amine (3p)

Following the general procedure A, **3p** was obtained as a yellow solid (40.5 mg, 66% yield), mp: 180-182 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40–8.19 (m, 1H), 7.55 (s, 1H), 7.45–7.30 (m, 5H), 7.21 (d, J = 8.6 Hz, 1H), 5.46 (brs, 2H), 2.80 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8, 161.7, 161.3, 139.9, 139.4, 134.2, 132.9, 130.7, 129.5, 129.0, 128.7, 127.7, 127.0, 126.7, 125.5, 115.8, 28.1, 23.9. HRMS (ESI) m/z calcd for $C_{18}H_{14}ClN_3Na^+$ $(M+Na)^+$ 330.0768, found 330.0771.



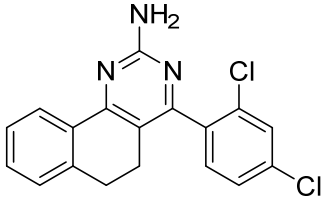
4-(*m*-Tolyl)-5,6-dihydrobenzo[*h*]quinazolin-2-amine (3q)

Following the general procedure A, **3q** was obtained as a yellow solid (31.0 mg, 54% yield), mp: 165-167 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32–8.22 (m, 1H), 7.40–7.29 (m, 5H), 7.27–7.18 (m, 2H), 5.31 (brs, 2H), 2.88–2.76 (m, 4H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.7, 161.6, 160.9, 139.5, 138.2, 138.0, 133.1, 130.5, 129.6, 129.1, 128.0, 127.6, 127.0, 125.6, 125.5, 116.0, 28.2, 24.0, 21.4. HRMS (ESI) m/z calcd for $C_{19}H_{17}N_3Na^+$ $(M+Na)^+$ 310.1315, found 310.1316.



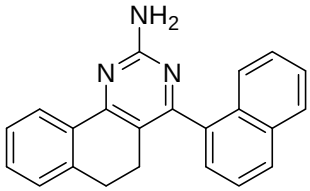
4-(3,4-Dimethylphenyl)-5,6-dihydrobenzo[*h*]quinazolin-2-amine (3r)

Following the general procedure A, **3r** was obtained as a yellow solid (30.1 mg, 50% yield), mp: 180-182 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37–8.19 (m, 1H), 7.42–7.31 (m, 3H), 7.29–7.17 (m, 3H), 5.39 (brs, 2H), 2.93–2.71 (m, 4H), 2.32 (d, J = 2.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 161.6, 160.8, 139.5, 137.6, 136.5, 135.7, 133.2, 130.4, 129.6, 129.3, 127.6, 126.9, 126.0, 125.5, 115.9, 28.2, 24.1, 19.8, 19.6. HRMS (ESI) m/z calcd for $C_{20}H_{19}N_3Na^+$ $(M+Na)^+$ 324.1471, found 324.1473.



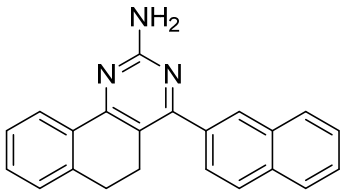
4-(2,4-Dichlorophenyl)-5,6-dihydrobenzo[*h*]quinazolin-2-amine (3s)

Following the general procedure A, **3s** was obtained as a yellow solid (52.5 mg, 77% yield), mp: 180-182 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40–8.20 (m, 1H), 7.48 (d, J = 2.0 Hz, 1H), 7.38–7.31 (m, 3H), 7.29 (d, J = 8.2 Hz, 1H), 7.22–7.14 (m, 1H), 5.56 (brs, 2H), 2.90–2.73 (m, 2H), 2.71–2.59 (m, 1H), 2.51–2.35 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.6, 161.7, 160.9, 139.6, 135.8, 135.0, 133.1, 132.6, 130.8, 130.7, 129.3, 127.8, 127.3, 127.0, 125.5, 116.9, 27.8, 22.9. HRMS (ESI) m/z calcd for $C_{18}H_{13}Cl_2N_3Na^+$ $(M+Na)^+$ 364.0379, found 364.0378.



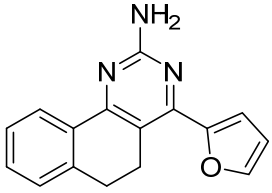
4-(Naphthalen-1-yl)-5,6-dihydrobenzo[*h*]quinazolin-2-amine (3t)

Following the general procedure A, **3t** was obtained as a yellow solid (34.9 mg, 54% yield), mp: 125-127 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43–8.27 (m, 1H), 8.00–7.84 (m, 2H), 7.65 (d, J = 8.4 Hz, 1H), 7.59–7.53 (m, 1H), 7.51–7.41 (m, 3H), 7.40–7.34 (m, 2H), 7.22–7.14 (m, 1H), 5.36 (brs, 2H), 2.74 (t, J = 7.3 Hz, 2H), 2.51–2.41 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 161.7, 160.7, 139.7, 135.9, 133.5, 133.0, 130.7, 130.6, 128.9, 128.4, 127.8, 127.0, 126.5, 126.1, 125.9, 125.6, 125.2, 117.6, 28.1, 23.4. HRMS (ESI) m/z calcd for $C_{22}H_{17}N_3Na^+$ $(M+Na)^+$ 346.1315, found 346.1319.



4-(Naphthalen-2-yl)-5,6-dihydrobenzo[*h*]quinazolin-2-amine (3u)

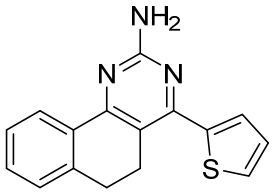
Following the general procedure A, **3u** was obtained as a yellow solid (41.3 mg, 64% yield), mp: 190-192 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38–8.23 (m, 1H), 8.00 (d, J = 1.7 Hz, 1H), 7.95–7.84 (m, 3H), 7.66 (dd, J = 8.4, 1.7 Hz, 1H), 7.55–7.47 (m, 2H), 7.39–7.32 (m, 2H), 7.23–7.15 (m, 1H), 5.47 (brs, 2H), 2.88 (dd, J = 8.1, 5.1 Hz, 2H), 2.78 (dd, J = 8.7, 5.5 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.3, 161.8, 161.1, 139.5, 135.6, 133.3, 133.1, 132.8, 130.5, 128.4, 128.2, 127.9, 127.6, 127.0, 126.7, 126.3, 126.1, 125.5, 116.1, 28.2, 24.1. HRMS (ESI) m/z calcd for $C_{22}H_{17}N_3Na^+$ $(M+Na)^+$ 346.1315, found 346.1318.



Phenyl(5-(thiophen-2-yl)-1*H*-pyrrol-2-yl)methanone (3v)

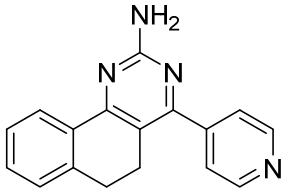
Following the general procedure A, **3v** was obtained as a yellow solid (21.0 mg, 40% yield), mp: 262-264 ºC; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.13 (dd, J = 7.6, 1.6 Hz, 1H), 7.89 (d, J = 1.7 Hz,

1H), 7.41–7.30 (m, 2H), 7.28 (dd, J = 7.3, 1.6 Hz, 1H), 7.08 (d, J = 3.4 Hz, 1H), 6.67 (dd, J = 3.4, 1.8 Hz, 1H), 6.50 (brs, 2H), 3.04 (dd, J = 8.5, 6.1 Hz, 2H), 2.84 (dd, J = 8.5, 6.1 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.4, 160.9, 153.7, 152.6, 145.2, 139.7, 133.3, 130.9, 128.2, 127.1, 125.4, 114.0, 113.1, 112.3, 27.7, 23.2. HRMS (ESI) m/z calcd for $C_{16}H_{13}N_3NaO^+$ $(M+Na)^+$ 286.0951, found 286.0952.



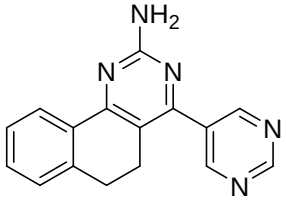
4-(Thiophen-2-yl)-5,6-dihydrobenzo[*h*]quinazolin-2-amine (3w)

Following the general procedure A, **3w** was obtained as a yellow solid (30.7 mg, 55% yield), mp: 236-238 ºC; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.14 (dd, J = 7.5, 1.7 Hz, 1H), 7.74 (d, J = 5.1 Hz, 1H), 7.55 (d, J = 3.7 Hz, 1H), 7.44–7.32 (m, 2H), 7.30 (d, J = 7.0 Hz, 1H), 7.23–7.16 (m, 1H), 6.56 (brs, 2H), 3.10–2.93 (m, 2H), 2.93–2.77 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.2, 160.8, 157.6, 142.9, 139.5, 133.4, 130.9, 129.9, 129.7, 128.5, 128.2, 127.2, 125.5, 113.4, 27.8, 24.2. HRMS (ESI) m/z calcd for $C_{16}H_{13}N_3NaS^+$ $(M+Na)^+$ 302.0722, found 302.0725.



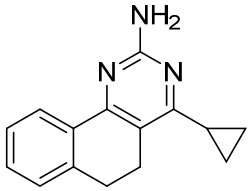
4-(Pyridin-4-yl)-5,6-dihydrobenzo[*h*]quinazolin-2-amine (3x)

Following the general procedure A, **3x** was obtained as a yellow solid (20.3 mg, 37% yield), mp: 212-214 ºC; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.71 (d, J = 5.0 Hz, 2H), 8.18 (dd, J = 7.4, 1.8 Hz, 1H), 7.61–7.51 (m, 2H), 7.45–7.34 (m, 2H), 7.29 (d, J = 7.1 Hz, 1H), 6.70 (brs, 2H), 2.84–2.67 (m, 4H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.9, 162.7, 160.7, 150.1, 146.1, 139.9, 133.2, 131.1, 128.4, 127.3, 125.5, 123.7, 114.7, 27.9, 23.6. HRMS (ESI) m/z calcd for $C_{17}H_{14}N_4Na^+$ $(M+Na)^+$ 297.1111, found 297.1111.



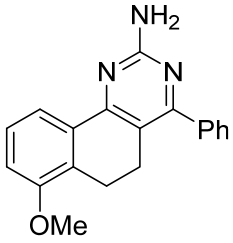
4-(Pyrimidin-5-yl)-5,6-dihydrobenzo[*h*]quinazolin-2-amine (3y)

Following the general procedure A, **3y** was obtained as a yellow solid (36.9 mg, 67% yield), mp: 195-197 ºC; ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.30 (s, 1H), 9.06 (s, 2H), 8.18 (d, J = 7.3 Hz, 1H), 7.44–7.35 (m, 2H), 7.30 (d, J = 6.5 Hz, 1H), 6.76 (brs, 2H), 2.81 (s, 4H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.8, 160.8, 159.6, 158.8, 157.0, 139.9, 133.1, 132.4, 131.2, 128.4, 127.3, 125.5, 115.3, 27.9, 23.5. HRMS (ESI) m/z calcd for $C_{16}H_{13}N_5Na^+$ $(M+Na)^+$ 298.1063, found 298.1065.



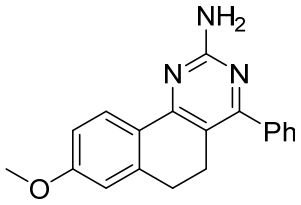
4-Cyclopropyl-5,6-dihydrobenzo[*h*]quinazolin-2-amine (3z)

Following the general procedure A, **3z** was obtained as a yellow solid (19.0 mg, 40% yield), mp: 240-242 ºC; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.11 (d, J = 7.4 Hz, 1H), 7.41–7.25 (m, 3H), 6.22 (brs, 2H), 2.86 (s, 4H), 2.22–2.05 (m, 1H), 1.05–0.96 (m, 2H), 0.96–0.86 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 168.8, 162.6, 157.9, 139.6, 133.5, 130.5, 128.3, 127.1, 125.4, 114.8, 27.9, 21.7, 12.8, 10.2. HRMS (ESI) m/z calcd for $C_{15}H_{16}N_3^+$ $(M+H)^+$ 238.1339, found 238.1342.



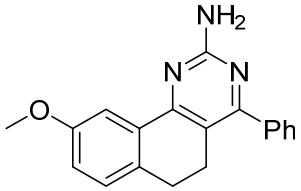
7-Methoxy-4-phenyl-5,6-dihydrobenzo[*h*]quinazolin-2-amine (4a)

Following the general procedure A, **4a** was obtained as a yellow solid (38.8 mg, 64% yield), mp: 198-200 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (dd, J = 7.9, 1.1 Hz, 1H), 7.59–7.51 (m, 2H), 7.50–7.38 (m, 3H), 7.31 (t, J = 8.0 Hz, 1H), 6.95 (d, J = 8.2 Hz, 1H), 5.47 (s, 2H), 3.83 (s, 3H), 2.79 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.3, 161.6, 161.0, 155.9, 138.2, 134.2, 128.8, 128.5, 128.1, 128.0, 127.1, 117.7, 115.8, 112.2, 55.5, 23.4, 20.2. HRMS (ESI) m/z calcd for $C_{19}H_{17}N_3NaO^+$ $(M+Na)^+$ 326.1264, found 326.1269.



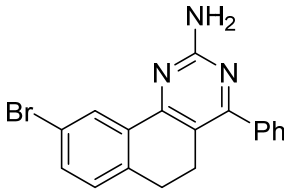
8-Methoxy-4-phenyl-5,6-dihydrobenzo[*h*]quinazolin-2-amine (4b)

Following the general procedure A, **4b** was obtained as a yellow solid (38.8 mg, 64% yield), mp: 169-171 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (d, J = 8.6 Hz, 1H), 7.52 (dd, J = 7.7, 1.9 Hz, 2H), 7.49–7.36 (m, 3H), 6.86 (dd, J = 8.6, 2.6 Hz, 1H), 6.71 (d, J = 2.6 Hz, 1H), 5.52 (brs, 2H), 3.81 (s, 3H), 2.83–2.77 (m, 2H), 2.77–2.70 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.8, 161.6, 161.3, 160.9, 141.5, 138.3, 128.7, 128.4, 128.1, 127.3, 125.9, 114.8, 112.7, 112.3, 55.1, 28.5, 23.9. HRMS (ESI) m/z calcd for $C_{19}H_{17}N_3NaO^+$ $(M+Na)^+$ 326.1264, found 326.1268.



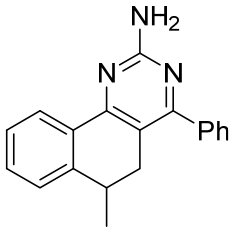
9-Methoxy-4-phenyl-5,6-dihydrobenzo[*h*]quinazolin-2-amine (4c)

Following the general procedure A, **4c** was obtained as a yellow solid (34.5 mg, 57% yield), mp: 180-182 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, J = 2.8 Hz, 1H), 7.59–7.52 (m, 2H), 7.51–7.37 (m, 3H), 7.12 (d, J = 8.3 Hz, 1H), 6.94 (dd, J = 8.3, 2.8 Hz, 1H), 5.38 (brs, 2H), 3.89 (s, 3H), 2.85–2.78 (m, 2H), 2.76–2.68 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 161.6, 160.9, 158.7, 138.2, 134.0, 131.8, 128.9, 128.7, 128.5, 128.2, 117.5, 116.1, 109.3, 55.4, 27.3, 24.3. HRMS (ESI) m/z calcd for $C_{19}H_{17}N_3NaO^+$ $(M+Na)^+$ 326.1264, found 326.1270.



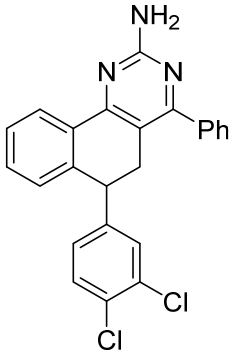
9-Bromo-4-phenyl-5,6-dihydrobenzo[*h*]quinazolin-2-amine (4d)

Following the general procedure A, **4d** was obtained as a yellow solid (33.7 mg, 48% yield), mp: 234-236 ºC; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.30 (d, J = 2.2 Hz, 1H), 7.57–7.52 (m, 3H), 7.49–7.45 (m, 3H), 7.24 (d, J = 8.1 Hz, 1H), 6.67 (brs, 2H), 2.73 (s, 4H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 165.8, 162.6, 158.8, 139.0, 138.5, 135.6, 133.2, 130.6, 129.4, 129.1, 128.5, 127.8, 120.2, 114.4, 27.4, 23.7. HRMS (ESI) m/z calcd for $C_{18}H_{14}BrN_3Na^+$ $(M+Na)^+$ 374.0263, found 374.0268.



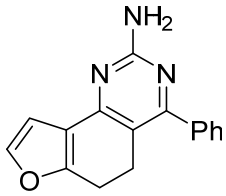
6-Methyl-4-phenyl-5,6-dihydrobenzo[*h*]quinazolin-2-amine (4e)

Following the general procedure A, **4e** was obtained as a yellow solid (37.3 mg, 65% yield), mp: 166-168 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (dd, J = 7.6, 1.6 Hz, 1H), 7.58–7.51 (m, 2H), 7.51–7.32 (m, 5H), 7.29–7.25 (m, 1H), 5.33 (brs, 2H), 3.07–2.87 (m, 2H), 2.76–2.62 (m, 1H), 1.19 (d, J = 6.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.9, 161.6, 160.8, 144.3, 138.2, 132.2, 130.8, 128.9, 128.5, 128.2, 126.8, 126.1, 125.7, 114.7, 32.2, 31.5, 19.9. HRMS (ESI) m/z calcd for $C_{19}H_{17}N_3Na^+$ $(M+Na)^+$ 310.1315, found 310.1318.



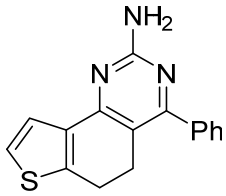
6-(3,4-Dichlorophenyl)-4-phenyl-5,6-dihydrobenzo[*h*]quinazolin-2-amine (4f)

Following the general procedure A, **4f** was obtained as a yellow solid (46.7 mg, 56% yield), mp: 225-227 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (dd, J = 7.6, 1.6 Hz, 1H), 7.48–7.32 (m, 7H), 7.28 (d, J = 8.3 Hz, 1H), 7.17 (d, J = 2.1 Hz, 1H), 7.00–6.82 (m, 2H), 5.46 (brs, 2H), 4.08 (t, J = 7.2 Hz, 1H), 3.10 (d, J = 7.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.9, 161.8, 160.6, 142.9, 140.4, 137.7, 133.0, 132.4, 131.0, 130.6, 130.3, 130.1, 129.0, 128.3, 128.3, 127.7, 127.7, 127.7, 125.9, 113.7, 43.2, 31.7. HRMS (ESI) m/z calcd for $C_{24}H_{17}Cl_2N_3Na^+$ $(M+Na)^+$ 440.0692, found 440.0697.



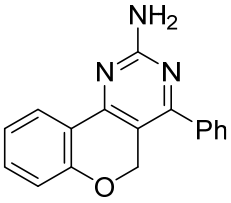
4-Phenyl-5,6-dihydrofuro[2,3-*h*]quinazolin-2-amine (4g)

Following the general procedure A, **4g** was obtained as a yellow solid (22.1 mg, 42% yield), mp: 180-182 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53–7.40 (m, 5H), 7.37 (d, J = 2.0 Hz, 1H), 6.86 (d, J = 2.0 Hz, 1H), 5.51 (brs, 2H), 2.99 (t, J = 8.0 Hz, 2H), 2.83 (t, J = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.1, 161.6, 159.7, 159.2, 142.7, 138.6, 128.7, 128.3, 128.2, 119.0, 112.1, 106.8, 24.2, 22.0. HRMS (ESI) m/z calcd for $C_{16}H_{13}N_3NaO^+$ $(M+Na)^+$ 286.0951, found 286.0957.



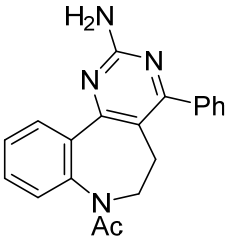
4-Phenyl-5,6-dihydrothieno[2,3-*h*]quinazolin-2-amine (4h)

Following the general procedure A, **4h** was obtained as a yellow solid (40.7 mg, 73% yield), mp: 211-213 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, J = 5.2 Hz, 1H), 7.54–7.49 (m, 2H), 7.48–7.39 (m, 3H), 7.14 (d, J = 5.2 Hz, 1H), 5.45 (brs, 2H), 2.99–2.88 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.8, 161.7, 159.0, 145.1, 138.5, 135.6, 128.8, 128.4, 128.2, 124.5, 123.1, 113.1, 24.8, 23.5. HRMS (ESI) m/z calcd for $C_{16}H_{13}N_3NaS^+$ $(M+Na)^+$ 302.0722, found 302.0729.



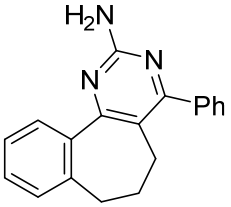
4-Phenyl-5*H*-chromeno[4,3-*d*]pyrimidin-2-amine (4i)

Following the general procedure A, **4i** was obtained as a yellow solid (27.5 mg, 50% yield), mp: 174-176 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (dd, J = 7.8, 1.7 Hz, 1H), 7.55–7.45 (m, 5H), 7.38 (t, J = 7.7 Hz, 1H), 7.10 (t, J = 7.5 Hz, 1H), 6.96 (d, J = 8.2 Hz, 1H), 5.36 (brs, 2H), 5.19 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.4, 162.4, 157.6, 157.6, 136.8, 132.9, 129.7, 128.6, 128.2, 125.3, 122.2, 121.8, 117.1, 111.1, 65.3. HRMS (ESI) m/z calcd for $C_{17}H_{13}N_3NaO^+$ $(M+Na)^+$ 298.0951, found 298.0958.



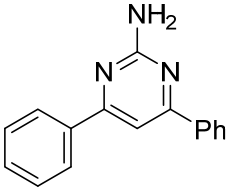
1-(2-Amino-4-phenyl-5,6-dihydro-7*H*-benzo[b]pyrimido[4,5-*d*]azepin-7-yl)ethan-1-one (4j)

Following the general procedure A, **4j** was obtained as a white solid (35.0 mg, 53% yield), mp: 132-134 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95–7.76 (m, 1H), 7.60–7.52 (m, 4H), 7.51–7.42 (m, 3H), 7.32–7.26 (m, 1H), 5.69 (brs, 2H), 5.11–4.86 (m, 1H), 3.52 (dd, J = 12.7, 6.2 Hz, 1H), 2.75 (dd, J = 14.7, 5.2 Hz, 1H), 2.37 (td, J = 14.3, 6.4 Hz, 1H), 1.74 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.0, 167.0, 165.9, 161.6, 139.7, 137.9, 137.3, 131.0, 129.6, 129.1, 129.0, 128.7, 128.4, 128.3, 117.5, 52.0, 25.6, 22.8. HRMS (ESI) m/z calcd for $C_{20}H_{18}N_3NaO^+$ $(M+Na)^+$ 353.1373, found 353.1380.



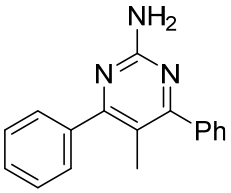
4-Phenyl-6,7-dihydro-5*H*-benzo[6,7]cyclohepta[1,2-*d*]pyrimidin-2-amine (4k)

Following the general procedure A, **4k** was obtained as a white solid (41.9 mg, 73% yield), mp: 190-192 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (dd, J = 5.6, 3.4 Hz, 1H), 7.63–7.53 (m, 2H), 7.54–7.38 (m, 5H), 7.32–7.21 (m, 1H), 5.88 (brs, 2H), 2.72 (t, J = 6.9 Hz, 2H), 2.34 (t, J = 6.9 Hz, 2H), 2.29–2.12 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.1, 166.5, 161.4, 139.9, 138.6, 138.5, 129.7, 128.7, 128.5, 128.4, 128.2, 128.1, 126.6, 118.7, 33.2, 31.2, 24.8. HRMS (ESI) m/z calcd for $C_{19}H_{17}N_3Na^+$ $(M+Na)^+$ 310.1315, found 310.1322.



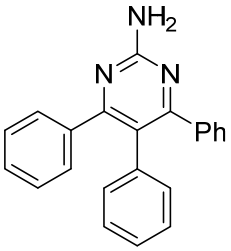
4,6-Diphenylpyrimidin-2-amine (4l)

Following the general procedure A, **4l** was obtained as a yellow solid (25.7 mg, 52% yield), mp: 94-96 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07–8.00 (m, 4H), 7.51–7.45 (m, 6H), 7.42 (s, 1H), 5.58 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.2, 163.6, 137.7, 130.4, 128.7, 127.1, 104.2. HRMS (ESI) m/z calcd for $C_{16}H_{13}N_3Na^+$ $(M+Na)^+$ 270.1002, found 270.1004.



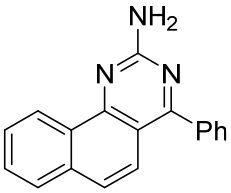
5-Methyl-4,6-diphenylpyrimidin-2-amine (4m)

Following the general procedure A, **4m** was obtained as a white solid (24.0 mg, 46% yield), mp: 181-183 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, J = 7.8 Hz, 4H), 7.50–7.34 (m, 6H), 5.57 (brs, 2H), 2.10 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.0, 160.8, 139.0, 128.7, 128.5, 128.2, 114.7, 16.3. HRMS (ESI) m/z calcd for $C_{17}H_{15}N_3Na^+$ $(M+Na)^+$ 284.1158, found 284.1165.



4,5,6-Triphenylpyrimidin-2-amine (4n)

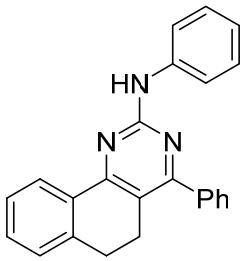
Following the general procedure A, **4n** was obtained as a yellow solid (14.2 mg, 22% yield), mp: 233-235 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29–7.17 (m, 10H), 7.12–7.02 (m, 3H), 6.96–6.76 (m, 2H), 5.64 (brs, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.8, 161.7, 138.7, 136.7, 131.5, 129.2, 128.4, 127.9, 127.7, 126.5, 122.1. HRMS (ESI) m/z calcd for $C_{22}H_{17}N_3Na^+$ $(M+Na)^+$ 346.1315, found 346.1322.



4-phenylbenzo[*h*]quinazolin-2-amine (6a)

Yellow solid, 37% yield (10.0 mg), mp: 194-196 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.13 (d, J = 7.4 Hz, 1H), 7.81 (d, J = 1.4 Hz, 1H), 7.76–7.61 (m, 5H), 7.59–7.50 (m, 3H), 7.47 (d, J = 9.0 Hz, 1H), 5.52

(s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.1, 160.0, 153.4, 137.6, 135.6, 129.8, 129.6, 129.6, 129.3, 128.5, 127.6, 126.6, 125.0, 123.5, 123.2, 115.1. HRMS (ESI) m/z calcd for $C_{18}H_{13}N_3Na^+$ $(M+Na)^+$ 294.1002, found 294.1007.



N,4-diphenyl-5,6-dihydrobenzo[*h*]quinazolin-2-amine (6b)

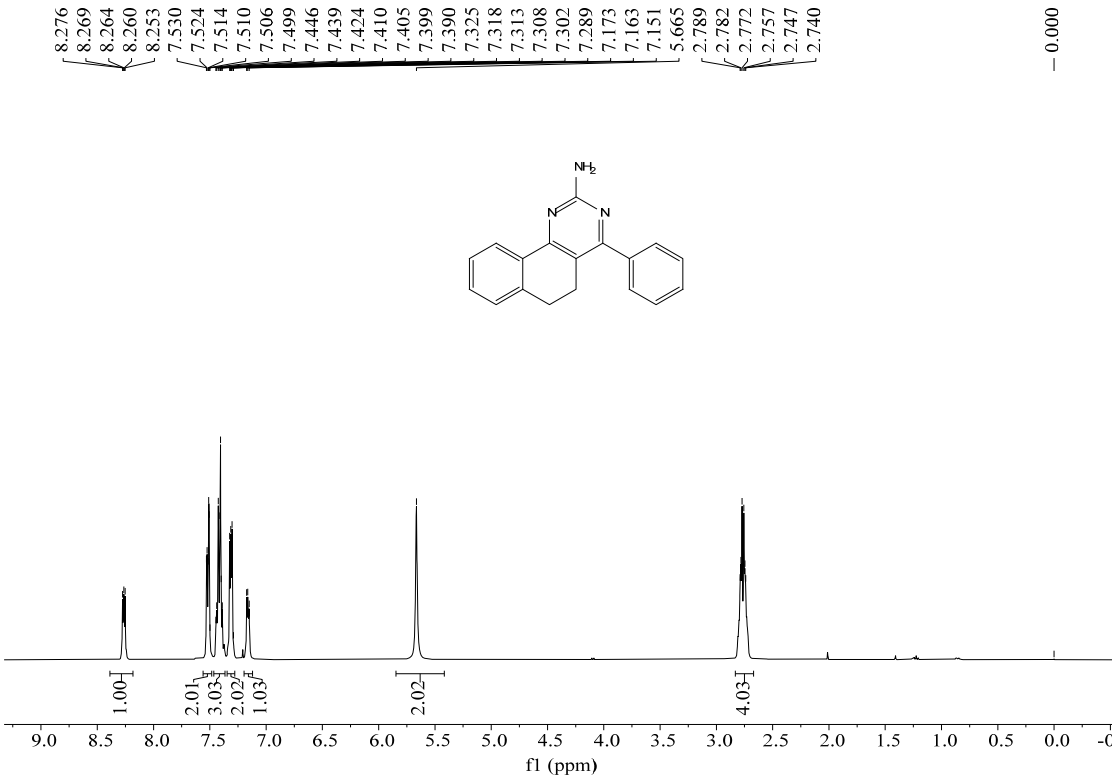
Yellow solid, 70% yield (24.4 mg), mp:185-187 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (dd, J = 6.6, 2.7 Hz, 1H), 7.76 (d, J = 8.0 Hz, 2H), 7.62 (d, J = 7.2 Hz, 2H), 7.52–7.44 (m, 3H), 7.43–7.37 (m, 2H), 7.34 (t, J = 7.9 Hz, 2H), 7.29 (s, 1H), 7.23 (t, J = 4.3 Hz, 1H), 7.01 (t, J = 7.4 Hz, 1H), 2.95–2.88 (m, 2H), 2.87–2.78 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.2, 160.8, 158.4, 140.2, 139.4, 138.2, 133.3, 130.6, 129.0, 128.8, 128.7, 128.2, 127.7, 127.1, 125.8, 121.6, 118.4, 117.0, 28.1, 24.2. HRMS (ESI) m/z calcd for $C_{24}H_{19}N_3Na^+$ $(M+Na)^+$ 372.1471, found 372.1480.

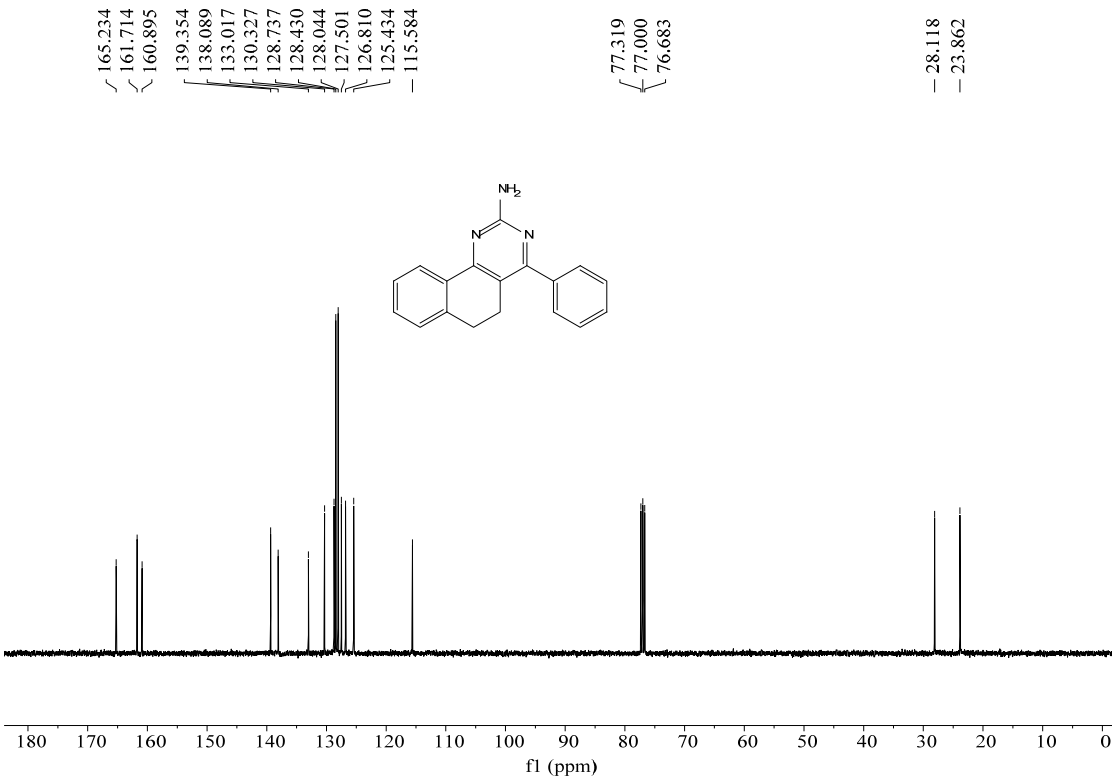
References

[1] Zhu, Z.; Tang, X.; Li, J.; Li, X.; Wu, W.; Deng, G.; Jiang, H. *Org. Lett.* **2017**, *19*, 1370.

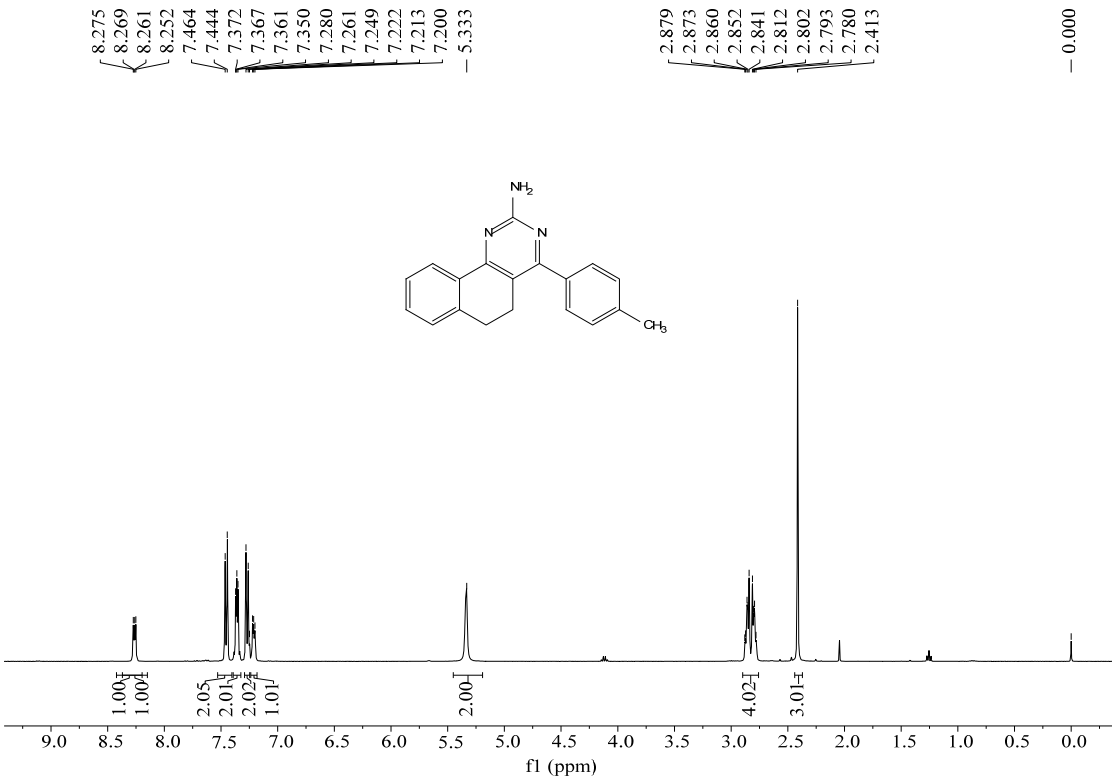
Copies of ^{1}H and ^{13}C NMR spectra of all products

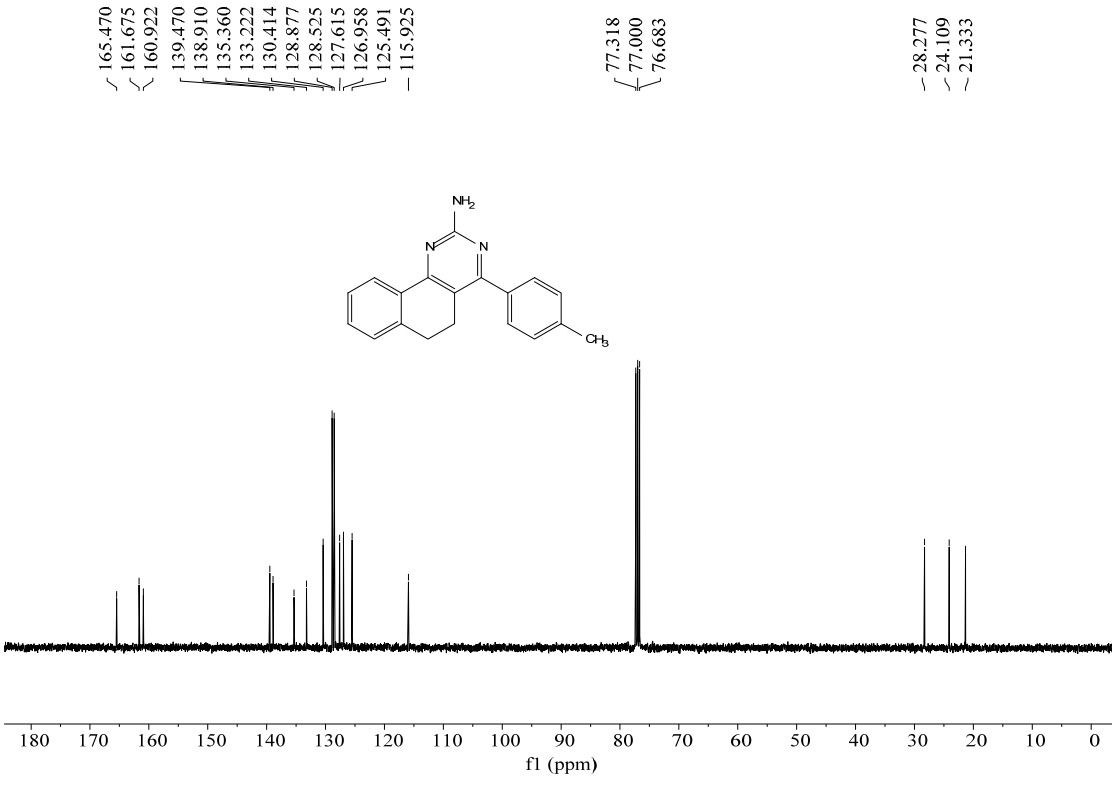
^{1}H and ^{13}C NMR spectra of **3a**



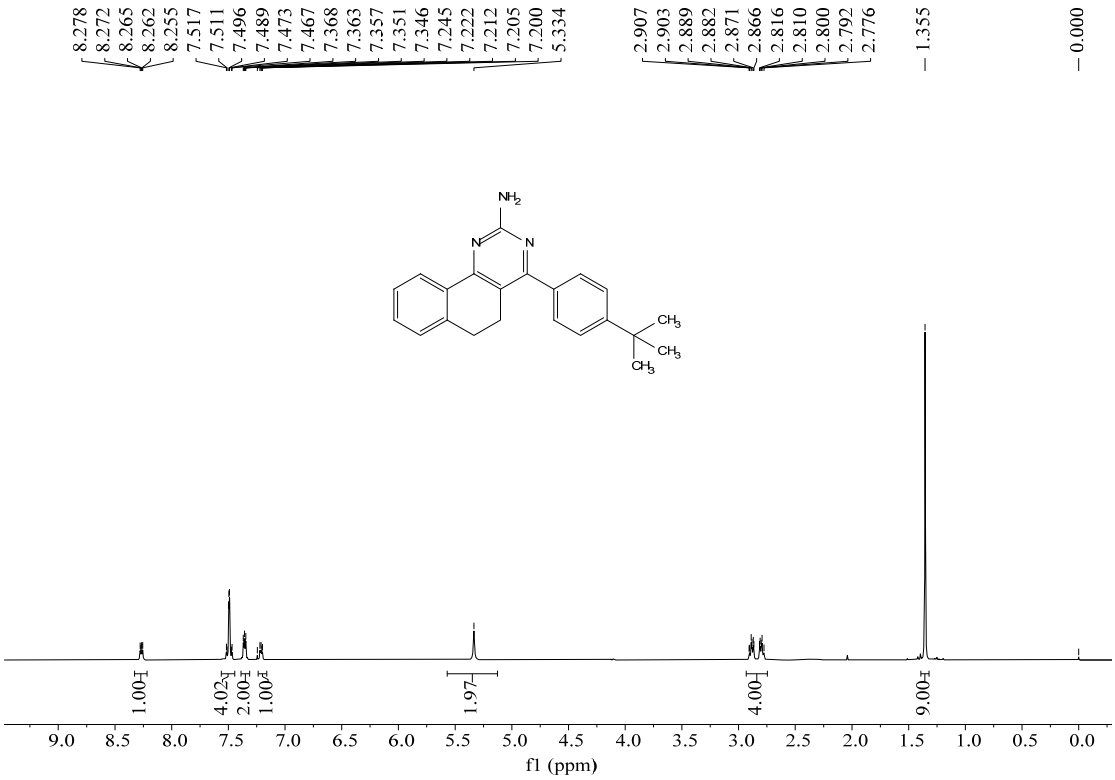


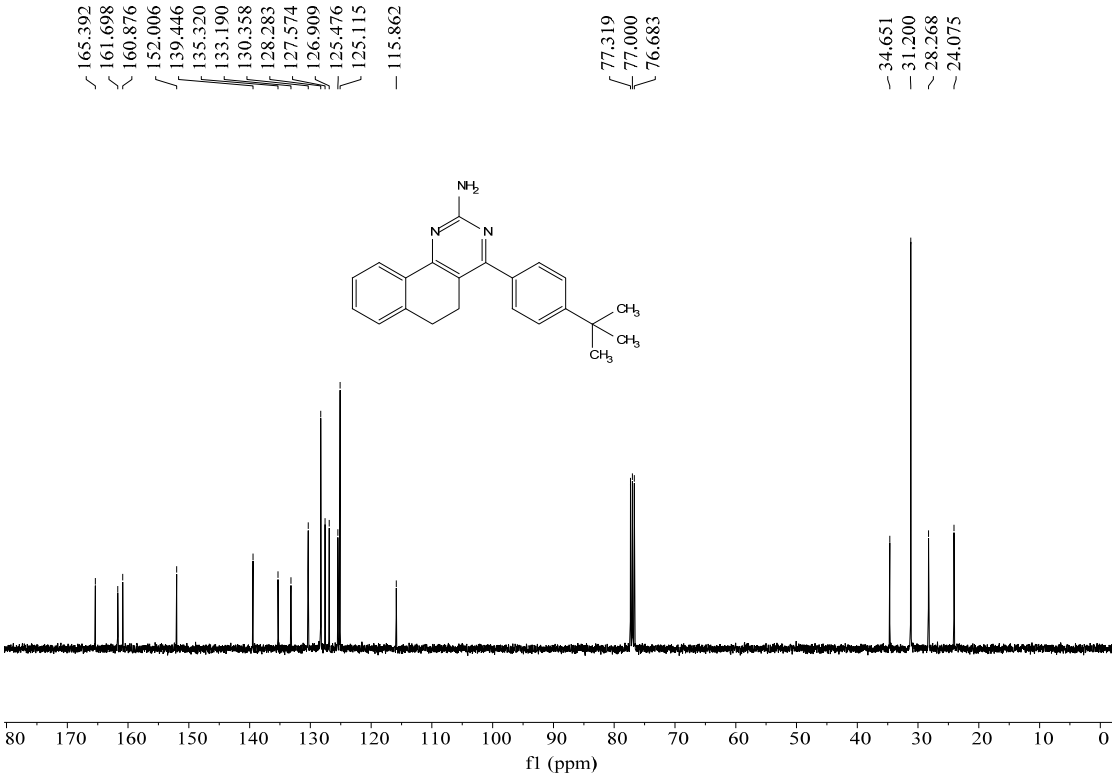
^{1}H and ^{13}C NMR spectra of **3b**



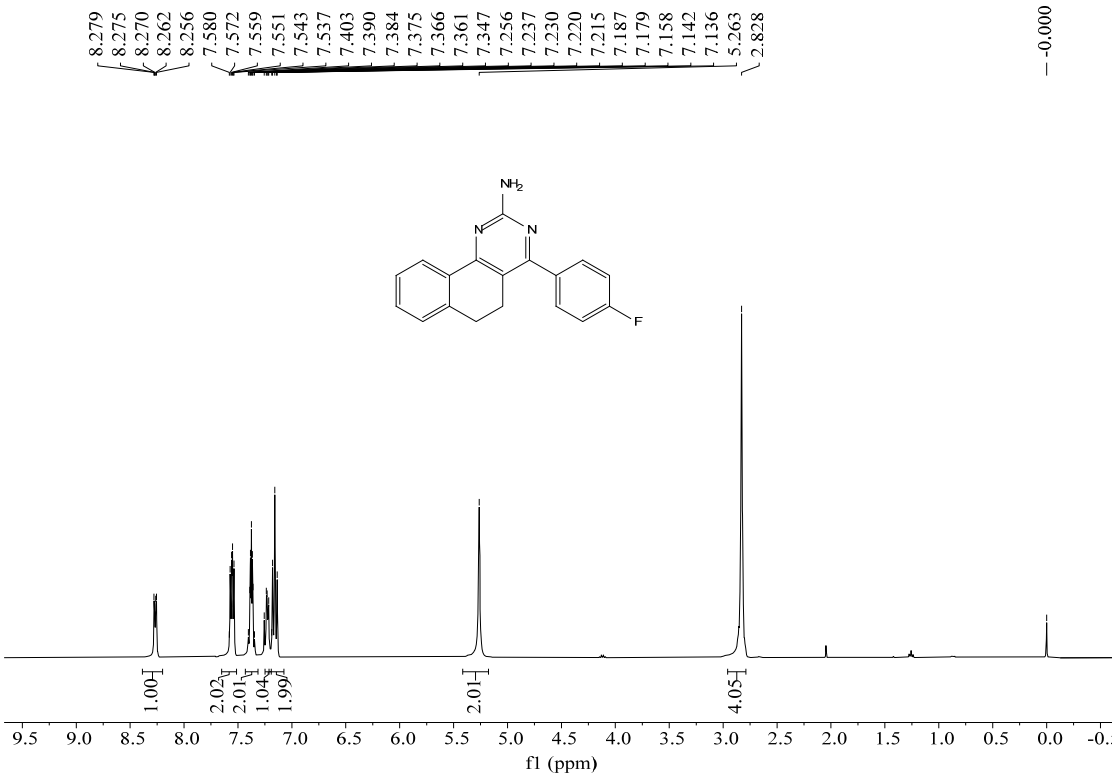


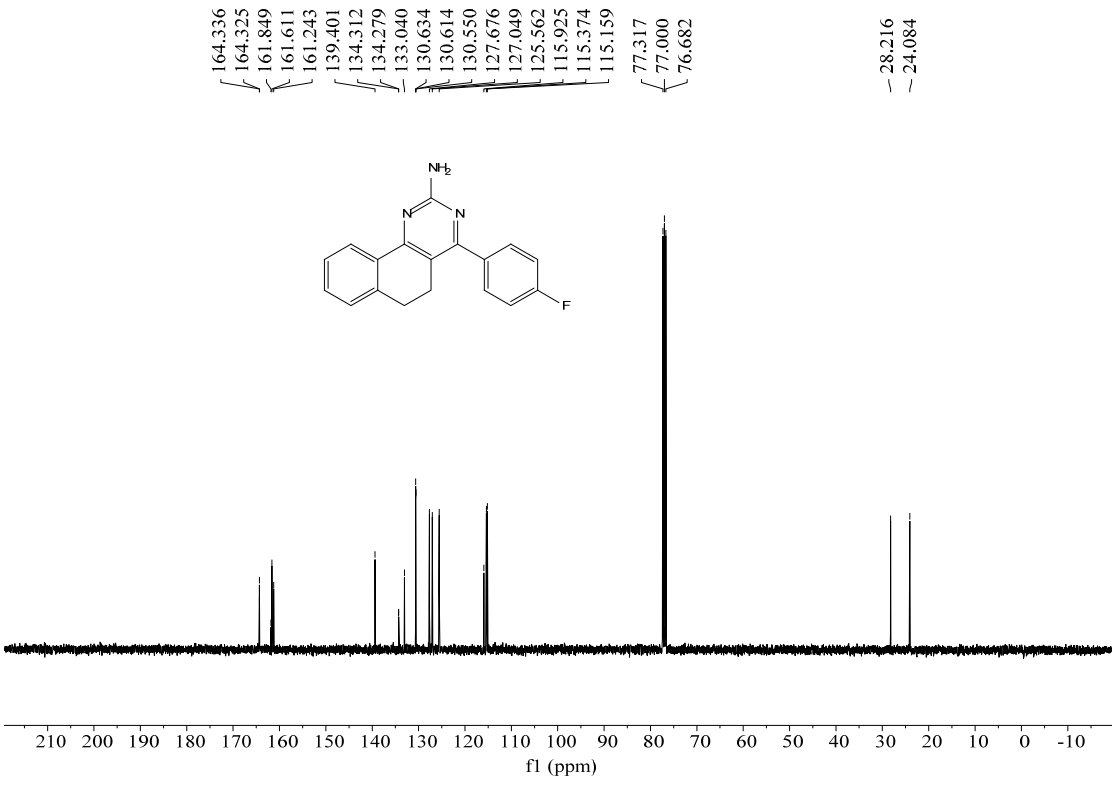
^{1}H and ^{13}C NMR spectra of **3c**



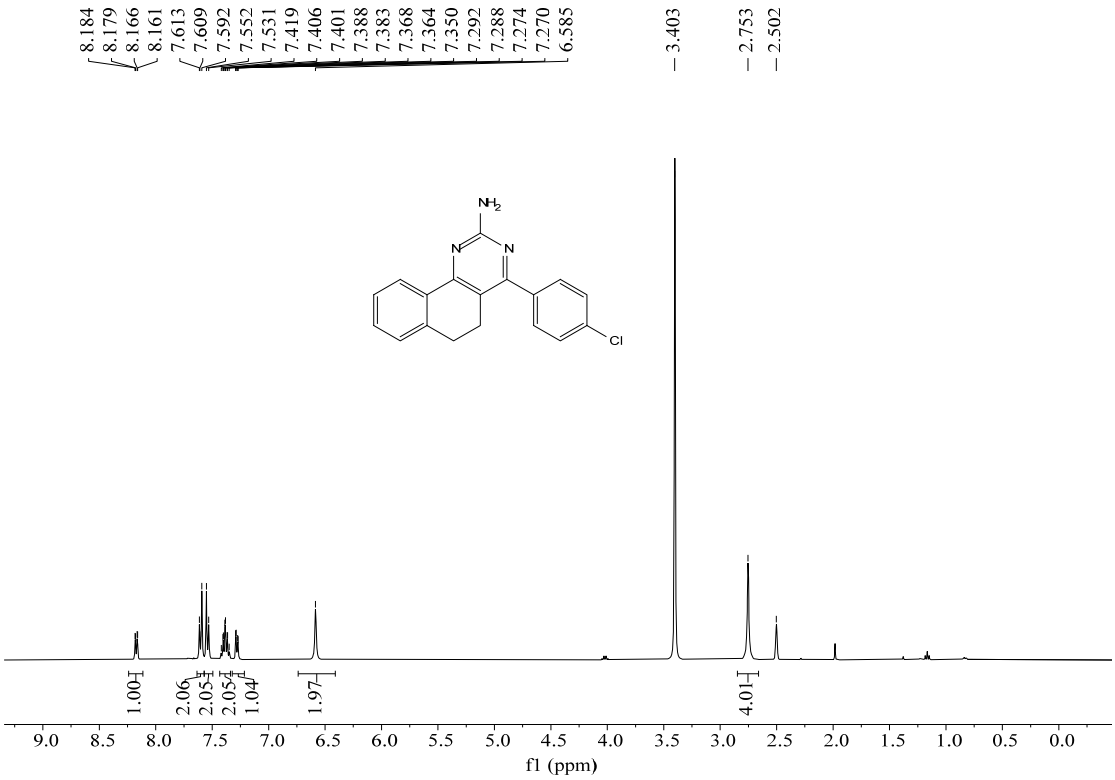


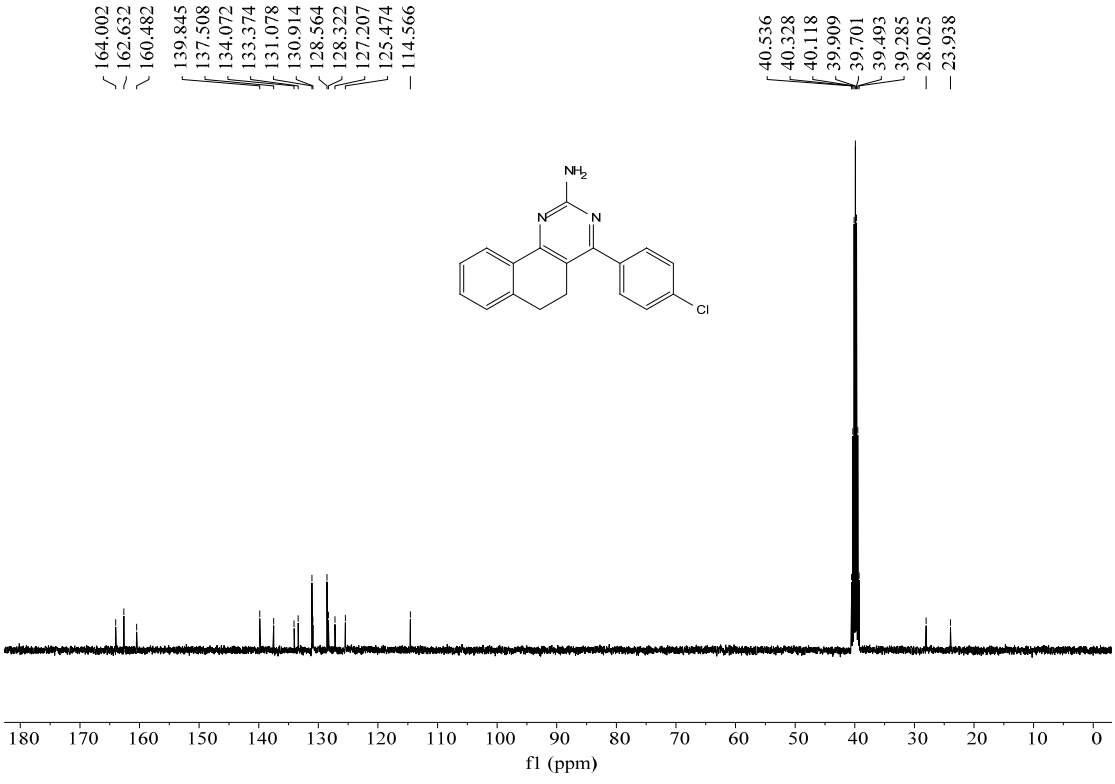
^{1}H and ^{13}C NMR spectra of **3d**



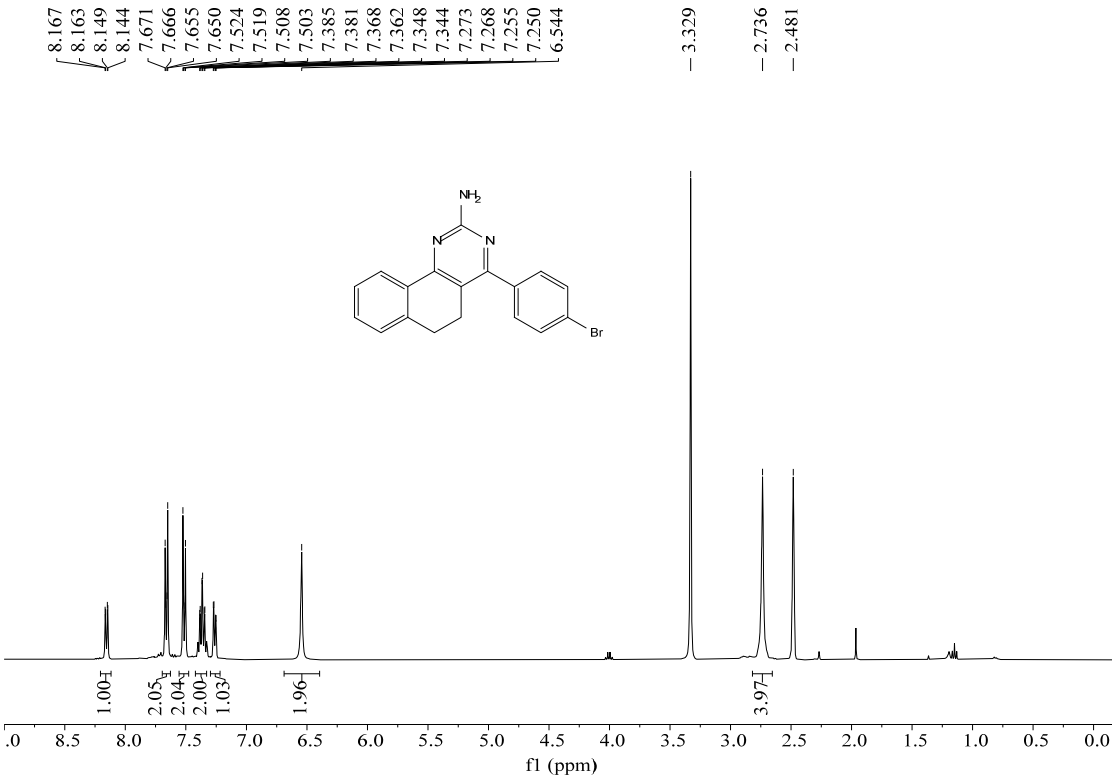


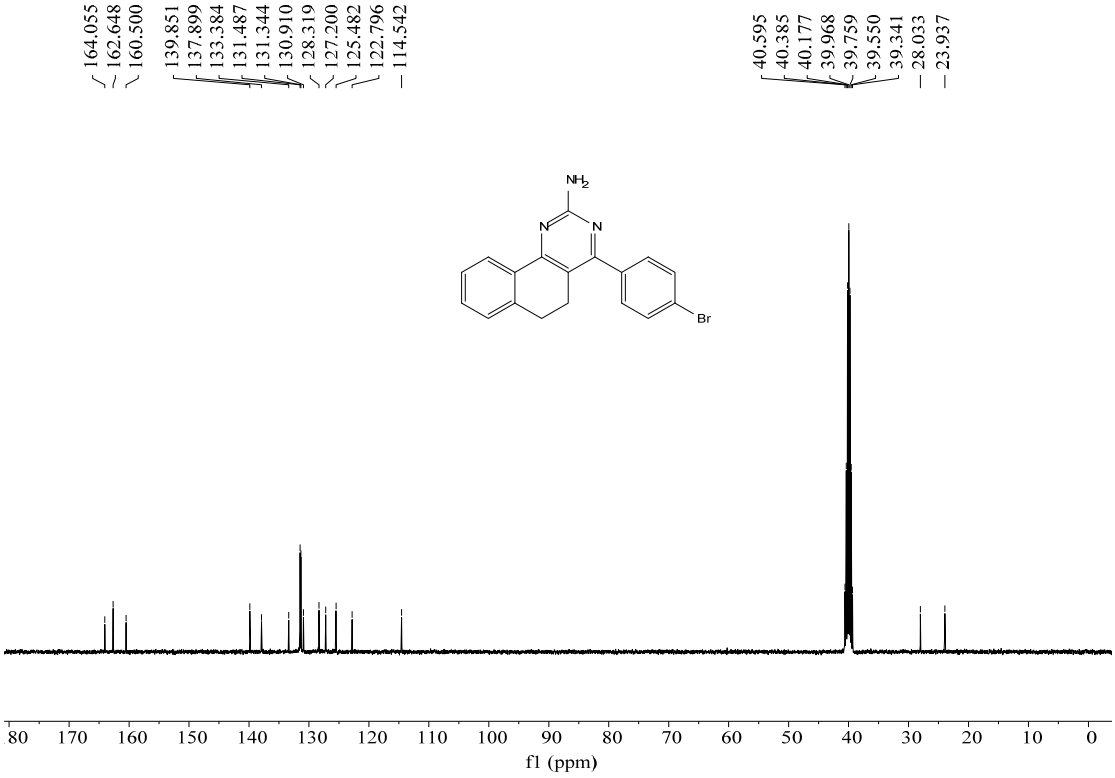
^{1}H and ^{13}C NMR spectra of **3e**



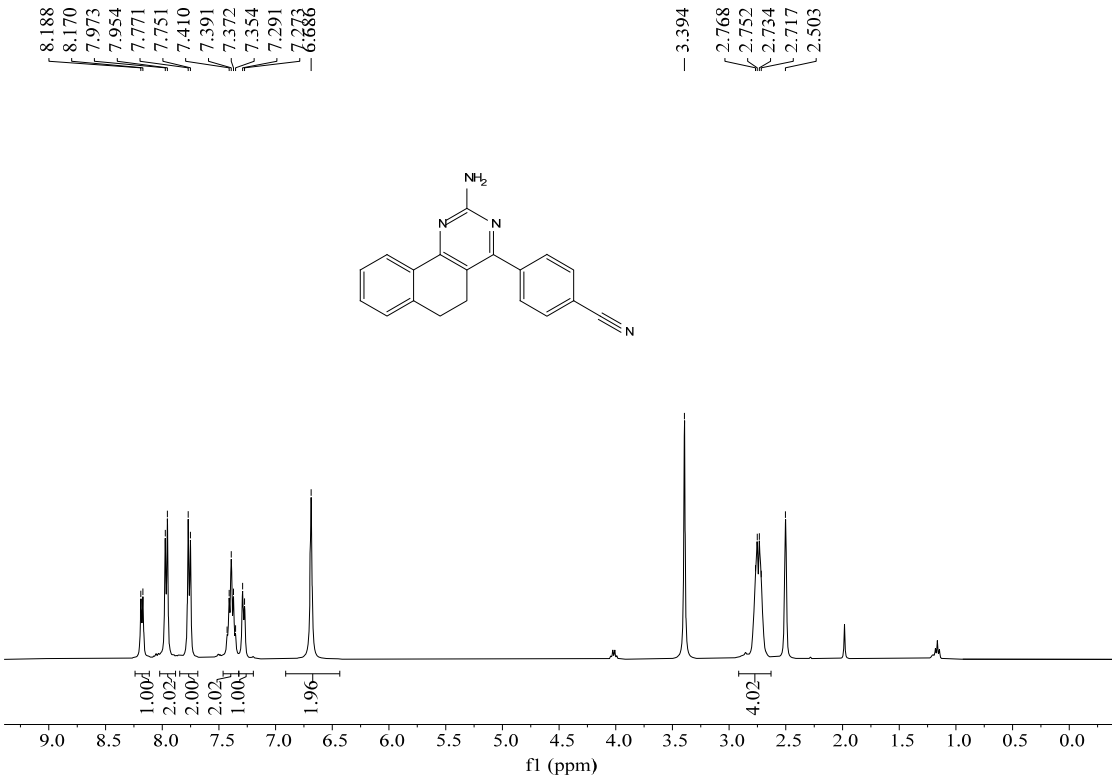


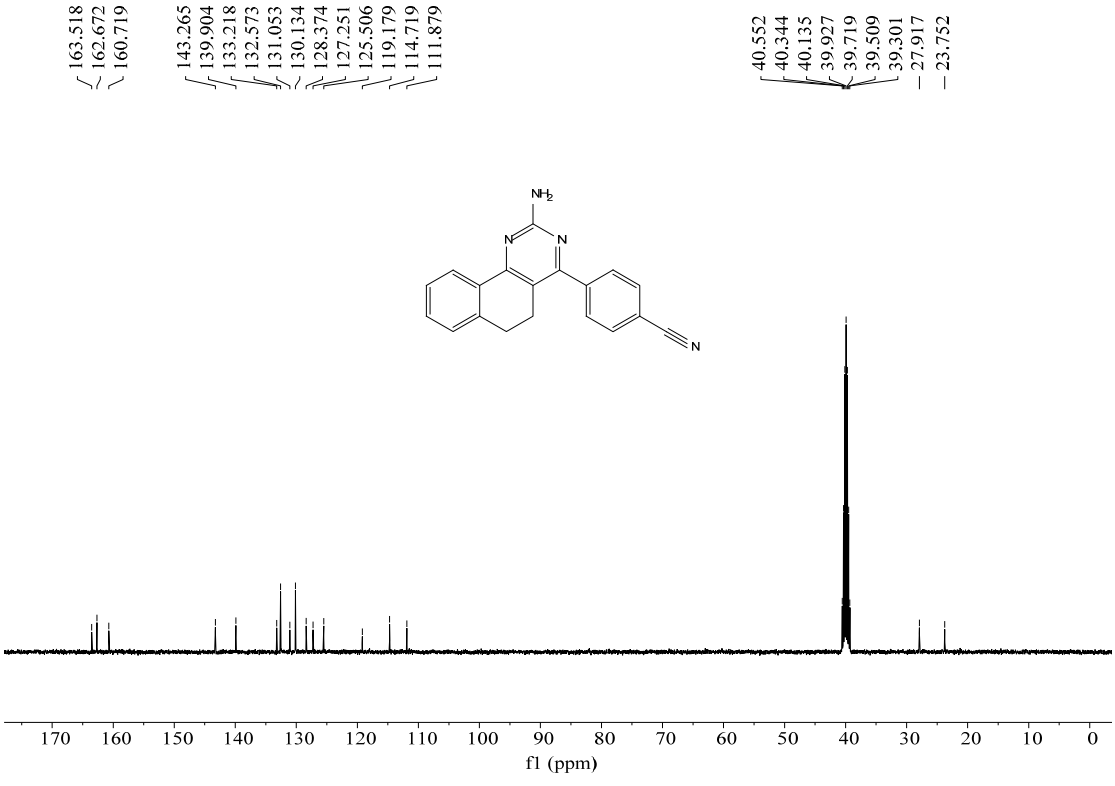
^{1}H and ^{13}C NMR spectra of **3f**



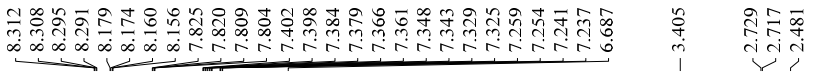


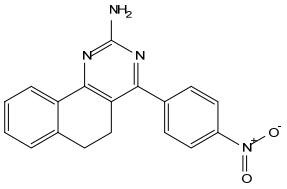
^{1}H and ^{13}C NMR spectra of **3g**

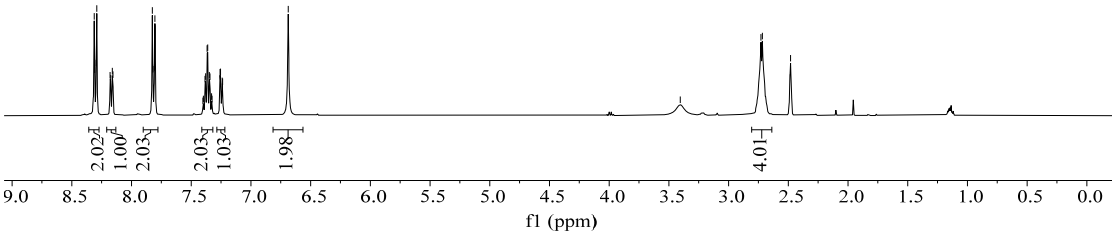


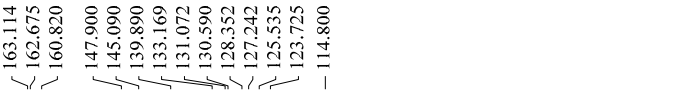


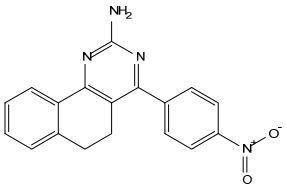
^{1}H and ^{13}C NMR spectra of **3h**

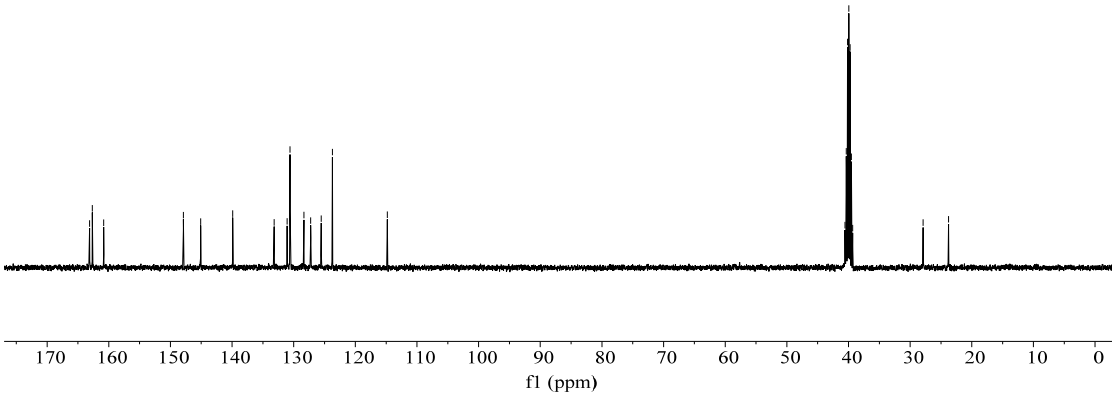




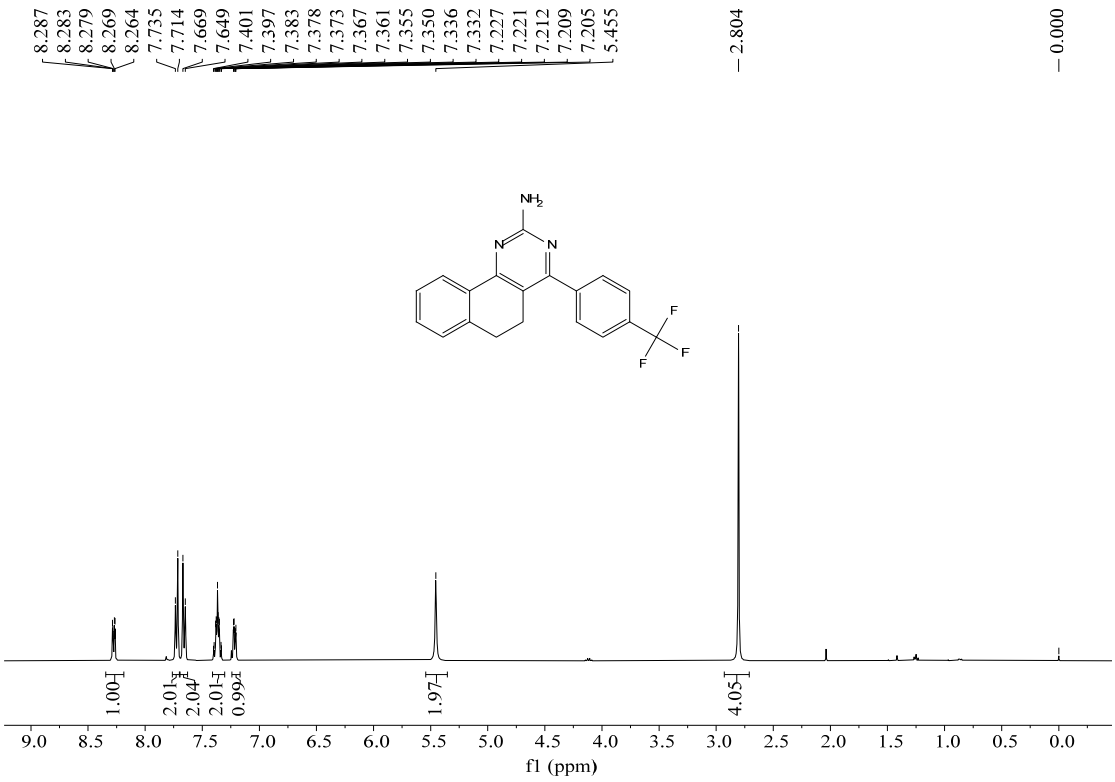


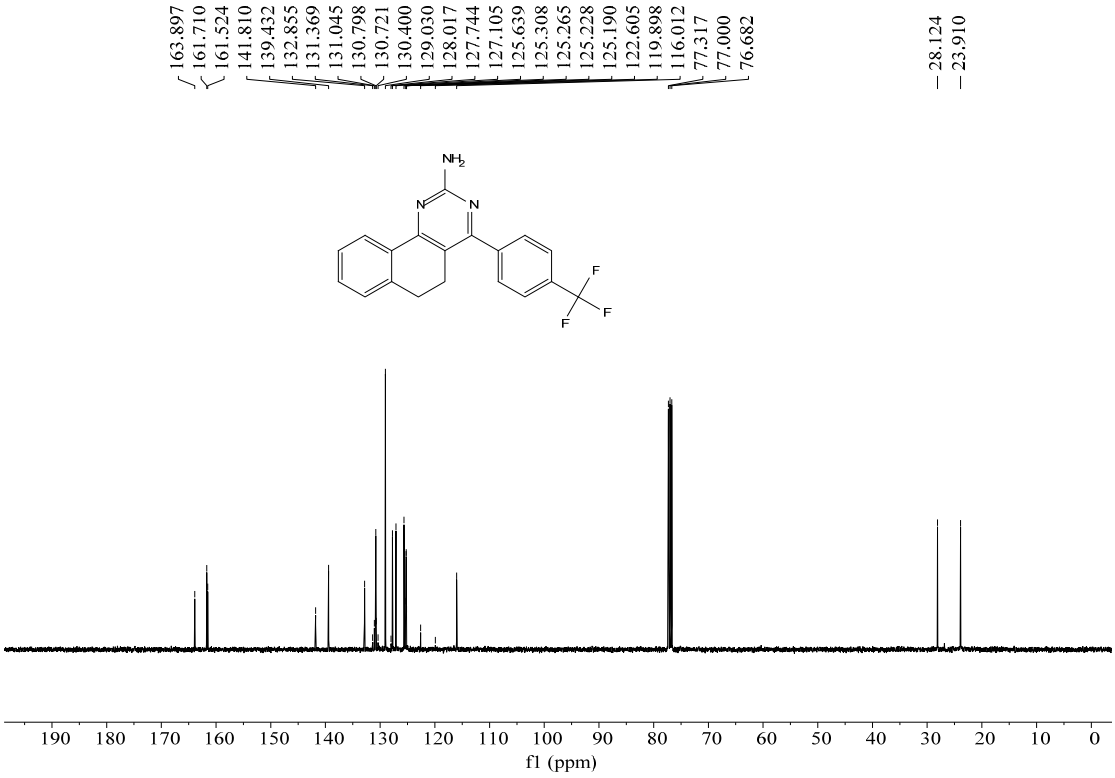




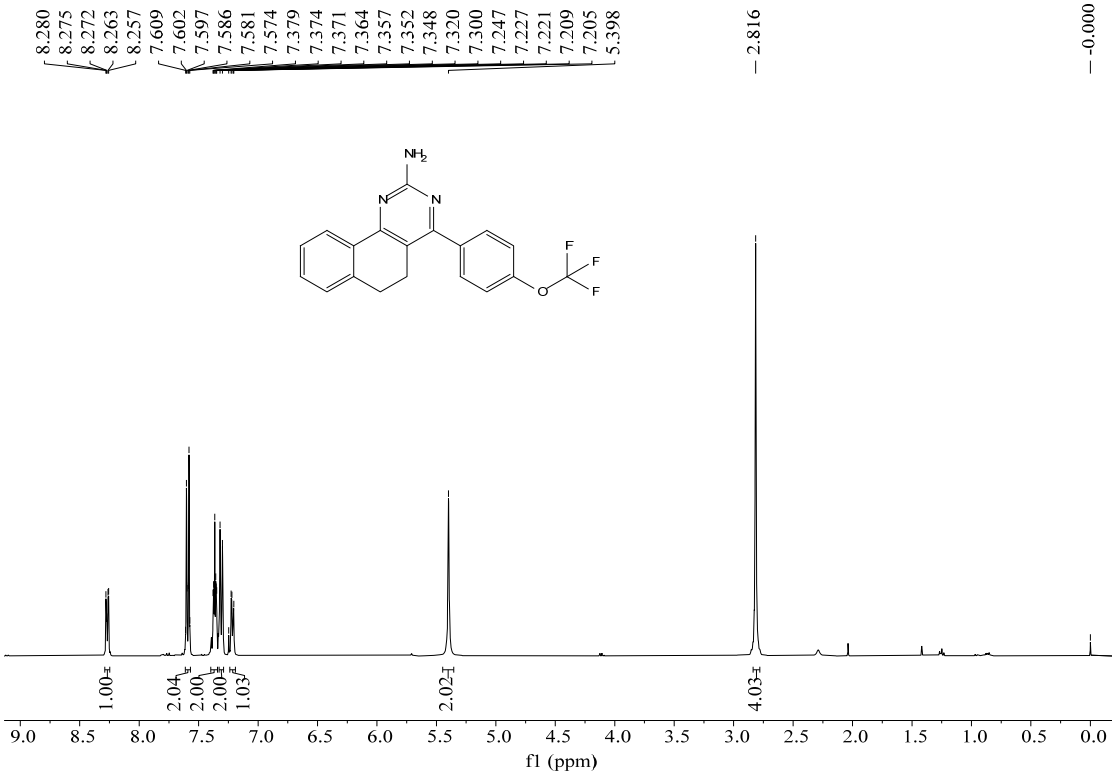


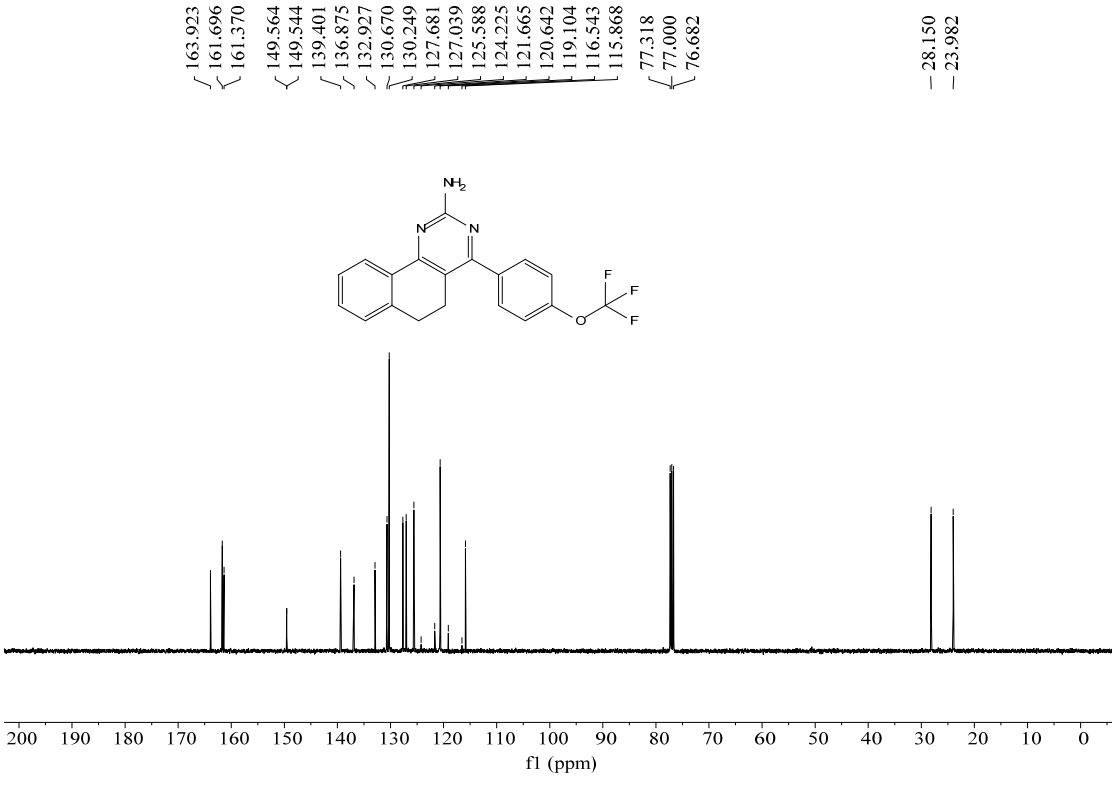
^{1}H and ^{13}C NMR spectra of **3i**



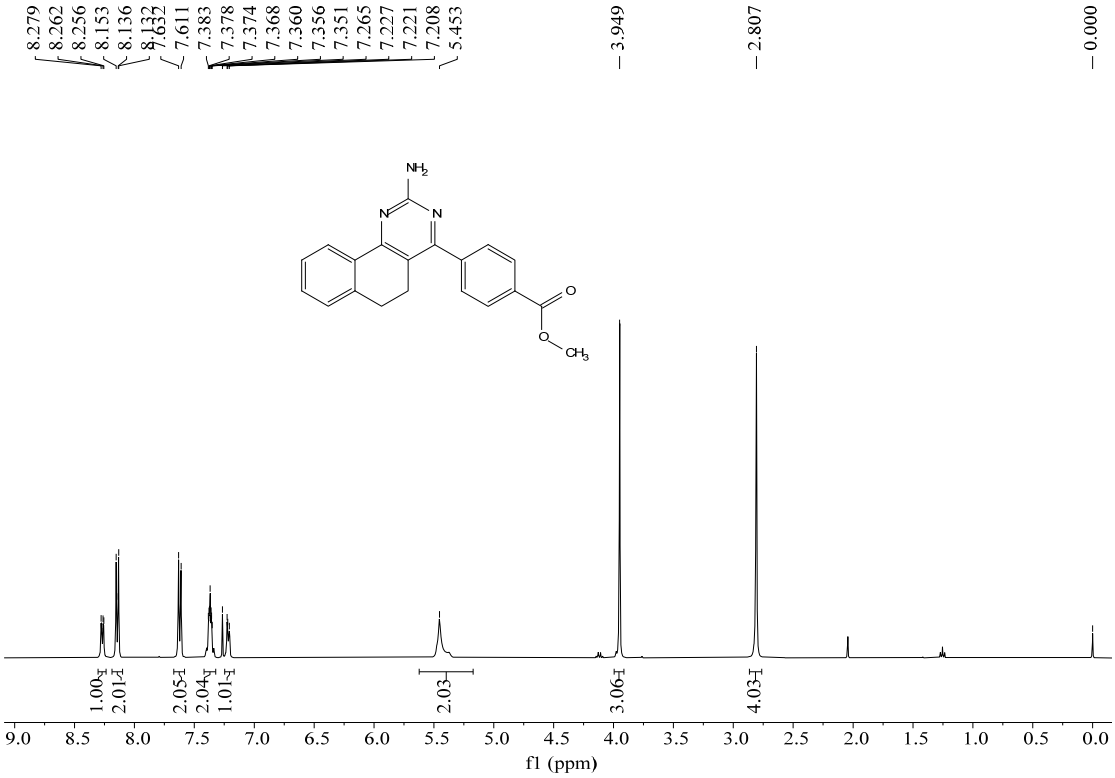


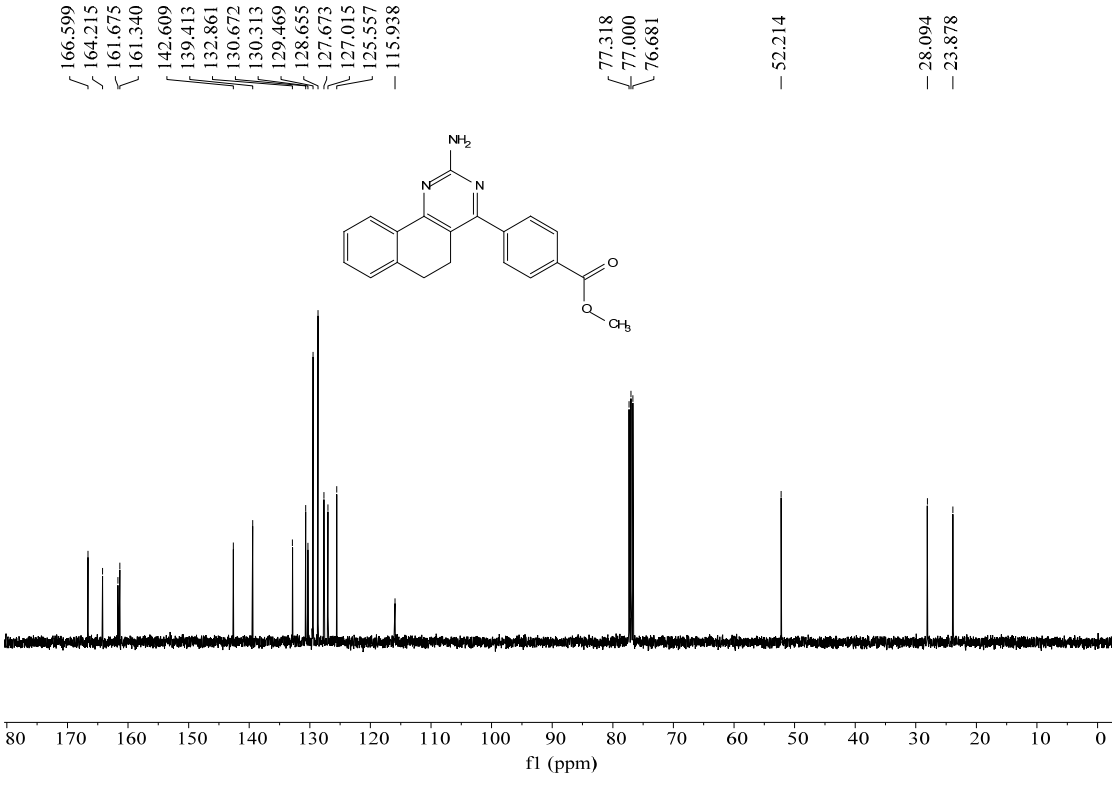
^{1}H and ^{13}C NMR spectra of **3j**



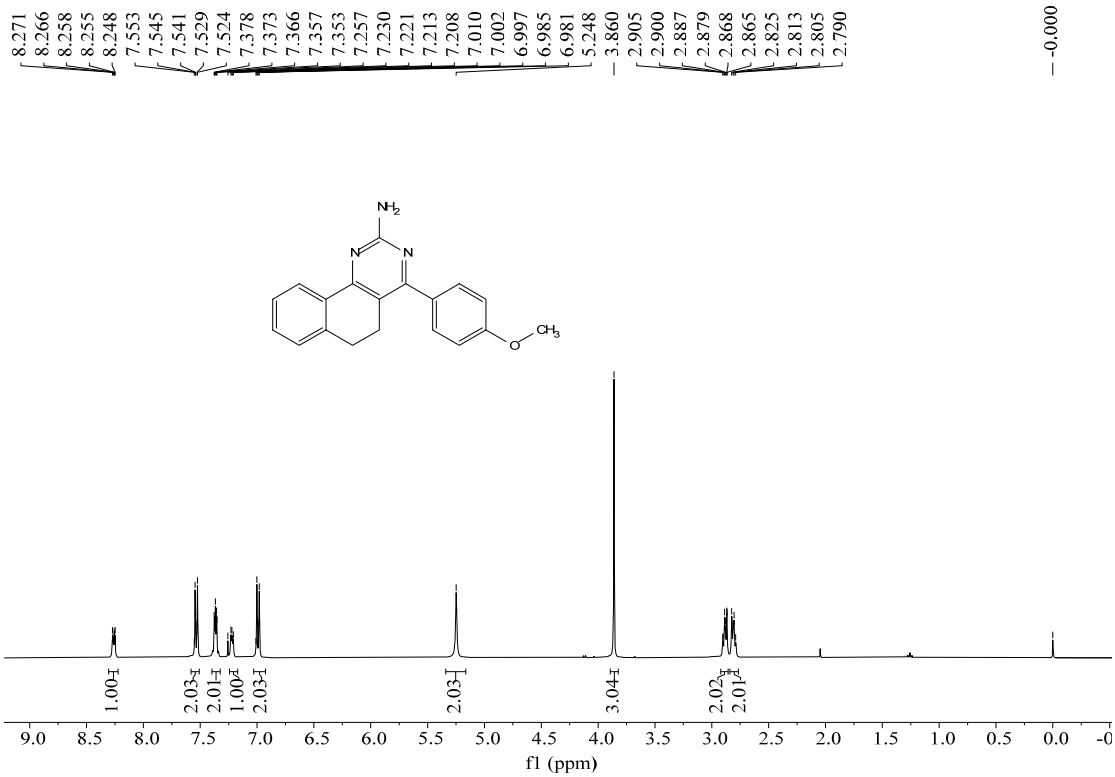


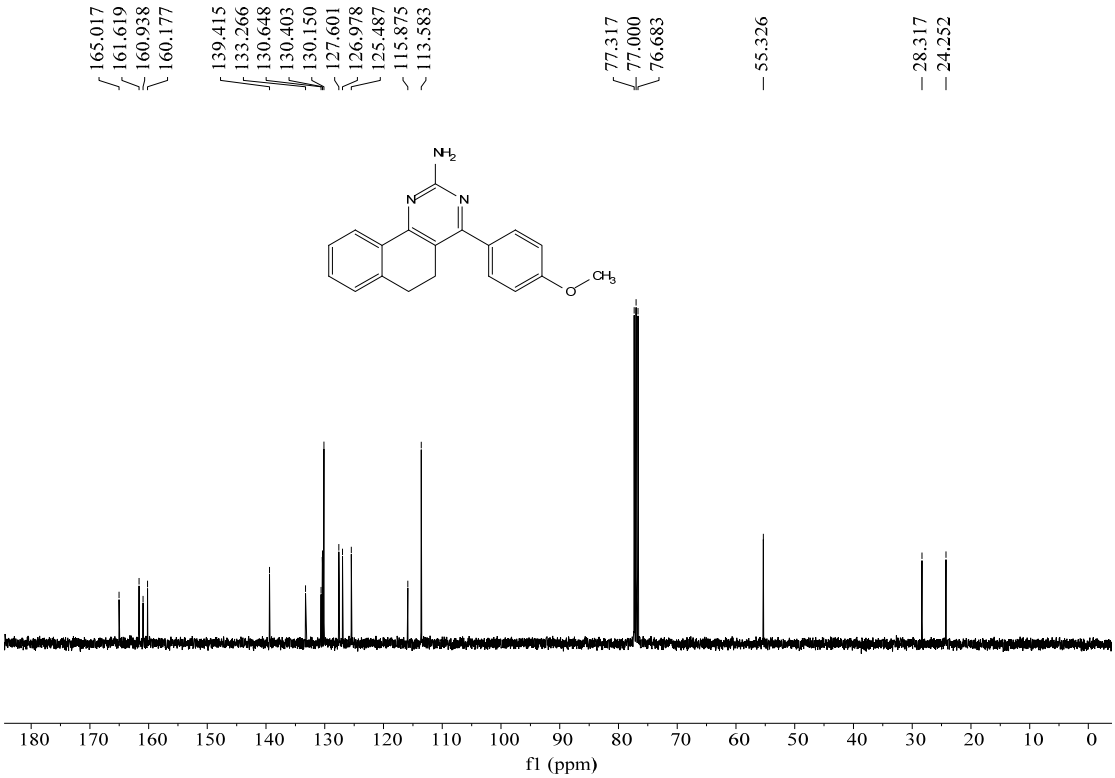
^{1}H and ^{13}C NMR spectra of **3k**



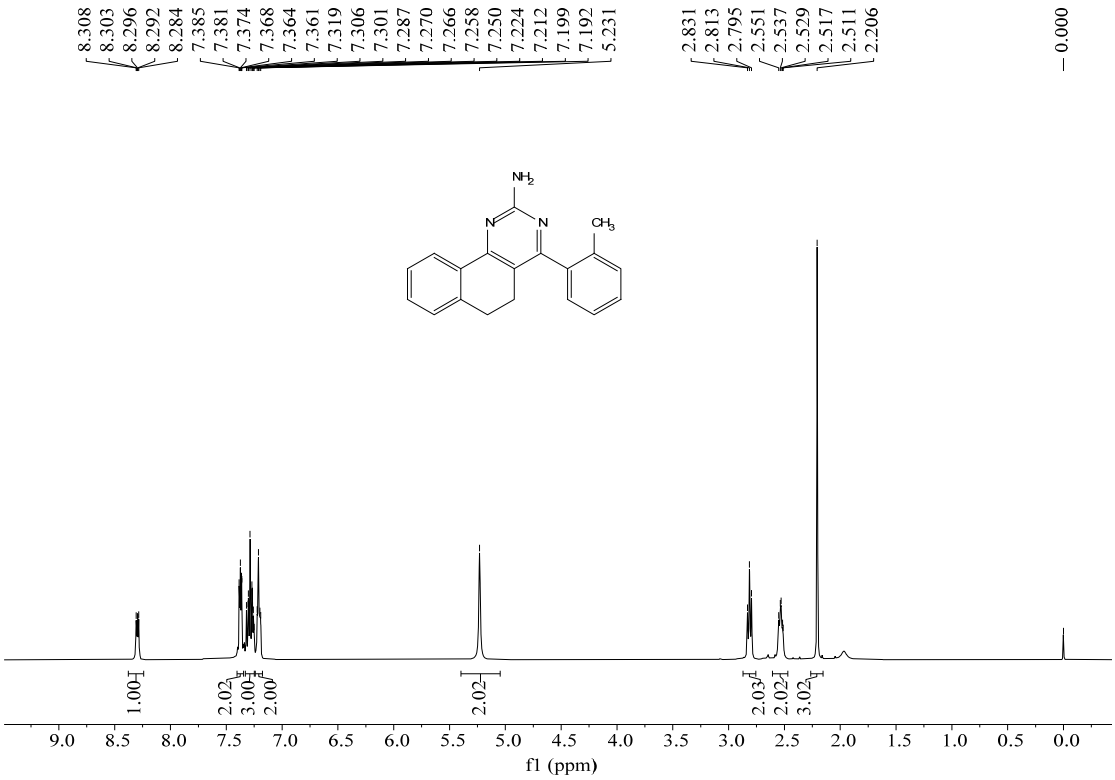


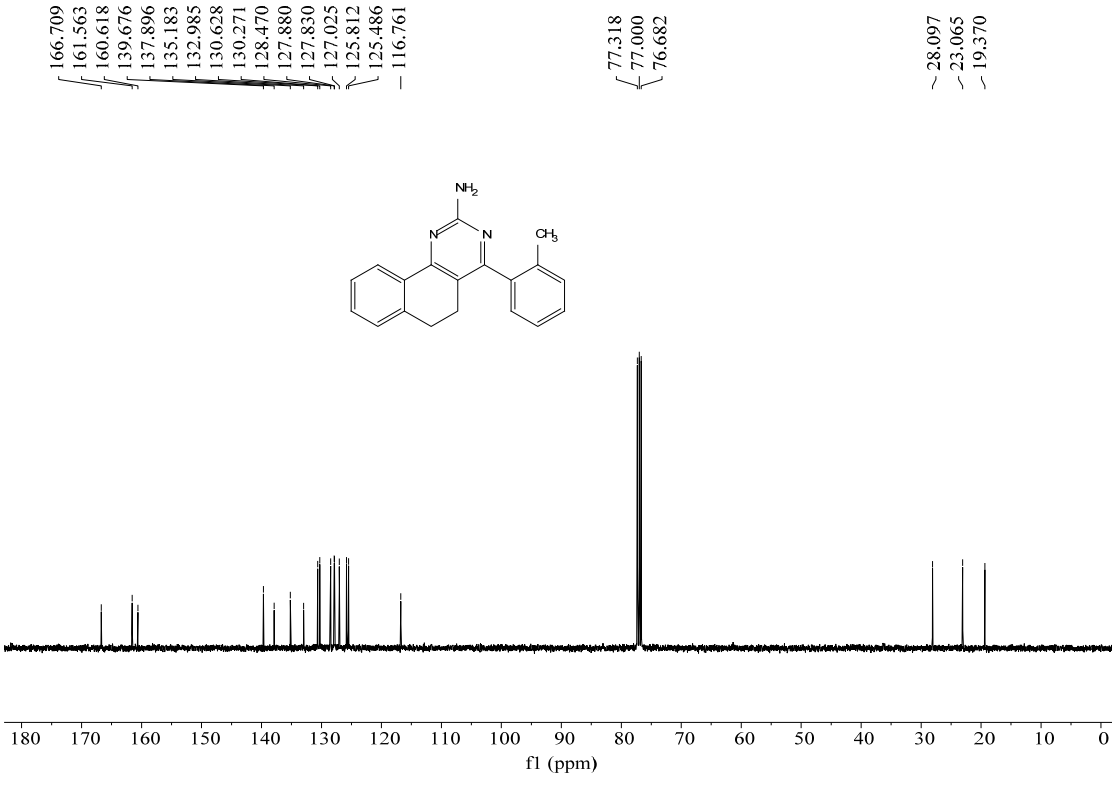
^{1}H and ^{13}C NMR spectra of **3l**



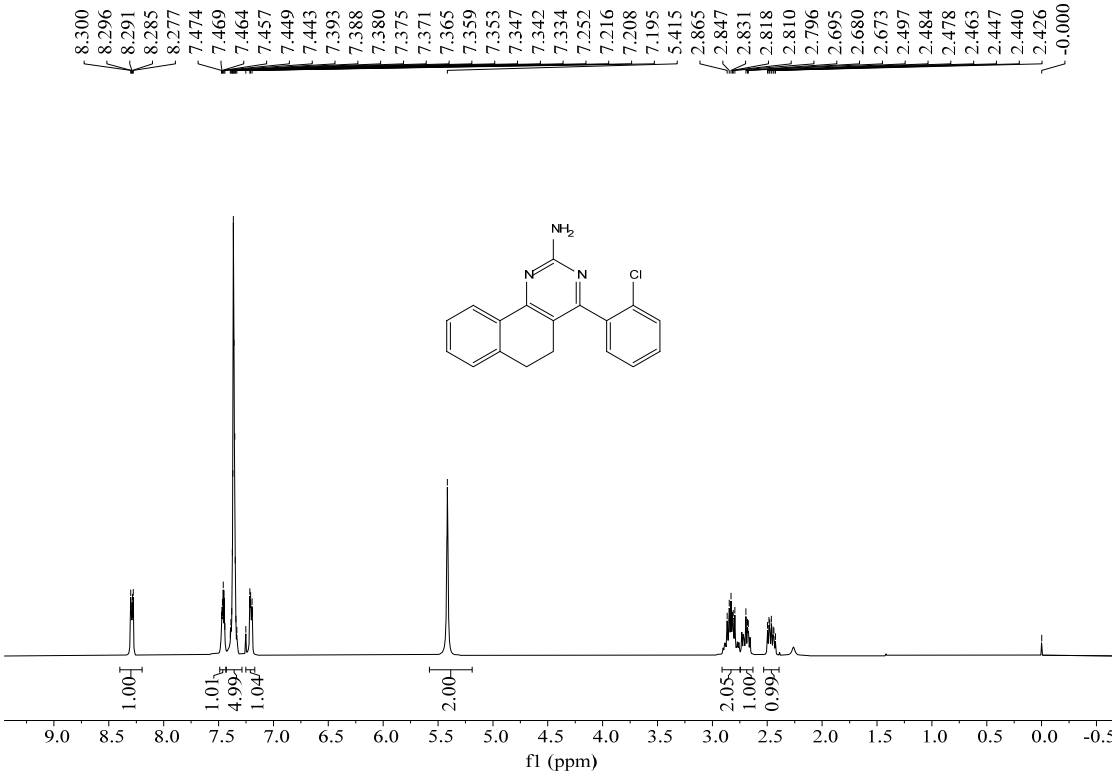


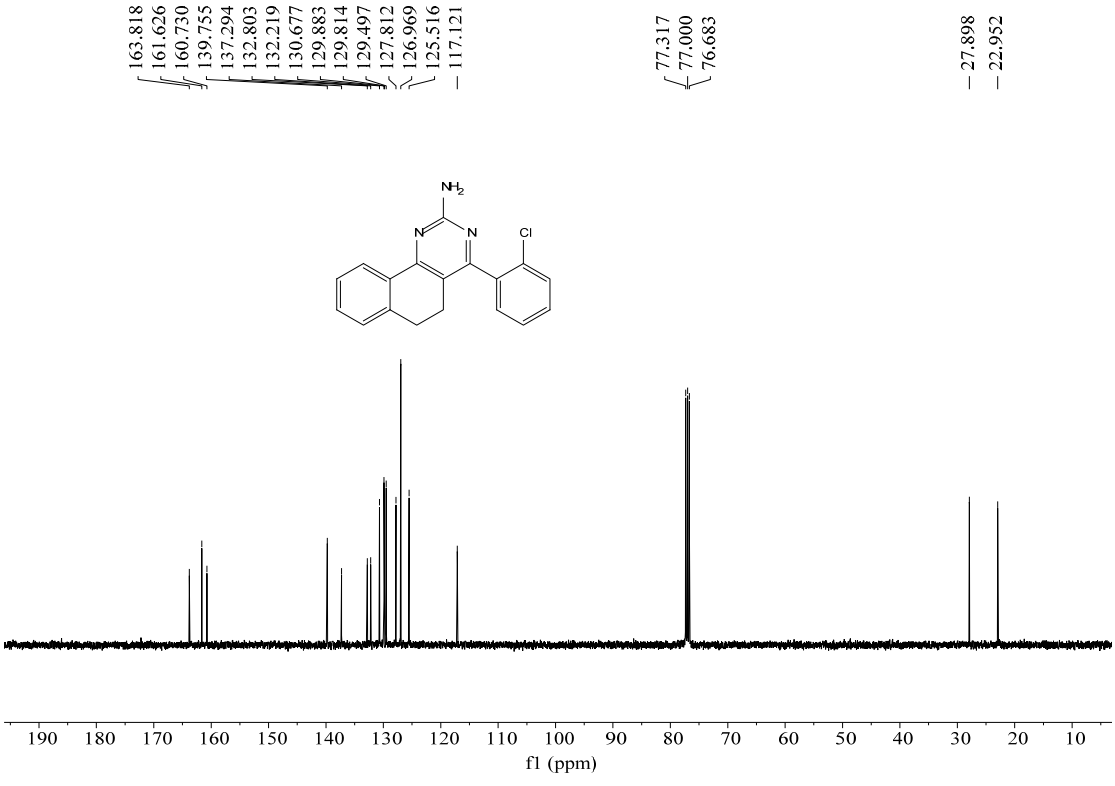
^{1}H and ^{13}C NMR spectra of **3m**



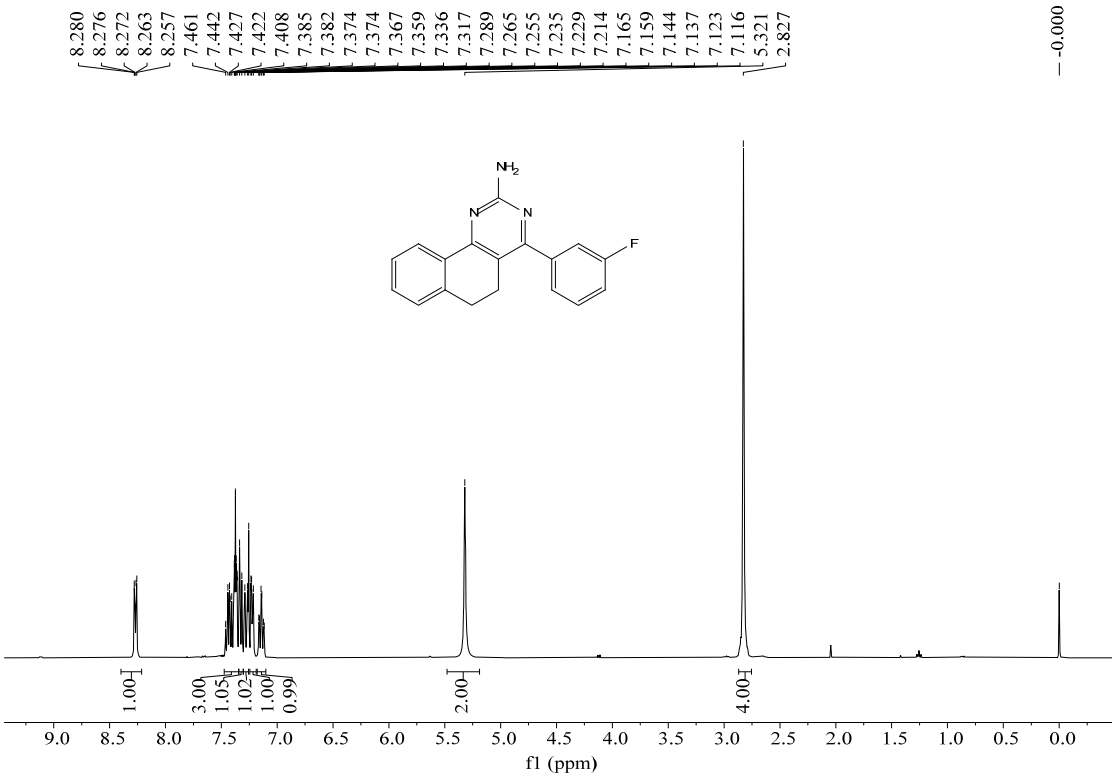


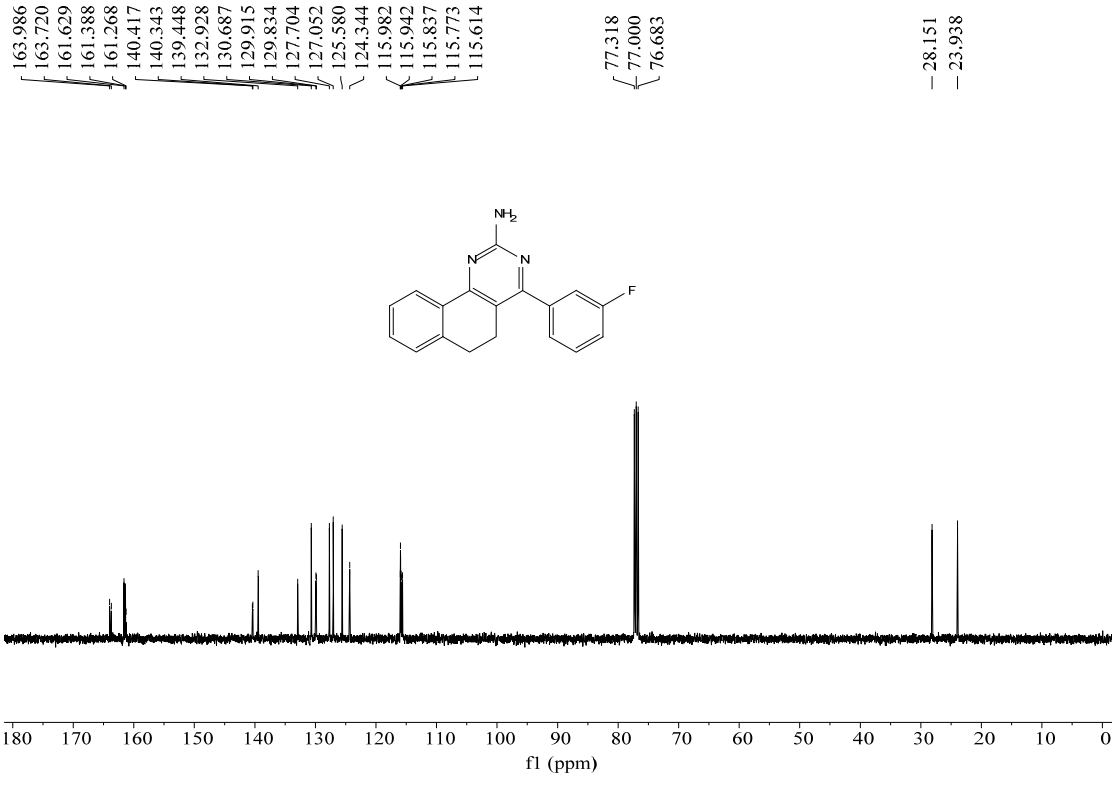
^{1}H and ^{13}C NMR spectra of **3n**



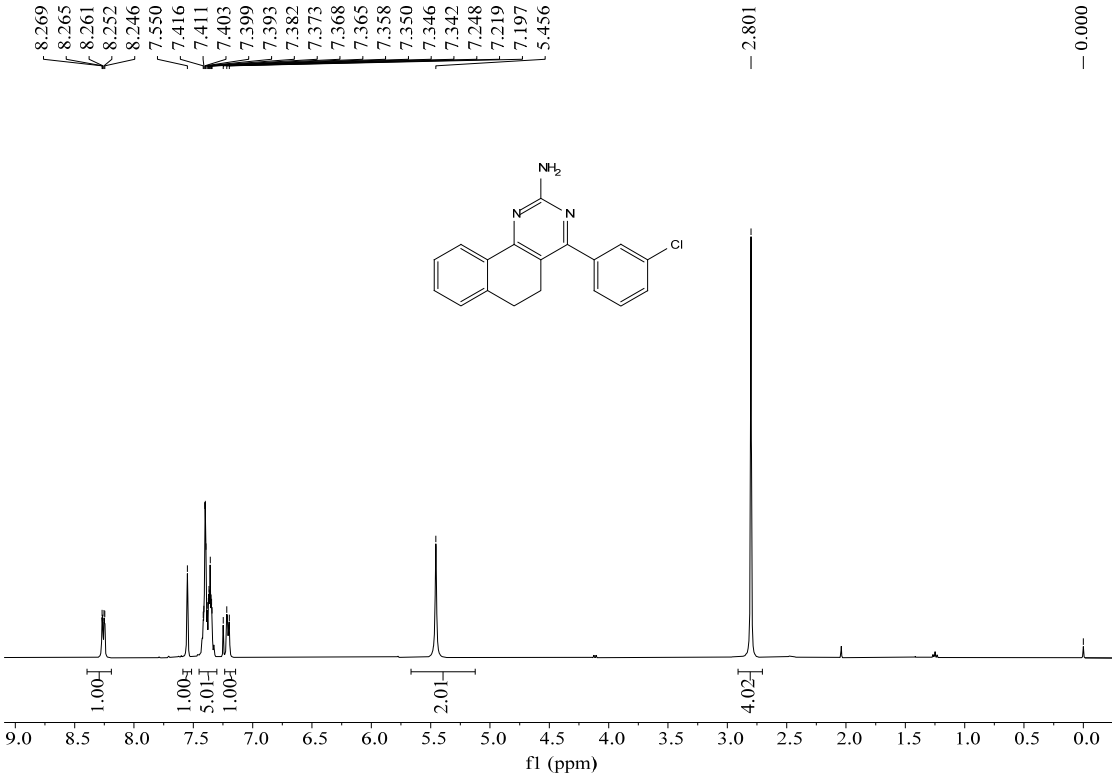


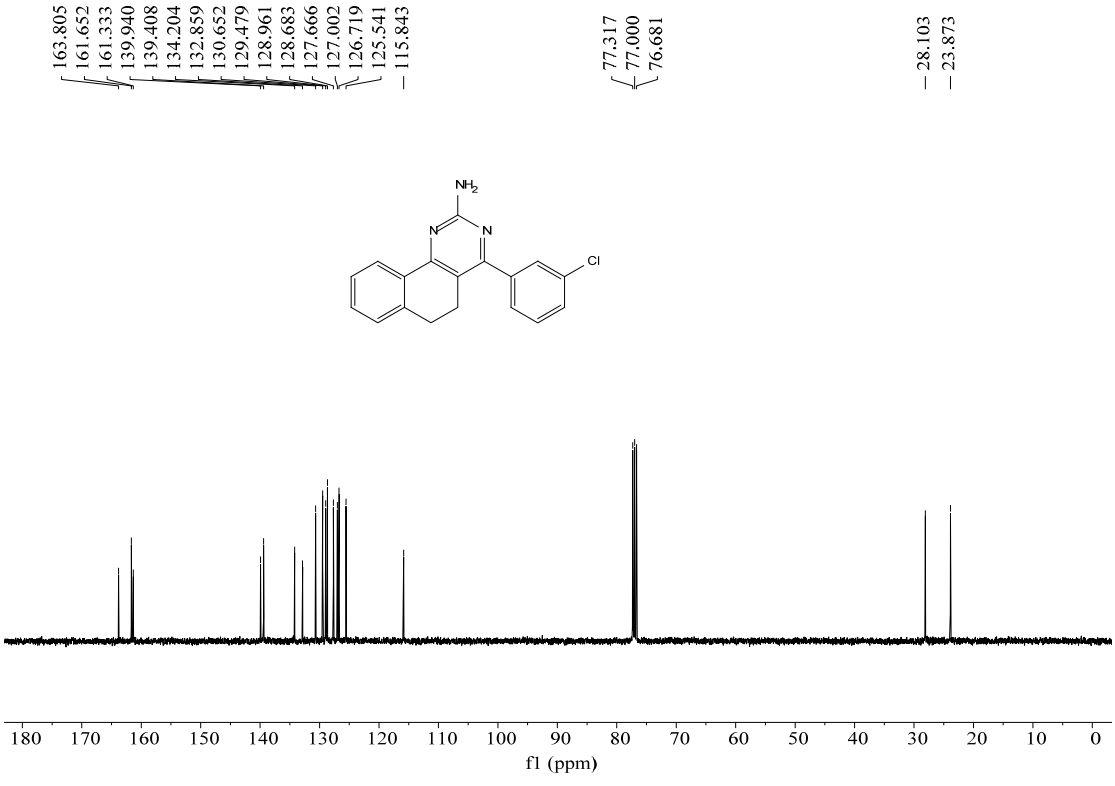
^{1}H and ^{13}C NMR spectra of **3o**



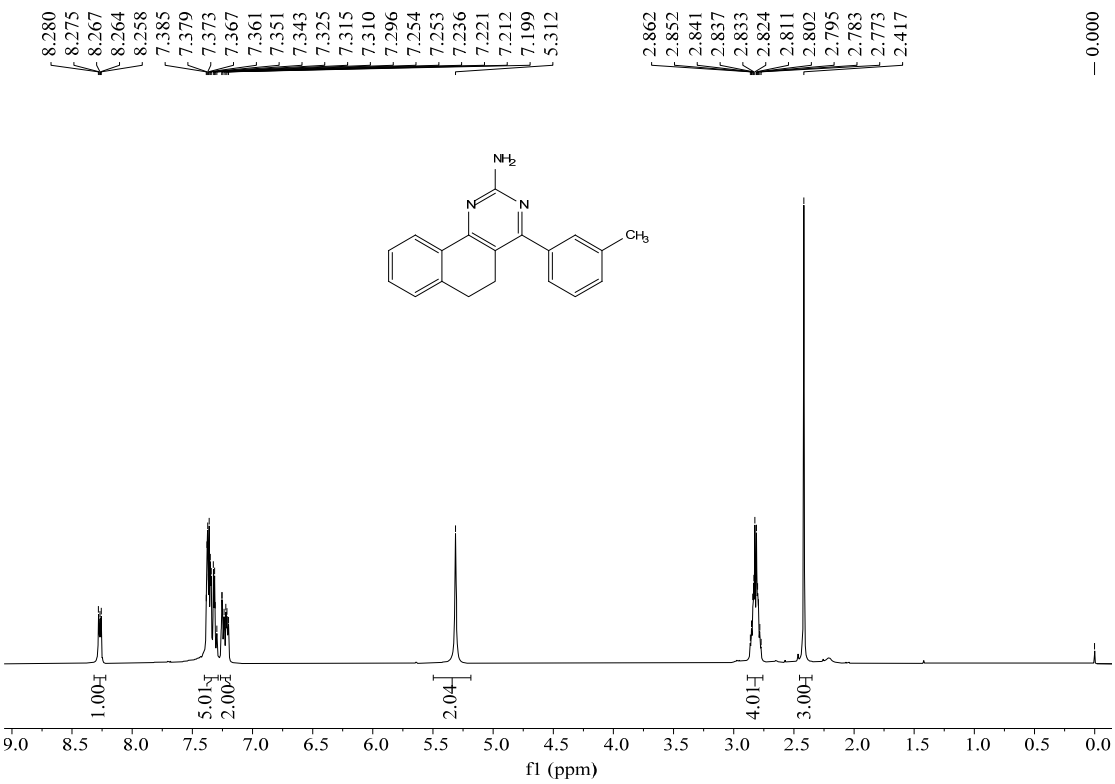


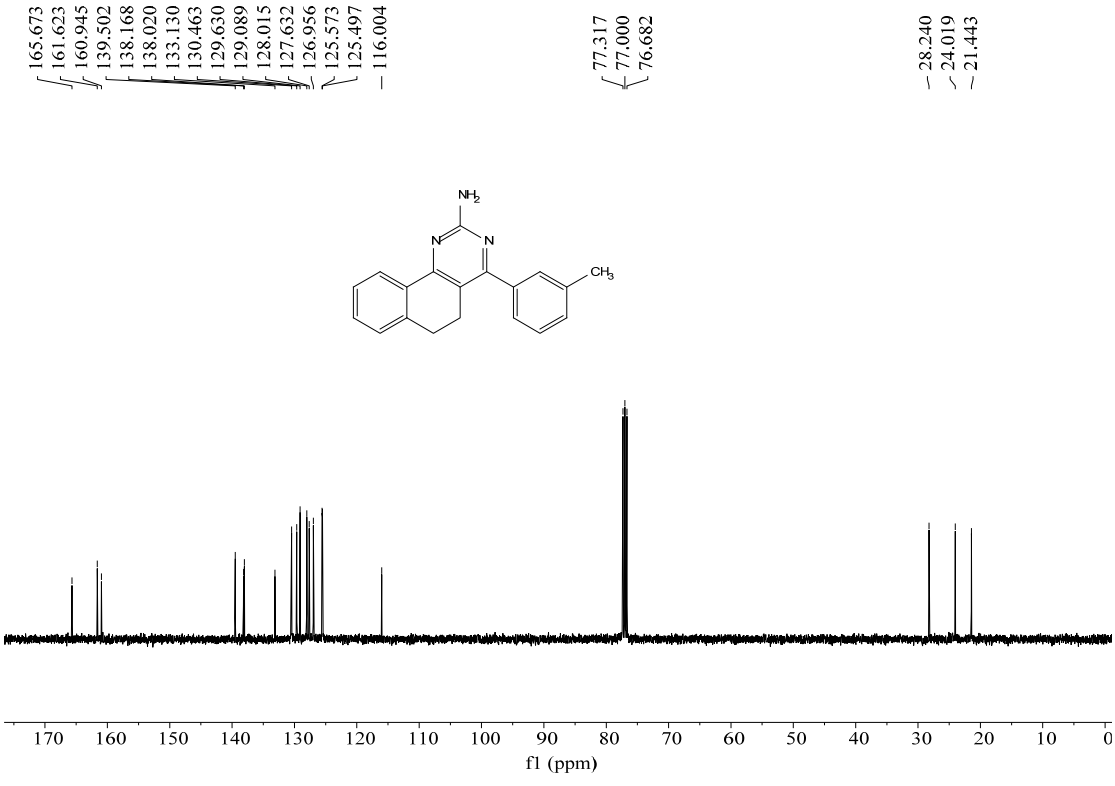
^{1}H and ^{13}C NMR spectra of **3p**



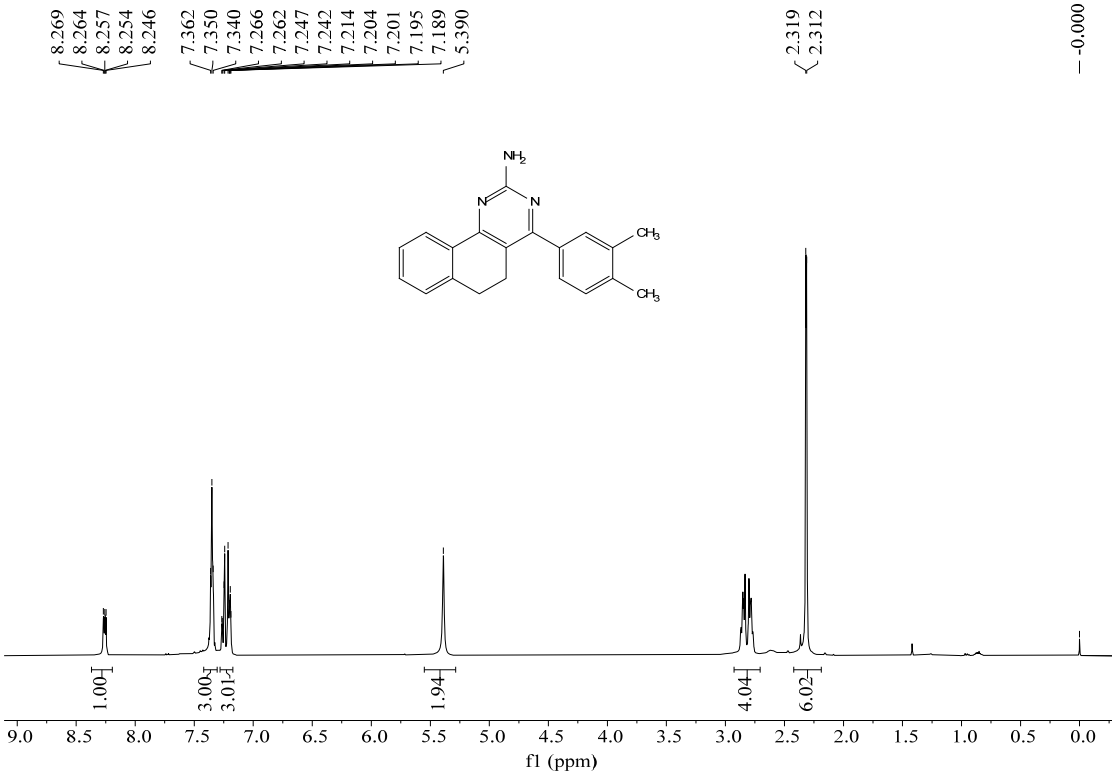


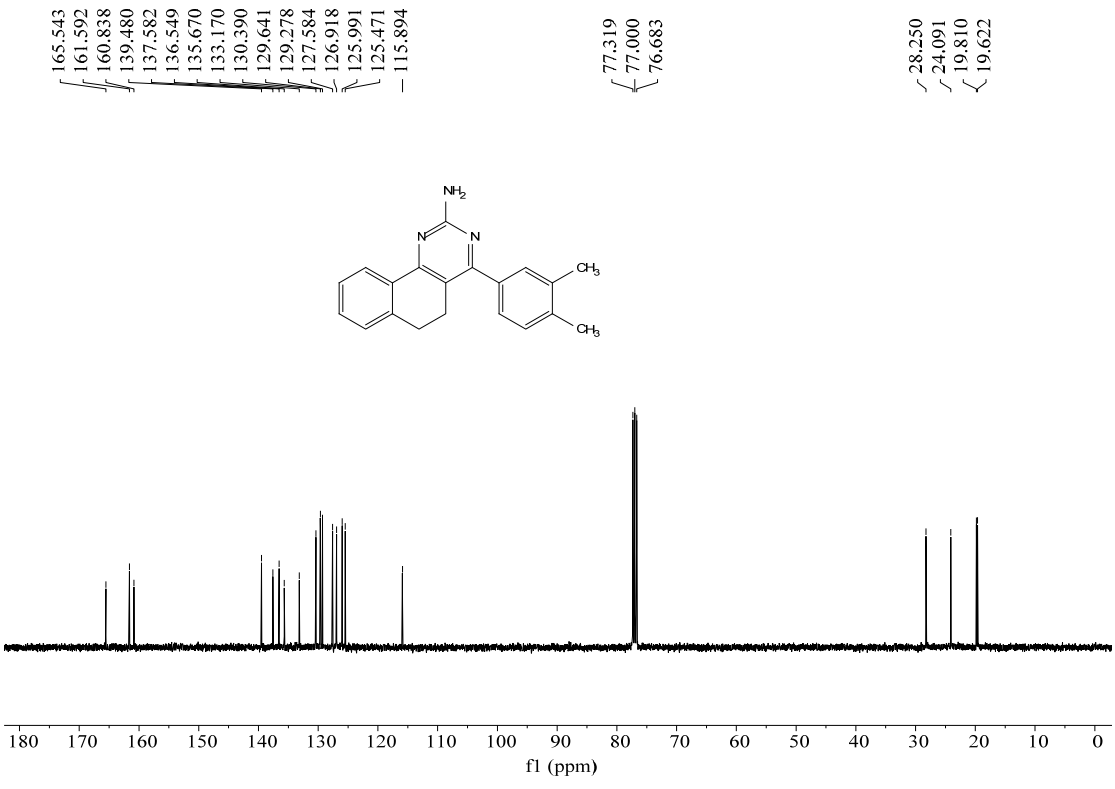
^{1}H and ^{13}C NMR spectra of **3q**



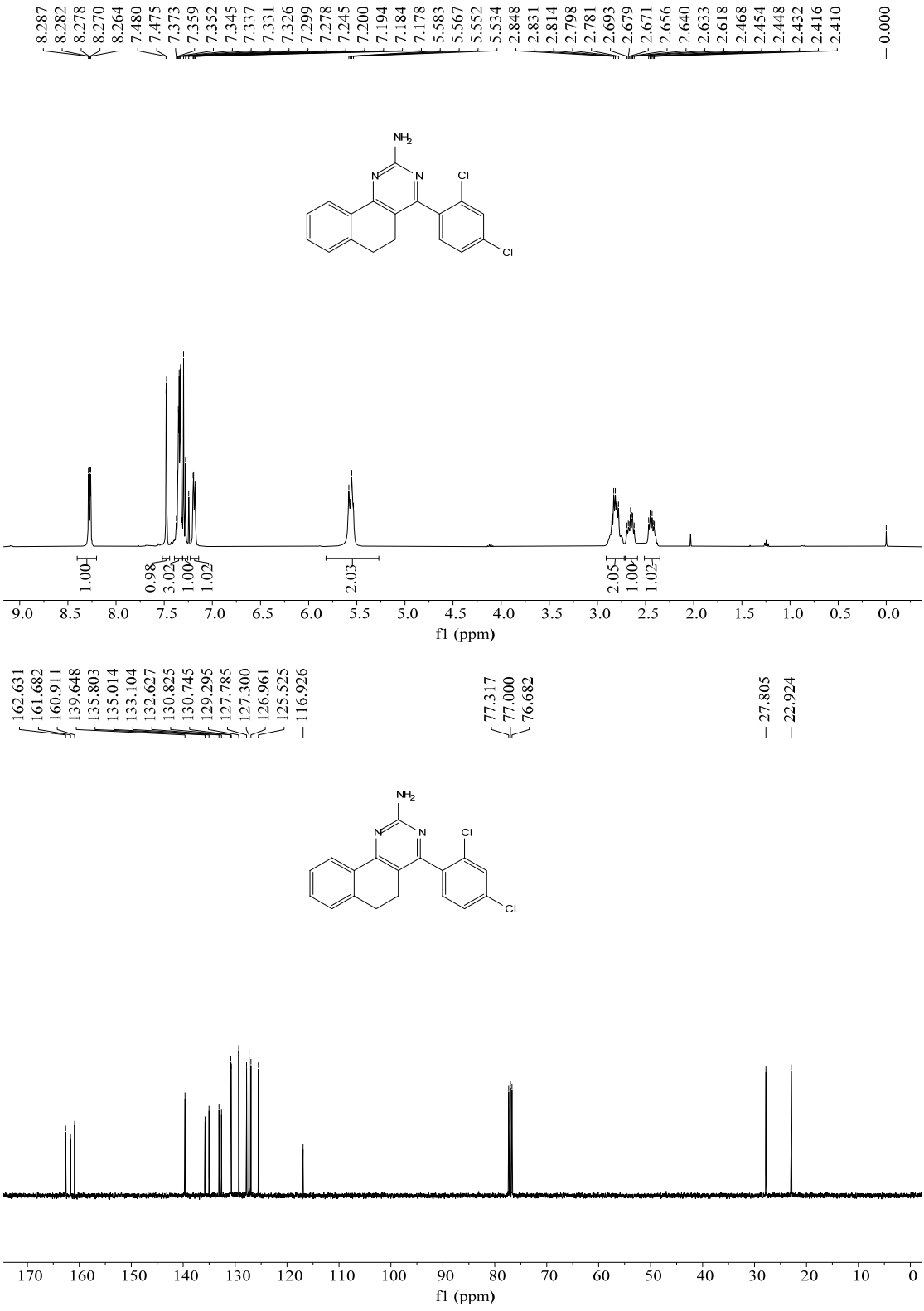


^{1}H and ^{13}C NMR spectra of **3r**

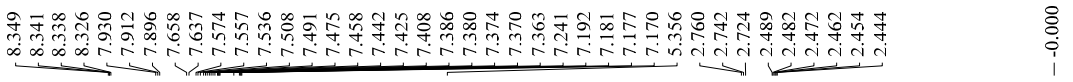


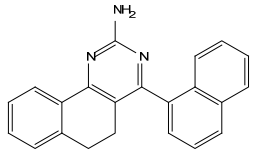


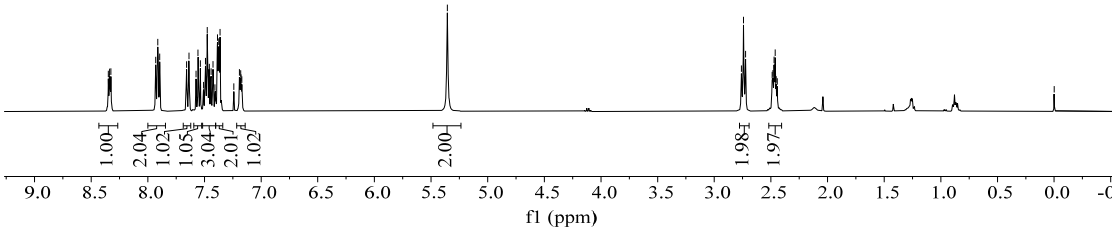
^{1}H and ^{13}C NMR spectra of **3s**

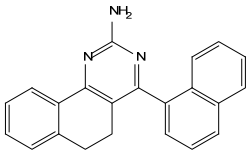


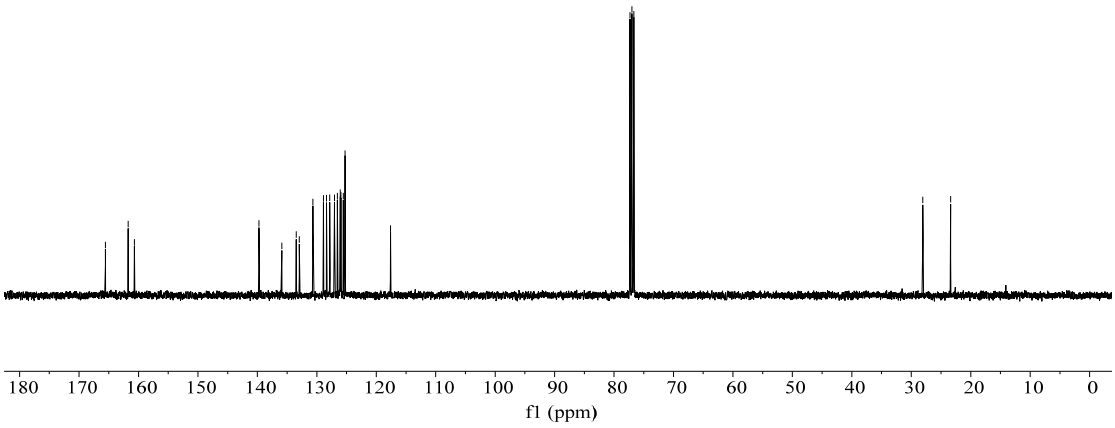
^{1}H and ^{13}C NMR spectra of **3t**



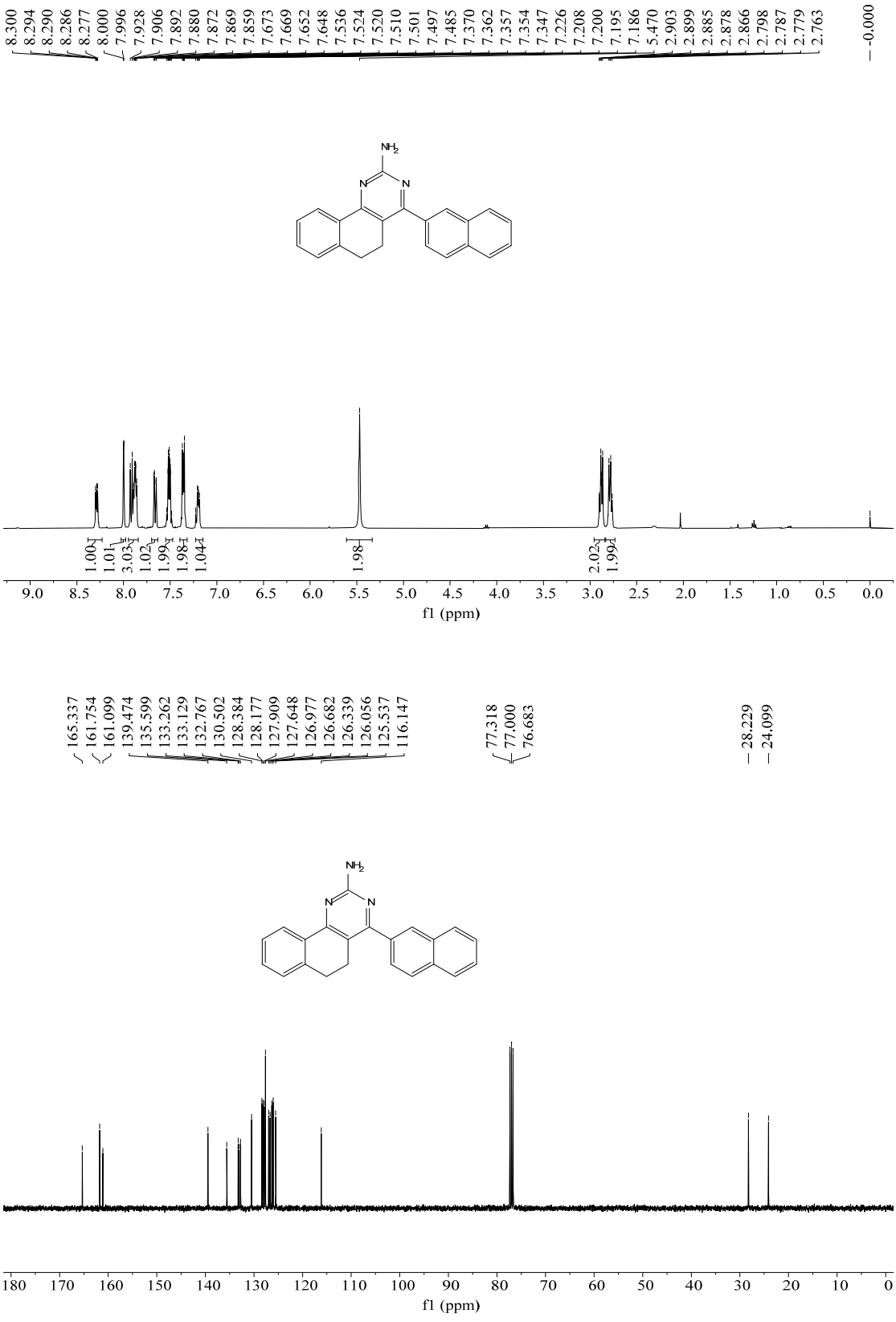




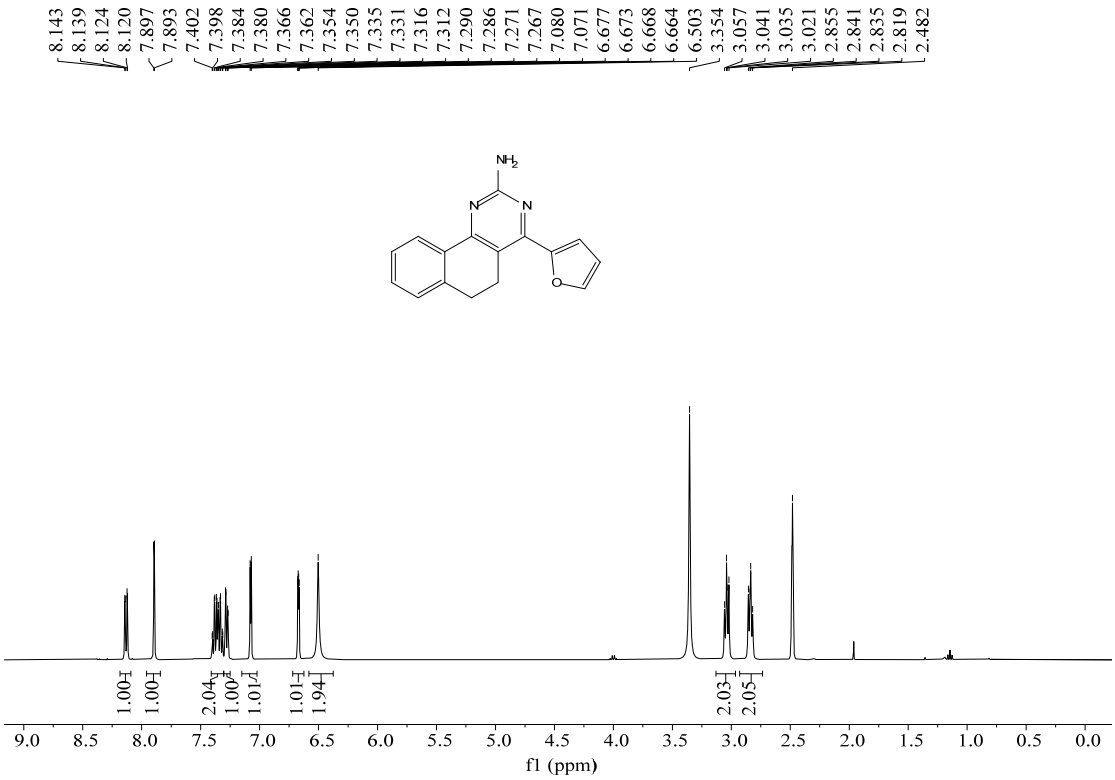


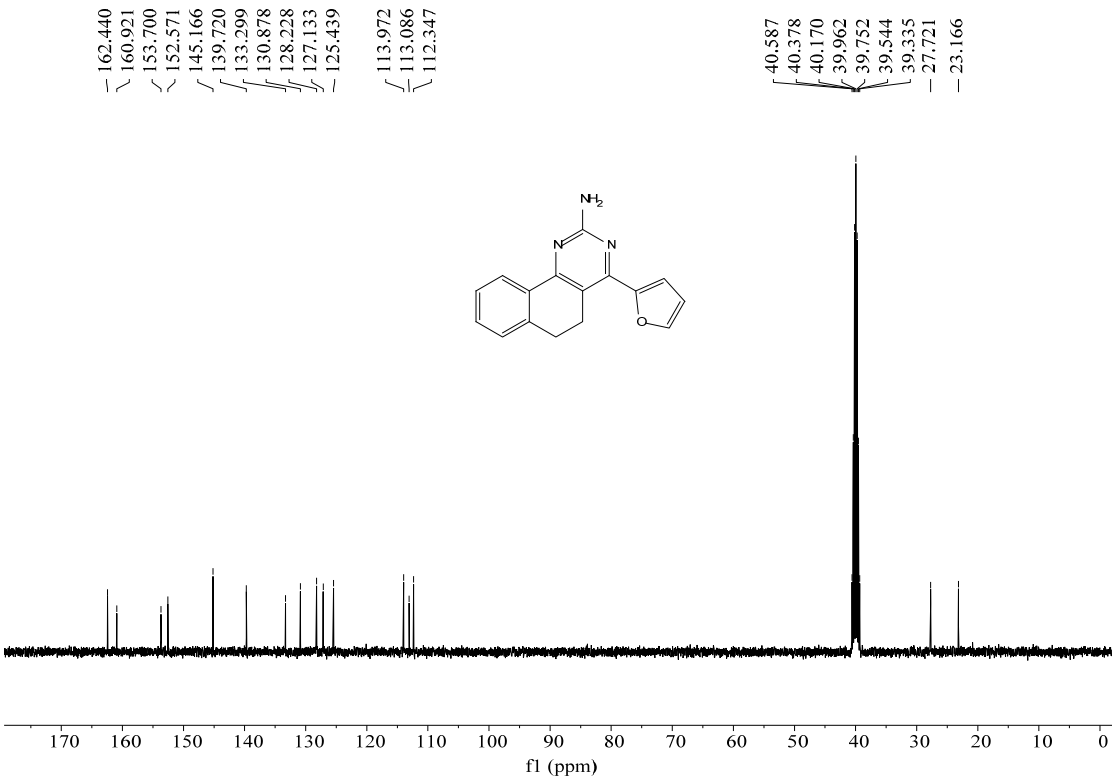


^{1}H and ^{13}C NMR spectra of **3u**

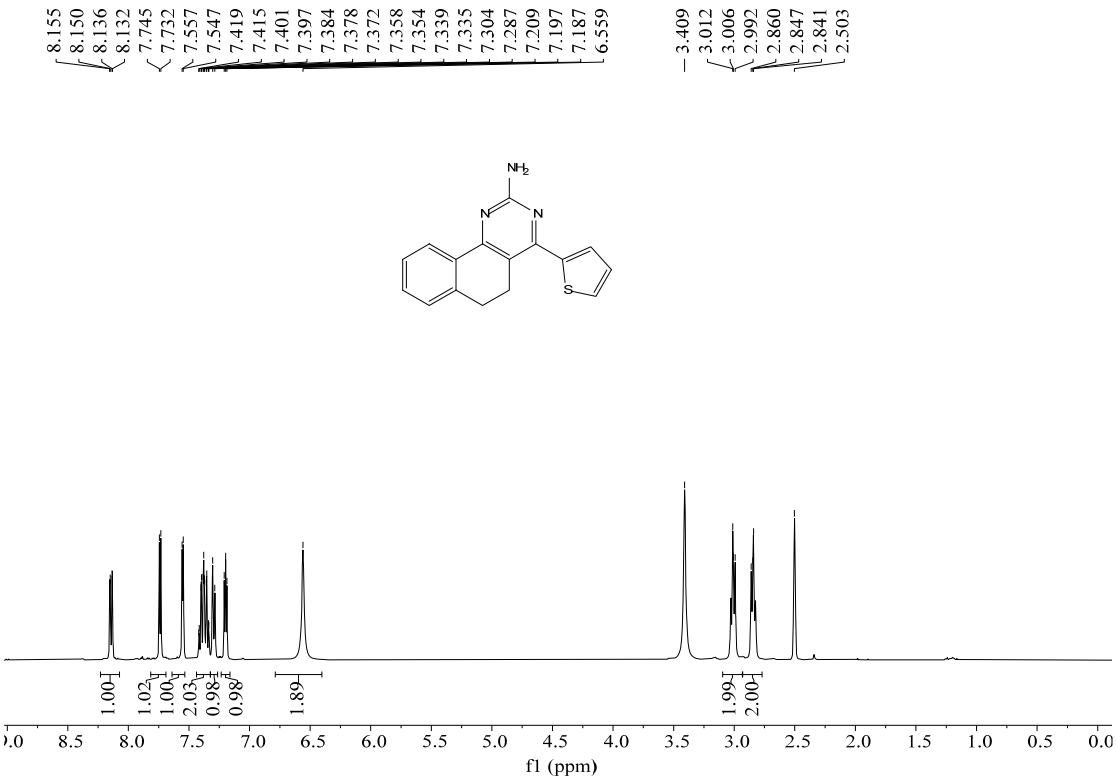


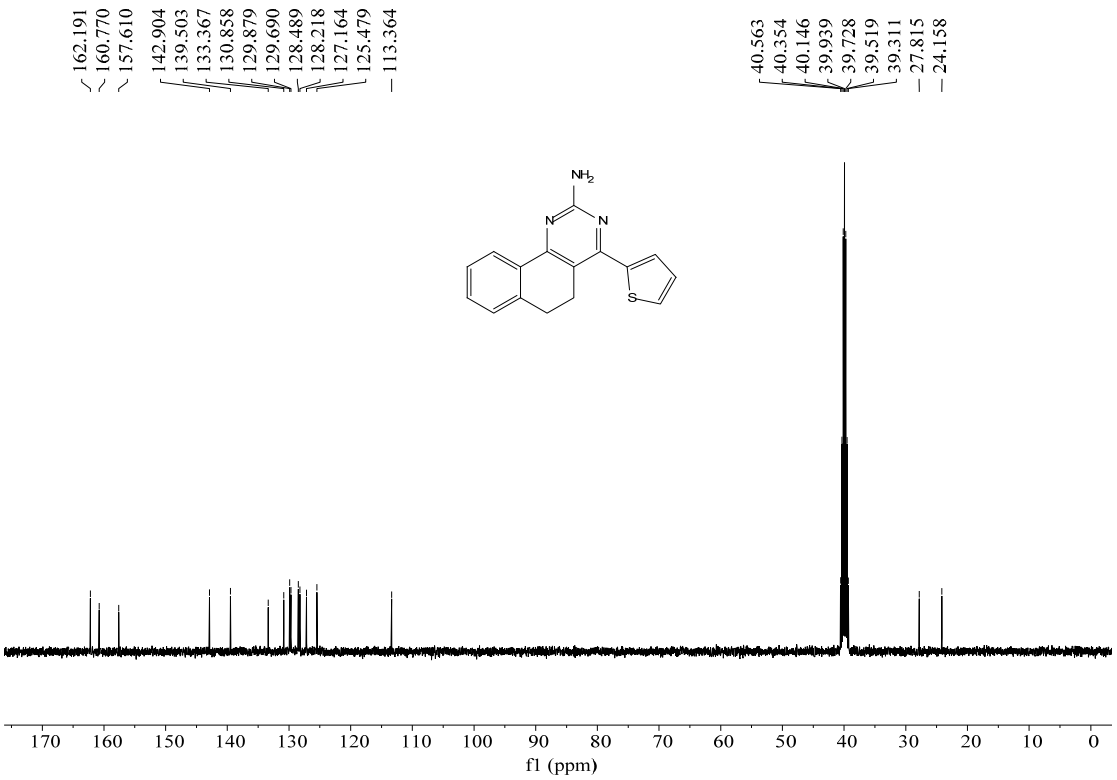
^{1}H and ^{13}C NMR spectra of **3v**



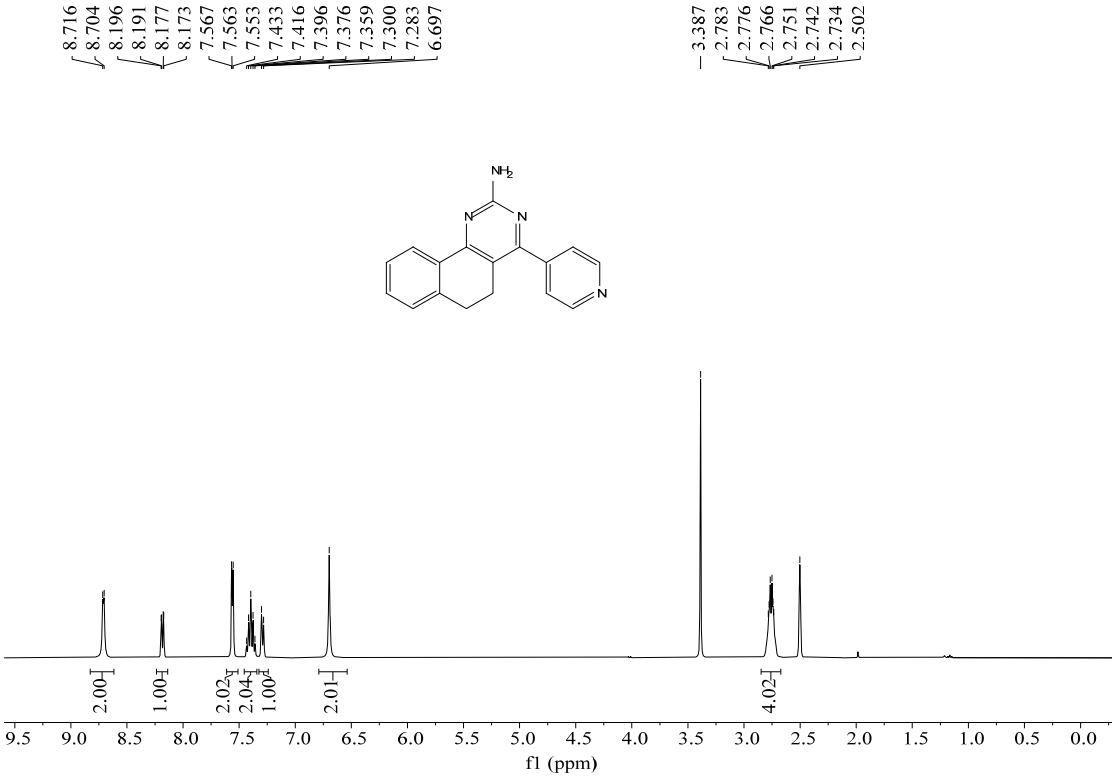


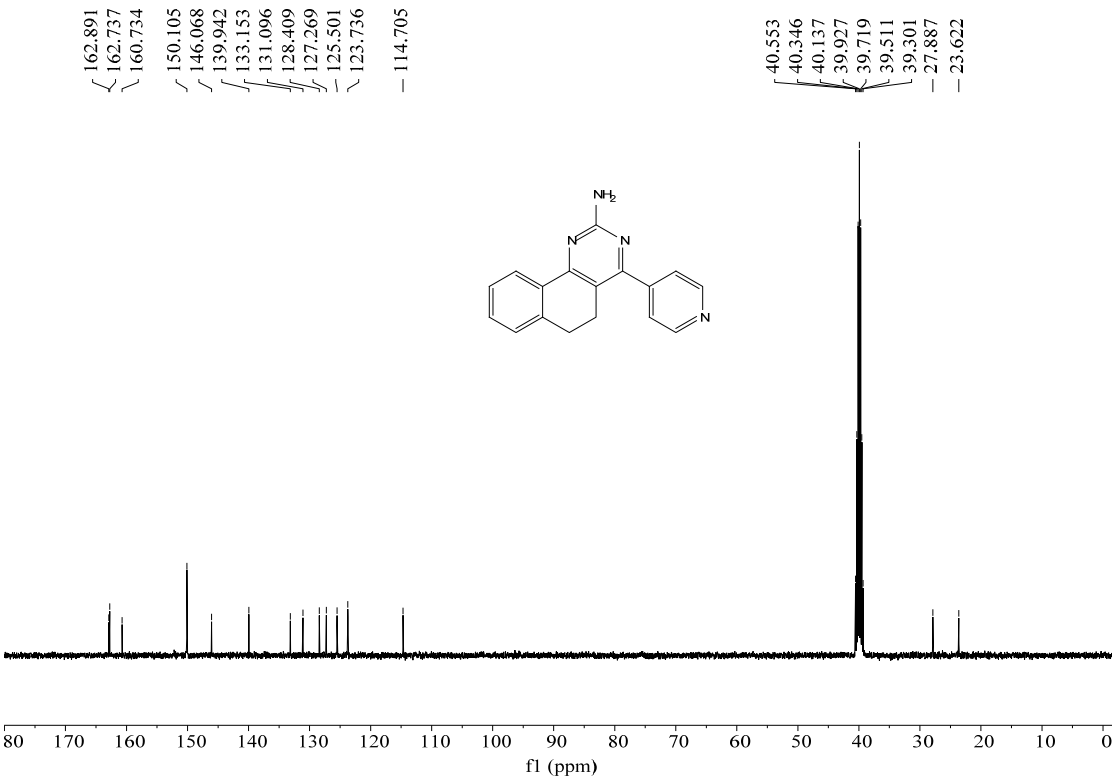
^{1}H and ^{13}C NMR spectra of **3w**



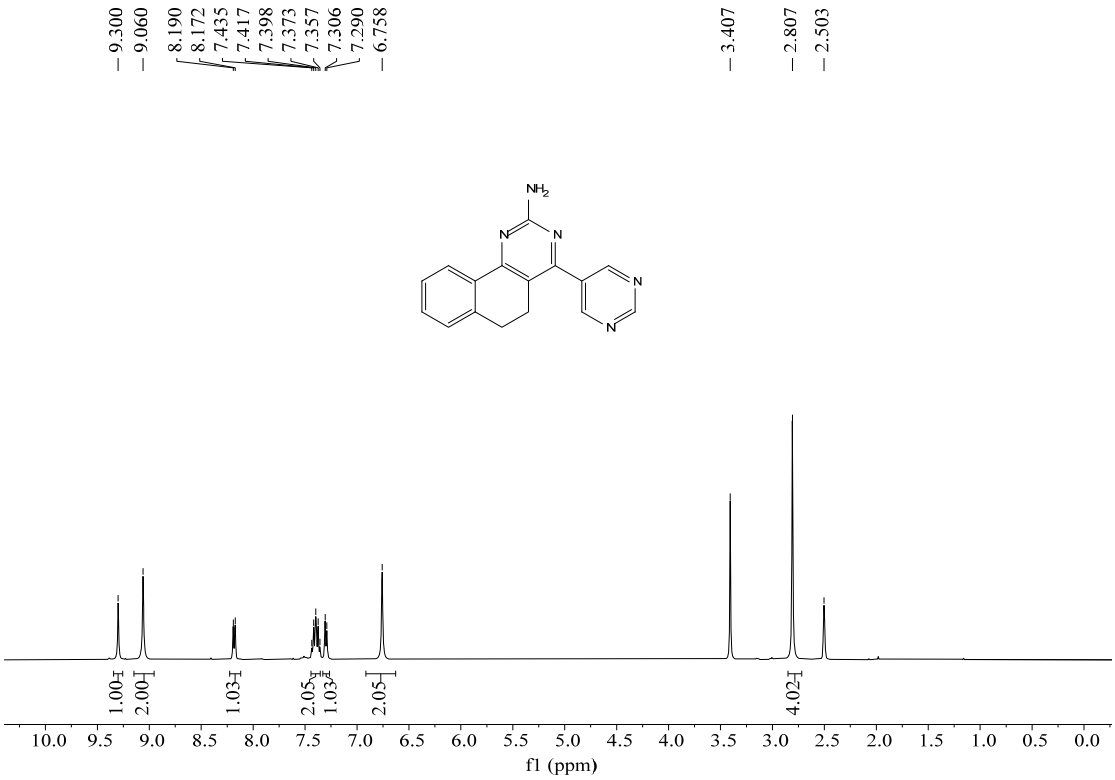


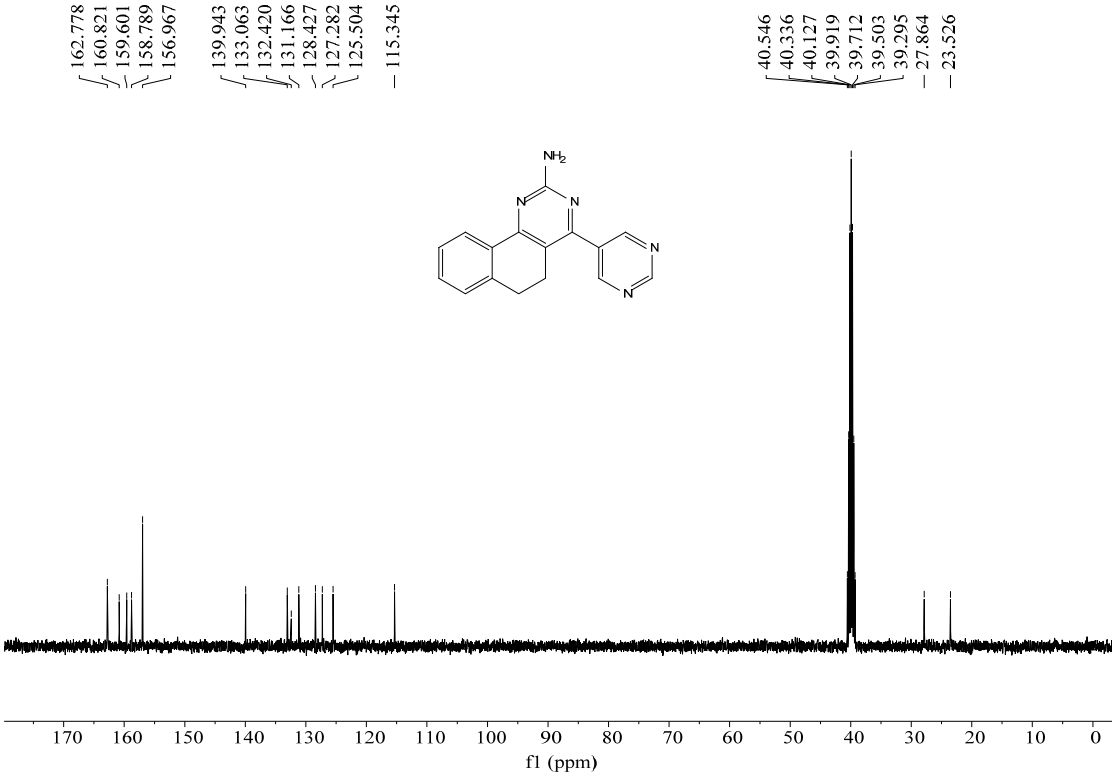
^{1}H and ^{13}C NMR spectra of **3x**



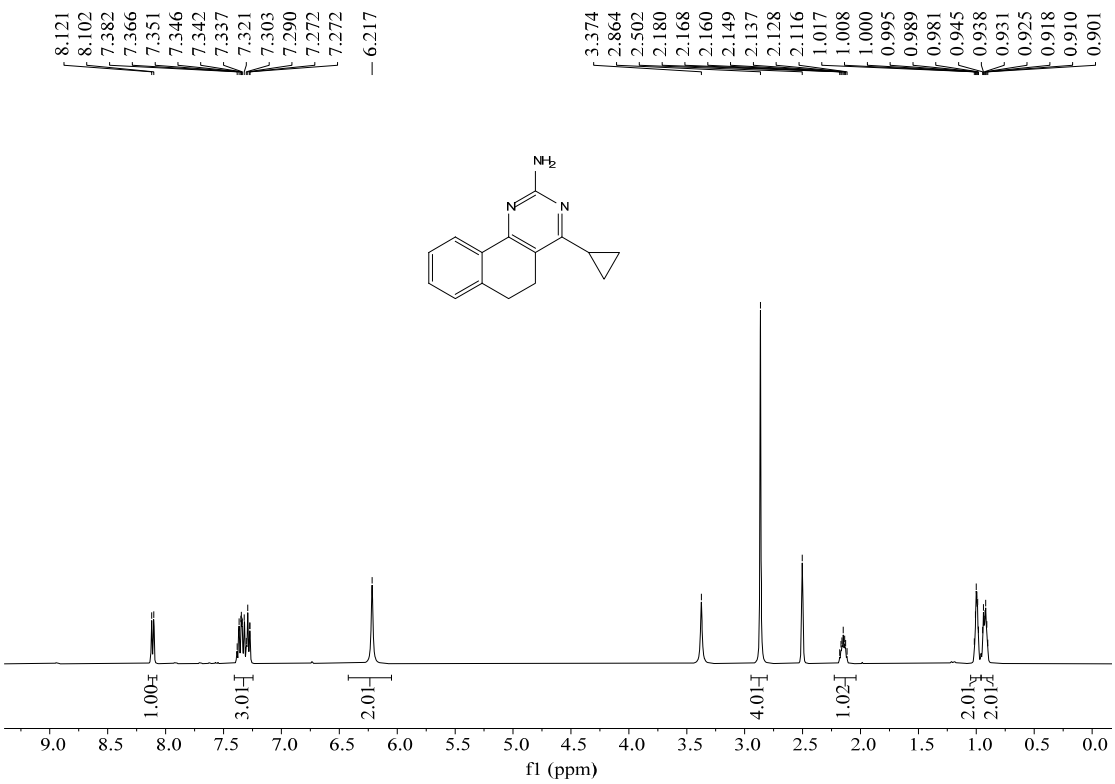


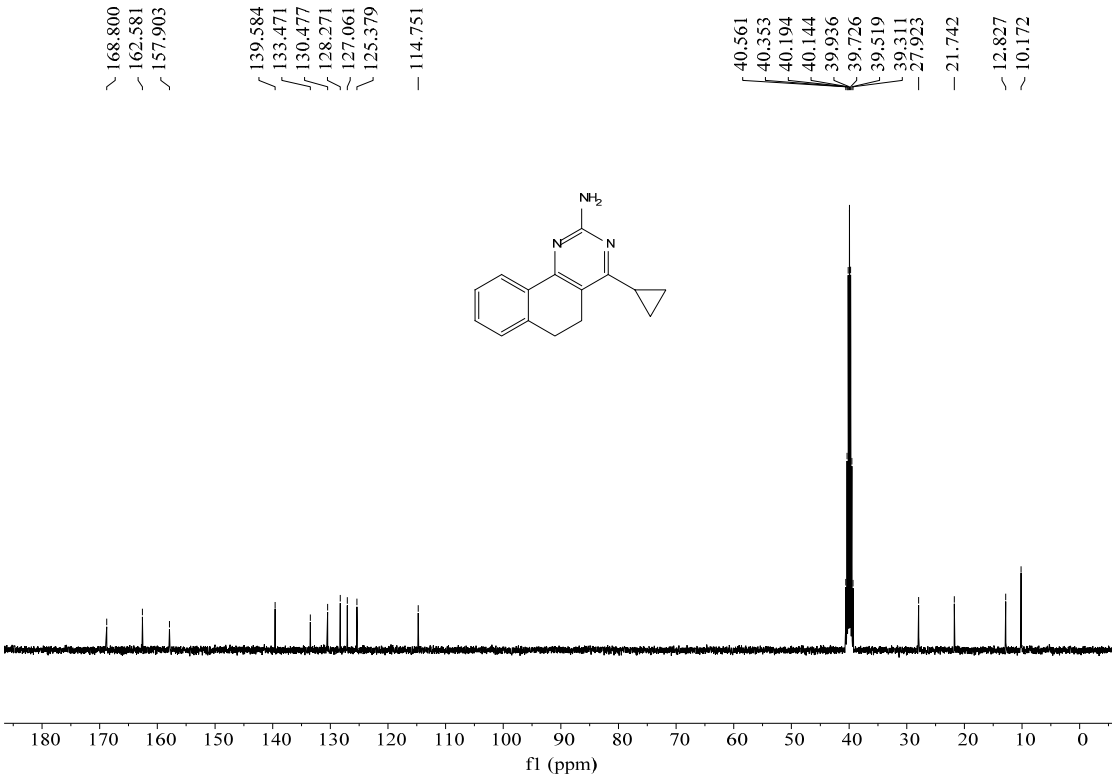
^{1}H and ^{13}C NMR spectra of **3y**



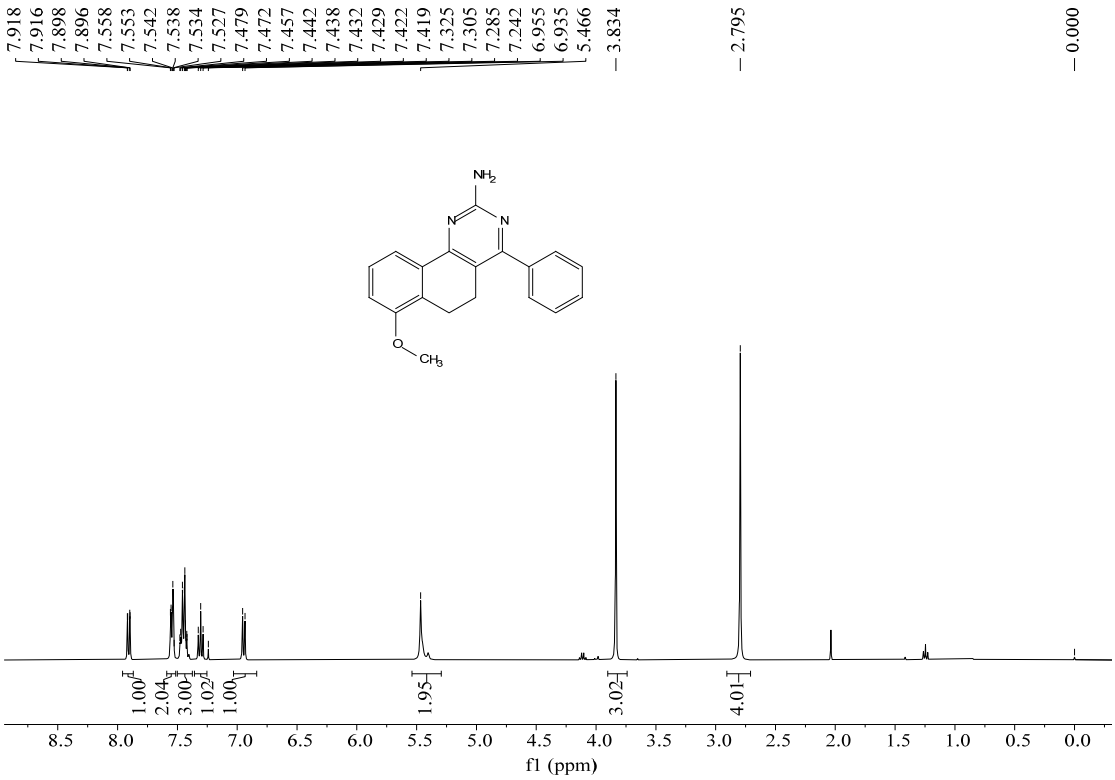


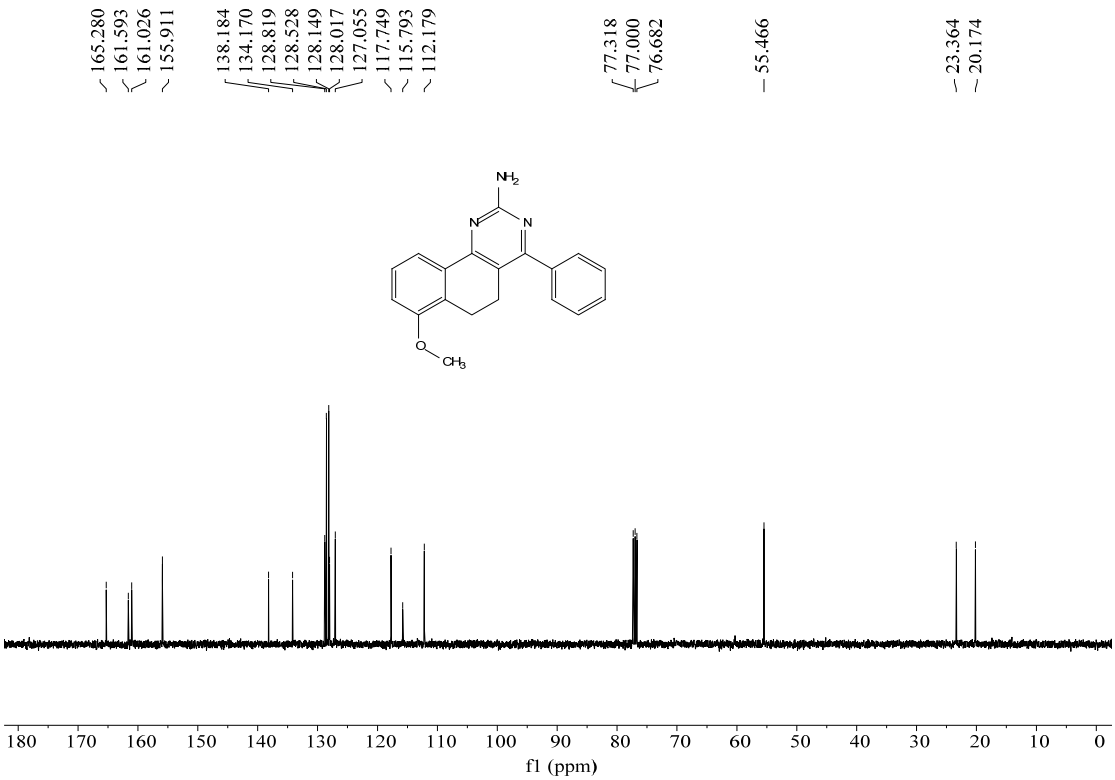
^{1}H and ^{13}C NMR spectra of **3z**



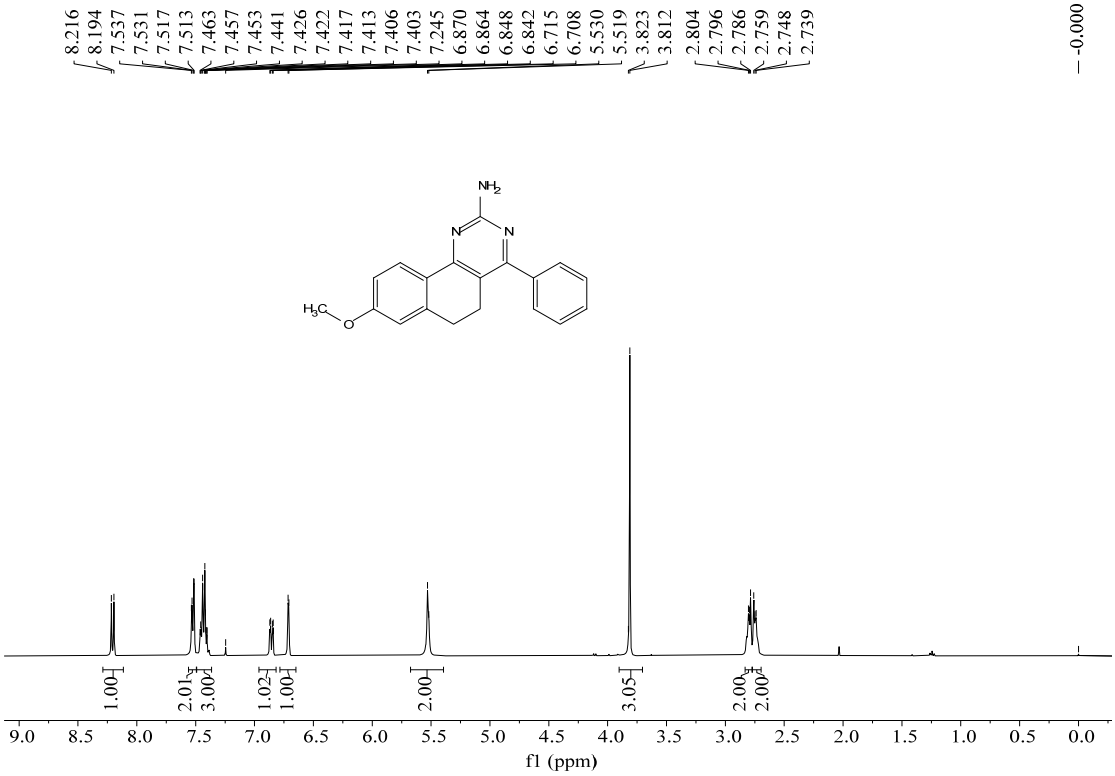


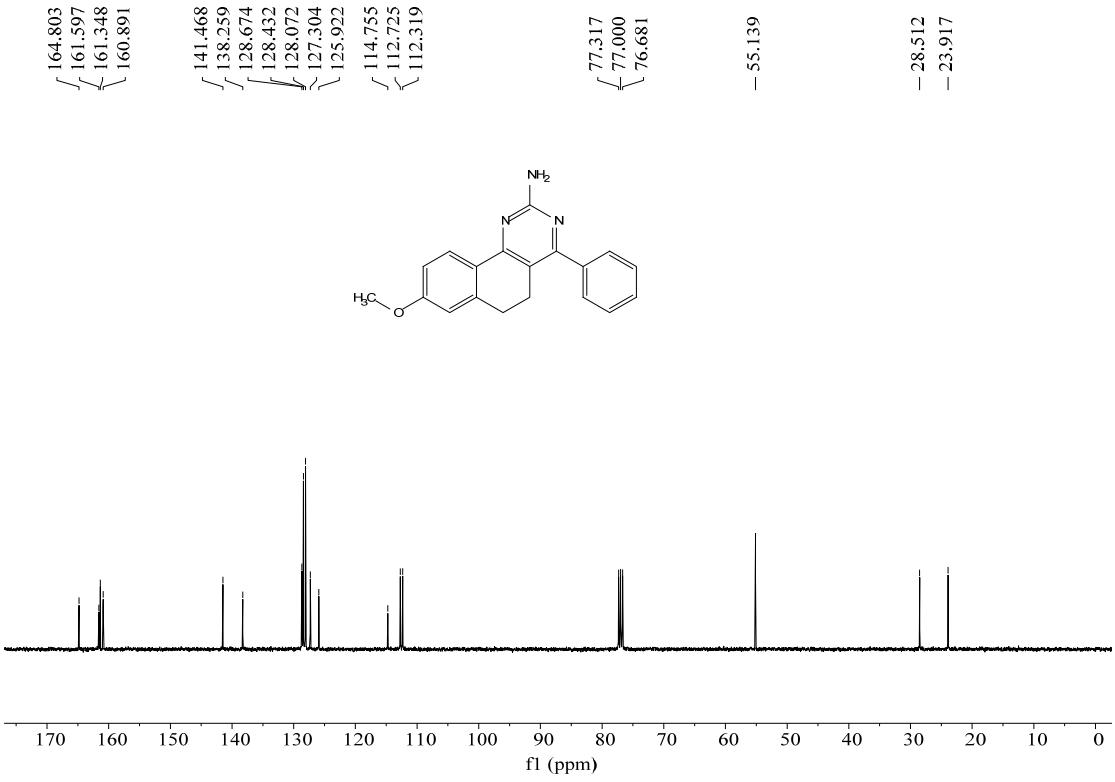
^{1}H and ^{13}C NMR spectra of **4a**



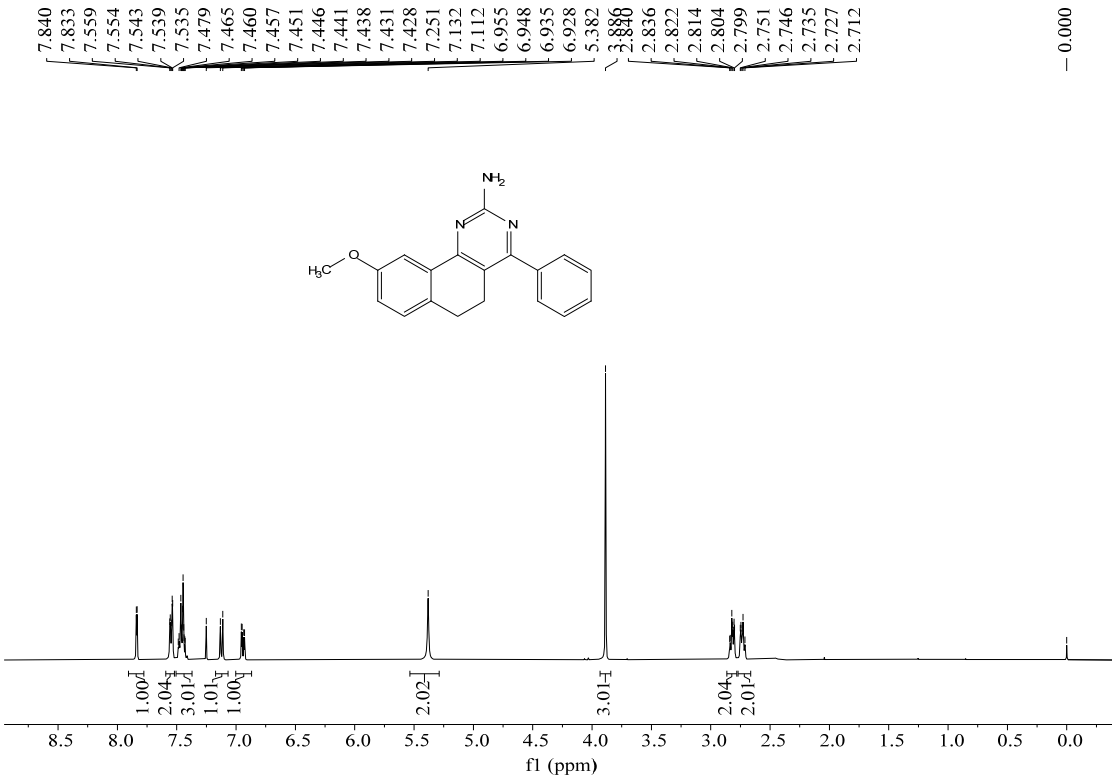


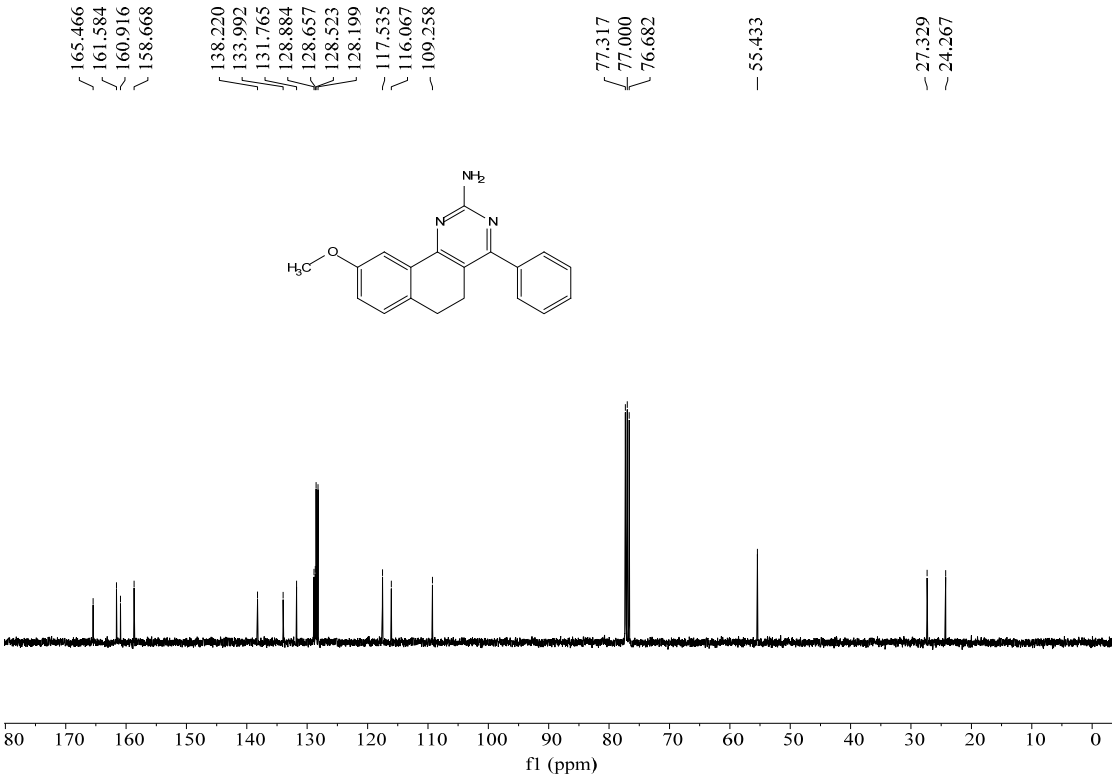
^{1}H and ^{13}C NMR spectra of **4b**



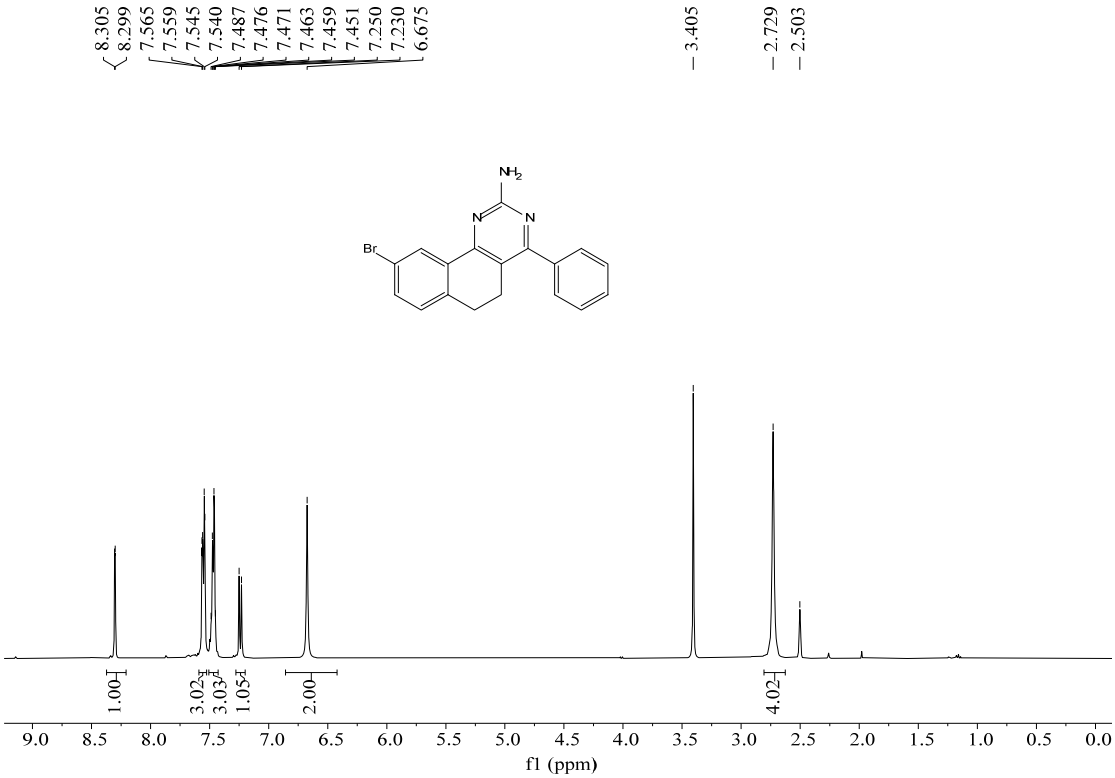


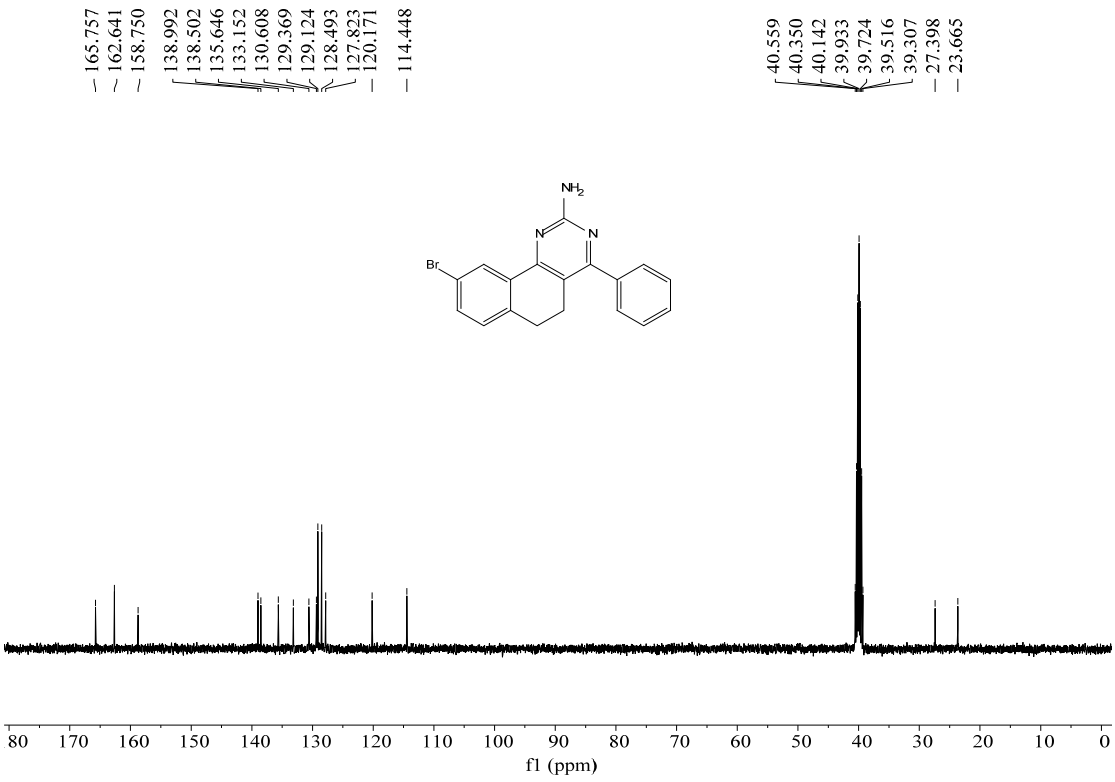
^{1}H and ^{13}C NMR spectra of **4c**



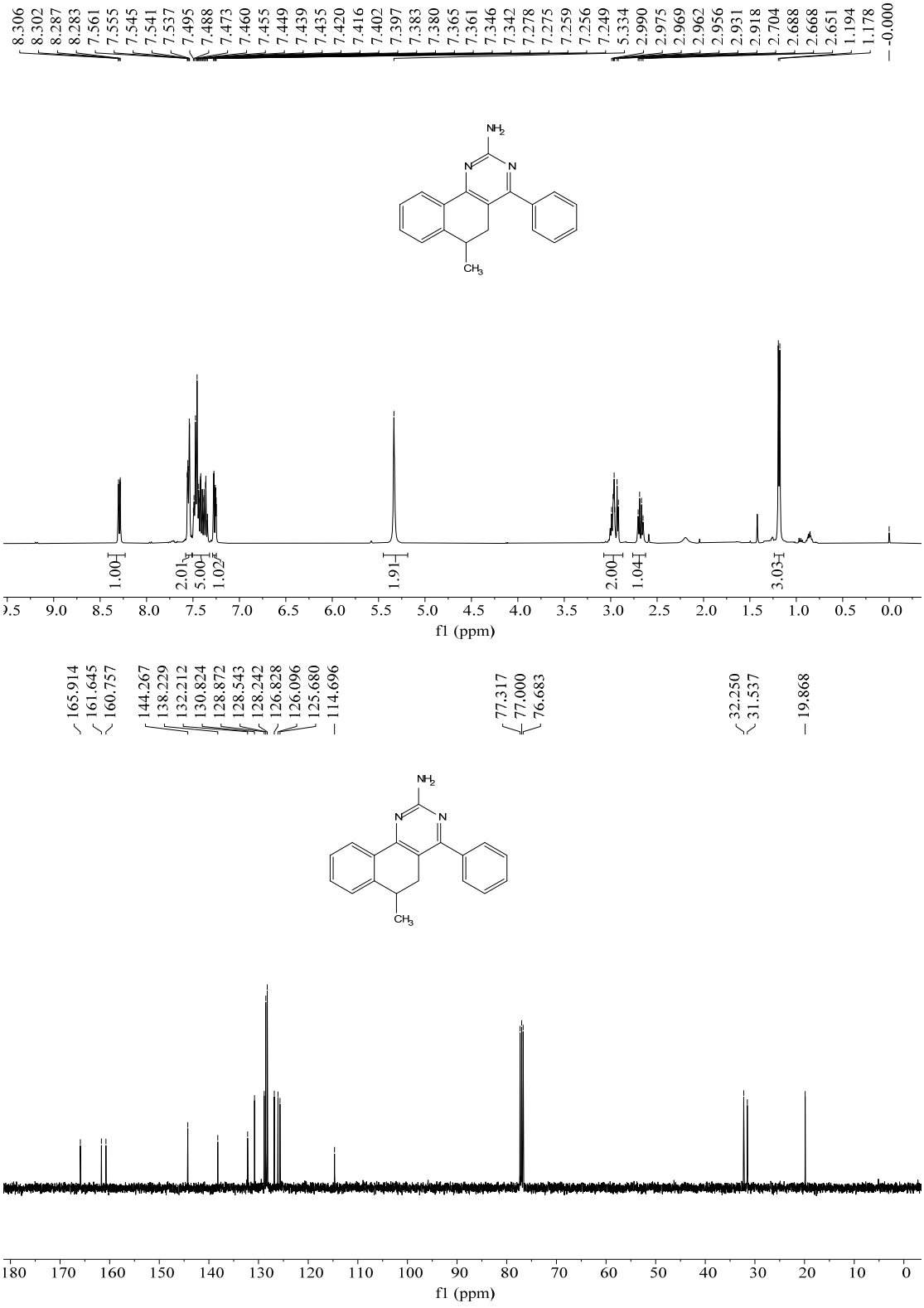


^{1}H and ^{13}C NMR spectra of **4d**

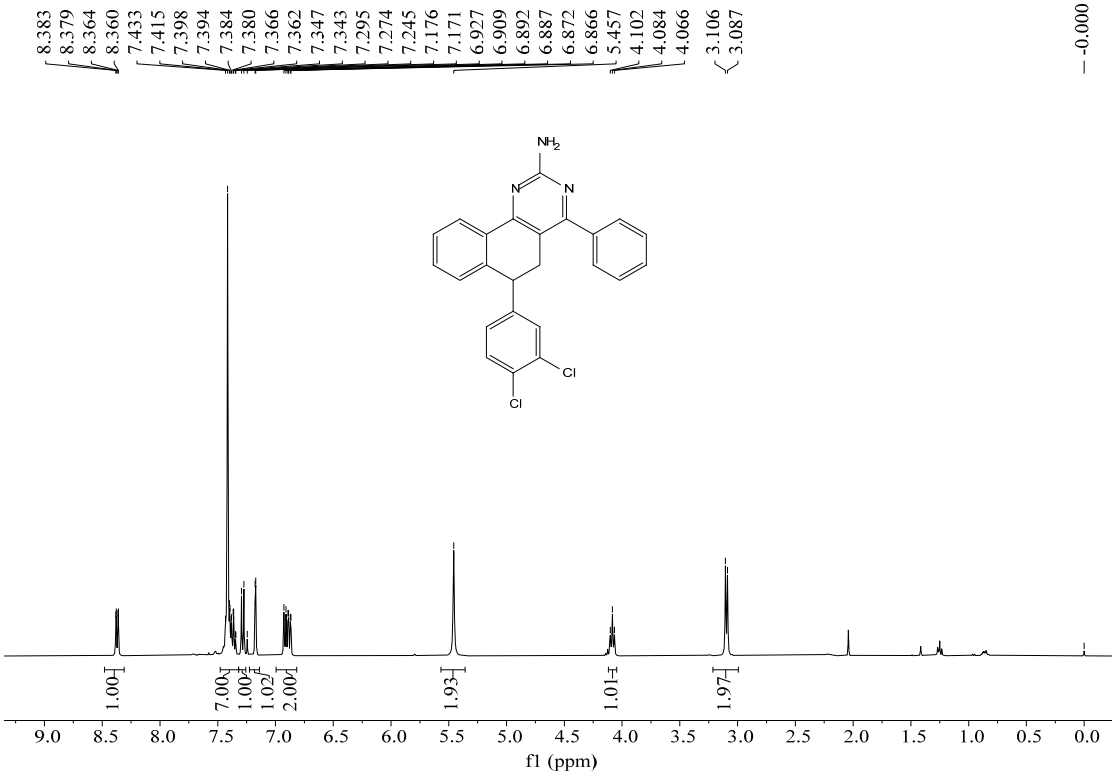


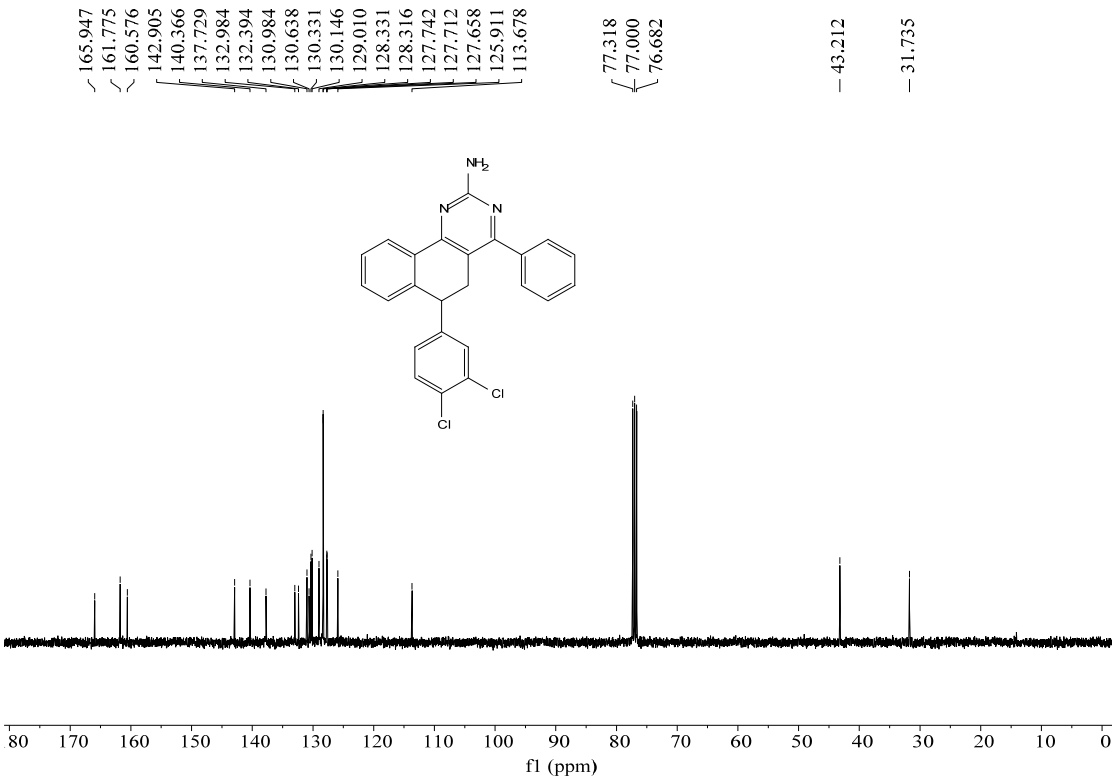


^{1}H and ^{13}C NMR spectra of **4e**

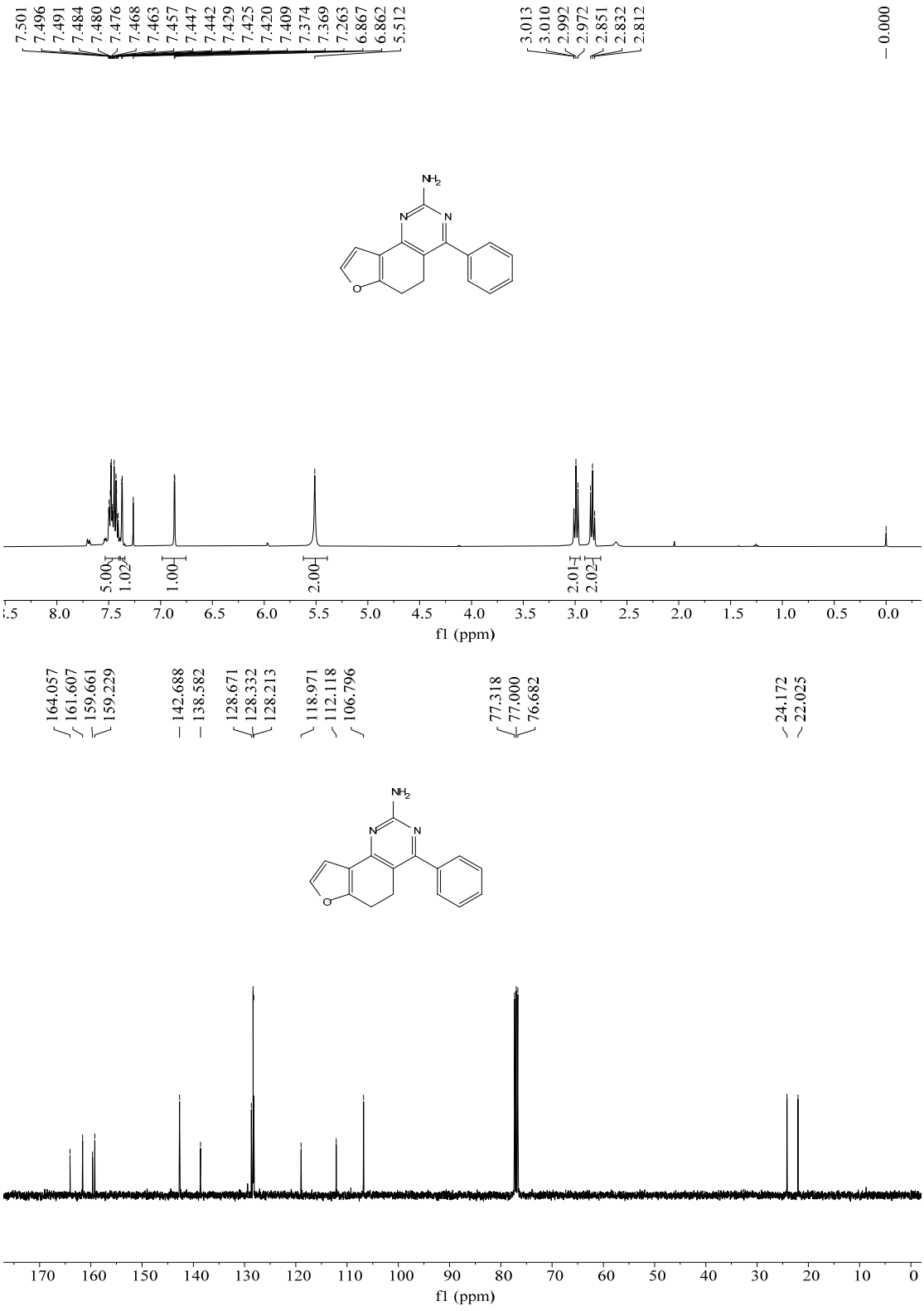


^{1}H and ^{13}C NMR spectra of **4f**

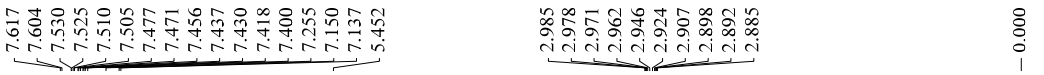


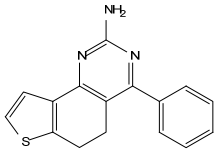


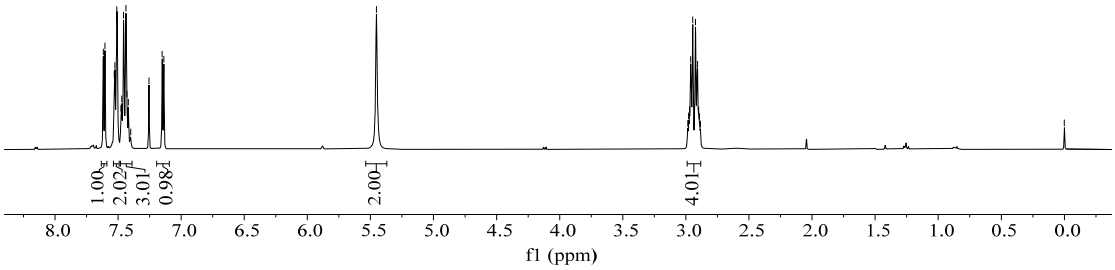
^{1}H and ^{13}C NMR spectra of **4g**

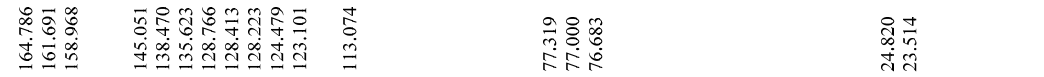


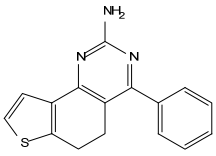
^{1}H and ^{13}C NMR spectra of **4h**

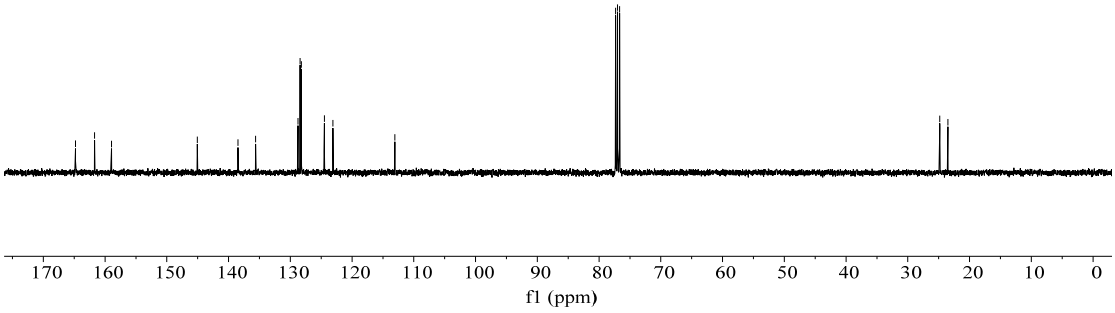




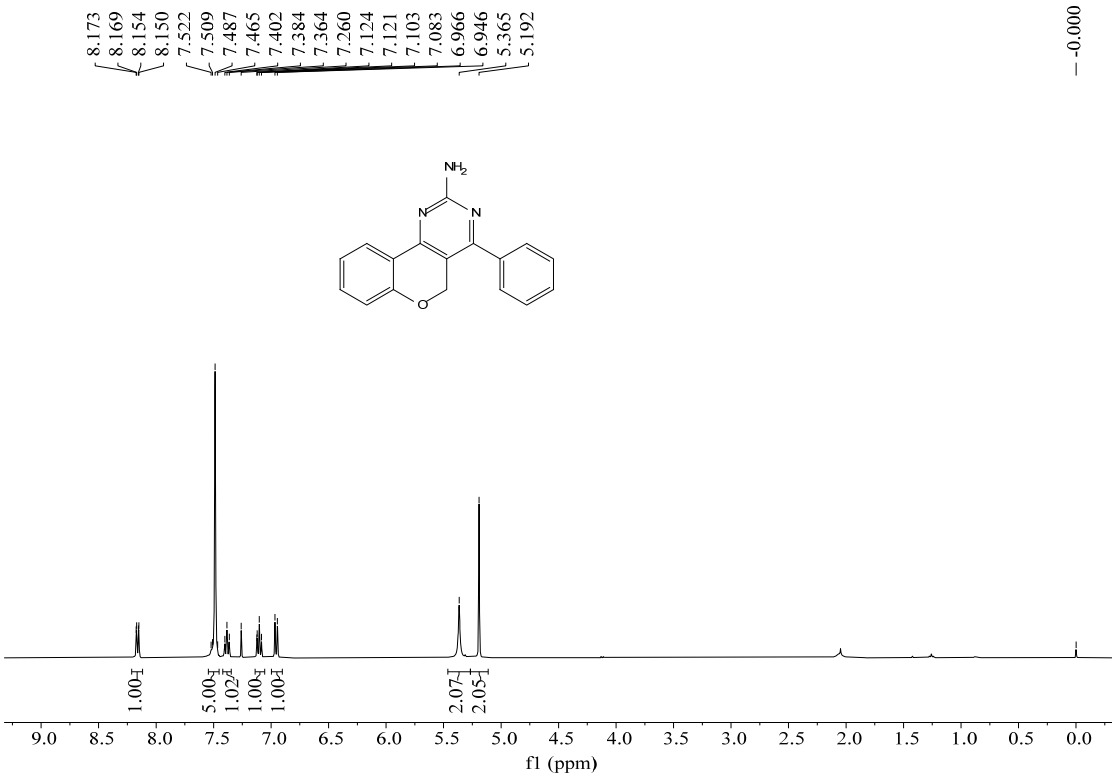


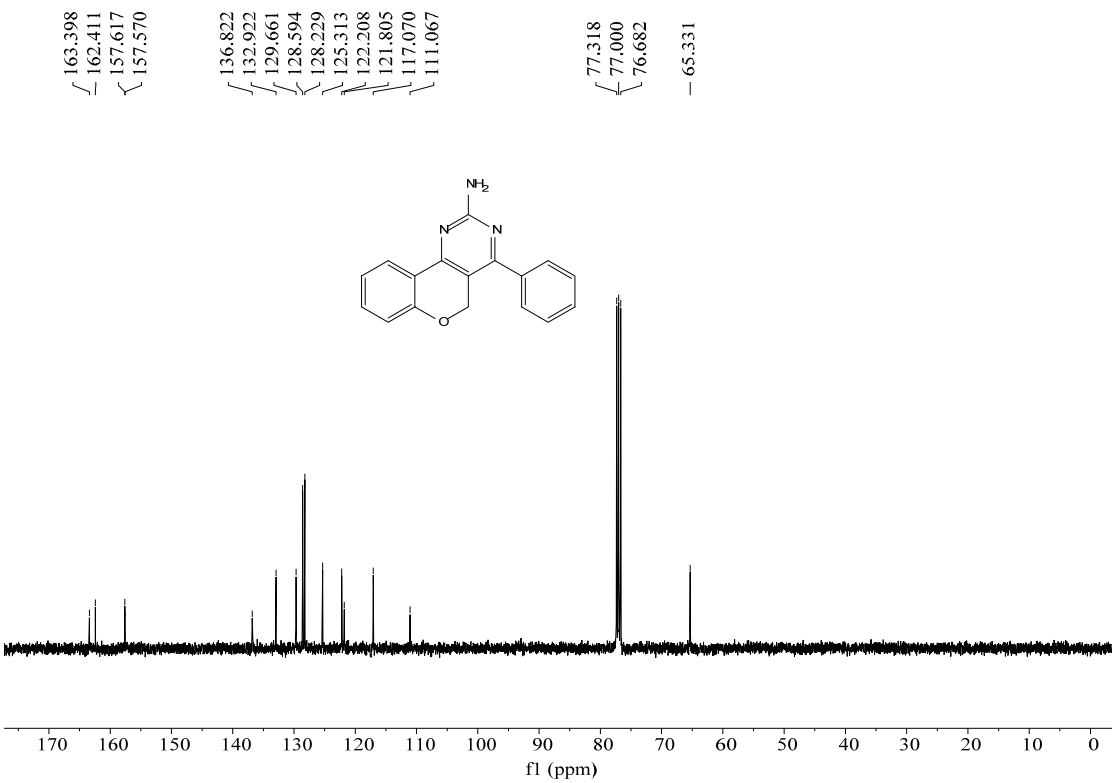




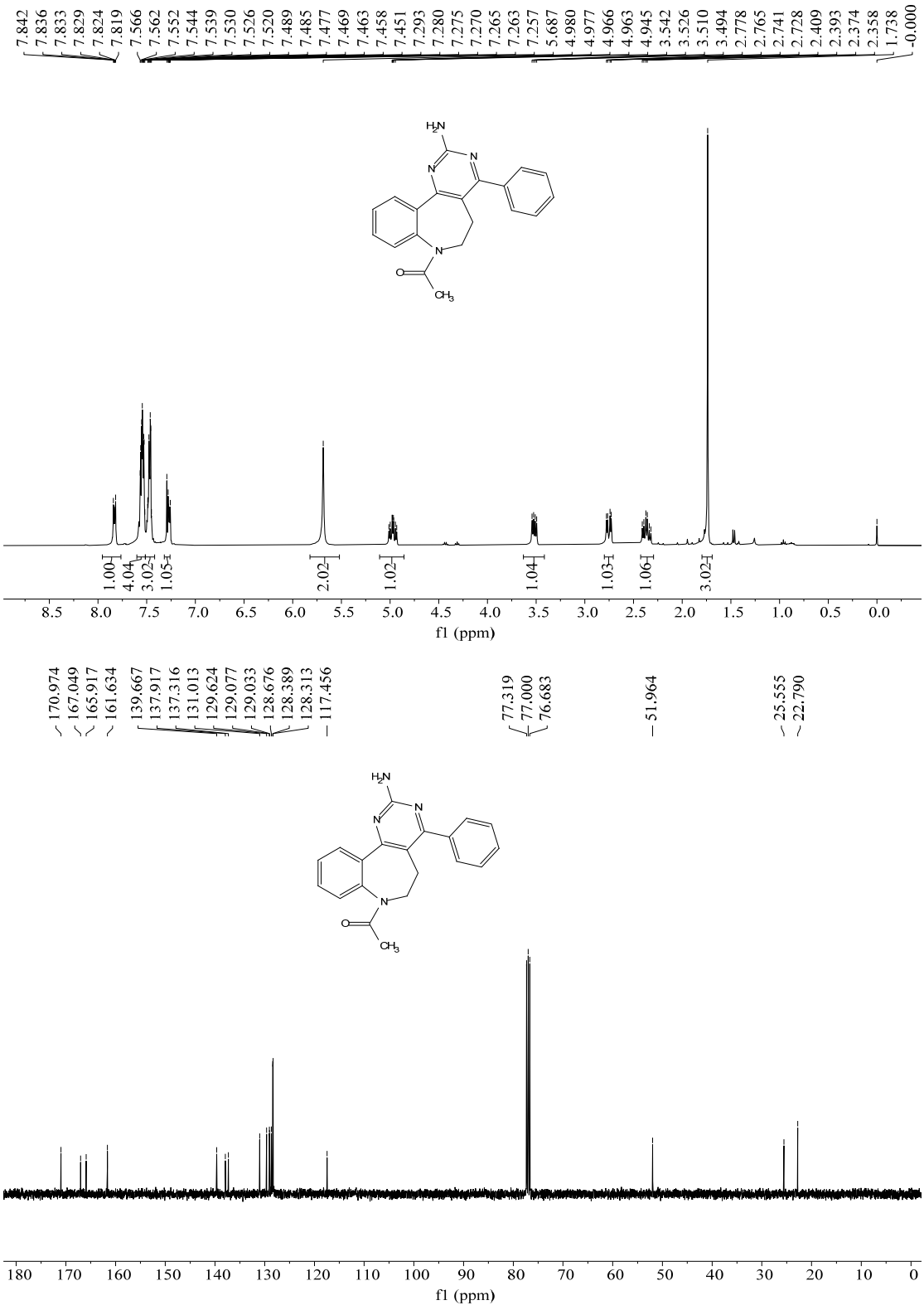


^{1}H and ^{13}C NMR spectra of **4i**

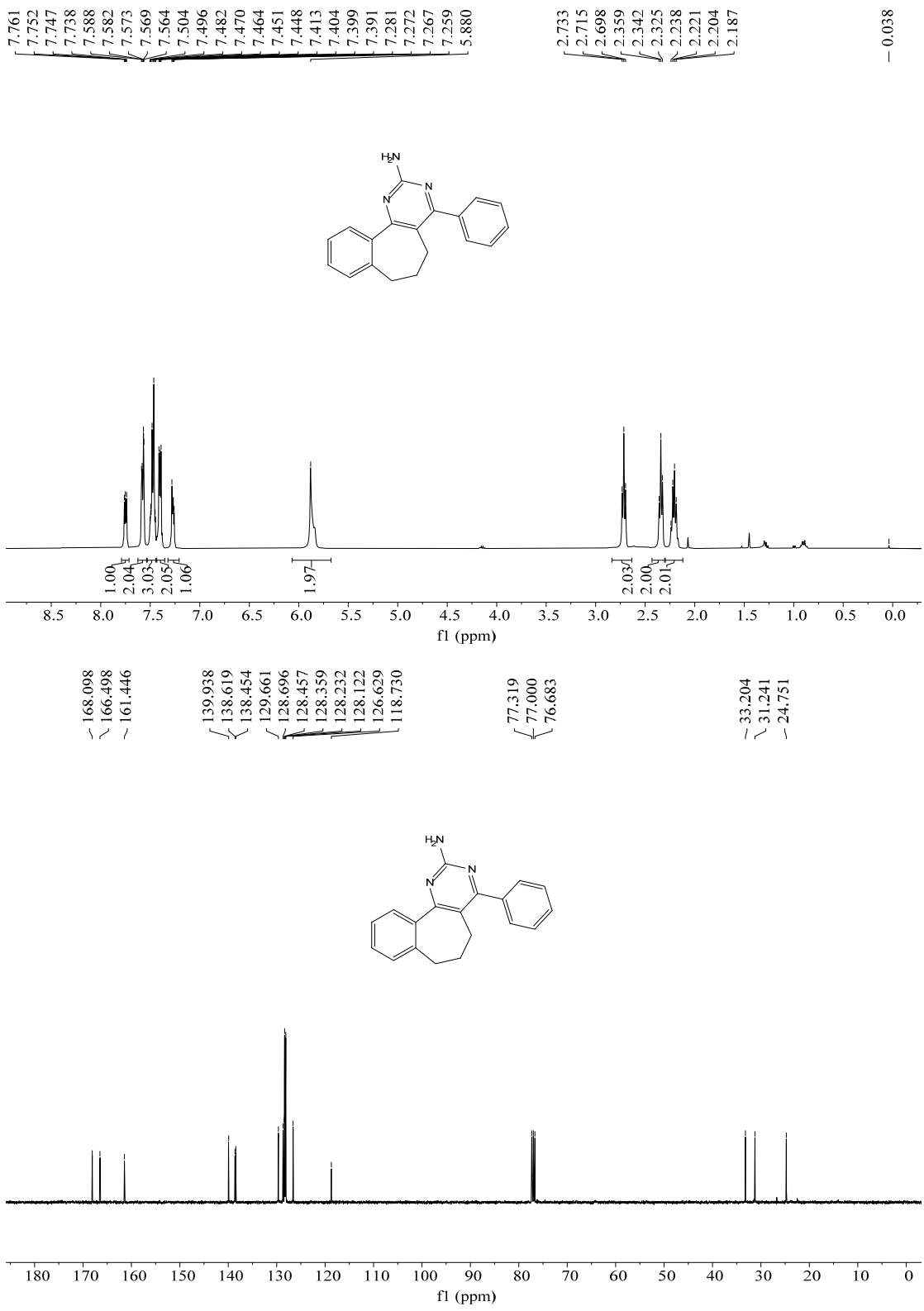




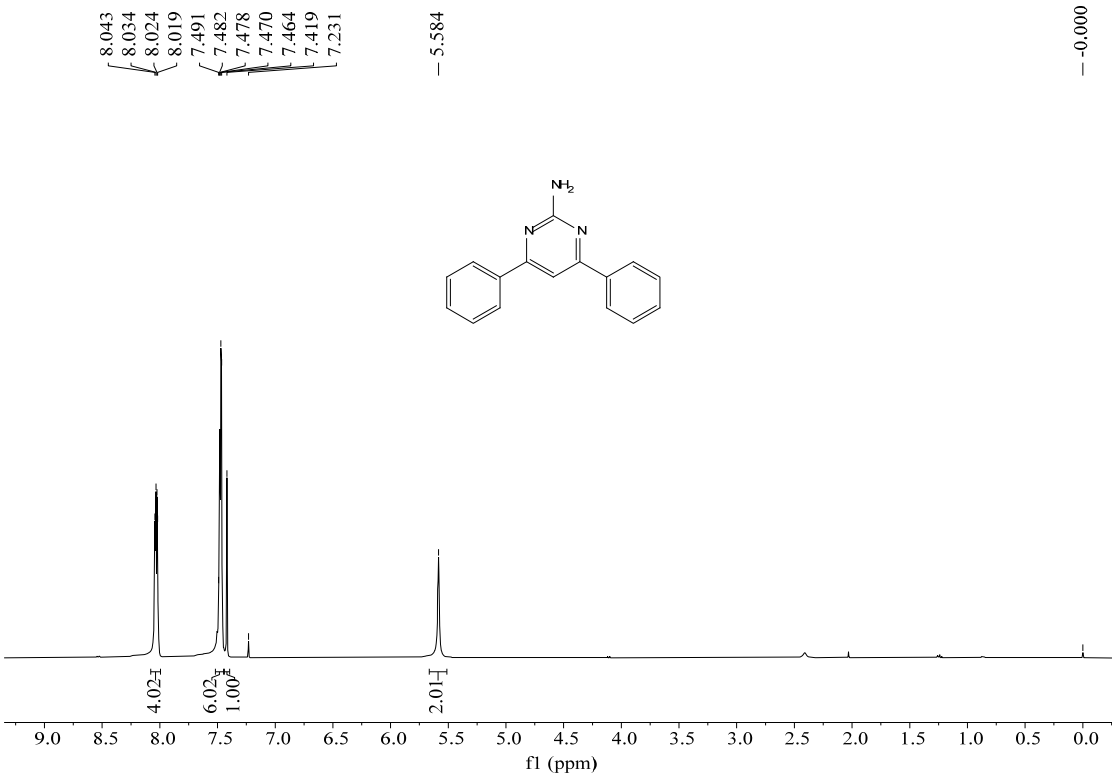
^{1}H and ^{13}C NMR spectra of **4j**

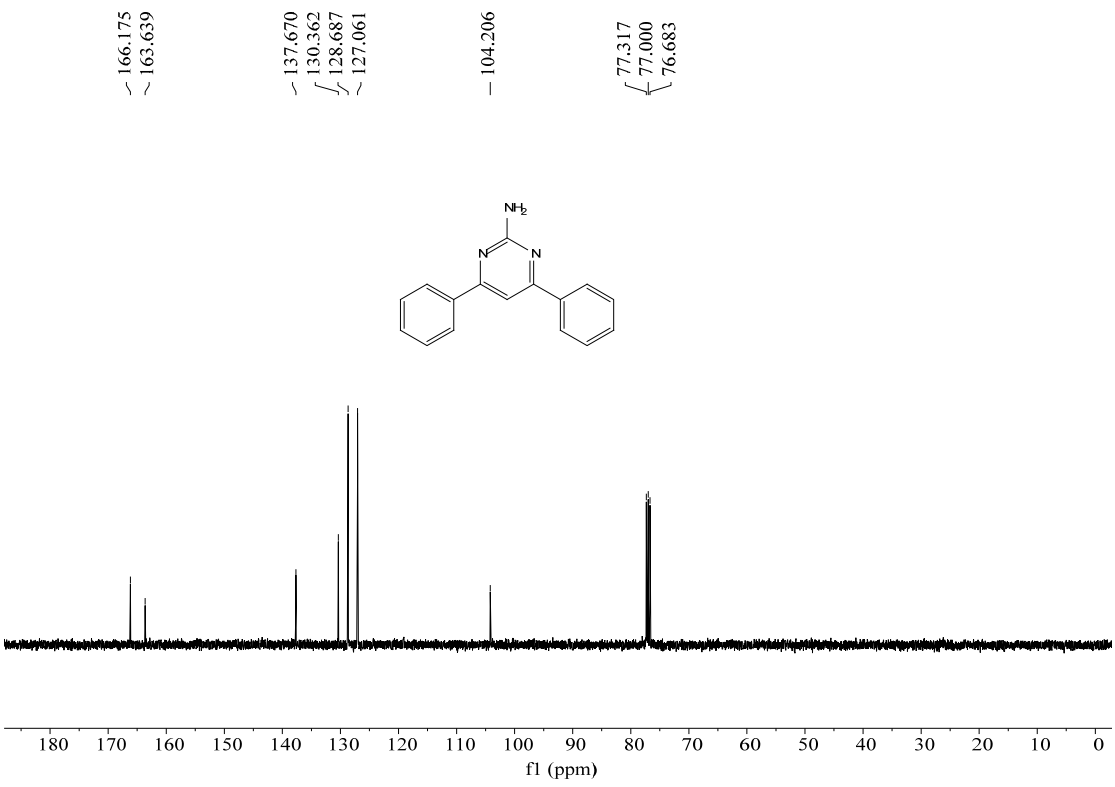


^{1}H and ^{13}C NMR spectra of **4k**

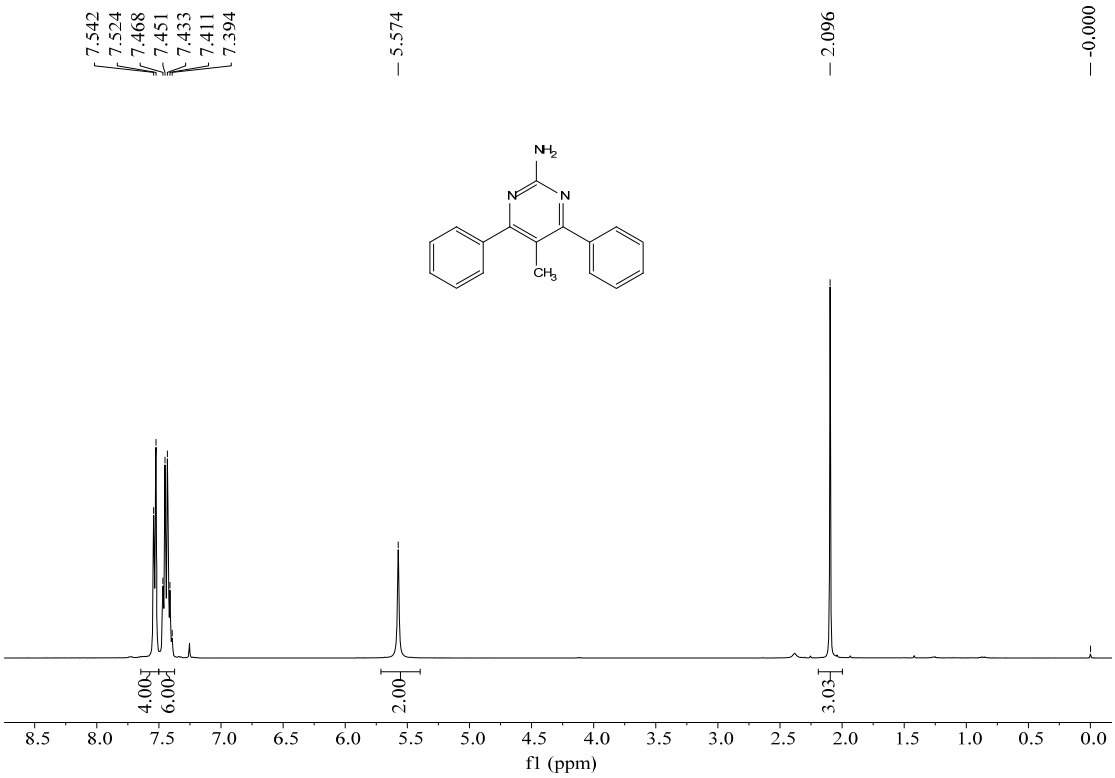


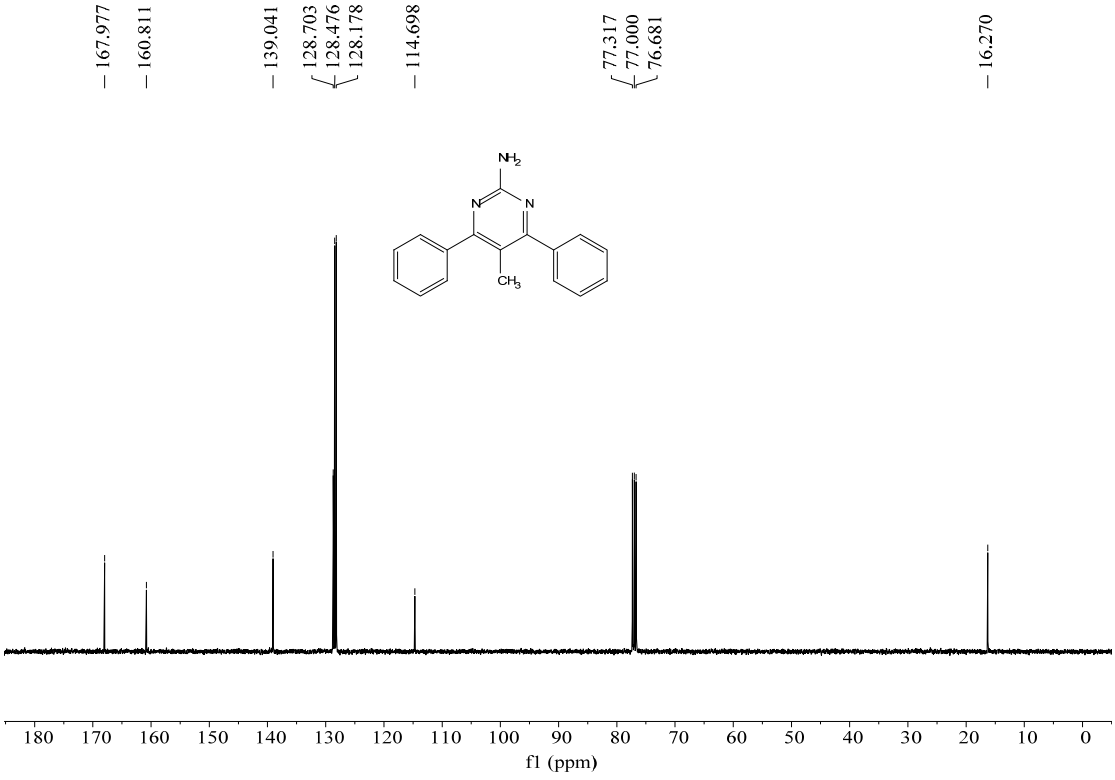
^{1}H and ^{13}C NMR spectra of **4l**



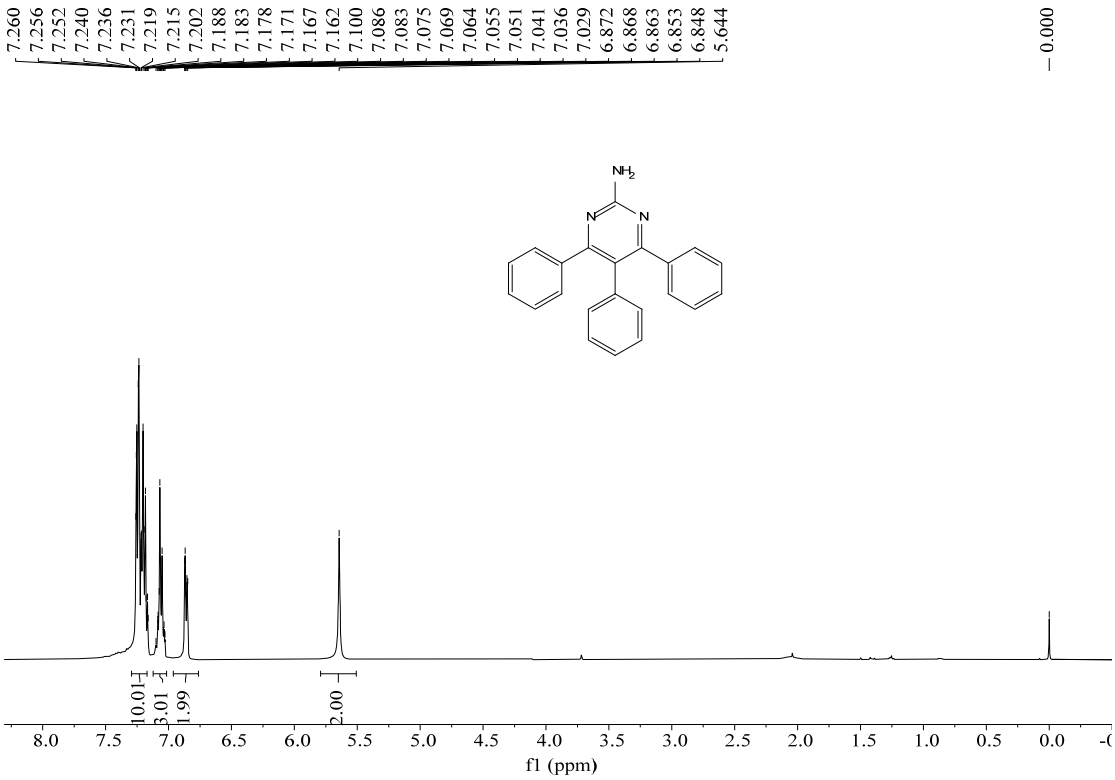


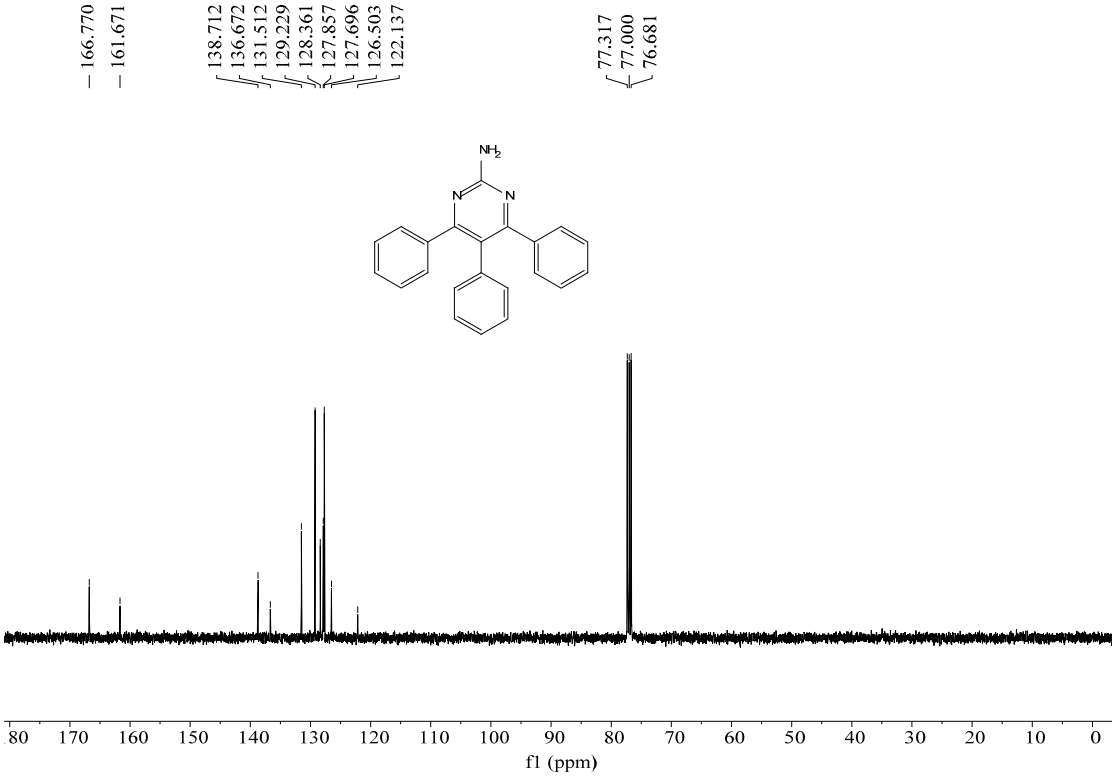
^{1}H and ^{13}C NMR spectra of **4m**



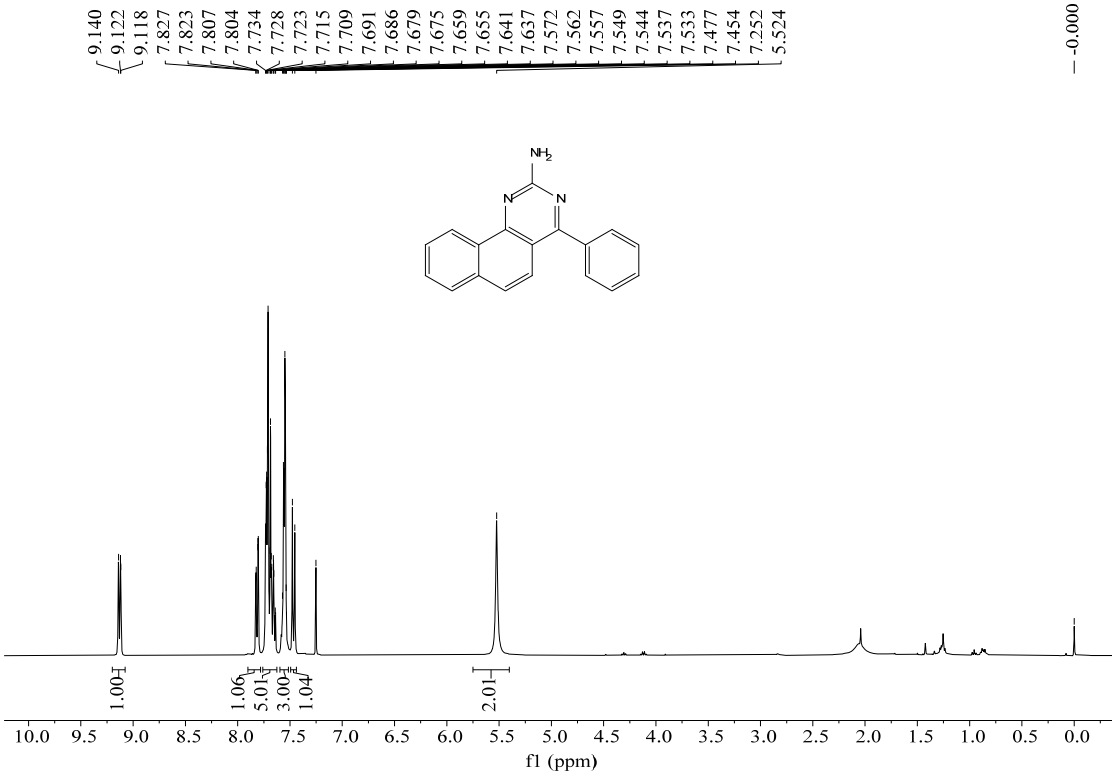


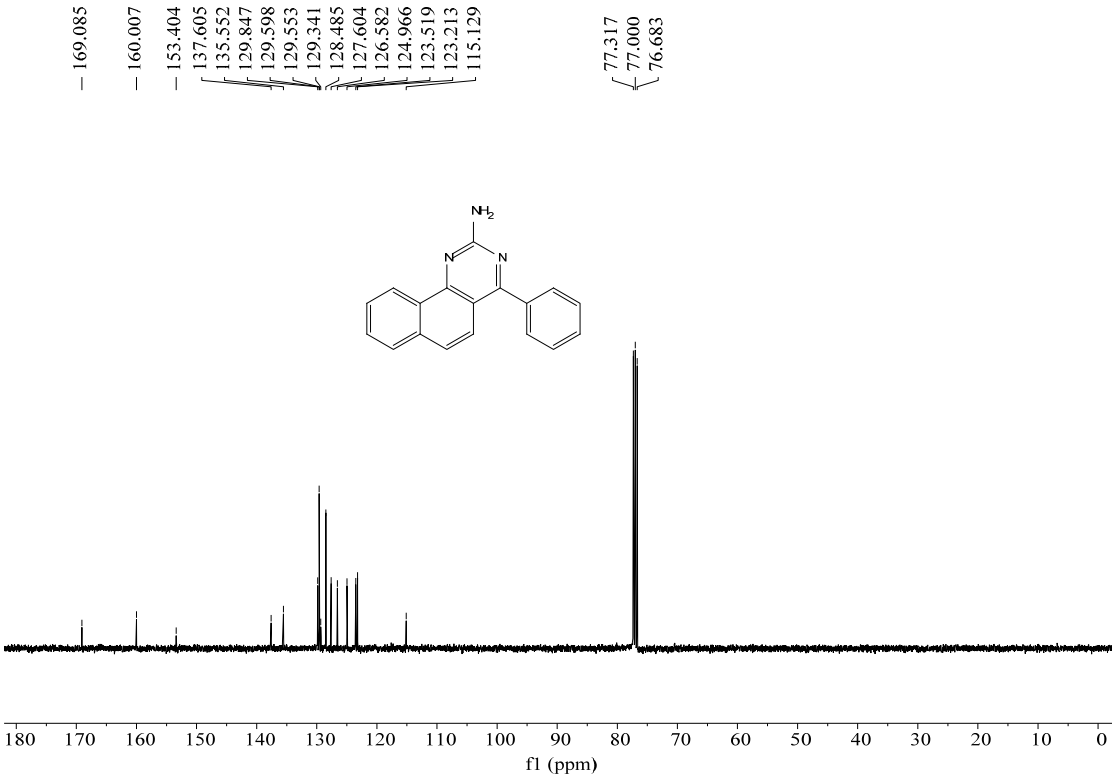
^{1}H and ^{13}C NMR spectra of **4n**





^{1}H and ^{13}C NMR spectra of **6a**





^{1}H and ^{13}C NMR spectra of **6b**