Electronic Supplementary Information

Metal-free Intramolecular Oxidative Decarboxylative Amination of Primary α-Amino Acids with Product Selectivity

Yizhe Yan and Zhiyong Wang*

Hefei National Laboratory for Physical Sciences at Microscale, CAS Key Laboratory of Soft Matter Chemistry and Department of Chemistry, University of Science and Technology of China, Hefei, 230026, P. R. China. Fax: (+86) 551-360-3185; E-mail: zwang3@ustc.edu.cn

Contents

General information

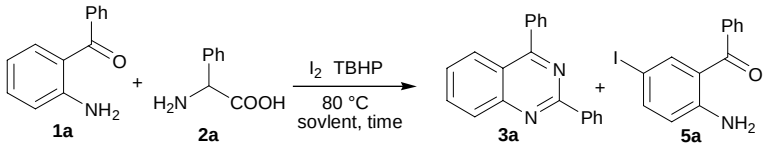
Unless otherwise indicated, all compounds and reagents were purchased from commercial suppliers and used without further purification. All chemical shifts (δ) are given in ppm. NMR spectra were recorded on Brucker AVANCE 300 or NMR spectrometer or Brucker AVANCE III 400 NMR spectrometer. HRMS was recorded on a Micromass UK LTD GCT spectrometer.

General procedure for the synthesis of quinazolines

1a (39.4 mg, 0.2 mmol), **2a** (45.3 mg, 0.3 mmol), I_2 (25.4 mg, 0.1 mmol) and TBHP (55 μL of 70 % aqueous solution, 0.4 mmol) in DMA (0.5 mL) were heated at 80 °C for 18 h in a sealed tube. The completion of the reaction was monitored by TLC and purified by column chromatography over silica gel to give the pure product **3a** as a light yellow solid (44 mg, 78 % yield).

Further optimizing for the reaction conditions

Table ESI-1 Further optimizing for the reaction conditions [a]

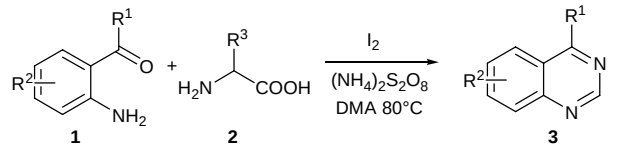


Entry	Sovlent	Time(h)	Yield(%)[b]	
			3a	**5a**
1	H_2O	18	0	85
2	MeOH	18	0	96
3	EtOH	18	0	84
4	*i*-PrOH	18	0	66
5	THF	18	0	41
6	Et_2O	18	0	98
7	CH_2Cl_2	18	0	90
8	DMA	0.5	6	0
9	DMA	1	33	0
10	DMA	2	49	0
11	DMA	4	64	0
12	DMA	6	67	0
13	DMA	12	79	0
14	DMA	18	85	0
15	DMA	36	85	0

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.3 mmol), I_2 (0.1 mmol), TBHP (0.4 mmol), sovlent (0.5 mL), 80 °C. [b] Determined by GC-MS analysis using an internal strandard.

Further investigation for oxidative decarboxylative coupling

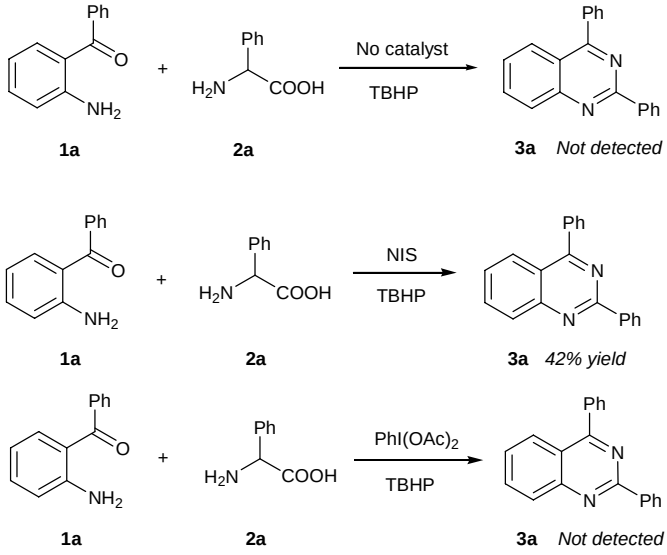
Table ESI-2 $I_2/(NH_4)_2S_2O_8$-mediated oxidative decarboxylative coupling [a]



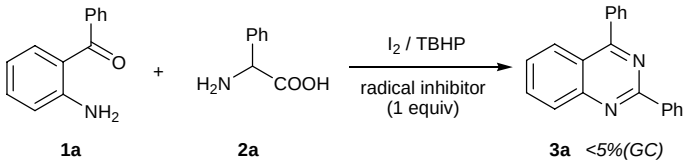
Entry	R^1	R^2	R^3	Product	Yield(%)[b]
1	Ph	H	Ph	**3r**	45
2	Ph	H	Me	**3r**	50
3	Ph	H	*i*-Pr	**3r**	60
4	4-F-Ph	H	*i*-Pr	**3s**	58
5	4-Br-Ph	H	*i*-Pr	**3t**	56
6	4-Me-Ph	H	*i*-Pr	**3u**	55
7	Ph	5-Cl	*i*-Pr	**3v**	65
8	Ph	5-Br	*i*-Pr	**3w**	64
9[c]	Ph	H	*i*-Pr	**4r**	50

[a] Reaction conditions: **1** (0.2 mmol), **2** (0.3 mmol), I_2 (0.02 mmol), $(NH_4)_2S_2O_8$ (0.6 mmol), DMA (0.5 mL), 80 °C. [b] isolated yield. [c] 1 equiv. of iodine was used.

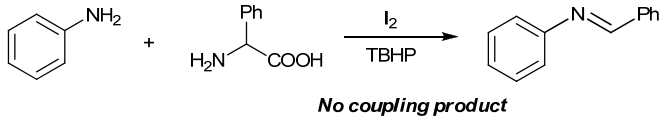
Control experiments about mechanism



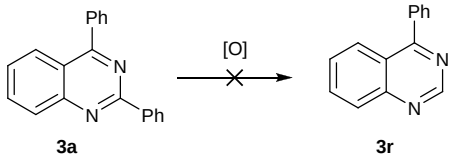
Scheme ESI-1 The effect of iodine



Scheme ESI-2 Radical trapping experiments



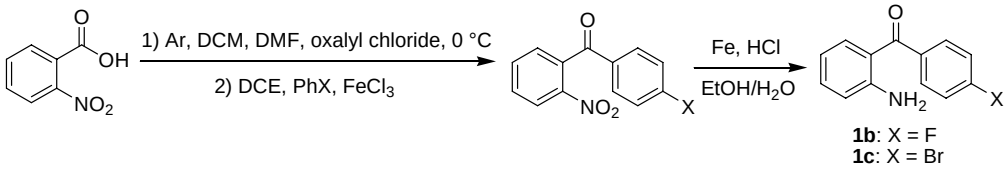
Scheme ESI-3 Intermolecular oxidative decarboxylative coupling of phenylglycine



Scheme ESI-4

Synthesis of substrates

Synthesis of **1b** and **1c** [1]



Scheme ESI-5 Synthesis of **1b** and **1c**

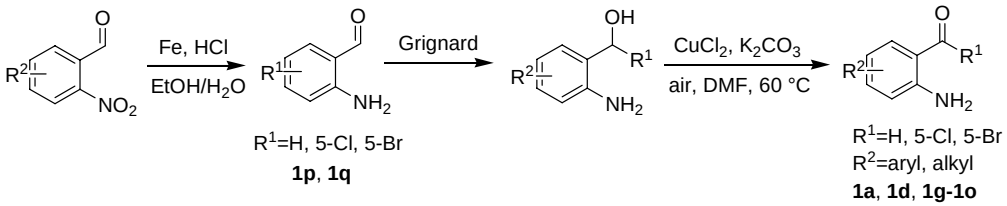
o-nitrobenzoic acid (5.014 g, 29.9 mmol) and anhydrous DMF (0.1 mL) were dissolved in dry DCM (105 mL) under argon. After cooling to 0 ºC, oxalyl chloride (5.2 mL, 60 mmol) was added slowly. The mixture was stirred at 0 °C for 30 min. Subsequently, the mixture was concentrated to leave the crude acid chloride as a light yellow oil. The oil was directly dissolved in 1, 2-dichloroethane (11.6 mL) and fluorobenzene (4.5 mL, 48 mmol). After cooling to 0 ºC. anhydrous iron (III) chloride (5.35 g, 33.0 mmol) was added to the reaction system, and the reaction was stirred at 0 ºC for 1 h. Then the reaction mixture was poured into ice-water (60 mL), and heated at 95 ºC to remove 1, 2-dichloroethane. When the temperature reached 75 ºC, isobutanol (20 mL) was added and the hot solution was washed with water. After cooling to room temperature, the precipitate was collected and washed with water to give the ((4-fluorophenyl)(2-nitrophenyl)methanone as a light brown solid.

Two drops of concentrated HCl were added to the solution of ((4-fluorophenyl)(2-nitrophenyl)methanone (999 mg, 4.0 mmol) in EtOH (12 mL) and water (3 mL) with iron powder (291 mg, 5.2 mmol). The reaction was refluxed at 80 ºC for 2 h, filtrated through silica gel and washed with EtOAc. The filtrate was extracted with EtOAc for three times,

washed with brine and dried over Na_2SO_4. The organic phase was concentrated in vacuum and purified by chromatographic column on silica gel, giving (2-aminophenyl)(4-fluorophenyl)methanone (**1b**) as a light yellow solid .

1c was synthesized according to the procedure for **1b**.

Synthesis of **1a**, **1d**, **1g-1q**



Scheme ESI-6 Synthesis of **1a**, **1d**, **1g-1q**

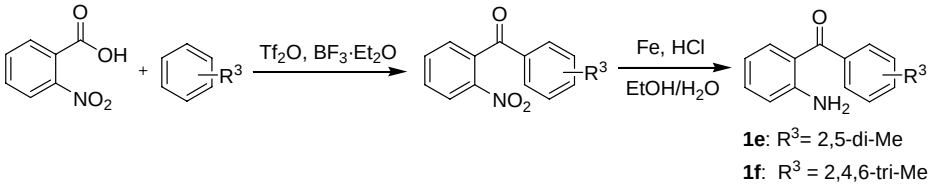
2-aminobenzaldehyde was synthesized with 2-nitrobenzaldehyde according to the procedure for (2-aminophenyl)(4-fluorophenyl)methanone.

Subsequently, phenylmagnesium bromide (51.6 mL, 1 M in THF, 51.6 mmol) was added to the solution of 2-aminobenzaldehyde (1.046 g, 8.6 mmol) in dry Et_2O (20 mL) dropwise. After the completion, the reaction was quenched with saturated NH_4Cl aqueous solution, and extracted with Et_2O for three times. The organic phase was washed with water and brine, and dried over Na_2SO_4. Then the organic phase was concentrated in vacuum, and purified by chromatographic column on silica gel, giving (2-aminophenyl)(phenyl)methanol as a light yellow solid.

(2-aminophenyl)(phenyl)methanol (426 mg, 2 mmol) was dissolved in DMF (15 mL) with $CuCl_2 \cdot H_2O$ (34.1 mg, 0.2 mmol) and K_2CO_3 (552 mg, 4 mmol). The mixture was stirred at 60 °C under air for 24 h. Then the reaction mixture was diluted with water, extracted with EtOAc for three times, washed with water for three times and brine once, and dried over Na_2SO_4. The organic phase was concentrated in vacuum, and purified by chromatographic column on silica gel, giving (2-aminophenyl)(phenyl)methanone (**1a)** as a light yellow solid.

1d, 1g-1q were synthesized according to the procedure for **1a**.

Synthesis of **1e** and **1f** [2]



Scheme ESI-7 Synthesis of **1e** and **1f**

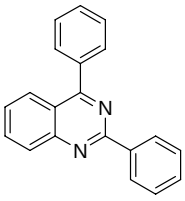
The mixture of 2-nitrobenzoic acid (1.997 g, 12 mmol) and trifluoroacetic anhydride (4 g, 19 mmol) was stirred and cooled in ice bath. Then boron trifluoride-ether (1.701 g, 12 mmol) was added to the solution dropwise. The deep red solution was dropped to *p*-xylene (1.988g, 18.75 mmol) in ice bath, and stirred for 2 h. Then the reaction mixture was poured onto ice and extracted with chloroform. The extract was washed with aqueous sodium hydroxide (40%), dried over Na_2SO_4, and concentrated to give a white solid. After recrystallization from EtOH, (2,5-dimethylphenyl)(2-nitrophenyl)methanone was obtained as white needles.

(2-aminophenyl)(2,5-dimethylphenyl)methanone (**1e**) was obtained according to the procedure for (2-aminophenyl)(4-fluorophenyl)methanone.

1f was synthesized according to the procedure for **1e**.

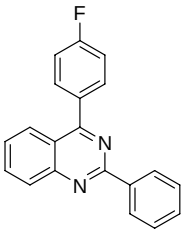
Characterization data for the products

2,4-diphenylquinazoline (3a) [3]



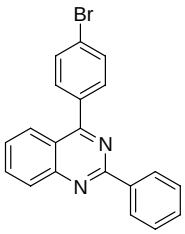
A light yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.72-8.68 (m, 2 H), 8.15 (d, *J* = 8.8 Hz, 1 H), 7.92-7.86 (m, 3 H), 7.61-7.50 (m, 7 H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 168.3, 160.3, 152.1, 138.3, 137.8, 133.6, 130.6, 130.3, 130.0, 129.3, 128.8, 128.6, 127.0, 121.8. HRMS calc. $C_{20}H_{14}N_2$: 282.1157, found: 282.1155.

4-(4-fluorophenyl)-2-phenylquinazoline (3b) [3]



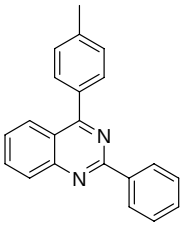
A light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.70-8.66 (m, 2 H), 8.15 (d, *J* = 8.8 Hz, 1 H), 8.08 (d, *J* = 8.4 Hz, 1 H), 7.92-7.86 (m, 3 H), 7.58-7.49 (m, 4 H), 7.31-7.24 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 167.2, 164.1 (d, *J* = 248.8 Hz) 160.3, 152.2, 138.2, 133.9 (d, *J* = 3.3 Hz), 133.7, 132.3 (d, *J* = 8.4 Hz), 130.7, 129.4, 128.8, 128.7, 127.2, 126.8, 121.7, 115.8 (d, *J* = 21.5 Hz). HRMS calc. $C_{20}H_{13}FN_2$: 300.1063, found: 300.1060.

4-(4-bromophenyl)-2-phenylquinazoline (3c) [3]



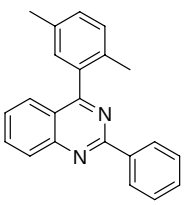
A light yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.69-8.65 (m, 2 H), 8.16 (d, *J* = 8.4 Hz, 1 H), 8.06 (d, *J* = 8.4 Hz, 1 H), 7.92-7.86 (m, 1 H), 7.79-7.71 (m, 4 H), 7.59-7.49 (m, 4 H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 167.2, 160.3, 152.2, 138.1, 136.7, 133.8, 131.90, 131.86, 130.7, 129.4, 128.8, 128.7, 127.3, 126.6, 124.7, 121.5. HRMS calc. $C_{20}H_{13}BrN_2$: 360.0262, found: 360.0261.

2-phenyl-4-*p*-tolylquinazoline (3d) [3]



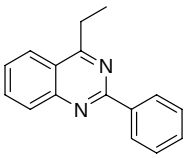
A white solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.71-8.68 (m, 2 H), 8.13 (d, *J* = 8.4 Hz, 2 H), 7.87-7.77 (m, 3 H), 7.52-7.47 (m, 4 H), 7.38 (d, *J* = 8.1 Hz, 2 H), 2.48 (s, 3 H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 168.4, 160.3, 152.1, 140.3, 138.4, 135.0, 133.5, 130.5, 130.3, 129.4, 129.3, 128.8, 128.6, 127.2, 127.0, 121.8, 21.6. HRMS calc. $C_{21}H_{16}N_2$: 296.1313, found: 296.1311.

4-(2,5-dimethylphenyl)-2-phenylquinazoline (3e) [3]



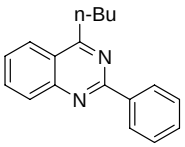
A light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.67-8.64 (m, 2 H), 8.14 (d, *J* = 8.4 Hz, 1 H), 7.88-7.85 (m, 1 H), 7.70-7.67 (m, 1 H), 7.52-7.48 (m, 4 H), 7.28-7.21 (m, 3 H), 2.40 (s, 3 H), 2.16 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 170.2, 160.5, 151.6, 138.4, 137.0, 135.3, 133.8, 133.4, 130.7, 130.6, 130.2, 130.1, 129.1, 128.9, 128.6, 127.3, 127.1, 122.8, 21.1, 19.6. HRMS calc. $C_{22}H_{18}N_2$: 310.1470, found: 310.1467.

4-ethyl-2-phenylquinazoline (3g) [3]



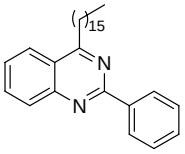
A light yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.68-8.64 (m, 2 H), 8.13-8.06 (m, 2 H), 7.88-7.81 (m, 1 H), 7.60-7.48 (m, 4 H), 3.38 (q, *J* = 7.5 Hz, 2 H), 1.54 (t, *J* = 7.5 Hz, 3 H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 172.2, 160.2, 150.7, 138.6, 133.4, 130.5, 129.5, 128.7, 128.6, 126.9, 124.6, 122.4, 27.8, 12.5. HRMS calc. $C_{16}H_{14}N_2$: 234.1157, found: 234.1156.

4-butyl-2-phenylquinazoline (3h) [3]



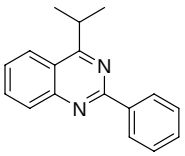
A yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.66-8.62 (m, 2 H), 8.13-8.05 (m, 2 H), 7.87-7.81 (m, 1 H), 7.59-7.48 (m, 4 H), 3.33 (t, *J* = 7.5 Hz, 2 H), 2.00-1.94 (m, 2 H), 1.54 (q, *J* = 7.5 Hz, 2 H), 1.02 (t, *J* = 7.5 Hz, 3 H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 171.6, 160.2, 150.8, 138.6, 133.3, 130.4, 129.5, 128.7, 128.6, 126.8, 124.7, 122.6, 34.4, 30.8, 22.9, 14.1. HRMS calc. $C_{18}H_{18}N_2$: 262.1470, found: 262.1473.

4-hexadecyl-2-phenylquinazoline (3i) [3]



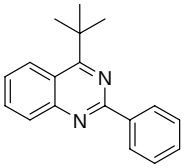
A yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.66-8.63 (m, 2 H), 8.12-8.06 (m, 2 H), 7.86- 7.81 (m, 1 H), 7.58-7.48 (m, 4 H), 3.32 (t, *J* = 7.6 Hz, 2 H), 2.00-1.94 (m, 2 H), 1.53-1.47 (m, 2 H), 1.42-1.36 (m, 2 H), 1.26-1.20 (m, 22 H), 0.88 (t, *J* = 6.4 Hz, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 171.6, 160.2, 150.9, 138.6, 133.3, 130.4, 129.6, 128.7, 128.6, 126.8, 124.7, 122.7, 34.7, 32.1, 29.85, 29.82, 29.74, 29.67, 29.5, 28.7, 22.8, 14.2. HRMS calc. $C_{30}H_{42}N_2$: 430.3348, found: 430.3345.

4-isopropyl-2-phenylquinazoline (3j) [3]



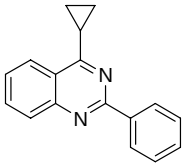
A yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.70-8.66 (m, 2 H), 8.17-8.07 (m, 2 H), 7.87- 7.80 (m, 1 H), 7.59-7.48 (m, 4 H), 4.00-3.90 (m, 1 H), 1.52 (s, 3 H), 1.50 (s, 3 H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 175.6, 151.1, 138.7, 133.2, 130.5, 129.7, 128.7, 128.6, 126.7, 124.2, 121.8, 31.3, 21.9. HRMS calc. $C_{17}H_{16}N_2$: 248.1313, found: 248.1317.

4-tert-butyl-2-phenylquinazoline (3k) [3]



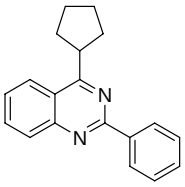
A yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.70-8.66 (m, 2 H), 8.44 (dd, J_1 = 8.8 Hz, J_2 = 0.8 Hz, 1 H), 8.11 (dd, J_1 = 8.4 Hz, J_2 = 0.4 Hz, 1 H), 7.82-7.78 (m, 1 H), 7.55-7.48 (m, 4 H), 1.72 (s, 9 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 176.5, 159.0, 152.2, 138.7, 132.4, 130.52, 130.48, 128.7, 128.6, 126.6, 125.7, 121.7, 40.7, 30.8. HRMS calc. $C_{18}H_{18}N_2$: 262.1470, found: 262.1469.

4-cyclopropyl-2-phenylquinazoline (3l) [3]



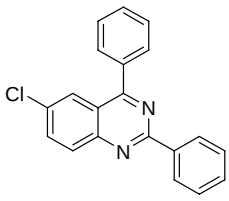
A yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.61-8.57 (m, 2 H), 8.27 (d, J = 8.4 Hz, 1 H), 8.05 (d, J = 8.4 Hz, 1 H), 7.86-7.79 (m, 1 H), 7.58-7.45 (m, 4 H), 2.83-2.74 (m, 1 H), 1.57-1.51 (m, 2 H), 1.28-1.21 (m, 2 H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 172.1, 159.9, 150.4, 138.6, 133.2, 130.3, 129.3, 128.53, 128.47, 126.6, 124.4, 123.0, 13.0, 12.2. HRMS calc. $C_{17}H_{14}N_2$: 246.1157, found: 246.1155.

4-cyclopentyl-2-phenylquinazoline (3m) [3]



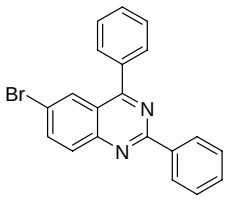
A yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.68-8.65 (m, 2 H), 8.18-8.15 (m, 1 H), 8.07 (d, J = 8.0 Hz, 1 H), 7.85-7.80 (m, 1 H), 7.58-7.47 (m, 4 H), 4.09-4.04 (m, 1 H), 2.25-2.14 (m, 4 H), 2.00-1.95 (m, 2 H), 1.85-1.80 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 174.5, 160.0, 151.0, 138.8, 133.1, 130.4, 129.5, 128.7, 128.6, 126.6, 124.7, 122.6, 42.7, 32.7, 26.4. HRMS calc. $C_{19}H_{18}N_2$: 274.1470, found: 274.1472.

6-chloro-2,4-diphenylquinazoline (3n) [3]



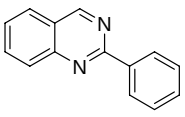
A white solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.69-8.66 (m, 2 H), 8.11-8.08 (m, 2 H), 7.88-7.78 (m, 3 H), 7.63-7.60 (m, 3 H), 7.56-7.51 (m, 3 H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 167.6, 160.6, 150.6, 137.9, 137.2, 134.6, 132.7, 131.0, 130.9, 130.3, 130.2, 128.8, 128.7, 125.9, 122.3. HRMS calc. $C_{20}H_{13}ClN_2$: 316.0767, found: 316.0764.

6-bromo-2,4-diphenylquinazoline (3o) [3]



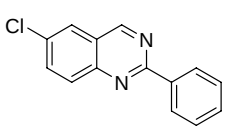
A white solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.69-8.65 (m, 2 H), 8.26-8.25 (m, 1 H), 8.04-8.00 (m, 1 H), 7.96-7.92 (m, 1 H), 7.88-7.84 (m, 2 H), 7.63-7.60 (m, 3 H), 7.55-7.50 (m, 3 H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 167.5, 160.6, 150.8, 137.9, 137.1, 131.1, 130.9, 130.3, 130.2, 129.2, 128.8, 128.7, 122.8, 120.7. HRMS calc. $C_{20}H_{13}BrN_2$: 360.0262, found: 360.0259.

2-phenylquinazoline (3p)



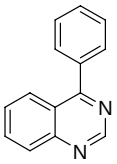
A yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.47 (s, 1 H), 8.64-8.61 (m, 2 H), 8.10 (dd, J_1 = 8.4 Hz, J_2 = 0.4 Hz, 1 H), 7.94-7.88 (m, 2 H), 7.64-7.59 (m, 1 H), 7.56-7.50 (m, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 161.2, 160.6, 150.9, 138.2, 134.3, 130.8, 128.80, 128.79, 128.7, 127.4, 127.3, 123.8. HRMS calc. $C_{14}H_{10}N_2$: 206.0844, found: 206.0845.

6-chloro-2-phenylquinazoline (3q) [3]



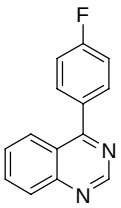
A light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.39 (s, 1 H), 8.62-8.58 (m, 2 H), 8.04 (d, *J* = 9.2 Hz, 1 H), 7.89 (d, *J* = 2.0 Hz, 1 H), 7.83-7.80 (m, 1 H), 7.56-7.50 (m, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 161.3, 159.7, 149.3, 137.5, 135.3, 133.0, 131.1, 130.5, 128.85, 128.78, 126.0, 124.1. HRMS calc. $C_{14}H_9ClN_2$: 240.0454, found: 240.0452.

4-phenylquinazoline (3r) [4]



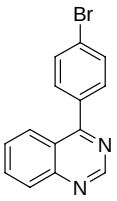
A needle-like solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.39 (s, 1 H), 8.24 (d, *J* = 8.8 Hz, 2 H), 7.95-7.90 (m, 1 H), 7.82-7.76 (m, 2 H), 7.64-7.56 (m, 4 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 168.6, 154.7, 151.1, 137.2, 133.9, 130.2, 130.1, 128.9, 128.8, 127.9, 127.2, 123.3. HRMS calc. $C_{14}H_{10}N_2$: 206.0844, found: 206.0841.

4-(4-fluorophenyl)quinazoline (3s)



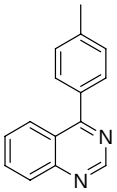
A light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.37 (s, 1 H), 8.13 (dd, J_1 = 13.2 Hz, J_2 = 8.4 Hz, 2 H), 7.96-7.91 (m, 1 H), 7.83-7.79 (m, 2 H), 7.67-7.62 (m, 1 H), 7.31-7.26 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 167.5, 164.2 (d, *J* = 249.2 Hz), 154.6, 151.2, 134.0, 133.3 (d, *J* = 3.2 Hz), 132.2 (d, *J* = 8.5 Hz), 129.1, 128.1, 126.9, 123.2, 116.0 (d, *J* = 21.8 Hz). HRMS calc. $C_{14}H_9FN_2$: 224.0750, found: 224.0754.

4-(4-bromophenyl)quinazoline (3t)



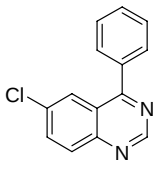
A white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.38 (s, 1 H), 8.16-8.07 (m, 2 H), 7.96-7.91 (m, 1 H), 7.75-7.61 (m, 5 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 167.4, 154.7, 151.8, 136.1, 134.0, 132.1, 131.7, 129.2, 128.1, 126.8, 125.0, 123.1. HRMS calc. $C_{14}H_9BrN_2$: 283.9949, found: 283.9946.

4-*p*-tolylquinazoline (3u) [5]



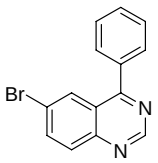
A yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.37 (s, 1 H), 8.18-8.09 (m, 2 H), 7.93-7.88 (m, 1 H), 7.71-7.69 (m, 2 H), 7.63-7.37 (m, 1 H), 7.39 (d, *J* = 8.0 Hz, 2 H), 2.48 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 168.6, 154.8, 151.3, 140.5, 134.5, 133.7, 130.1, 129.5, 129.0, 127.7, 127.3, 123.4, 21.6. HRMS calc. $C_{15}H_{12}N_2$: 220.1000, found: 220.1000.

6-chloro-4-phenylquinazoline (3v) [6]



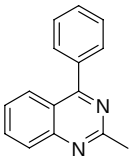
A light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.38 (s, 1 H), 8.12-8.06 (m, 2 H), 7.87-7.84 (m, 1 H), 7.79-7.75 (m, 2 H), 7.63-7.58 (m, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 167.8, 154.9, 149.7, 136.7, 134.9, 133.7, 130.8, 130.5, 130.0, 129.0, 126.0, 123.8. HRMS calc. $C_{14}H_9ClN_2$: 240.0454, found: 240.0455.

6-bromo-4-phenylquinazoline (3w)



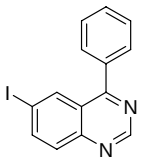
A light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.39 (s, 1 H), 8.28 (d, J = 1.2 Hz, 1 H), 8.00-7.96 (m, 2 H), 7.79-7.74 (m, 2 H), 7.63-7.58 (m, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 167.7, 155.0, 149.9, 137.4, 136.6, 130.8, 130.6, 130.0, 129.3, 129.0, 124.3, 121.8. HRMS calc. $C_{14}H_9BrN_2$: 283.9949, found: 283.9952.

2-methyl-4-phenylquinazoline (3x)



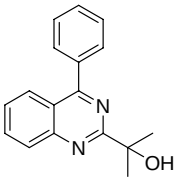
A yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.07-8.02 (m, 2 H), 7.90-7.87 (m, 1 H), 7.77-7.74 (m, 2 H), 7.59-7.52 (m, 4 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 168.8, 164.0, 154.8, 137.4, 133.8, 130.03, 130.00, 128.8, 128.2, 127.2, 126.9, 121.2, 26.7. HRMS calc. $C_{15}H_{12}N_2$: 220.1000, found: 220.1002.

6-iodo-4-phenylquinazoline (4r)



A yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.39 (s, 1 H), 8.49 (d, J = 2.0 Hz, 1 H), 8.15 (dd, J_1 = 2.0 Hz, J_2 = 8.8 Hz, 1 H), 7.85 (d, J = 8.8 Hz, 1 H), 7.78-7.75 (m, 2 H), 7.63-7.58 (m, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 167.4, 155.1, 150.3, 142.6, 136.7, 135.9, 130.8, 130.5, 130.0, 129.0, 124.8, 93.3. HRMS calc. $C_{14}H_9IN_2$: 331.9810, found: 331.9814.

2-(4-phenylquinazolin-2-yl)propan-2-ol (4y)



A white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.17-8.12 (m, 2 H), 7.95-7.90 (m, 1 H), 7.84-7.80 (m, 2 H), 7.63-7.58 (m, 4 H), 1.74 (s, 6 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 170.1, 169.3, 150.2, 137.2, 134.3, 130.5, 130.4, 128.8, 128.3, 127.7, 127.4, 121.5, 29.9. HRMS calc. $C_{15}H_{12}N_2$: 264.1263, found: 264.1260.

References

1 C. M. Counceller, C. C. Eichman, B. C. Wray, J. P. Stambuli, *Org. Lett.* **2008**, *10*, 1021.

2 D. G. Kawkins, O. Meth-Cohn, *J. Chem. Soc., Perkin Trans. 1* **1983**, 2077.

3 J. T. Zhang, C. M. Yu, S. J. Wang, C. F. Wan, Z. Y. Wang, *Chem. Commun.* **2010**, *46*, 5244.

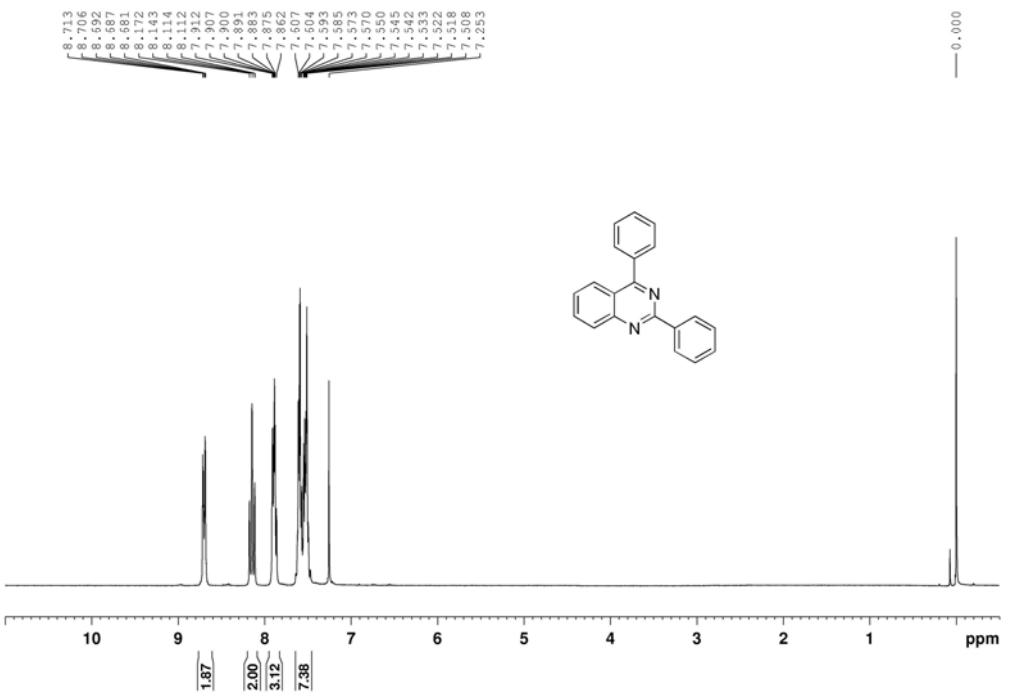
4 J. Bergman, A. Brynolf, B. Elman, E. Vuorinen, *Tetrahedron*, **1986**, *42*, 3697.

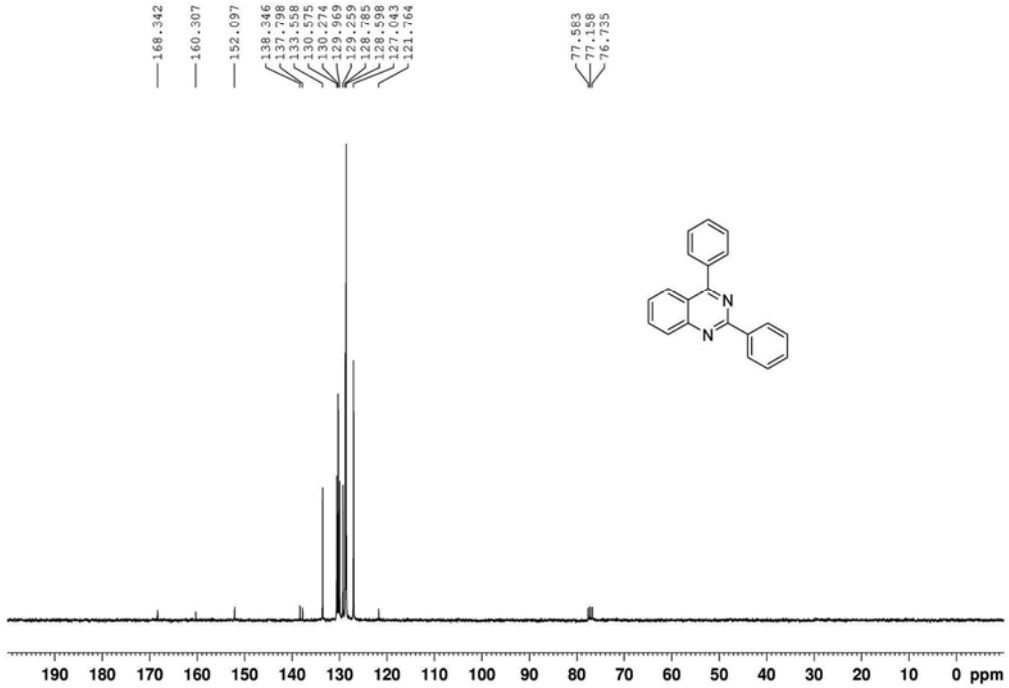
5 F.-A. Kang, Z. H. Sui, W. V. Murray, *J. Am. Chem. Soc.* **2008**, *130*, 11300.

6 M. Dabiri, P. Salehi, M. Bahramnejad. *Synth. Commun.* **2010**, *40*, 3214.

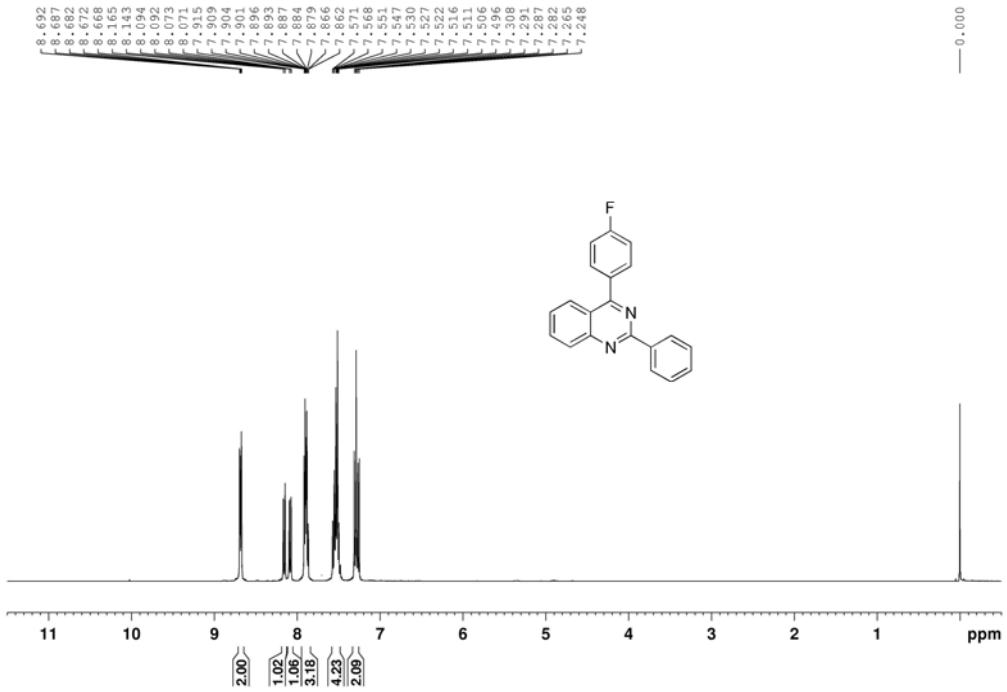
NMR spectra for the products

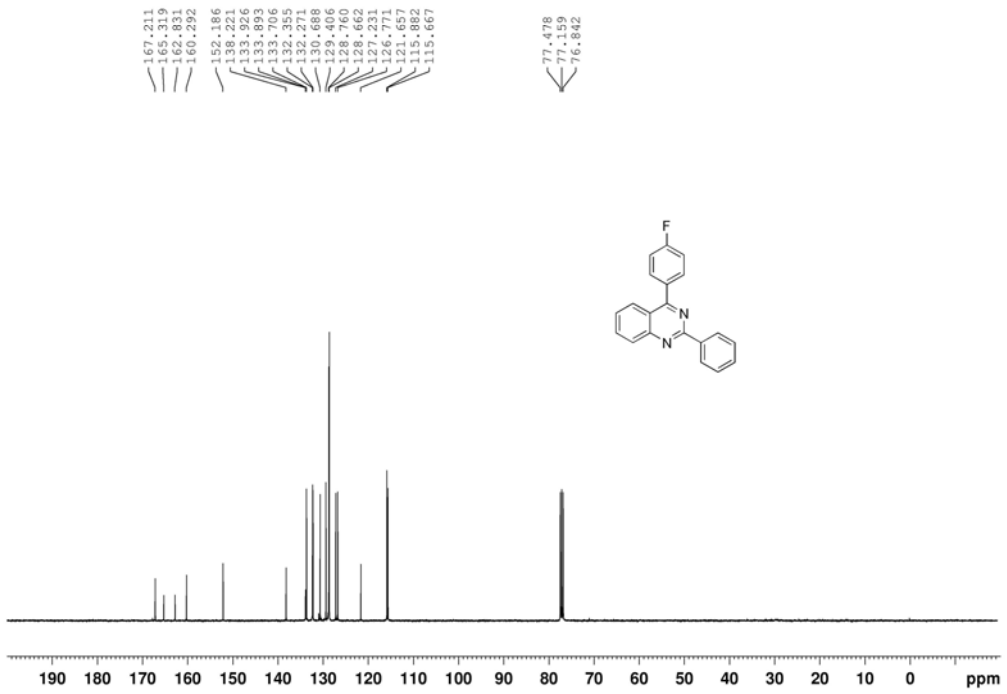
2,4-diphenylquinazoline (3a)



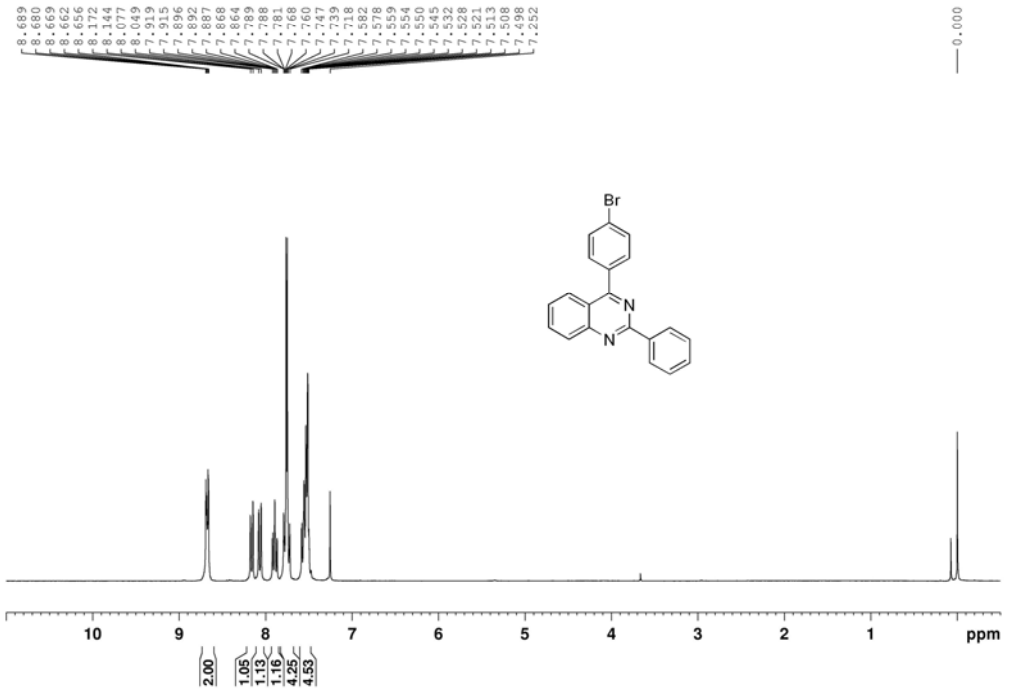


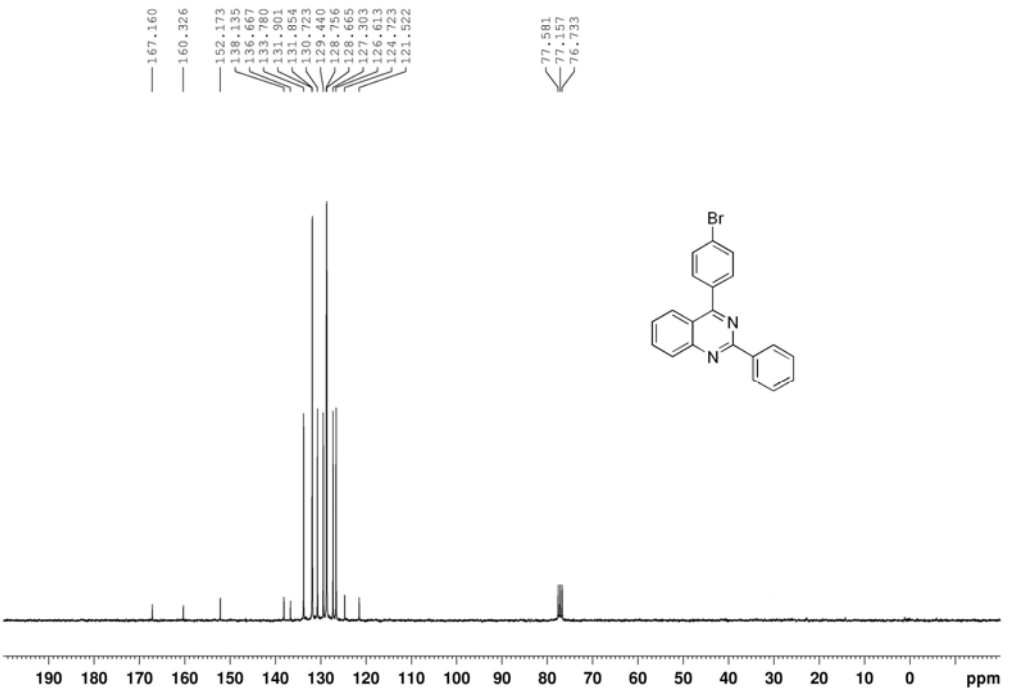
4-(4-fluorophenyl)-2-phenylquinazoline (3b)



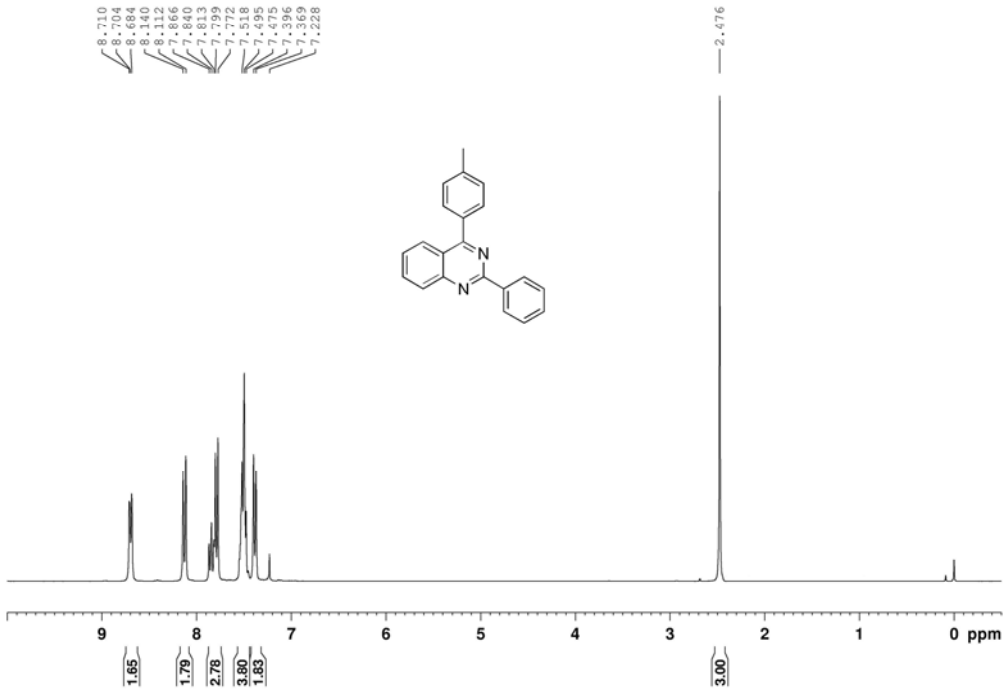


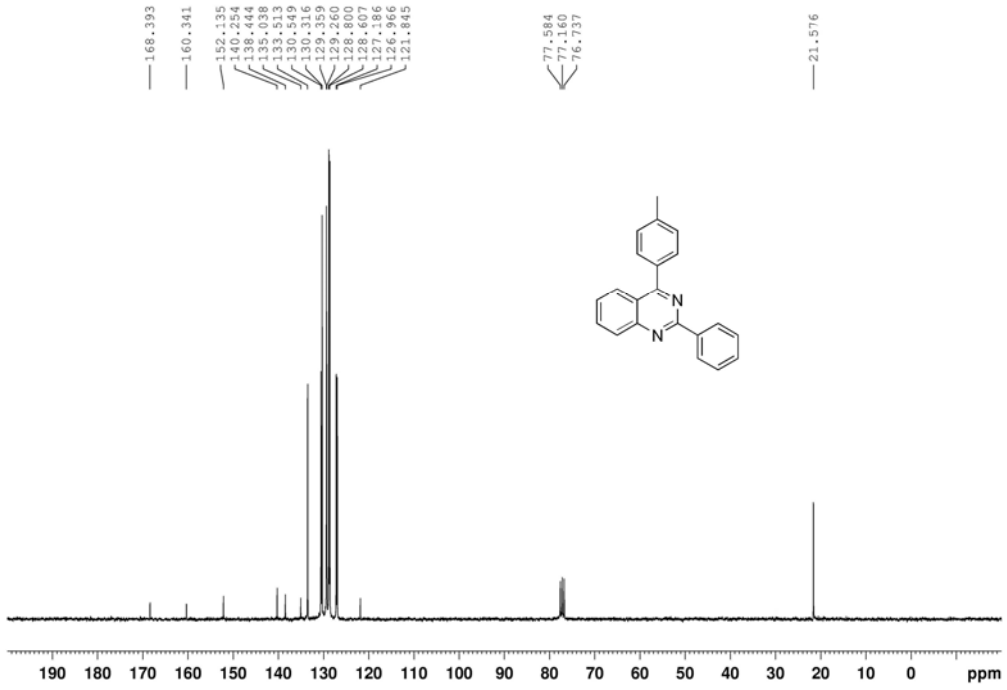
4-(4-bromophenyl)-2-phenylquinazoline (3c)



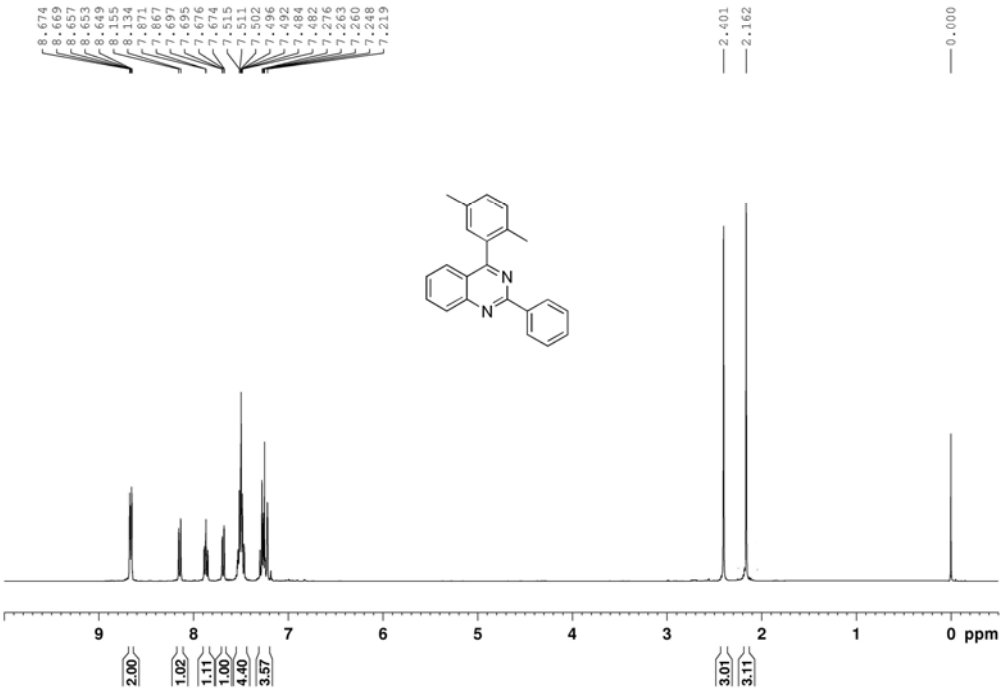


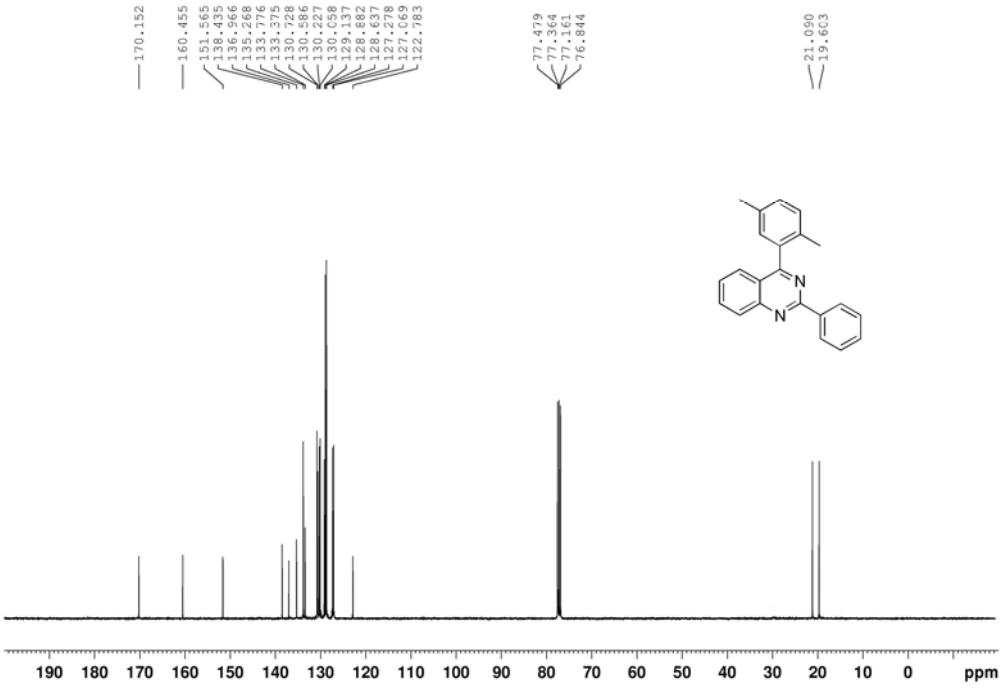
2-phenyl-4-*p*-tolylquinazoline (3d)



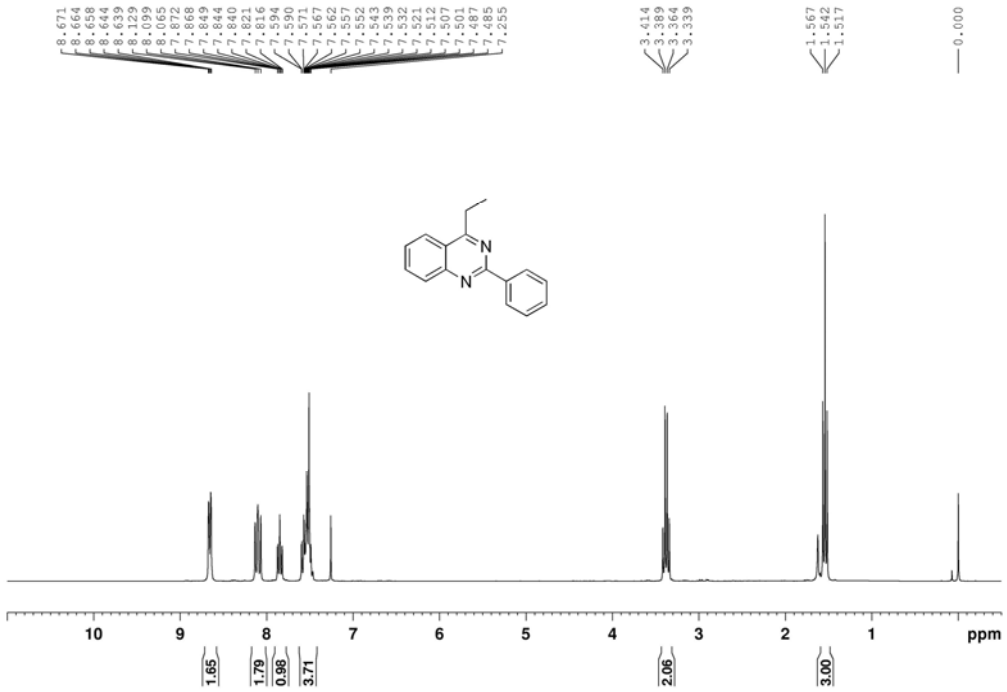


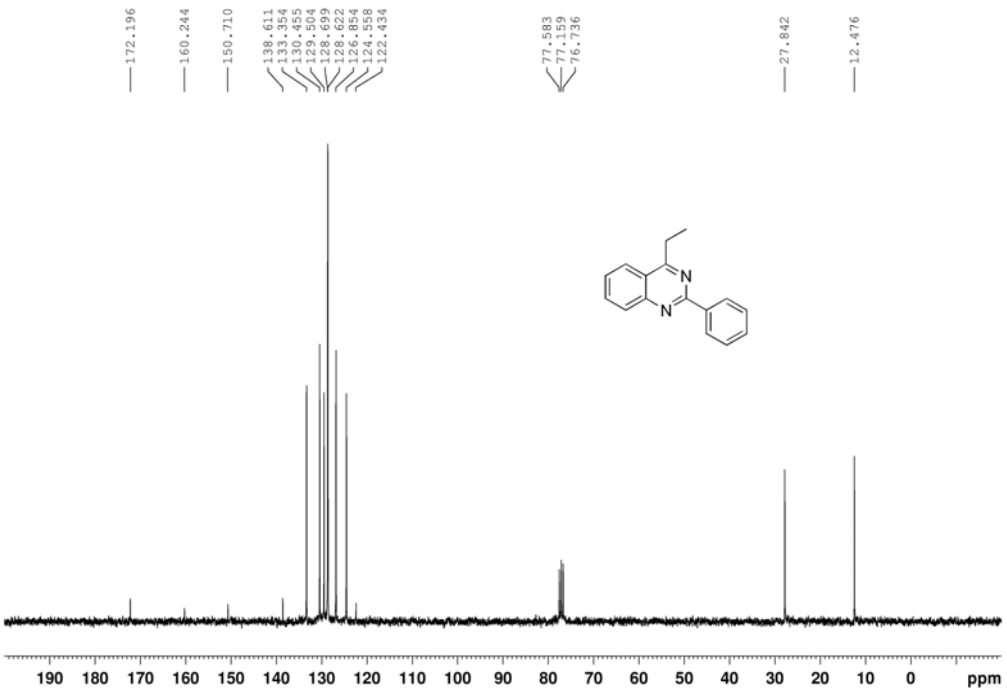
4-(2,5-dimethylphenyl)-2-phenylquinazoline (3e)



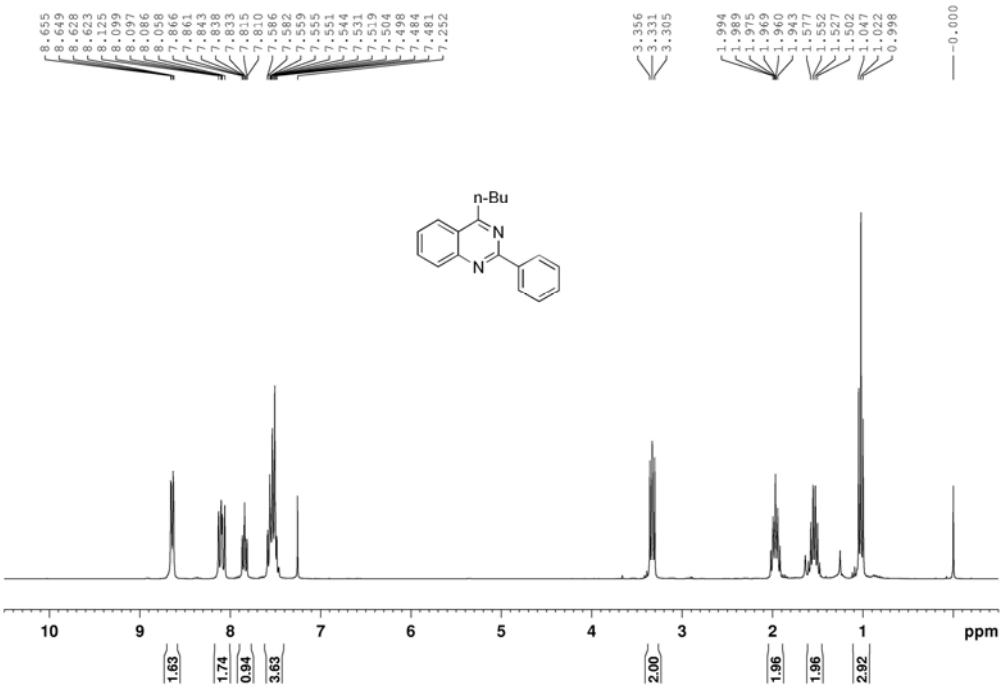


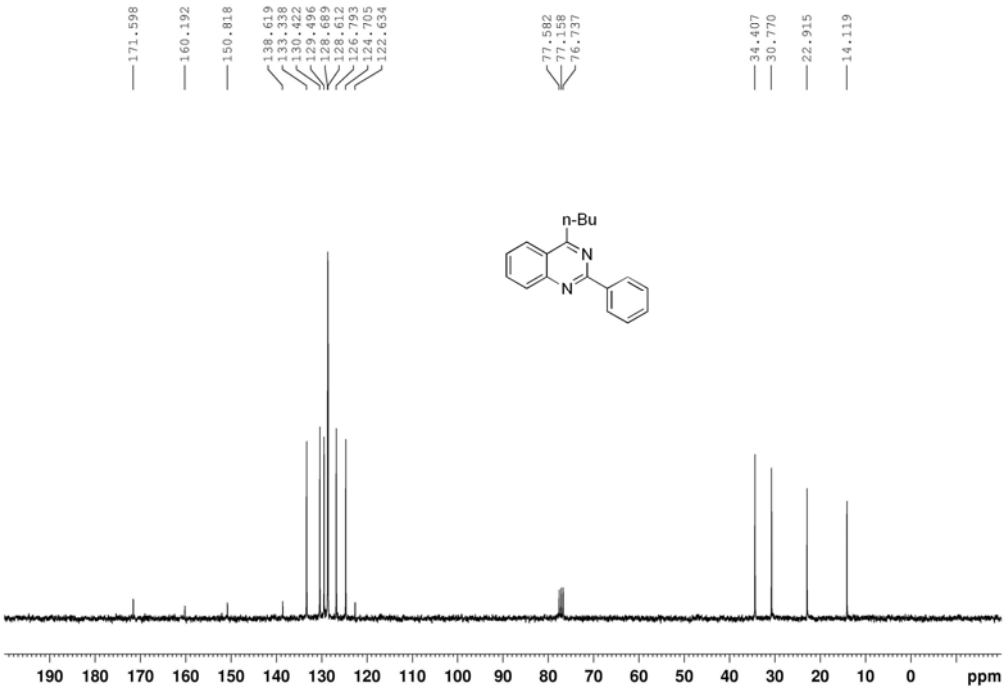
4-ethyl-2-phenylquinazoline (3g)



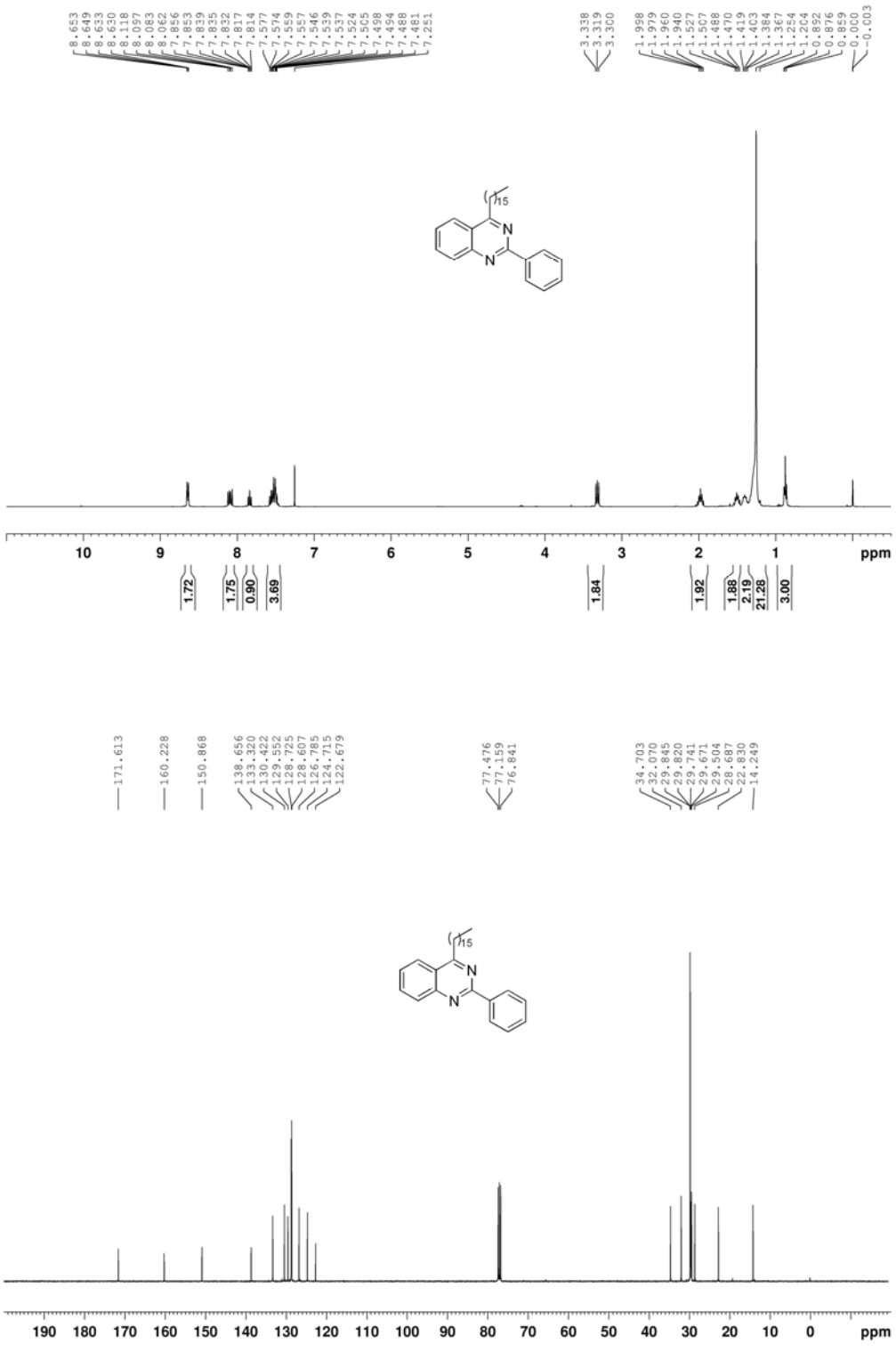


4-butyl-2-phenylquinazoline (3h)

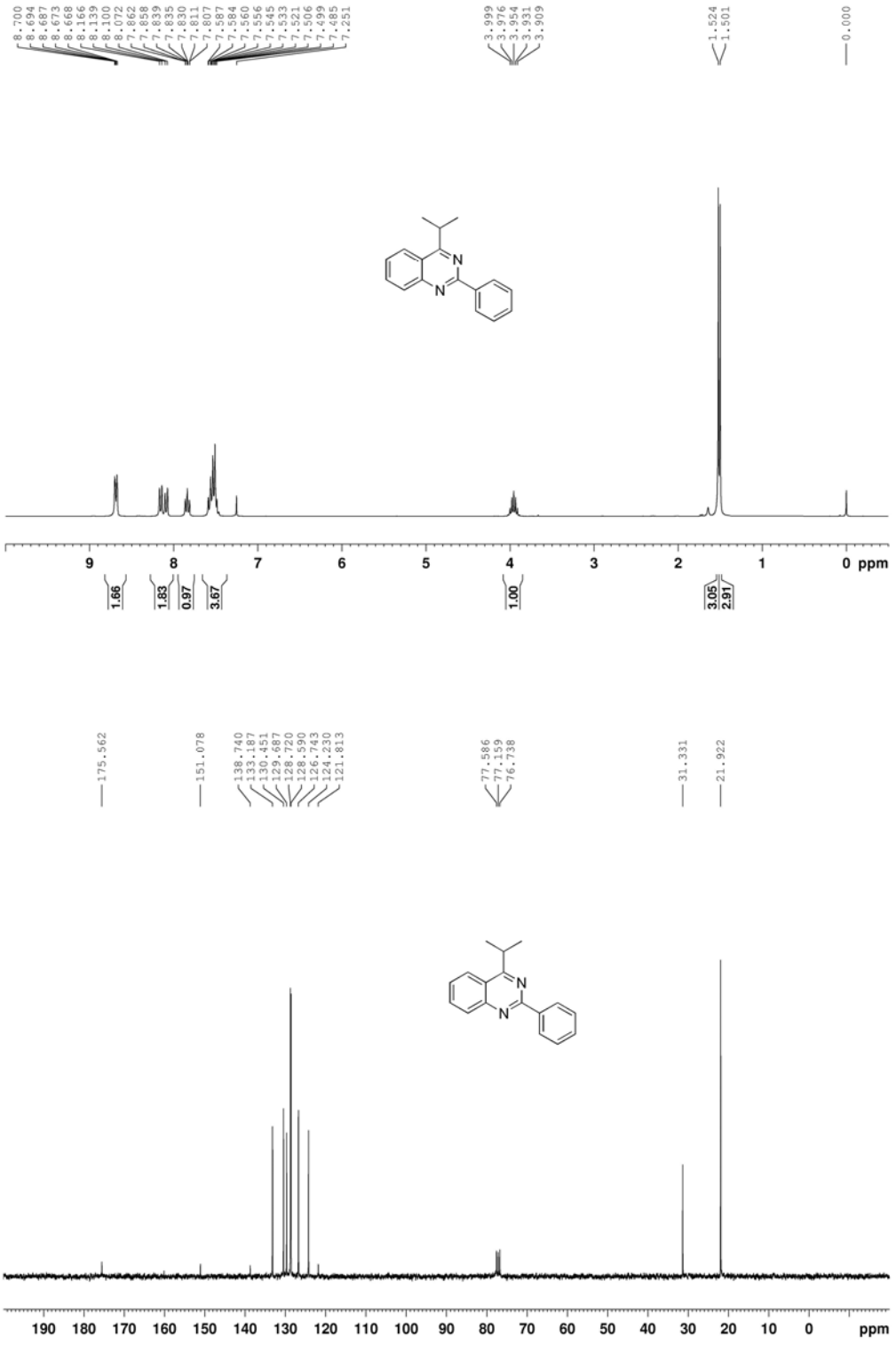




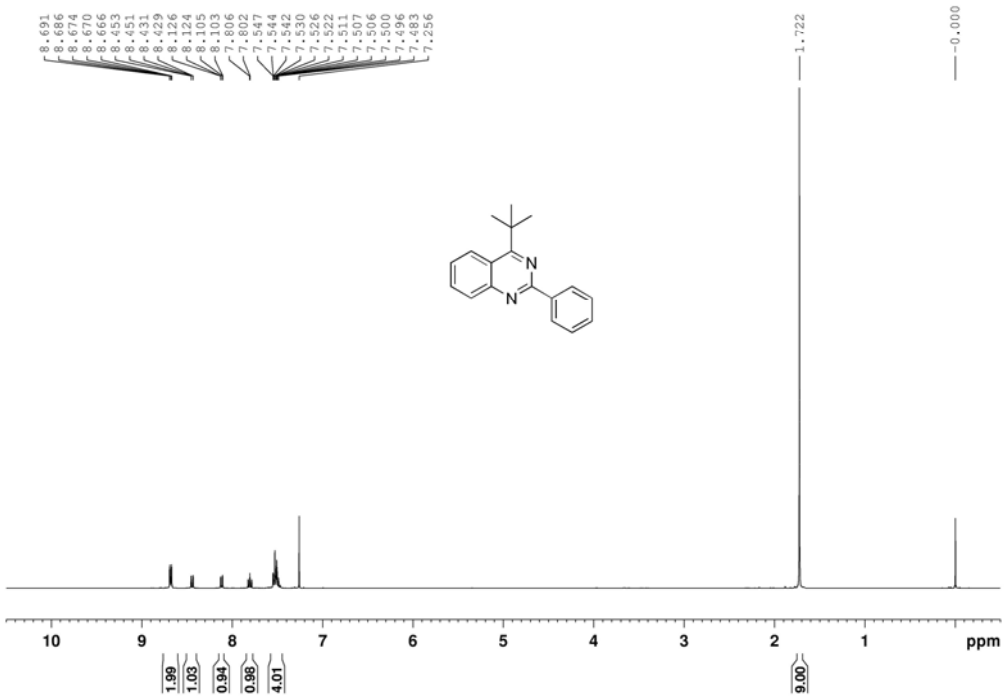
4-hexadecyl-2-phenylquinazoline (3i)

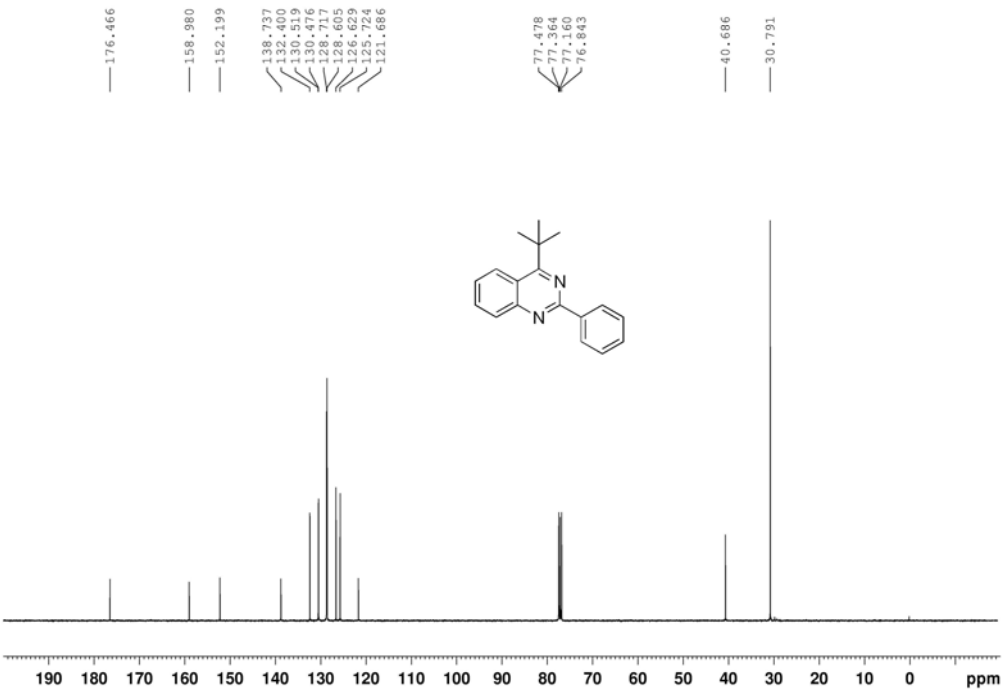


4-isopropyl-2-phenylquinazoline (3j)

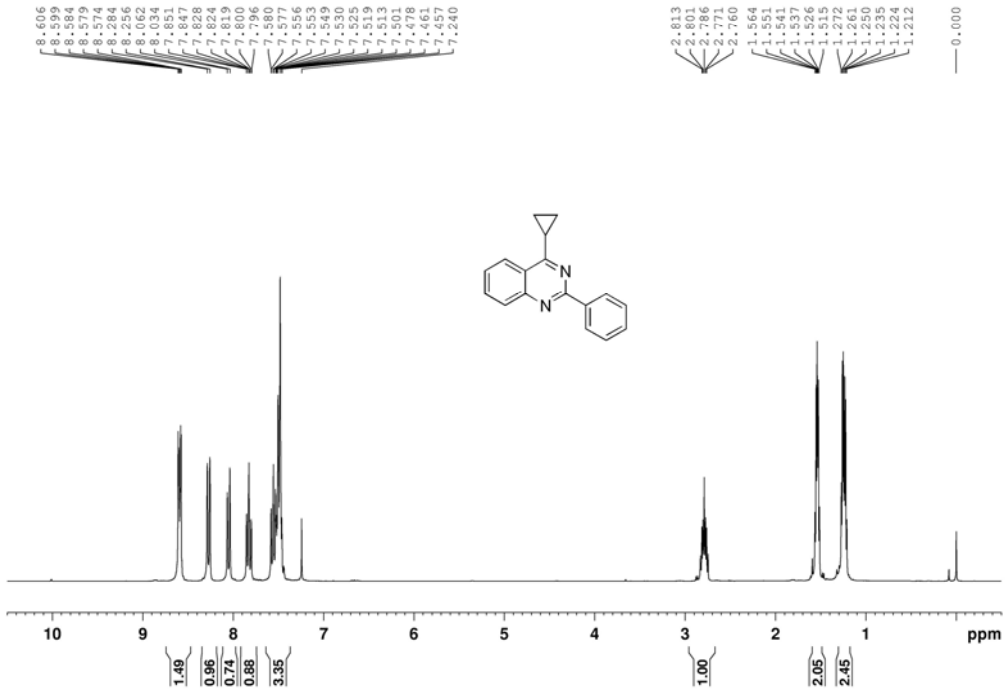


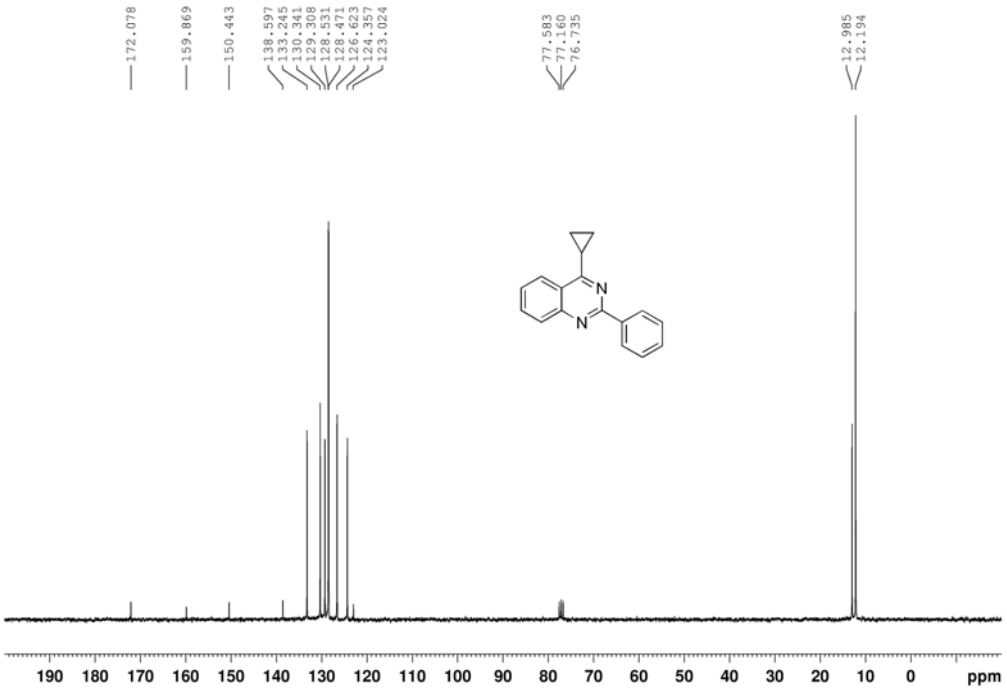
4-tert-butyl-2-phenylquinazoline (3k)



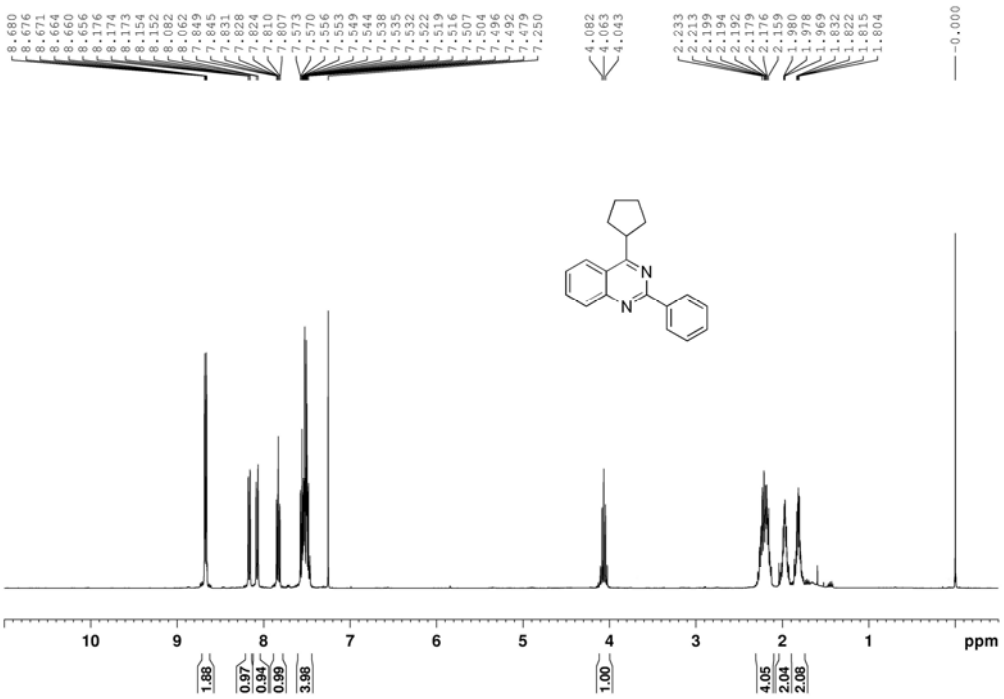


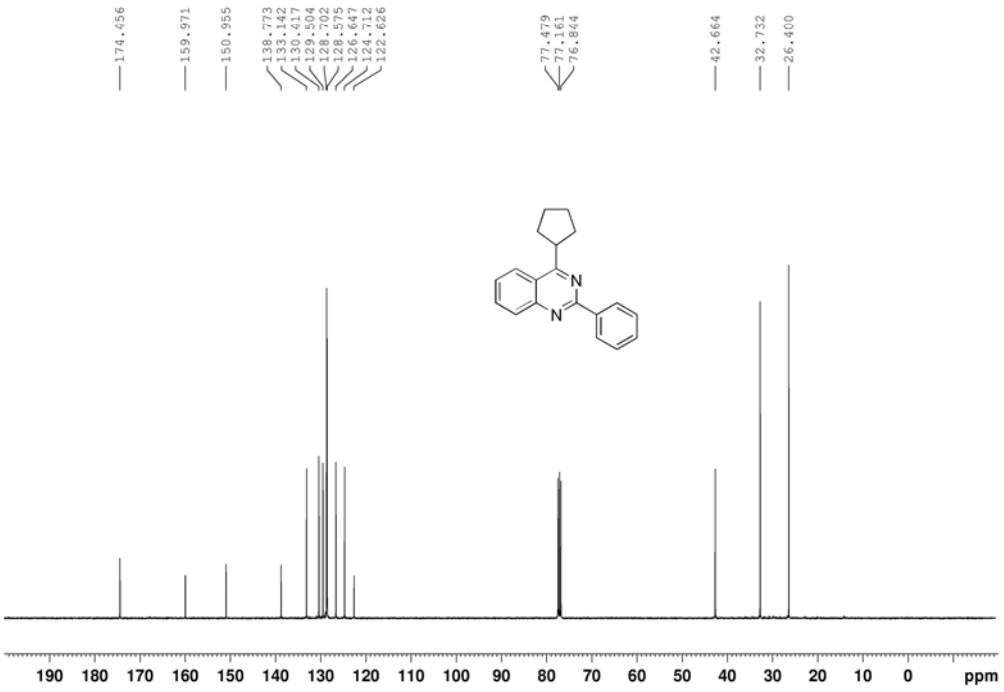
4-cyclopropyl-2-phenylquinazoline (3l)



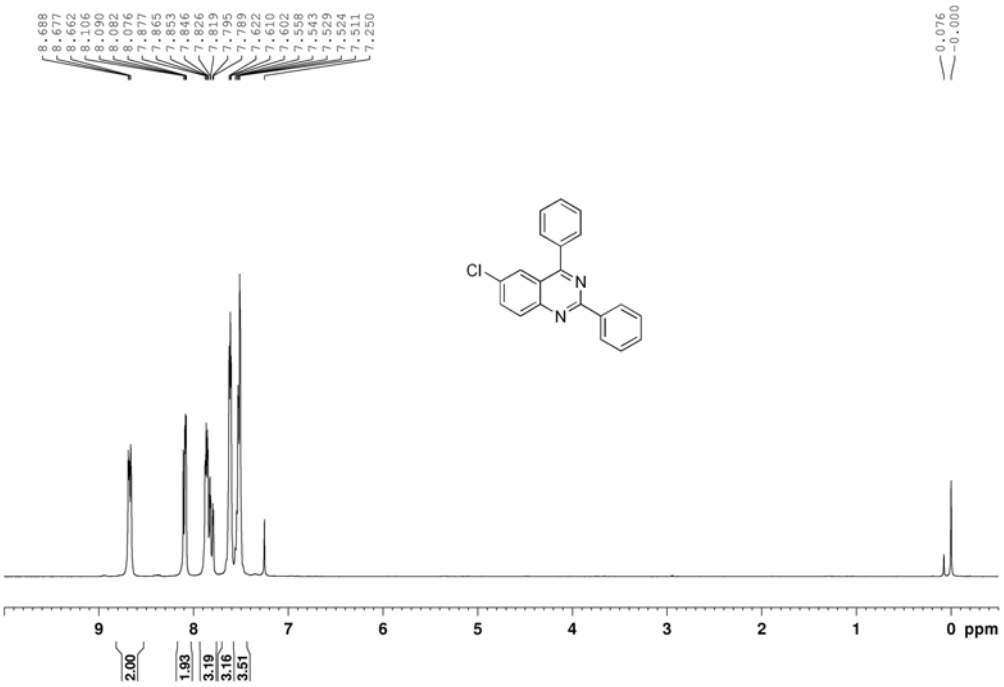


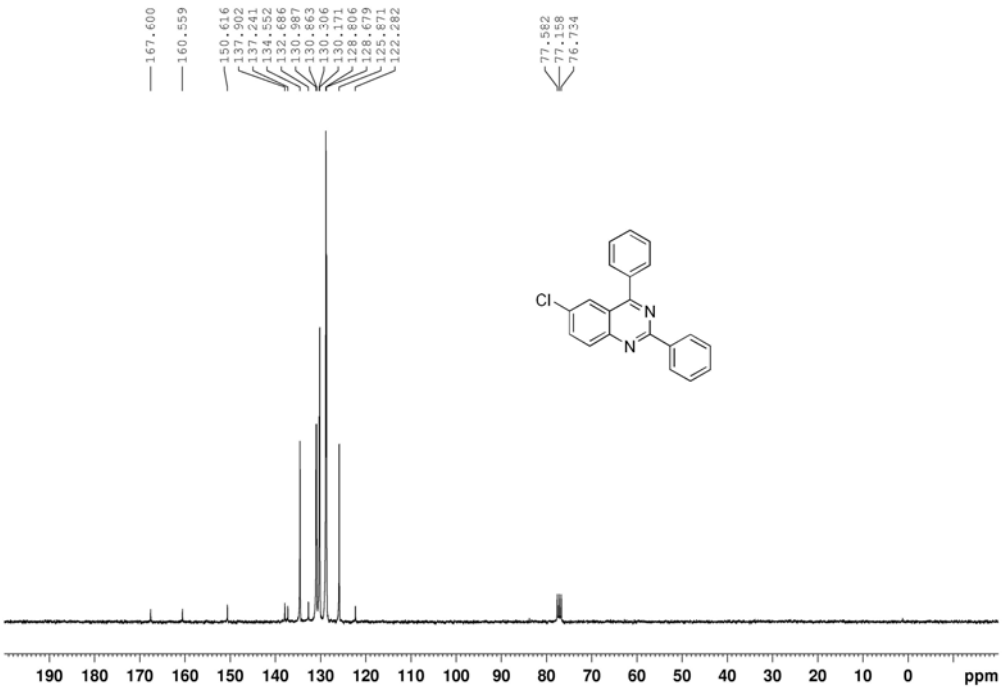
4-cyclopentyl-2-phenylquinazoline (3m)



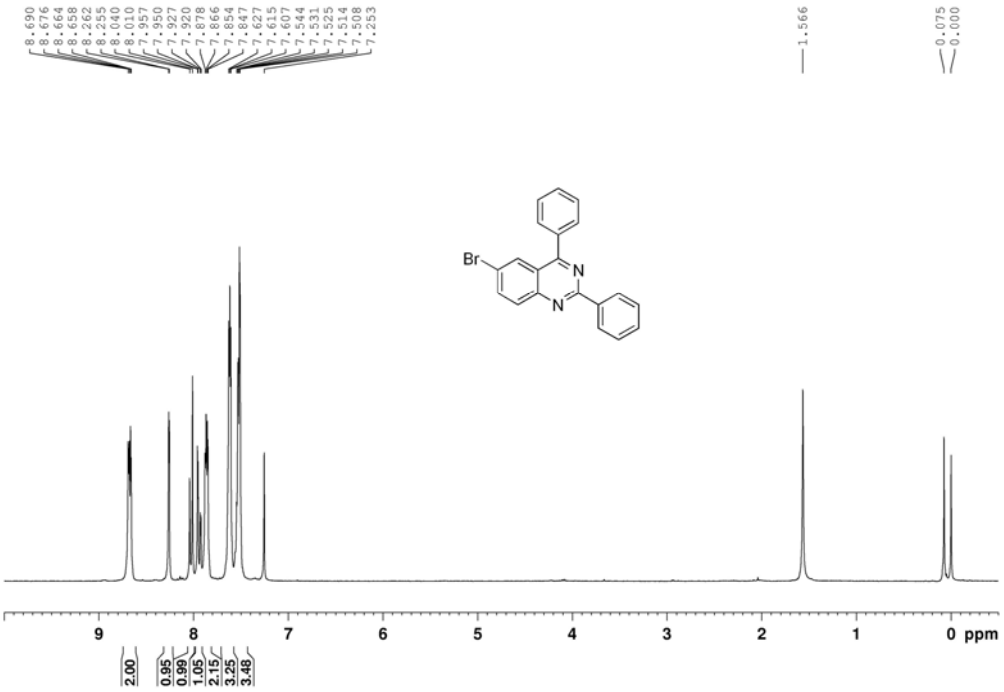


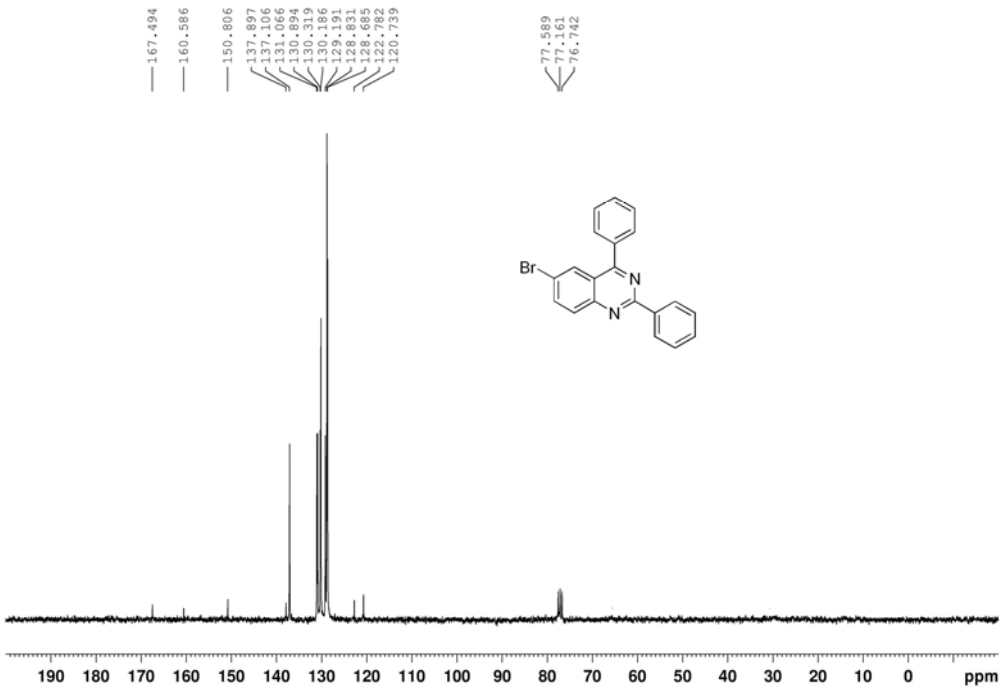
6-chloro-2,4-diphenylquinazoline (3n)



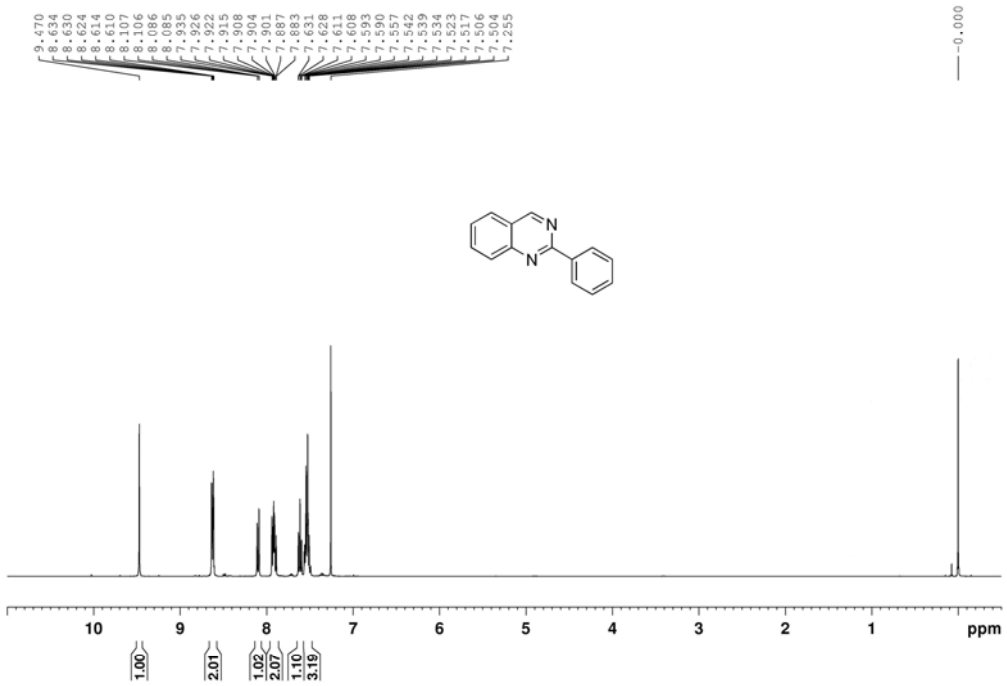


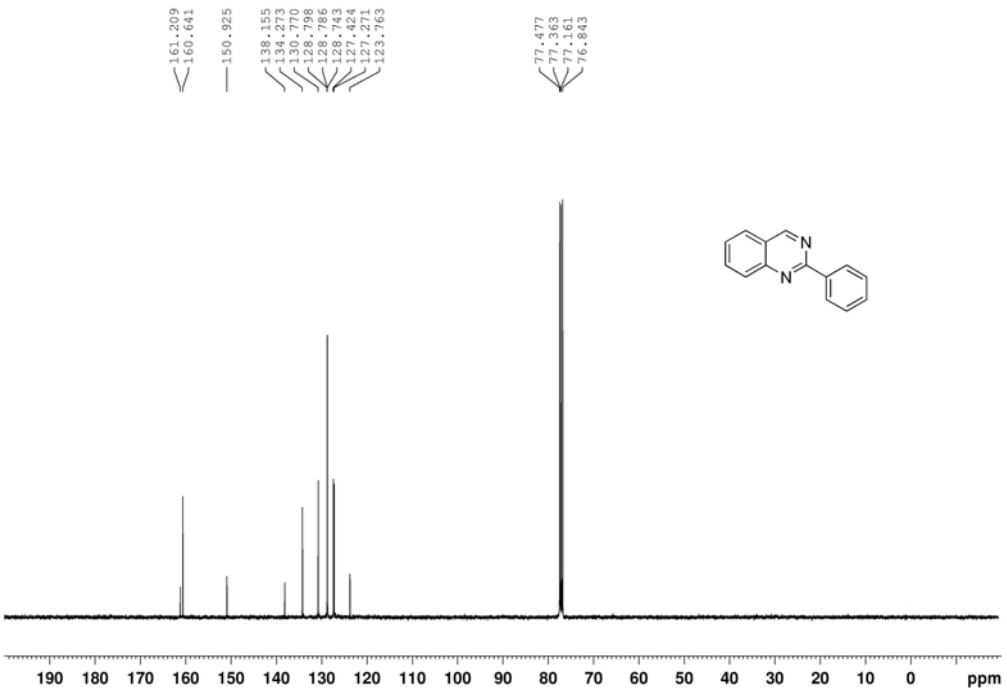
6-bromo-2,4-diphenylquinazoline (3o)



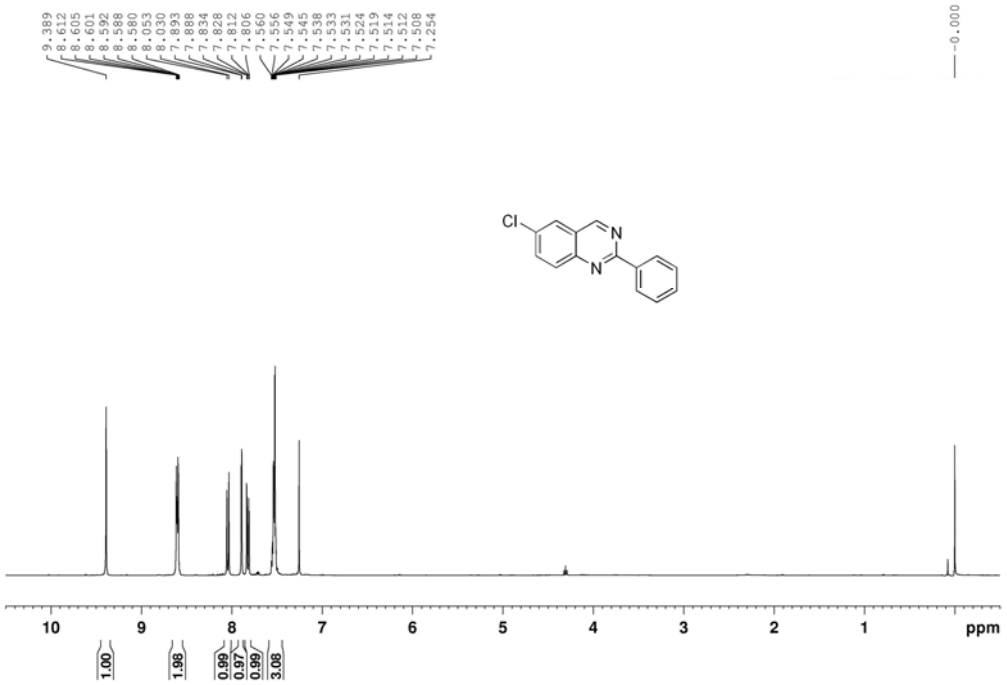


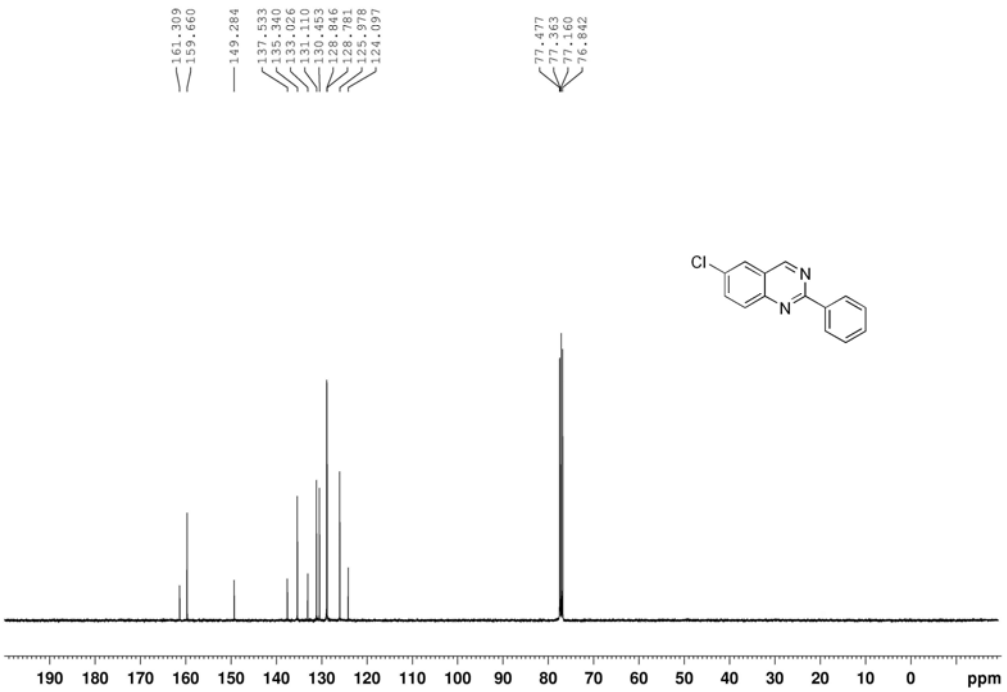
2-phenylquinazoline (3p)



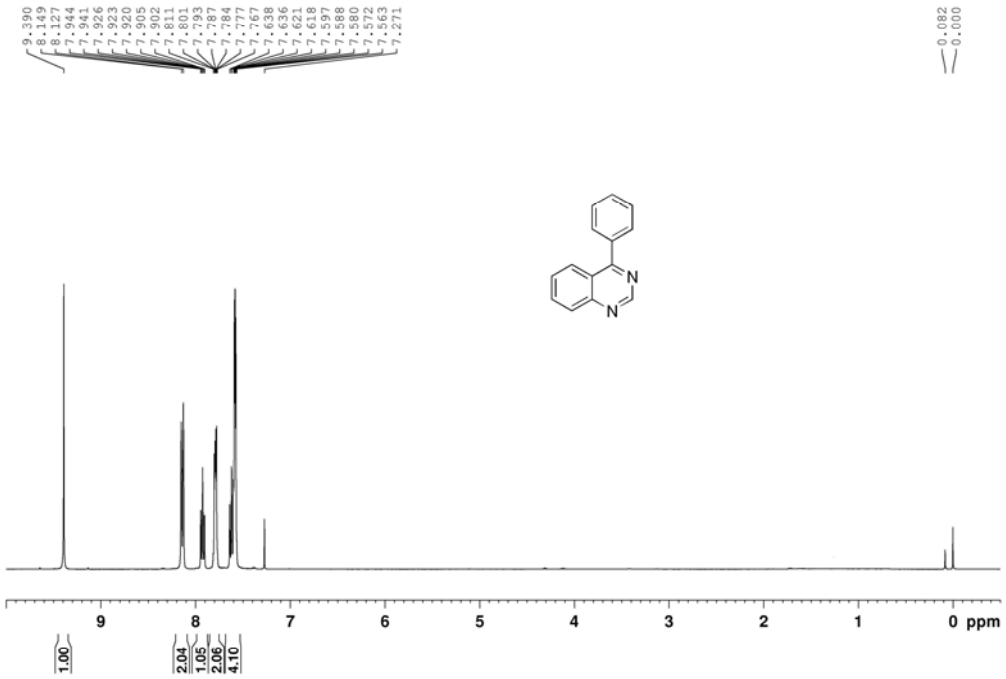


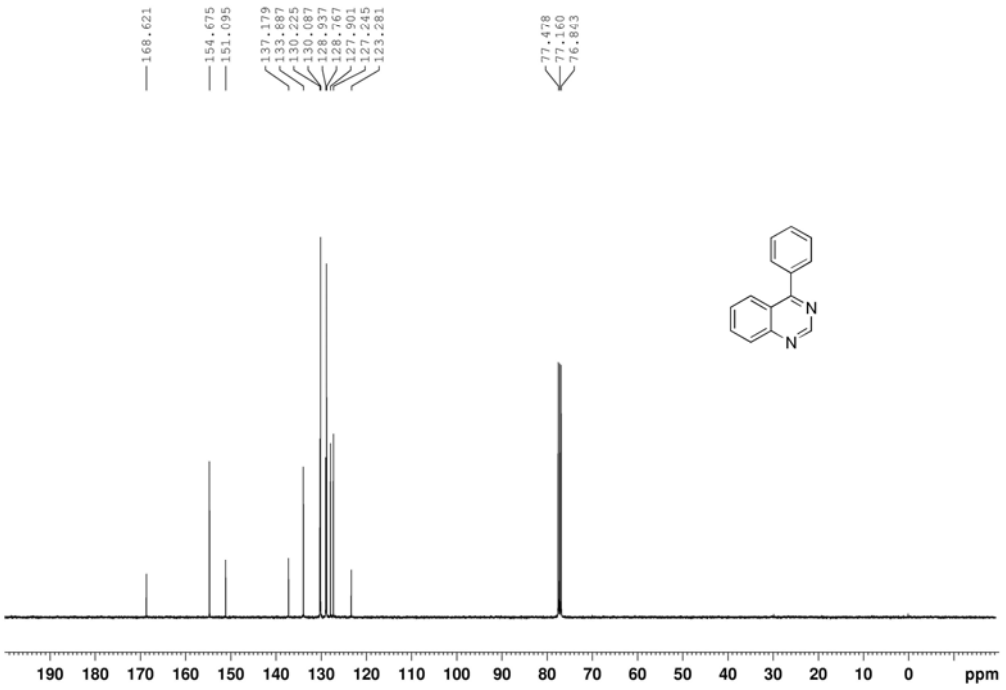
6-chloro-2-phenylquinazoline (3q)



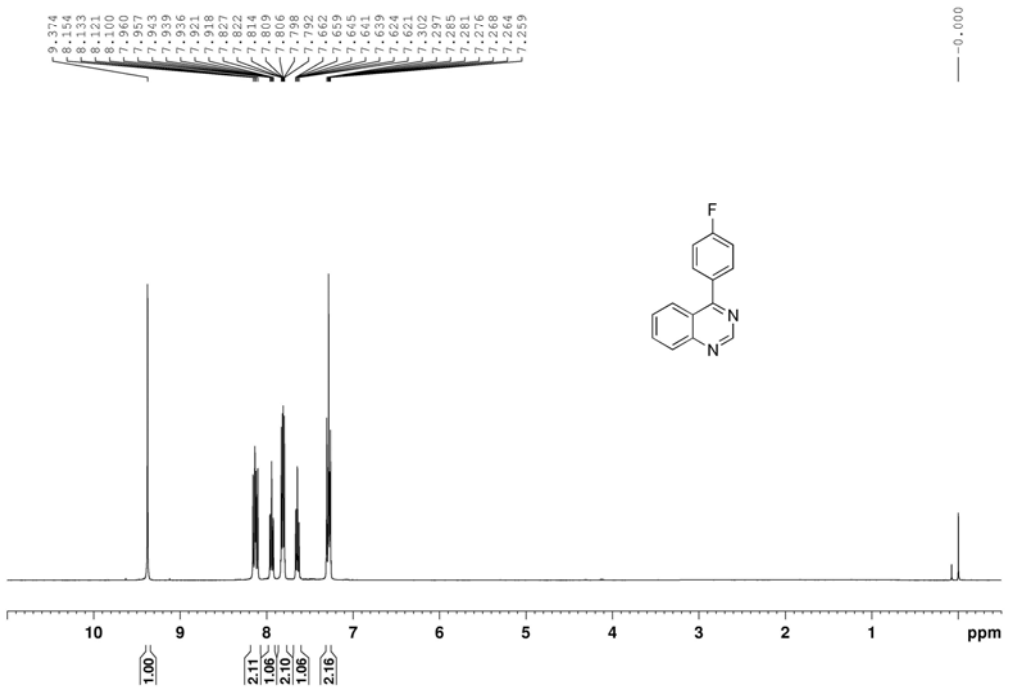


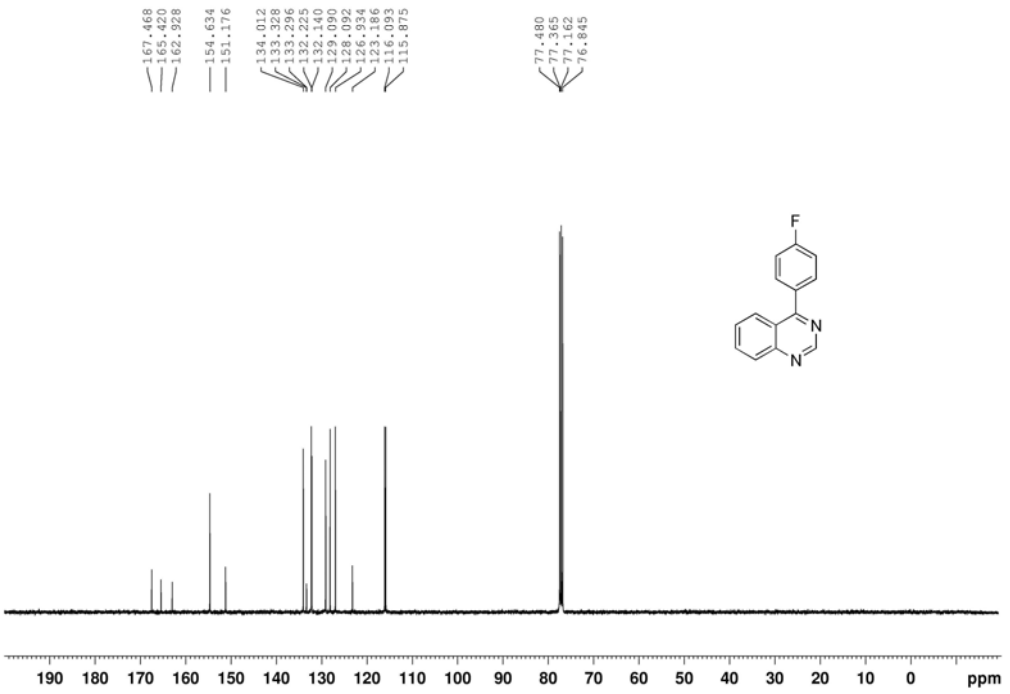
4-phenylquinazoline (3r)



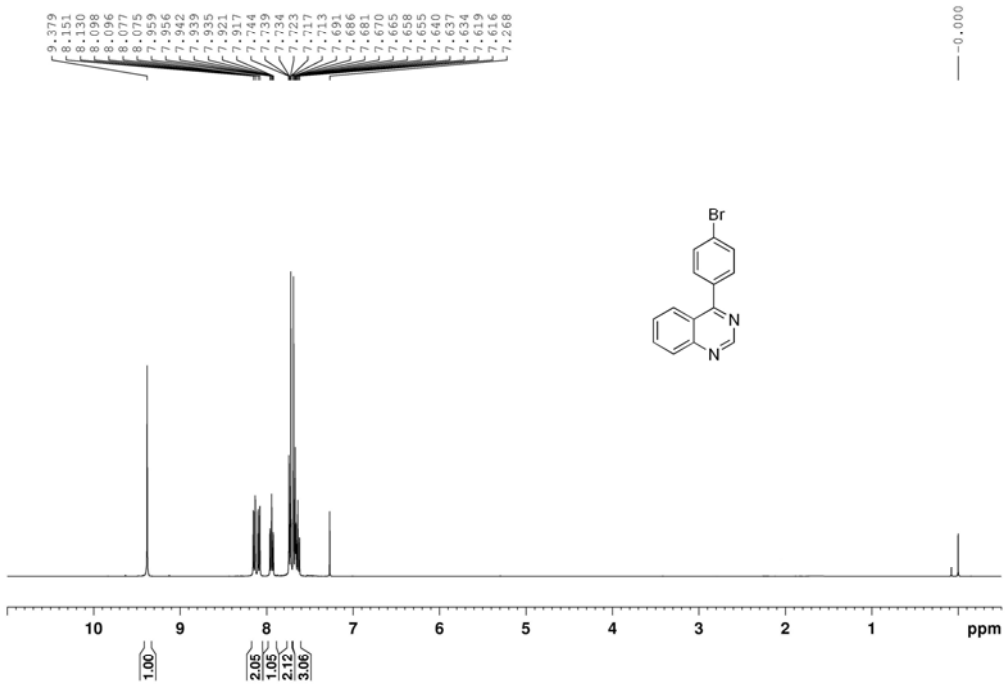


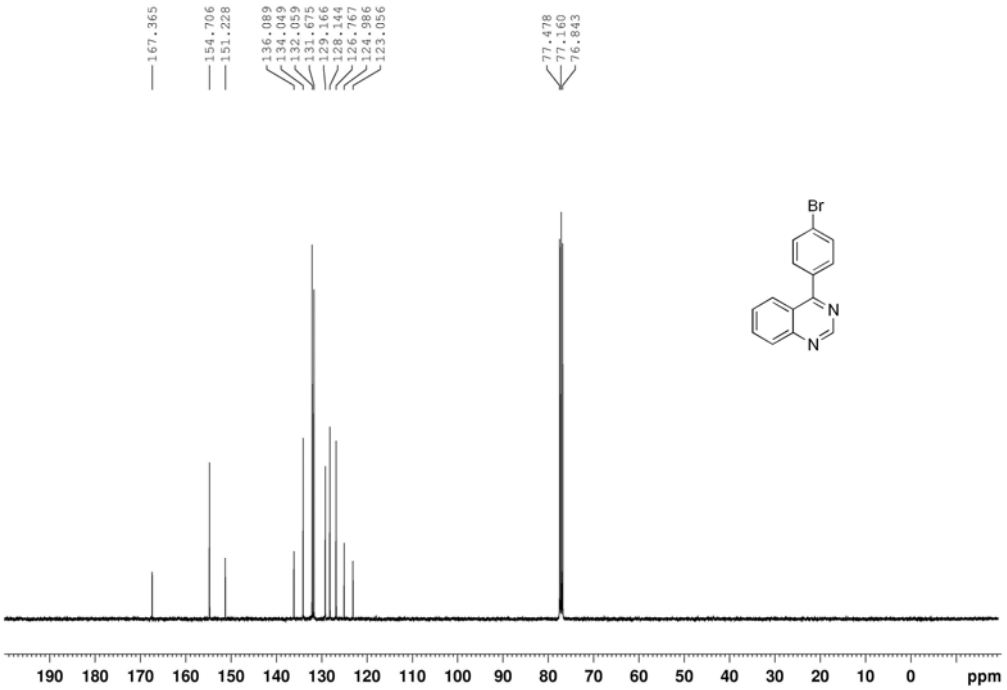
4-(4-fluorophenyl)quinazoline (3s)



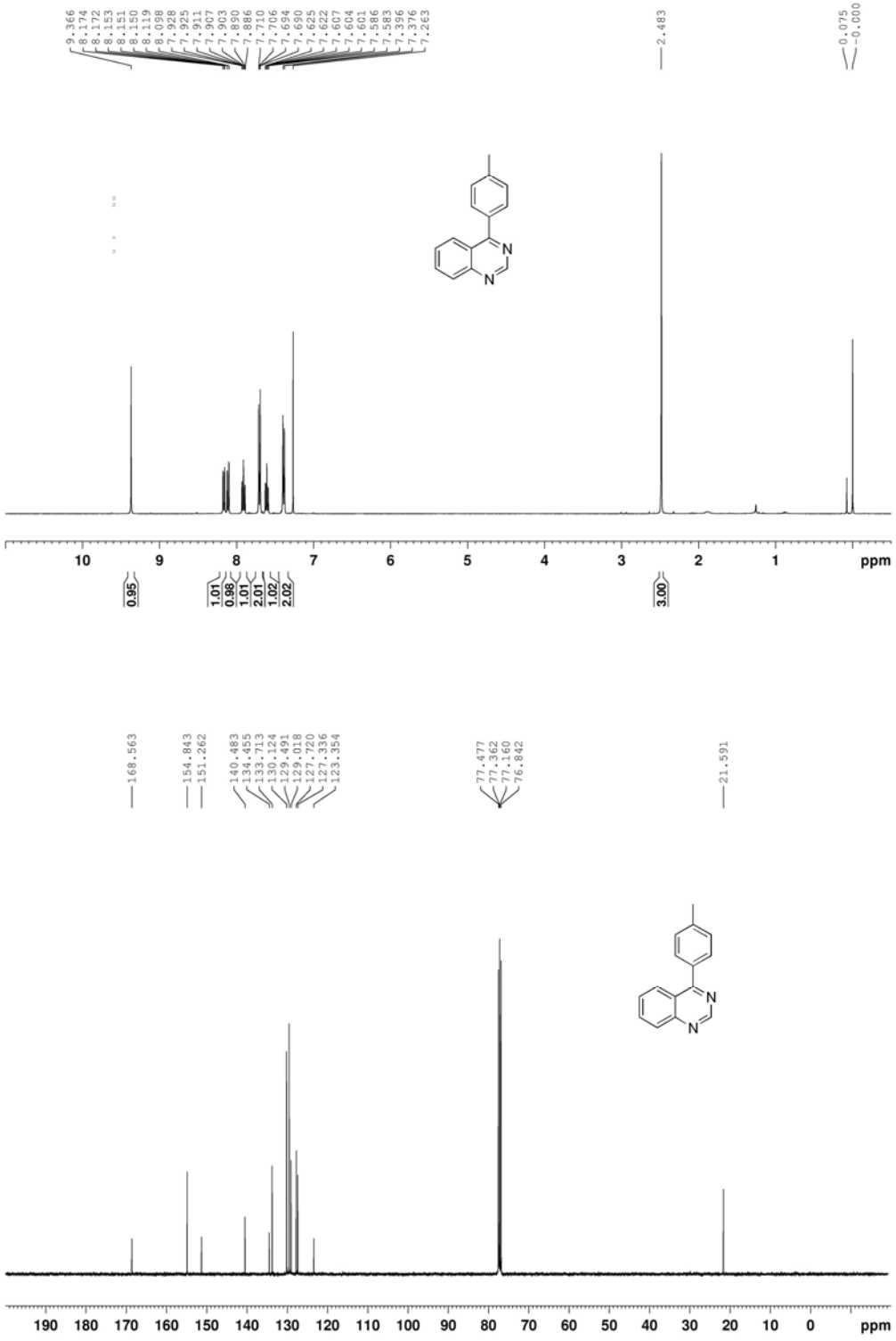


4-(4-bromophenyl)quinazoline (3t)

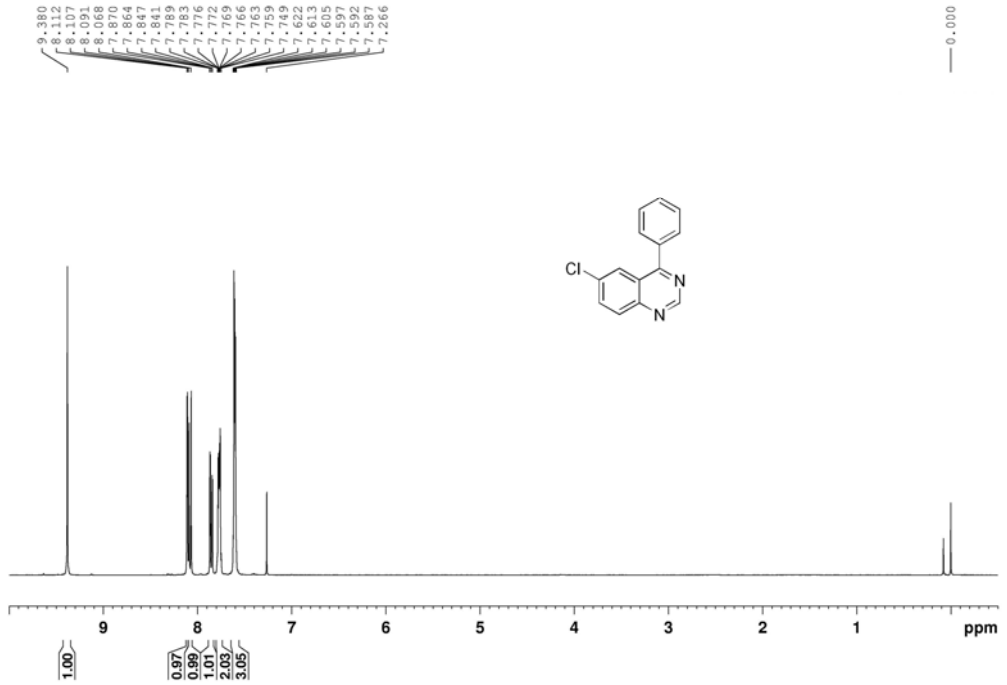


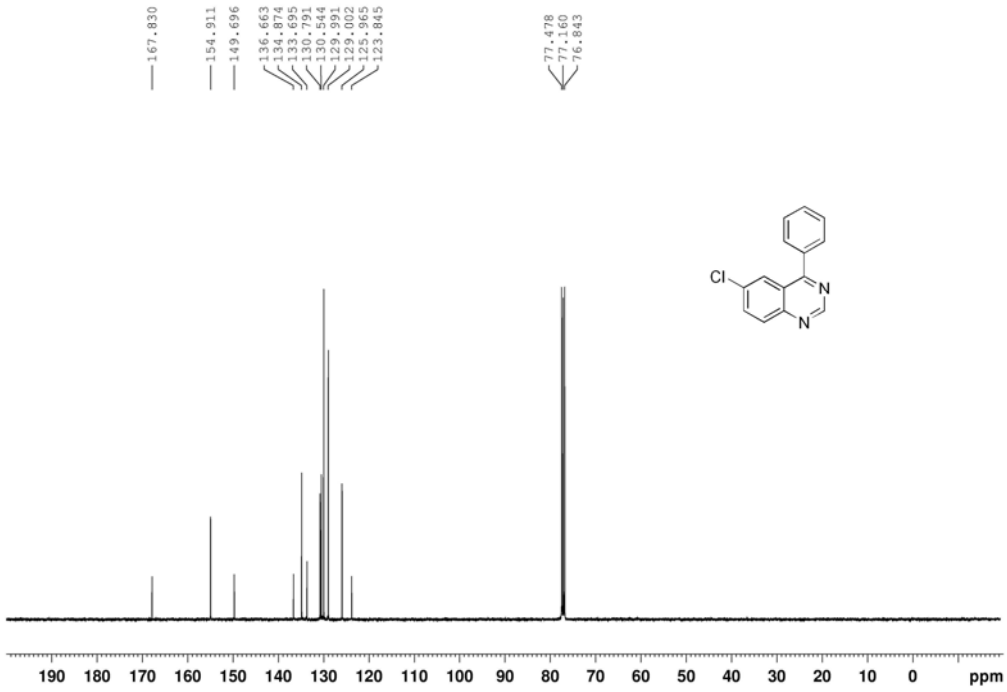


4-*p*-tolylquinazoline (3u)

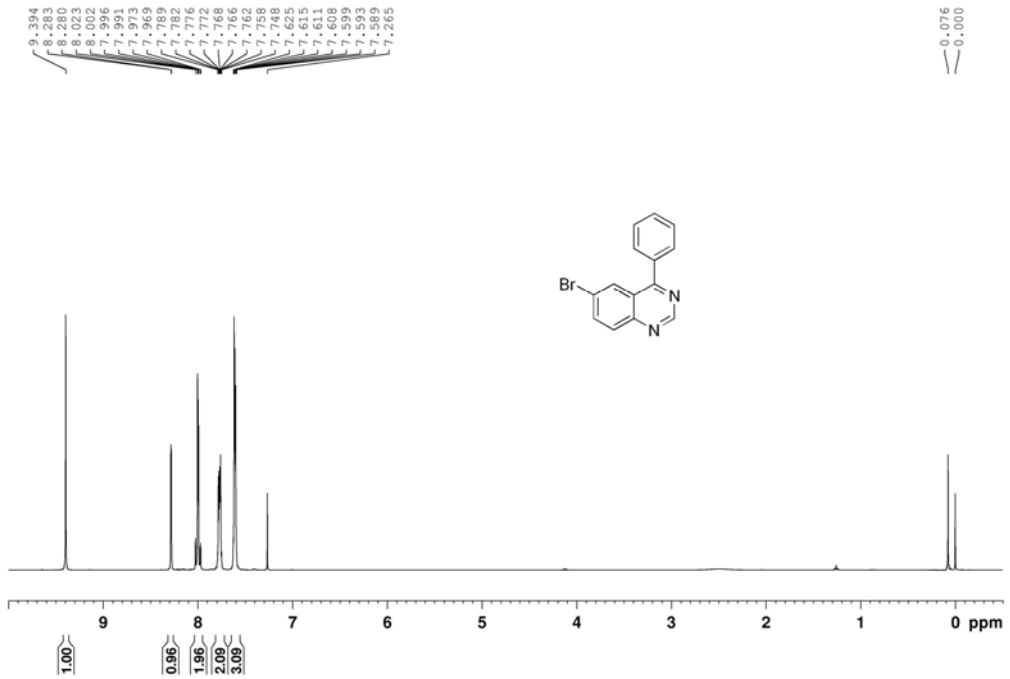


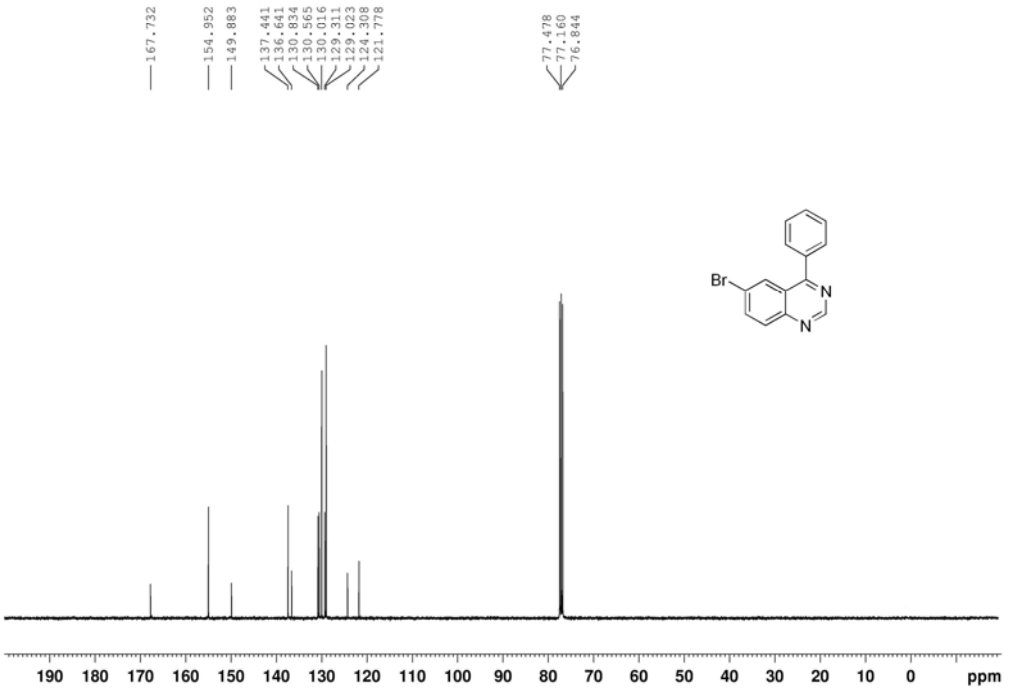
6-chloro-4-phenylquinazoline (3v)



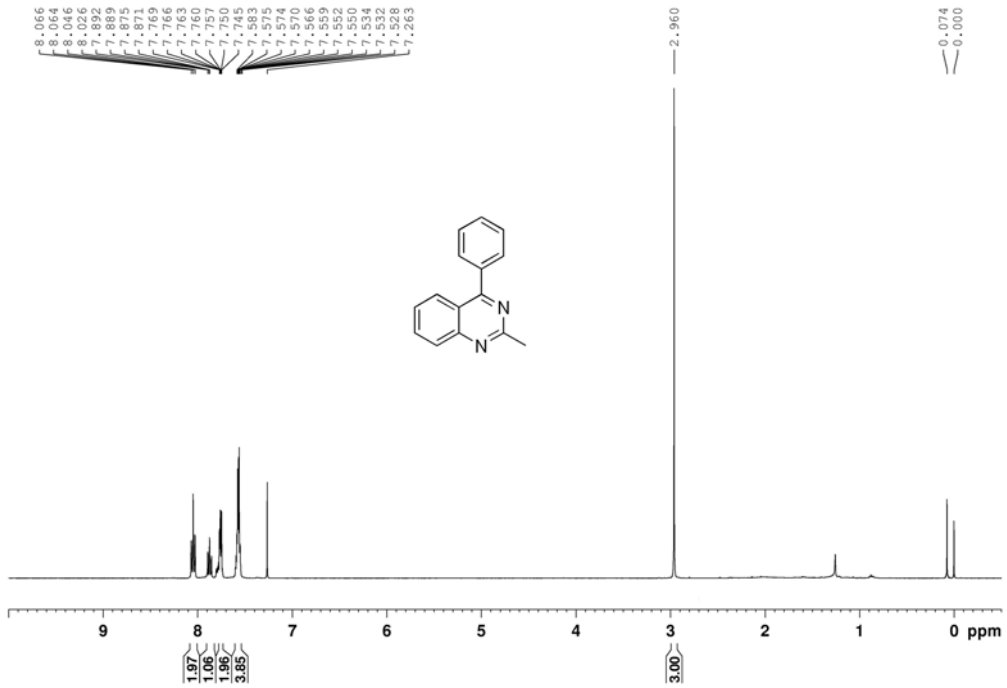


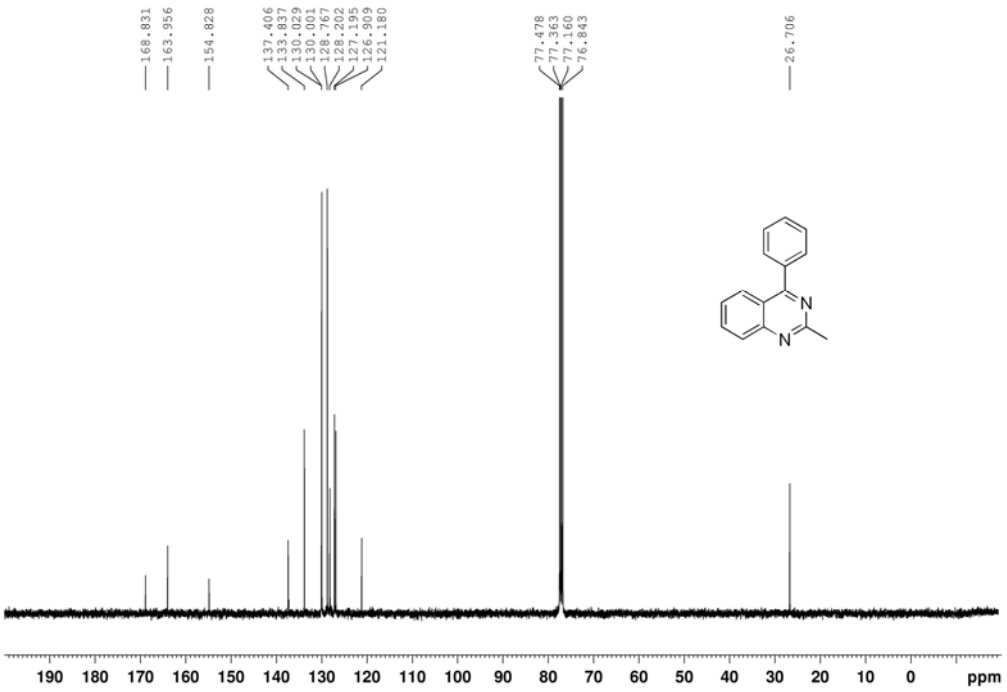
6-bromo-4-phenylquinazoline (3w)



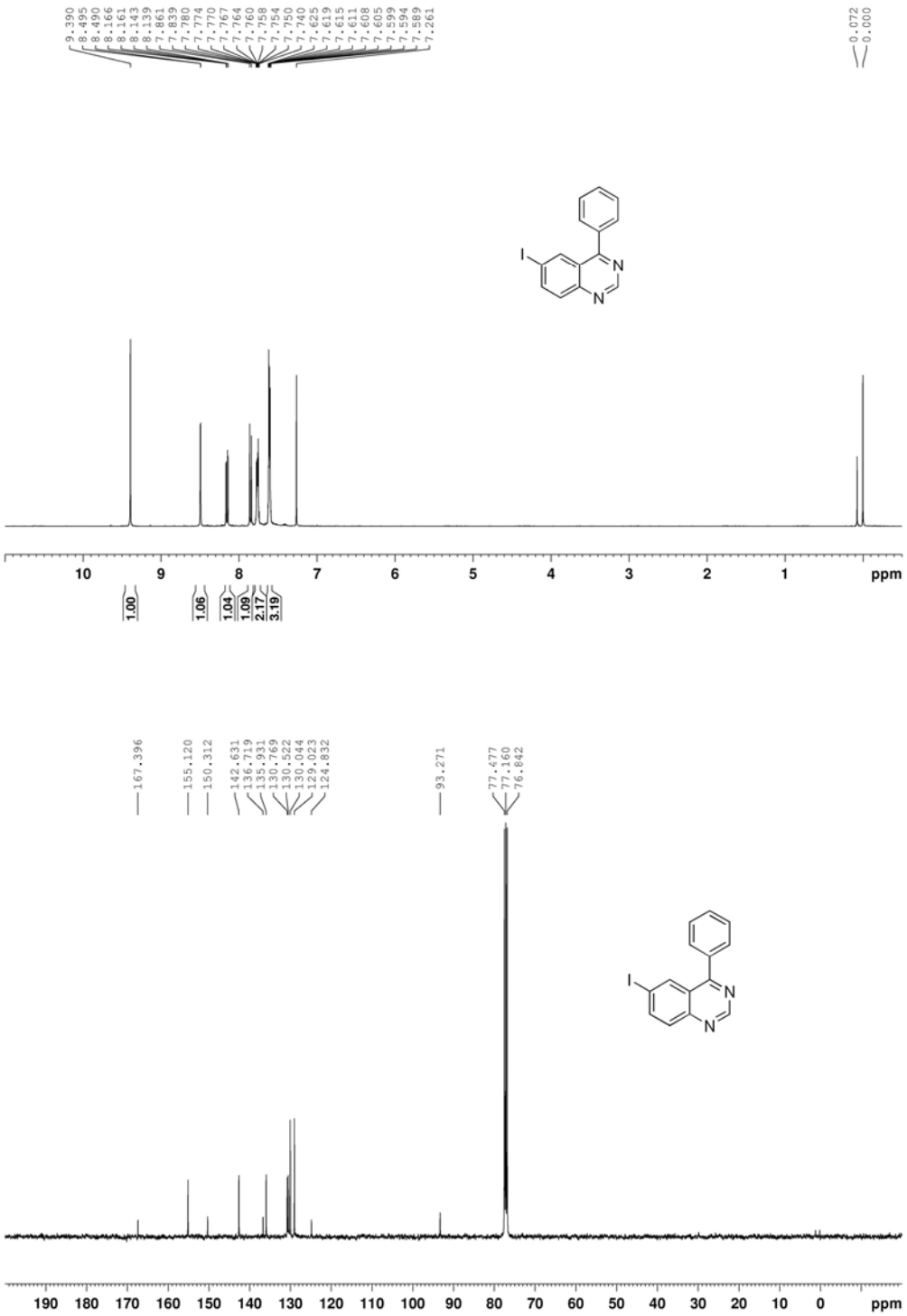


2-methyl-4-phenylquinazoline (3x)





6-iodo-4-phenylquinazoline (4r)



2-(4-phenylquinazolin-2-yl)propan-2-ol (4y)