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# Electrochemical synthesis of quinazolinone via $I_2$-catalyzed tandem oxidative in aqueous solution

Huiqing Hou,[a] Xinhua Ma,[a] Yingying Lin,[a] Jin Lin,[a] Weiming Sun,[a] Lei Wang,[c] Xiuzhi Xu[a*] and Fang Ke[a,b*]

[a.] *School of Pharmacy, Fujian Provincial Key Laboratory of Natural Medicine Pharmacology, Fujian Medical University, Fuzhou 350004, China. E-mail: kefang@mail.fjmu.edu.cn; Fax: +86-591-22862016; Tel: +86-591-22862016.*

[b.] *Faculty of Material and Chemical Engineering, Yibin University, Yibin 644000, China.*

[c.] *School of science, Xuchang University, Xuchang 461000, China.*

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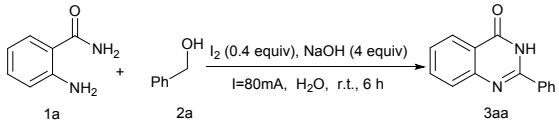
## 1. General information

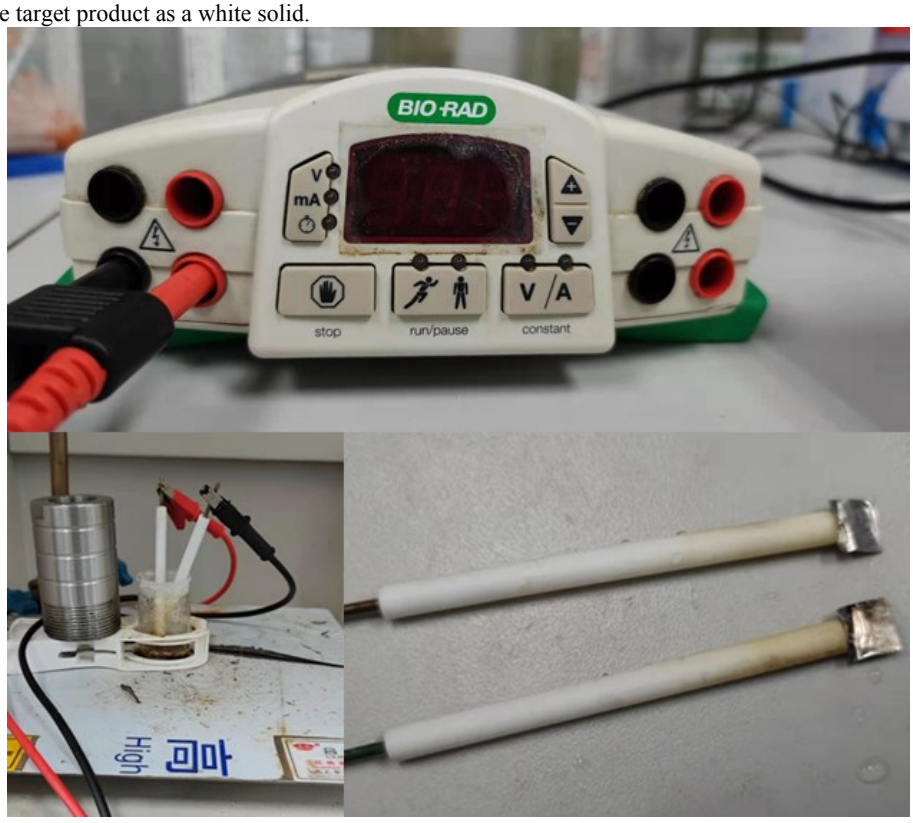
All reagents were purchased from commercial sources and used without further purification. All solvents were dried in a standard manner. Reactions were monitored by TLC on silica gel plates. Column chromatography was performed over silica gel (200-300 mesh) and a petroleum ether/ethyl. Shanghai chenhua CHI600E electrochemical workstation was used in the standard configuration as delivered, including proprietary software. All products were characterized by NMR. $^{1}H$ NMR spectra were recorded at 500 MHz or 400 MHz and $^{13}C$ NMR spectra were recorded at 126 MHz or 101 MHz (Bruker DPX) with DMSO-d6 as solvent. Chemical shifts are reported in ppm using TMS as internal standard. NMR by the services provided at the Shandong Liaocheng University. HPLC were recorded on an SHIMDZU LC-20A instrument with a HP5-MS 30 m x 0.25 mm capillary apolar columns. A549, HCT-116 and SGC-7901 cells were all obtained from the Cell Bank of the Chinese Academy of Sciences.

## 2. General procedure for the catalytic reactions

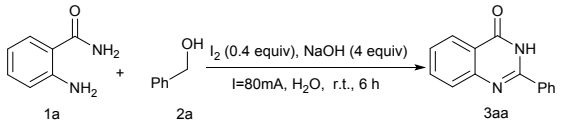



1a 2a 3aa

A dried 10 mL quartz tube equipped was charged with benzamides (0.5 mmol), alcohols (0.6 mmol), $I_2$ (0.2 mmol), NaOH (2.0 mmol) and water (3 mL). The mixture was stirred at room temperature with a voltage range of 6-8 V for 6 h with 80 mA. After the reaction was completed the solution of the crude product was concentrated in vacuo, and the residue was purified by column chromatography on a silica gel (petroleum ether/ethyl acetate=3/1) to afford the target product as a white solid.



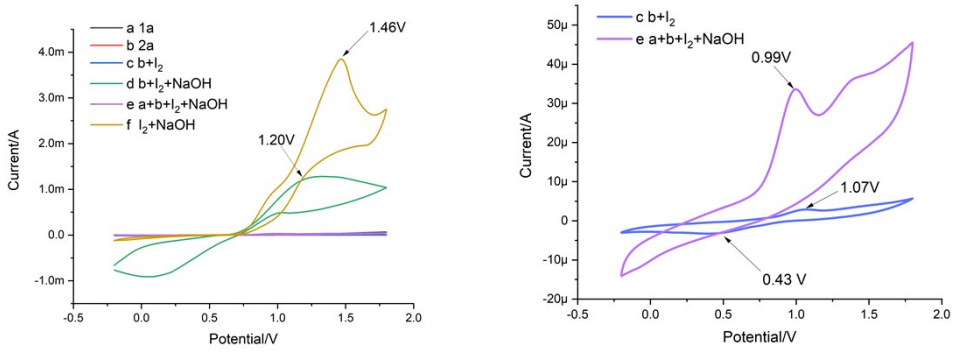

## 3. General procedure for the gram scale experiment

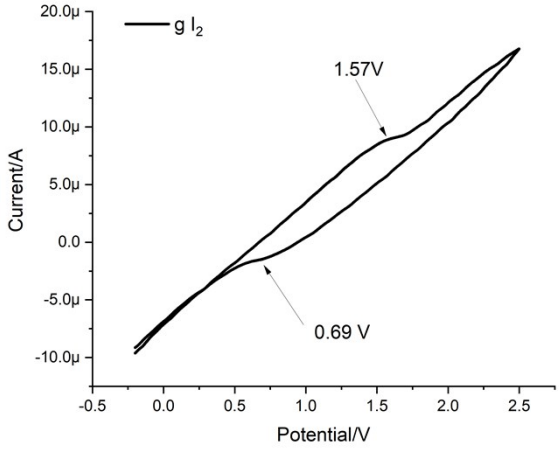



In 50 mL quartz tube equipped with *o*-aminobenzamide (5.0 mmol), benzyl alcohol (6.0 mmol), $I_2$ (2.0 mmol), NaOH (20.0 mmol) and water (20 mL). The mixture was stirred at room temperature for 6 h in the 80 mA circuit. After the reaction was completed the solution of the crude product was concentrated in vacuo. The product was purified by flash column chromatography on silica gel.

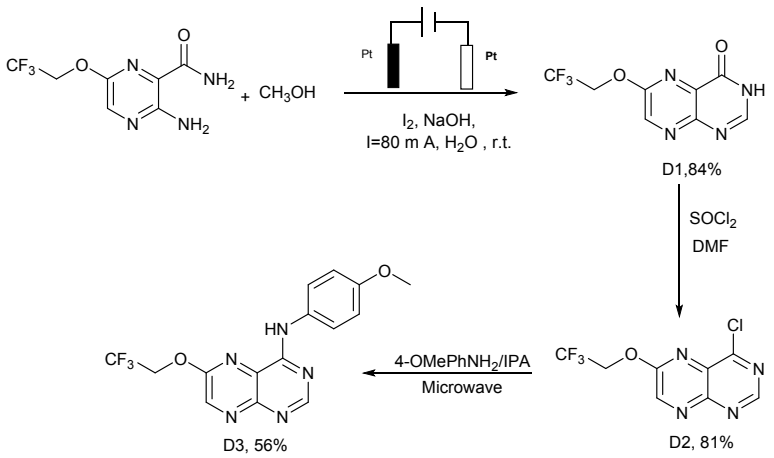
## 4. Cyclic voltammetry experiment

Cyclic voltammograms were measured using Shanghai chenhua CHI600E electrochemical workstation with electrochemical analysis software, using a conventional three-electrode cell. The working electrode was a glassy carbon working electrode, the counter and reference electrodes consisted of a Pt wire and a SCE, respectively. The glassy carbon working electrode was polished with a polishing cloth before each measurement. The concentration of all tested compounds was 1 mmol $L^{-1}$. The scan rate was 0.1 V/s.




## 5. Synthesis of *N*-(4-methoxyphenyl) -6- (2,2,2-trifluoroethoxy) pteridin -4-amine (A3).



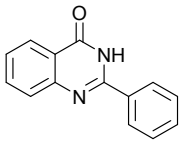

(1) The reaction of 3-amino-6-(2,2,2-trifluoroethoxy)pyrazine-2-carboxamide with formaldehyde (1.2 mmol) was carried out for 6 hours under the irradiation of 80 mA circuit with $I_2$ (40 mmol%), NaOH (2 mmol) as base and 4 mL water as solvent, the yield of 6-(2,2,2-trifluoroethoxy)pteridin-4(3*H*)-one was 84% .

(2) In a 100 mL flask, 6-trifluoroethoxy-4(3h)-Pteridine (2 mmol) , 10 mL thionyl dichloride, and 1-2 drops of DMF were added. Vacuum distillation removes dichlorothionyl and is then dried in vacuum for 30 minutes before being cooled to a yellow solid. It was slowly added into 10 mL ice water, then reaction mixture was added $NaHCO_3$ to adjust pH value to 7, and stirred for 10 minutes, filtered, and dried in a vacuum to obtain 6-(2,2,2-trifluoroethoxy)-4-chloro-pteridine as pale yellow powder. The yield was 81%.

(3) 6-trifluoroethoxy-4-chloro-pteridine (2 mmol) , aromatic amine (2 mmol) and isopropanol were added into 50 mL single-port round-bottom flask and stirred evenly for several minutes. Then a drying tube of anhydrous calcium chloride was connected to the upper end of the spherical condensing tube, and the optimal reaction conditions for dichloromethane dissolution were optimized by adjusting the microwave power and reaction time. After the reaction was followed by thin layer chromatography (TLC), it was cooled to 25 ℃ and then extracted with 50 mLwater and ethyl acetate (30 mL×3) to concentrate the organic phase of the pale yellow crude. The crude product is separated by silica gel column Chromatography (gradient elution of petroleum ether from 1:4 to 1:2 Ethyl acetate) and the final product is obtained.

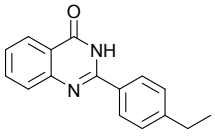
## Experimental procedures and characterization data

**(3aa) 2-phenylquinazolin-4(3*H*)-one[1]**




**$^1$H NMR (500 MHz, *DMSO-d6*)** δ 12.56 (s, 1H), 8.24-8.11 (m, 3H), 7.83 (t, *J* = 7.3 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.55 (ddd, *J* = 21.1, 13.9, 7.1 Hz, 4H). **$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 162.8, 152.8, 149.1, 135.1, 133.2, 131.9, 129.1, 128.2, 127.9, 127.0, 126.3, 121.4. **MS** [EI, m/z]: 222 [$M^+$].

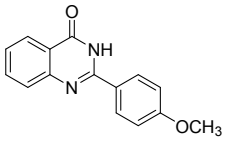
**(3ab) 2-(4-ethylphenyl)quinazolin-4(3*H*)-one[2]**




**$^1$H NMR (500 MHz, *DMSO-d6*)** δ 12.50 (s, 1H), 8.18-8.10 (m, 3H), 7.84 (ddd, *J* = 8.5, 7.2, 1.6 Hz, 1H), 7.74 (d, *J* = 7.7 Hz, 1H), 7.55-7.50 (m, 1H), 7.40 (d, *J* = 8.3 Hz, 2H), 2.70 (q, *J* = 7.6 Hz, 2H),

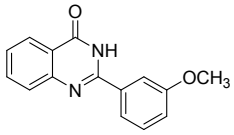
1.23 (t, *J* = 7.6 Hz, 3H).**$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 162.7, 152.7, 149.3, 148.1, 135.1, 130.7, 128.5, 128.3, 127.9, 126.9, 126.3, 121.4, 28.5, 15.8. **MS** [EI, m/z]: 250 [$M^+$].

**(3ac) 2-(4-methoxyphenyl)quinazolin-4(3*H*)-one[1]**



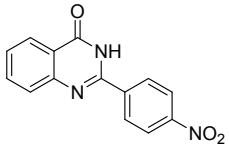

**$^{1}$H NMR (500 MHz, *DMSO-d6*)** δ 12.43 (s, 1H), 8.20 (d, *J* = 8.9 Hz, 2H), 8.14 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.85-7.79 (m, 1H), 7.71 (d, *J* = 8.1 Hz, 1H), 7.50 (dd, *J* = 11.0, 3.9 Hz, 1H), 7.10 (d, *J* = 8.9 Hz, 2H), 3.86 (s, 3H). **$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 162.8, 162.3, 152.3, 149.4, 135.1, 129.9, 127.8, 126.6, 126.3, 125.2, 121.1, 114.5, 55.9. **MS** [EI, m/z]: 252 [$M^+$].

**(3ad) 2-(3-methoxyphenyl)quinazolin-4(3*H*)-one[3]**



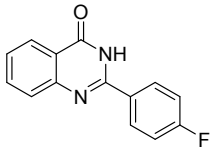

**$^{1}$H NMR (500 MHz, *DMSO-d6*)** δ 12.56 (s, 1H), 8.16 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.88-7.83 (m, 1H), 7.83- 7.72 (m, 3H), 7.57-7.51 (m, 1H), 7.47 (t, *J* = 8.0 Hz, 1H), 7.16 (dd, *J* = 8.1, 2.1 Hz, 1H), 3.87 (s, 3H). **$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 162.7, 159.8, 152.5, 149.1, 135.1, 134.5, 130.2, 128.0, 127.1, 126.3, 121.5, 120.6, 118.1, 113.0, 55.8. **MS** [EI, m/z]: 252 [$M^+$].

**(3ae) 2-(4-nitrophenyl)quinazolin-4(3*H*)-one[4]**



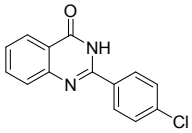

**$^{1}$H NMR (500 MHz, *DMSO-d6*)** δ 12.86 (s, 1H), 8.44-8.37 (m, 4H), 8.19 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.89 (ddd, *J* = 8.5, 7.2, 1.5 Hz, 1H), 7.81 (d, *J* = 7.8 Hz, 1H), 7.61- 7.57 (m, 1H). **$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 151.2, 149.5, 148.8, 139.0, 135.3, 129.8, 128.5, 128.3, 127.9, 126.4, 124.1, 121.7. **MS** [EI, m/z]: 267 [$M^+$].

**(3af) 2-(4-fluorophenyl)quinazolin-4(3*H*)-one[1]**



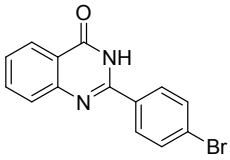

**$^{1}$H NMR (500 MHz, *DMSO-d6*)** δ 12.58 (s, 1H), 8.28-8.23 (m, 2H), 8.15 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.84 (ddd, *J* = 8.5, 7.2, 1.6 Hz, 1H), 7.74 (d, *J* = 7.7 Hz, 1H), 7.55-7.50 (m, 1H), 7.43-7.36 (m, 2H). **$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 165.5, 163.5, 162.8, 152.0, 149.1, 135.1, 130.8 (130.87, 130.79, d, *J* = 9.0 Hz), 129.7, 127.8, 127.1, 126.3, 121.3, 116.2. **MS** [EI, m/z]: 240 [$M^+$].

**(3ag) 2-(4-chlorophenyl)quinazolin-4(3*H*)-one[5]**



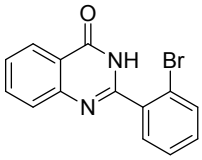
**$^1$H NMR (500 MHz, *DMSO-d6*)** δ 12.61 (s, 1H), 8.21 (d, *J* = 8.6 Hz, 2H), 8.16 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.90-7.83 (m, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 8.6 Hz, 2H), 7.55 (t, *J* = 7.5 Hz, 1H). **$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 136.8, 135.4, 135.1, 133.3, 132.0, 130.1, 129.2, 128.0, 127.3, 126.3, 121.5, 120.0. **MS** [EI, m/z]: 256 [$M^+$].

**(3ah) 2-(4-bromophenyl)quinazolin-4(3*H*)-one[4]**



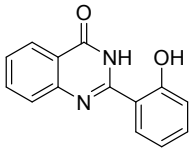
**$^1$H NMR (500 MHz, *DMSO-d6*)** δ 12.63 (s, 1H), 8.19-8.09 (m, 3H), 7.89-7.81 (m, 1H), 7.76 (t, *J* = 9.2 Hz, 3H), 7.57-7.51 (m, 1H). **$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 162.6, 151.9, 149.0, 135.2, 132.4, 132.1, 130.3, 128.0, 127.3, 126.3, 125.7, 121.5. **MS** [EI, m/z]: 300 [$M^+$].

**(3ai) 2-(2-bromophenyl)quinazolin-4(3*H*)-one[6]**



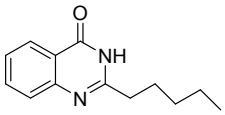
**$^1$H NMR (500 MHz, *DMSO-d6*)** δ 12.62 (s, 1H), 8.19 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.89-7.84 (m, 1H), 7.78 (dd, *J* = 8.0, 0.9 Hz, 1H), 7.72 (d, *J* = 7.9 Hz, 1H), 7.65 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.60-7.52 (m, 2H), 7.49 (td, *J* = 7.7, 1.8 Hz, 1H). **$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 161.9, 153.8, 149.0, 136.3, 135.1, 133.1, 132.1, 131.2, 128.1, 127.9, 127.5, 126.3, 121.7, 121.4. **MS** [EI, m/z]: 300 [$M^+$].

**(3aj) 2-(2-hydroxyphenyl)quinazolin-4(3*H*)-one[7]**



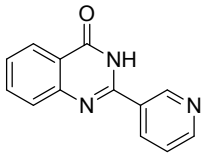
**$^1$H NMR (500 MHz, *DMSO-d6*)** δ 13.80 (s, 1H), 12.50 (s, 1H), 8.23 (dd, *J* = 8.0, 1.4 Hz, 1H), 8.17 (d, *J* = 7.6 Hz, 1H), 7.89-7.85 (m, 1H), 7.78 (d, *J* = 8.1 Hz, 1H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.50-7.44 (m, 1H), 7.02 (dd, *J* = 8.3, 0.8 Hz, 1H), 6.97 (t, *J* = 7.5 Hz, 1H). **$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 160.6, 154.2, 146.5, 135.6, 134.2, 128.2, 127.5, 126.5, 121.2, 119.3, 118.4, 114.3. **MS** [EI, m/z]: 238 [$M^+$].

**(3ak) 2-pentylquinazolin-4(3*H*)-one[8]**



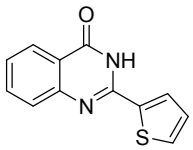
**$^1$H NMR (500 MHz, *DMSO-d6*)** δ 12.18 (s, 1H), 8.08 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.77 (ddd, *J* = 8.5, 7.2, 1.6 Hz, 1H), 7.60 (d, *J* = 7.8 Hz, 1H), 7.49-7.43 (m, 1H), 2.62-2.56 (m, 2H), 1.77-1.68 (m, 2H), 1.35 - 1.28 (m, 4H), 0.87 (t, *J* = 6.9 Hz, 3H). **$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 162.3, 158.0, 149.4, 134.8, 127.2, 126.4, 126.1, 121.2, 34.9, 31.2, 27.0, 22.3, 14.3. **MS** [EI, m/z]: 216 [$M^+$].

**(3al) 2-(pyridin-3-yl)quinazolin-4(3*H*)-one[9]**



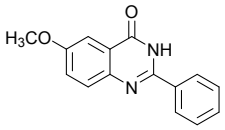
**$^1$H NMR (500 MHz, *DMSO-d6*)** δ 12.76 (s, 1H), 9.30 (d, *J* = 2.0 Hz, 1H), 8.77 (dd, *J* = 4.7, 1.2 Hz, 1H), 8.55-8.47 (m, 1H), 8.18 (d, *J* = 7.3 Hz, 1H), 7.92-7.84 (m, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.64-7.53 (m, 2H). **$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 162.6, 152.3, 151.2, 149.2, 149.0, 135.9, 135.2, 129.2, 128.1, 127.5, 126.4, 124.0, 121.6. **MS** [EI, m/z]: 223 [$M^+$].

**(3am) 2-(thiophen-2-yl)quinazolin-4(3*H*)-one[5]**



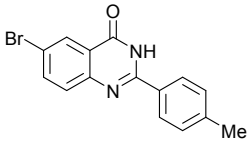
**$^1$H NMR (500 MHz, *DMSO-d6*)** δ 12.49 (s, 1H), 8.61 (dd, *J* = 2.9, 1.2 Hz, 1H), 8.14 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.88 (dd, *J* = 5.1, 1.2 Hz, 1H), 7.85-7.80 (m, 1H), 7.75-7.67 (m, 2H), 7.54-7.48 (m, 1H). **$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 162.5, 149.3, 148.7, 135.8, 135.1, 129.1, 127.8 (d, *J* = 14.1 Hz), 127.5, 126.9, 126.3, 121.4. **MS** [EI, m/z]: 228 [$M^+$].

**(3an)6-methoxy-2-phenylquinazolin-4(3*H*)-one[10]**



**$^1$H NMR (500 MHz, *DMSO-d6*)** δ 12.53 (s, 1H), 8.16 (d, *J* = 6.7 Hz, 2H), 7.71 (d, *J* = 8.9 Hz, 1H), 7.55 (q, *J* = 7.5, 6.5 Hz, 4H), 7.46 (dd, *J* = 8.9, 2.9 Hz, 1H), 3.90 (s, 3H). **$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 162.5, 158.2, 143.7, 133.2, 131.6, 129.7, 129.1, 128.0, 124.6, 122.2, 106.3, 56.1. **MS** [EI, m/z]: 252 [$M^+$].

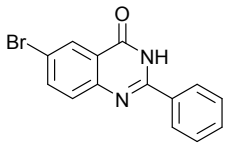
**(3ao)6-bromo-2-(p-tolyl)quinazolin-4(3*H*)-one[11]**



**$^1$H NMR (500 MHz, *DMSO-d6*)** δ 12.67 (s, 1H), 8.22 (s, 1H), 8.09 (d, *J* = 8.1 Hz, 2H), 8.01-7.95 (m, 1H), 7.68 (d, *J* = 8.7 Hz, 1H), 7.37 (d, *J* = 7.9 Hz, 2H), 2.40 (s, 3H). **$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 161.7, 153.3, 148.3, 142.3, 137.9, 130.3, 130.1, 129.7, 128.4, 128.2, 122.9, 119.2, 21.5. **MS** [EI, m/z]:

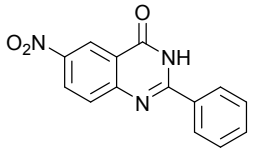
314 [M$^+$].

**(3ap) 6-bromo-2-phenylquinazolin-4(3*H*)-one[2]**



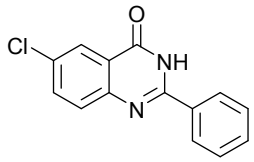

**$^1$H NMR (500 MHz, *DMSO-d6*)** δ 12.75 (s, 1H), 8.24 (d, *J* = 2.2 Hz, 1H), 8.17 (d, *J* = 7.2 Hz, 2H), 7.99 (dd, *J* = 8.7, 2.4 Hz, 1H), 7.71 (d, *J* = 8.7 Hz, 1H), 7.62 (t, *J* = 7.2 Hz, 1H), 7.56 (t, *J* = 7.3 Hz, 2H). **$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 153.4, 148.2, 137.9, 132.9, 132.1, 130.4, 129.1, 128.5, 128.3, 123.1, 119.4. **MS** [EI, m/z]: 300 [M$^+$].

**(3aq) 6-nitro-2-phenylquinazolin-4(3*H*)-one[12]**



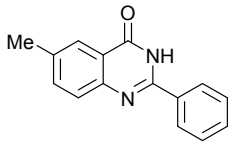

**$^1$H NMR (500 MHz, *DMSO-d6*)** δ 13.02 (s, 1H), 8.88-8.79 (m, 1H), 8.62-8.52 (m, 1H), 8.22 (d, *J* = 7.5 Hz, 2H), 7.92 (d, *J* = 8.9 Hz, 1H), 7.62 (dt, *J* = 32.9, 7.1 Hz, 3H). **$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 156.2, 145.1, 132.8, 132.5, 129.7, 129.2, 129.0, 128.7, 122.5, 121.4. **MS** [EI, m/z]: 267[M$^+$].

**(3ar) 6-chloro-2-phenylquinazolin-4(3*H*)-one[12]**



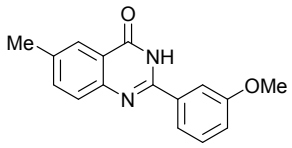

**$^1$H NMR (500 MHz, *DMSO-d6*)** δ 12.74 (s, 1H), 8.18 (d, *J* = 7.4 Hz, 2H), 8.10 (d, *J* = 2.2 Hz, 1H), 7.88 (dd, *J* = 8.7, 2.3 Hz, 1H), 7.78 (d, *J* = 8.7 Hz, 1H), 7.59 (dt, *J* = 24.7, 7.1 Hz, 3H). **$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 135.2, 132.1, 131.3, 130.2, 129.1, 128.3, 125.3, 122.7. **MS** [EI, m/z]: 256 [M$^+$].

**(3as) 6-methyl-2-phenylquinazolin-4(3*H*)-one[3]**



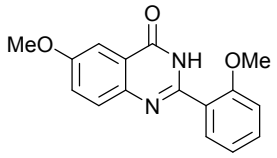

**$^1$H NMR (500 MHz, *DMSO-d6*)** δ 12.49 (s, 1H), 8.17 (dd, J = 8.3, 1.5 Hz, 2H), 7.96 (s, 1H), 7.69-7.65 (m, 2H), 7.59-7.53 (m, 3H), 2.47 (s, 3H). **$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 162.7, 152.0, 147.2, 136.8, 136.4, 133.2, 131.7, 129.1, 128.1, 127.9, 125.7, 121.2, 21.3. **MS** [EI, m/z]: 236 [M$^+$].

**(3at) 2-(3-methoxyphenyl)-6-methylquinazolin-4(3*H*)-one[13]**



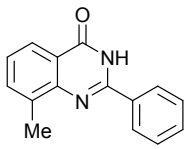

**$^1$H NMR (500 MHz, *DMSO-d6*)** δ 12.48 (s, 1H), 7.96 (s, 1H), 7.78 (d, *J* = 7.9 Hz, 1H), 7.75-7.72 (m, 1H), 7.67 (d, *J* = 1.9 Hz, 2H), 7.45 (t, *J* = 8.0 Hz, 1H), 3.87 (s, 3H), 2.47 (s, 3H). **$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 162.6, 159.8, 151.7, 147.1, 136.9, 134.5, 130.2, 127.9, 125.7, 121.2, 120.4, 117.9, 112.8, 55.8, 21.3. **MS** [EI, m/z]: 266 [$M^+$].

**(3au) 6-methoxy-2-(2-methoxyphenyl)quinazolin-4(3*H*)-one[14]**



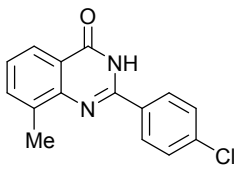

**$^1$H NMR (500 MHz, *DMSO-d6*)** δ 12.06 (s, 1H), 7.69 (dd, *J* = 7.6, 1.8 Hz, 1H), 7.66 (d, *J* = 9.0 Hz, 1H), 7.54 (d, *J* = 3.0 Hz, 2H), 7.44 (dd, *J* = 8.9, 3.1 Hz, 1H), 7.19 (dd, *J* = 8.5, 0.9 Hz, 1H), 7.09 (td, *J* = 7.5, 1.0 Hz, 1H), 3.89 (s, 3H), 3.86 (s, 3H). **$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 161.5, 158.2, 157.5, 150.6, 144.0, 132.5, 130.9, 129.6, 124.4, 123.1, 122.2, 120.9, 112.3, 106.2, 56.2, 56.1. **MS** [EI, m/z]: 282[$M^+$].

**(3av) 8-methyl-2-phenylquinazolin-4(3*H*)-one[15]**



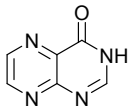

**$^1$H NMR (500 MHz, *DMSO-d6*)** δ 12.55 (s, 1H), 8.23 (d, *J* = 6.8 Hz, 2H), 8.00 (d, *J* = 7.8 Hz, 1H), 7.71 (d, *J* = 7.2 Hz, 1H), 7.63-7.53 (m, 3H), 7.41 (t, *J* = 7.6 Hz, 1H), 2.63 (s, 3H). **$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 163.0, 151.5, 147.6, 136.9, 135.4, 133.4, 131.8, 129.1, 128.2, 126.6, 124.0, 121.3, 17.6. **MS** [EI, m/z]: 236 [$M^+$].

**(3aw) 2-(4-chlorophenyl)-8-methylquinazolin-4(3*H*)-one[16]**



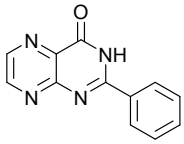

**$^1$H NMR (500 MHz, *DMSO-d6*)** δ 12.61 (s, 1H), 8.25 (d, *J* = 8.6 Hz, 2H), 8.00 (d, *J* = 7.9 Hz, 1H), 7.71 (d, *J* = 7.2 Hz, 1H), 7.65 (d, *J* = 8.6 Hz, 2H), 7.42 (t, *J* = 7.6 Hz, 1H), 2.62 (s, 3H). **$^{13}$C NMR (126 MHz, *DMSO-d6*) δ** 163.0, 150.5, 147.4, 136.7, 136.1, 135.5, 133.6, 132.2, 130.0, 129.2, 126.8, 124.3, 124.0, 121.4, 17.6**. MS** [EI, m/z]: 270 [$M^+$].

**(3ax) pteridin-4(3*H*)-one[17]**



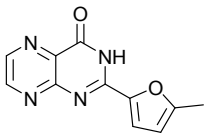
**$^{1}$H NMR (500 MHz, *DMSO-d6*)** δ 12.87 (s, 1H), 9.01 (d, *J* = 2.0 Hz, 1H), 8.85 (d, *J* = 2.0 Hz, 1H), 8.37 (s, 1H). **$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 160.8, 155.8, 150.6, 149.8, 144.9, 135.1. **MS** [EI, m/z]: 148[$M^+$].

**(3ay) 2-phenylpteridin-4(3*H*)-one[18]**



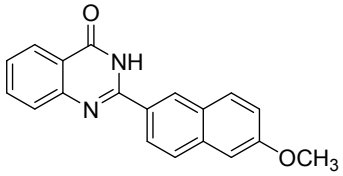
**$^{1}$H NMR (500 MHz, *DMSO-d6*)** δ 11.32 (s, 1H), 8.40 (s, 1H), 8.01-7.89 (m, 3H), 7.72-7.65 (m, 2H), 7.60 (t, *J* = 7.4 Hz, 2H). **$^{13}$C NMR (126 MHz, *DMSO-d6*)** δ 169.1, 164.9, 164.8, 156.2, 155.8, 149.6, 147.3, 133.9, 133.5, 131.9, 131.4, 129.5, 128.2, 123.8. **MS** [EI, m/z]: 224 [$M^+$].

**(3az) 2-(5-methylfuran-2-yl)quinazolin-4(3*H*)-one[19]**



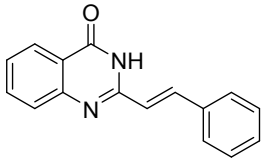
**$^{1}$H NMR (400 MHz, *DMSO-d6*)** δ 12.40 (s, 1H), 8.11 (dd, J = 7.9, 1.4 Hz, 1H), 7.80 (ddd, J = 8.5, 7.1, 1.6 Hz, 1H), 7.69 (d, J = 8.1 Hz, 1H), 7.56 (d, J = 3.4 Hz, 1H), 7.47 (ddd, J = 8.1, 7.1, 1.3 Hz, 1H), 6.38 (dd, J = 3.4, 1.1 Hz, 1H), 2.41 (d, J = 1.1 Hz, 3H).**$^{13}$C NMR (101 MHz, *DMSO-d6*)**δ 162.1, 156.6, 149.3, 144.9, 144.4, 135.1, 127.6, 126.7, 126.4, 121.5, 116.3, 109.4, 14.0. **MS** [EI, m/z]: 226 [$M^+$].

**(3ba) 2-(6-methoxynaphthalen-2-yl)quinazolin-4(3*H*)-one[20]**



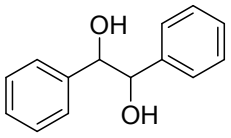
**$^{1}$H NMR (400 MHz, *DMSO-d6*)** δ 8.37 (s, 1H), 7.86 (dd, J = 8.8, 6.8 Hz, 2H), 7.68 (dd, J = 8.2, 1.9 Hz, 2H), 7.35 (d, J = 2.5 Hz, 1H), 7.27 (ddd, J = 8.5, 7.3, 1.8 Hz, 1H), 7.19-7.16 (m, 1H), 6.85-6.65 (m, 2H), 3.88 (s, 3H). **$^{13}$C NMR (101 MHz, *DMSO-d6*)** δ 164.2, 158.1, 148.5, 136.9, 134.9, 133.8, 130.0, 128.3, 127.9, 127.5, 126.3, 125.8, 119.4, 117.7, 115.4, 114.9, 106.3, 55.7. **MS** [EI, m/z]: 302 [$M^+$].

**(3bb)2-styrylquinazolin-4(3*H*)-one[21]**



**$^1$H NMR (400 MHz, *DMSO-d6*)** δ 12.57 (s, 1H), 8.77 (s, 1H), 8.29 (d, *J* = 8.8 Hz, 1H), 8.18 (d, *J* = 6.5 Hz, 1H), 7.97 (d, *J* = 11.5 Hz, 2H), 7.86 (t, *J* = 7.6 Hz, 1H), 7.78 (d, *J* = 7.6 Hz, 1H), 7.64-7.38 (m, 3H), 7.28 (dd, *J* = 8.9, 2.6 Hz, 1H). **$^{13}$C NMR (101 MHz, *DMSO-d6*)** δ 159.3, 152.8, 149.4, 136.3, 135.1, 131.1, 128.4, 127.5, 126.9, 126.4, 125.5, 112.0, 106.5. **MS** [EI, m/z]: 248 [$M^+$].

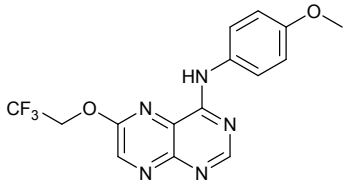
**(5a) 1,2-diphenylethane-1,2-diol [22]**




1,2-diphenylethane-1,2-diol

**$^1$H NMR (400 MHz, *DMSO-d6*)** δ 7.40-7.32 (m, 8H), 7.25 (tt, *J* = 5.8, 2.3 Hz, 2H), 5.28 (t, *J* = 5.8 Hz, 2H), 4.55 (s, 2H). **$^{13}$C NMR (101 MHz, *DMSO-d6)*** δ 143.00, 128.51, 127.10, 126.91, 63.46. **MS** [EI, m/z]: 214 [$M^+$].

**(A3) *N*-(4-methoxyphenyl) -6- (2,2,2-trifluoroethoxy) pteridin -4-amine[23]**




**$^1$H NMR (400 MHz, *DMSO-d6*)** δ 9.92 (s, 1H), 8.98 (s, 1H), 8.62 (s, 1H), 7.76-7.70 (m, 2H), 7.04 - 6.99 (m, 2H), 5.46 (q, *J* = 9.1 Hz, 2H), 3.79 (s, 3H). **$^{13}$C NMR (101 MHz, *DMSO-d6*)** δ 158.3, 156.8, 156.6, 155.1, 150.8, 144.9, 131.5, 125.8, 124.9, 123.0, 121.5, 114.2, 63.2, 62.8, 55.7. **MS** [EI, m/z]: 351 [$M^+$].

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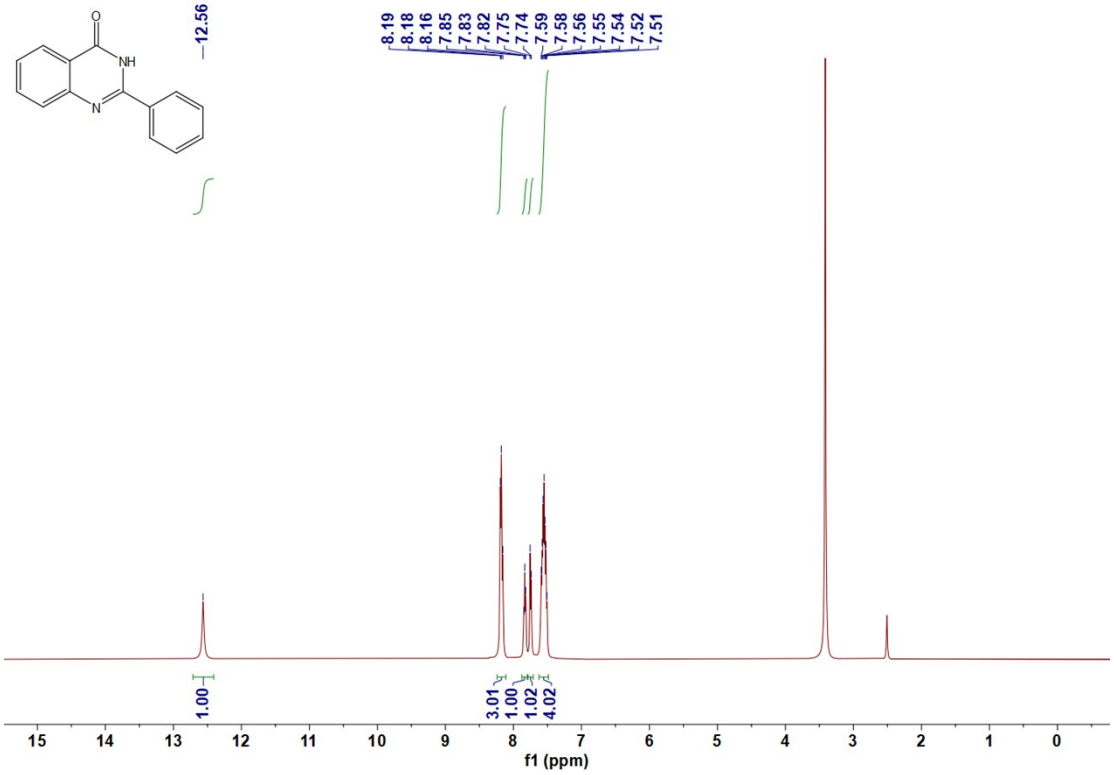
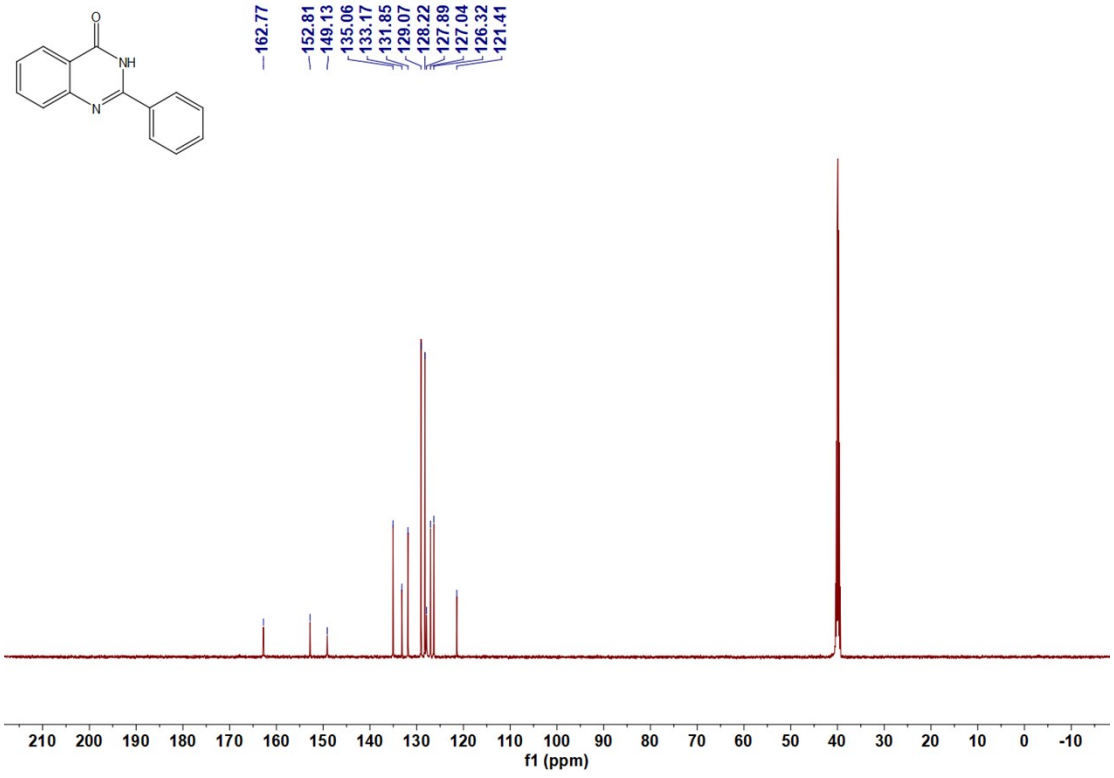
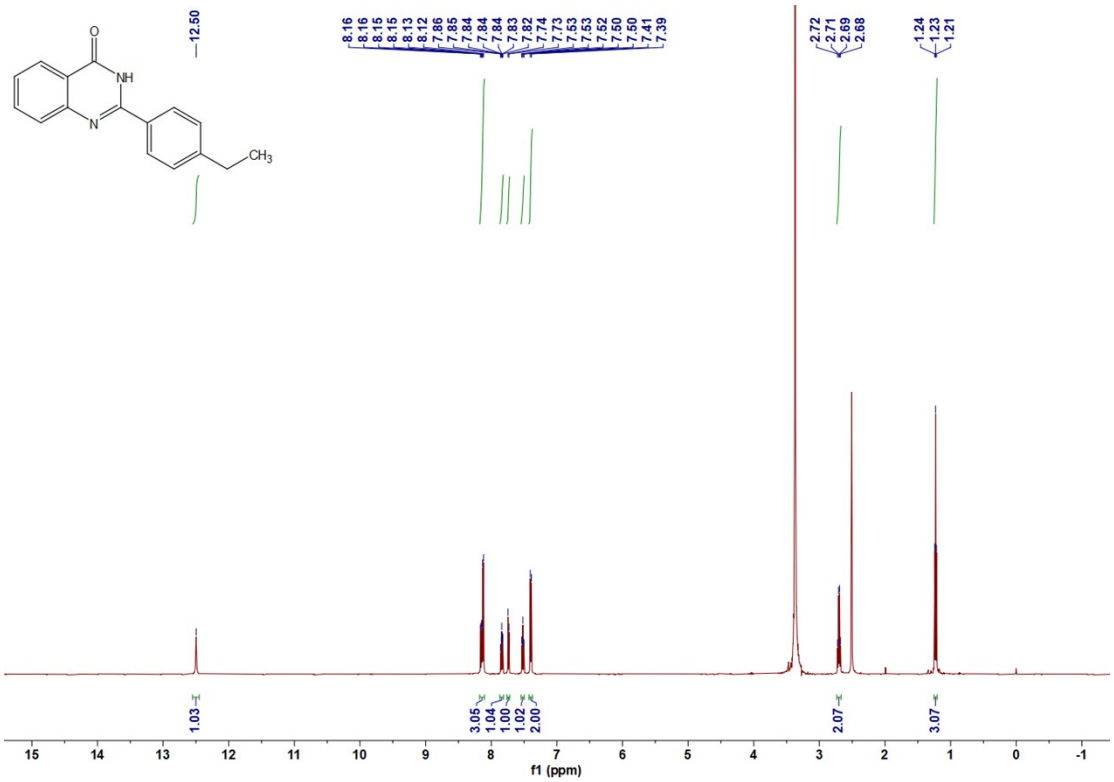
## $^{1}$H NMR and $^{13}$C NMR spectra for the products

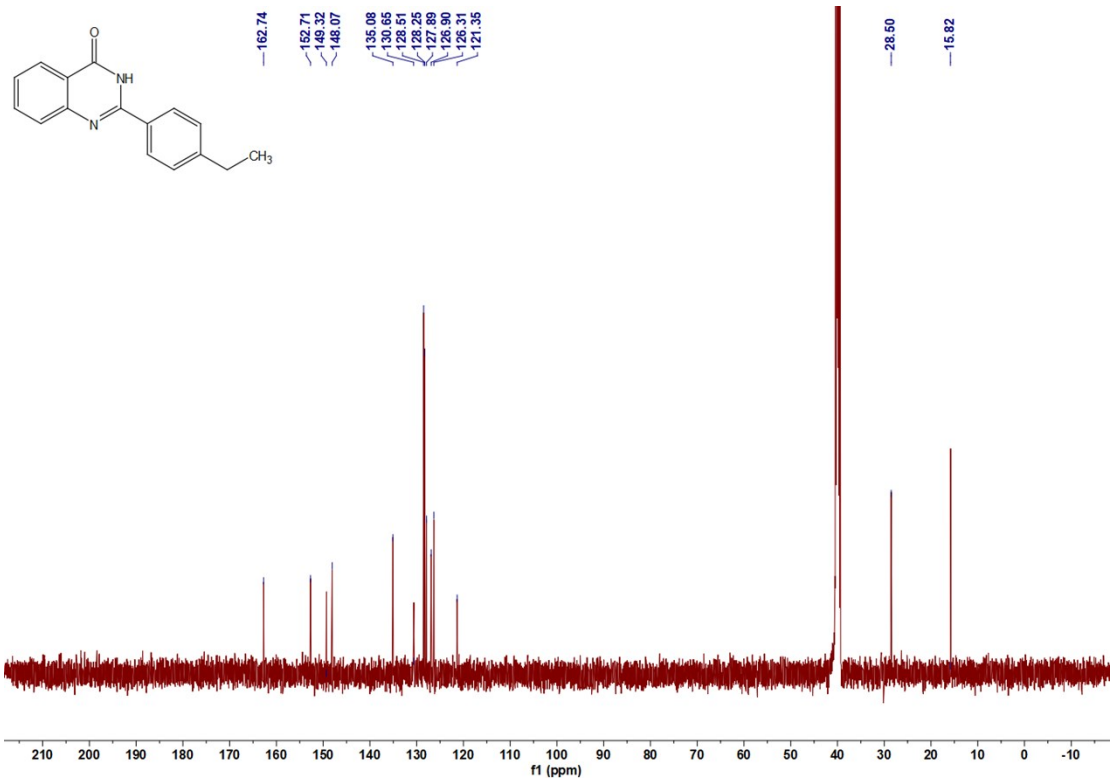
**(3aa) 2-phenylquinazolin-4(3*H*)-one**



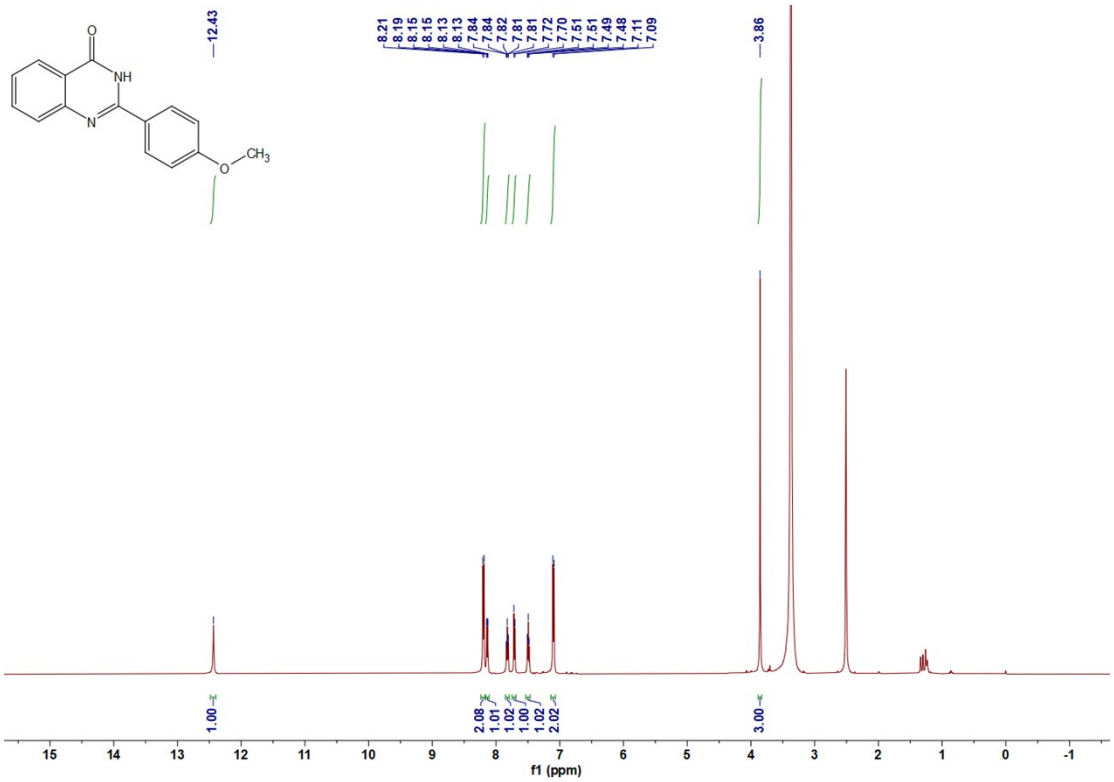



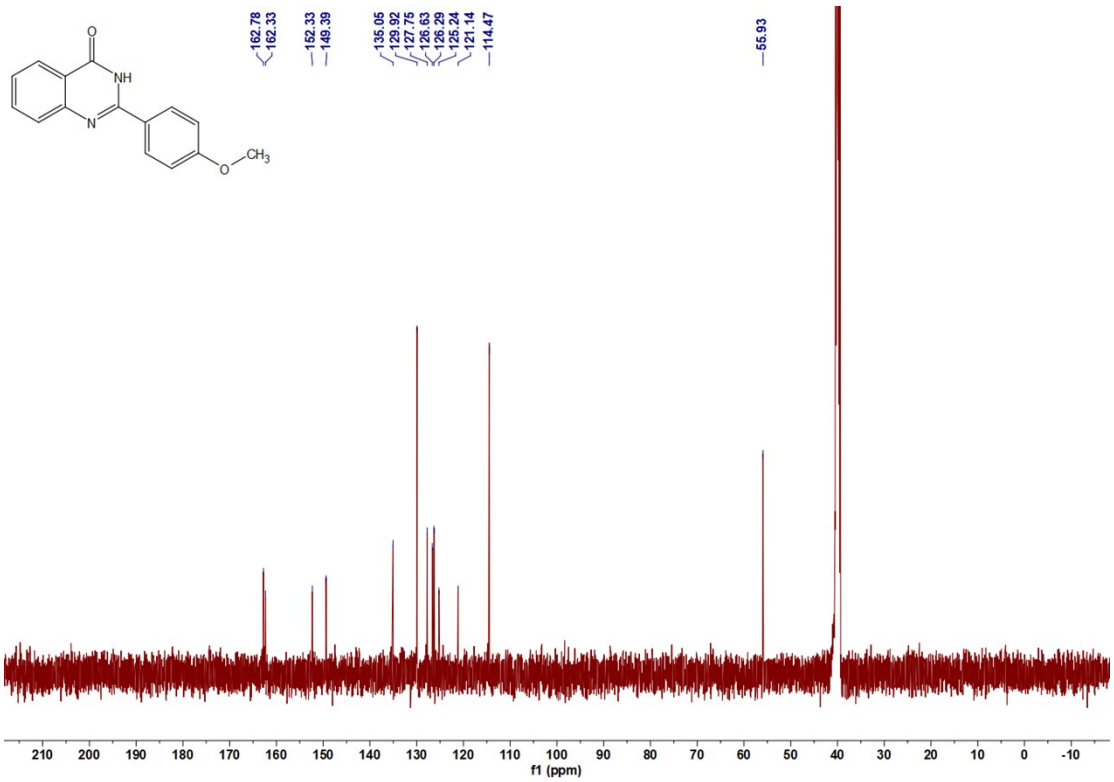
**(3ab) 2-(4-ethylphenyl)quinazolin-4(3*H*)-one**



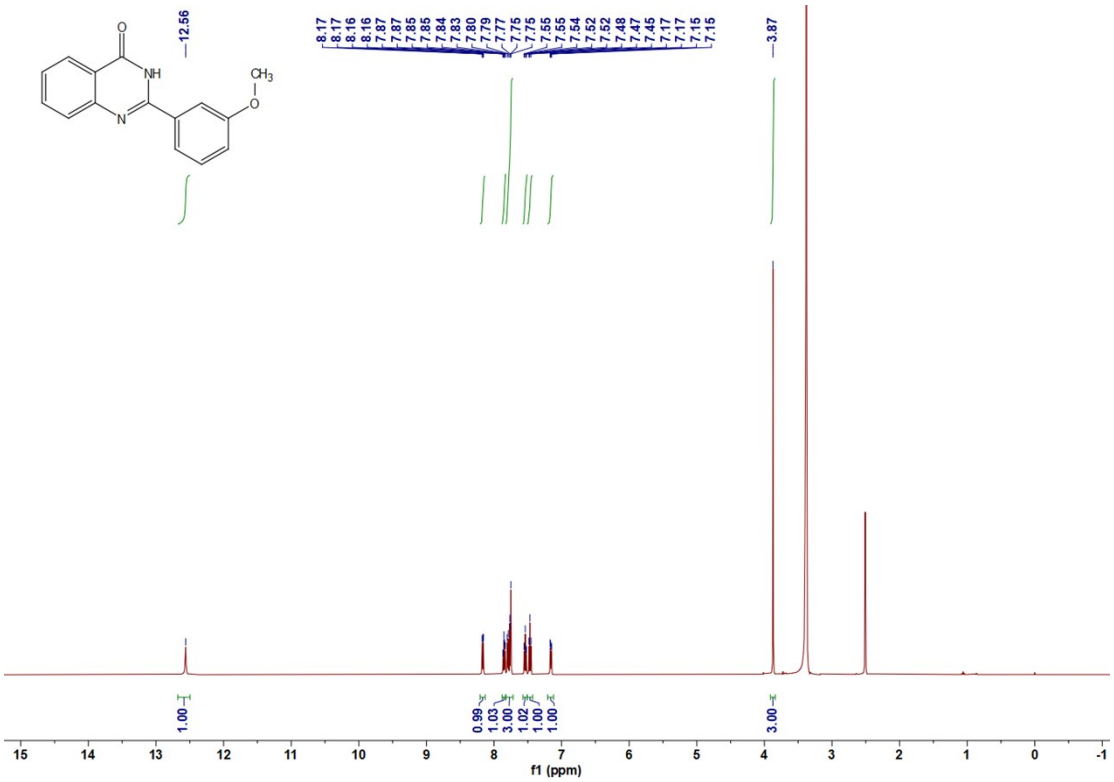



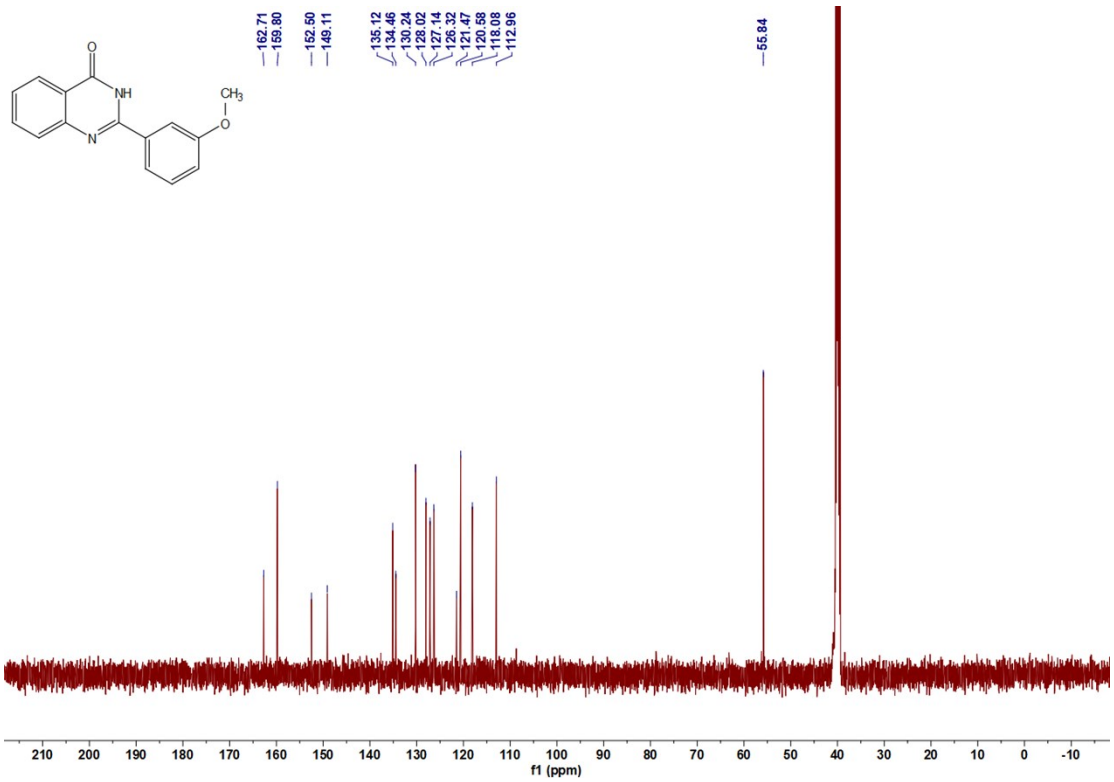
**(3ac) 2-(4-methoxyphenyl)quinazolin-4(3*H*)-one**



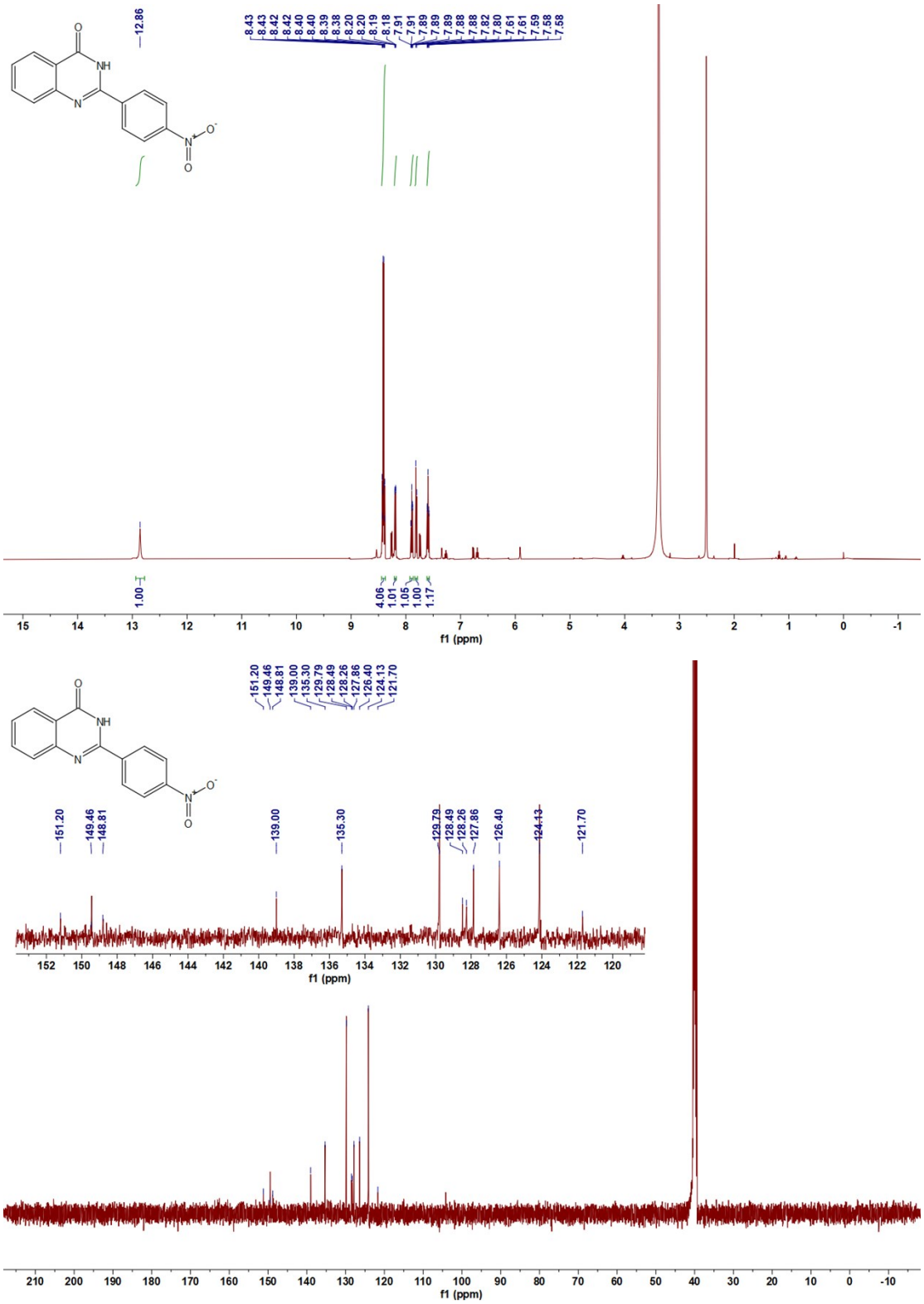



**(3ad) 2-(3-methoxyphenyl)quinazolin-4(3*H*)-one**

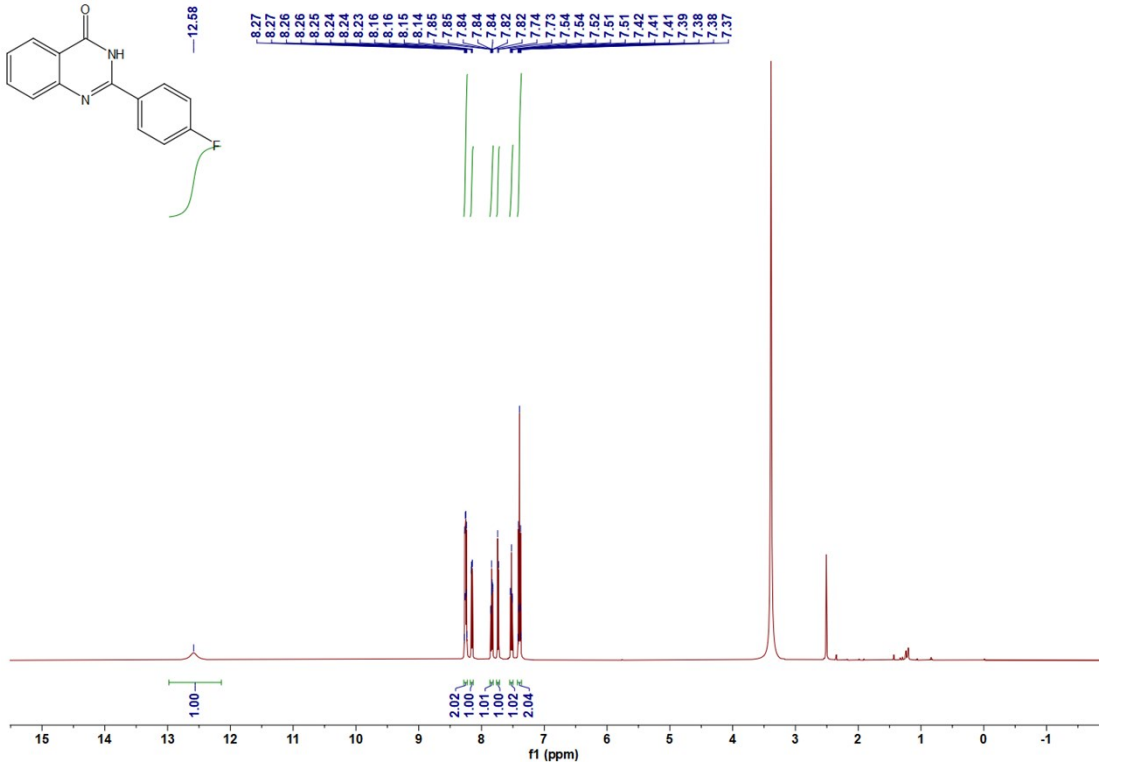


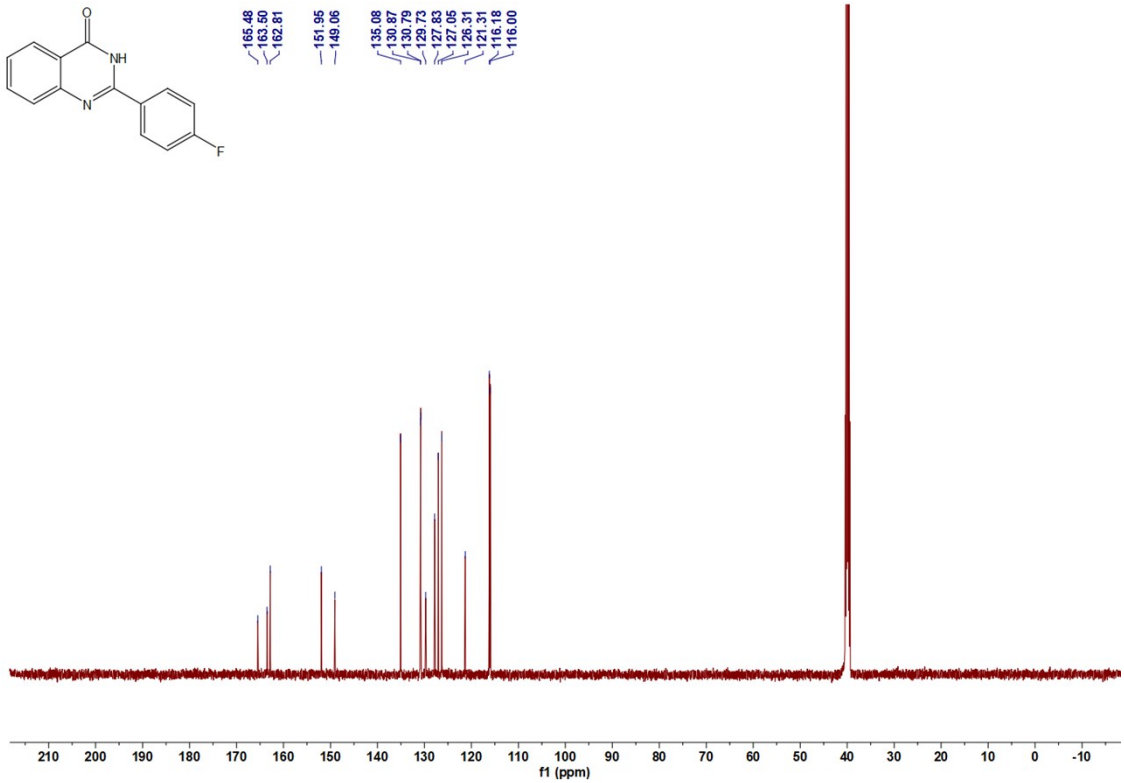



**(3ae) 2-(4-nitrophenyl)quinazolin-4(3*H*)-one**

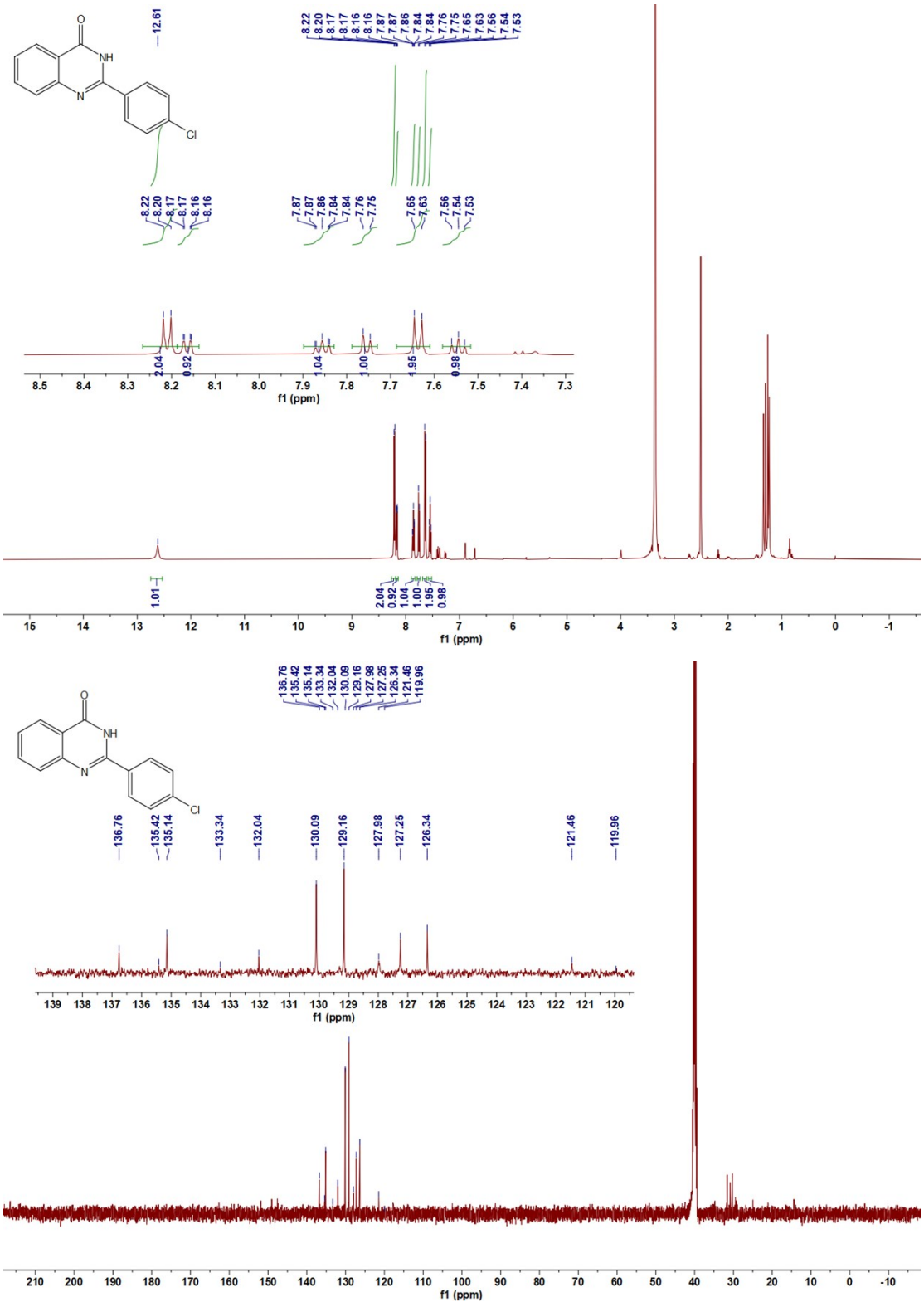


**(3af) 2-(4-fluorophenyl)quinazolin-4(3*H*)-one**

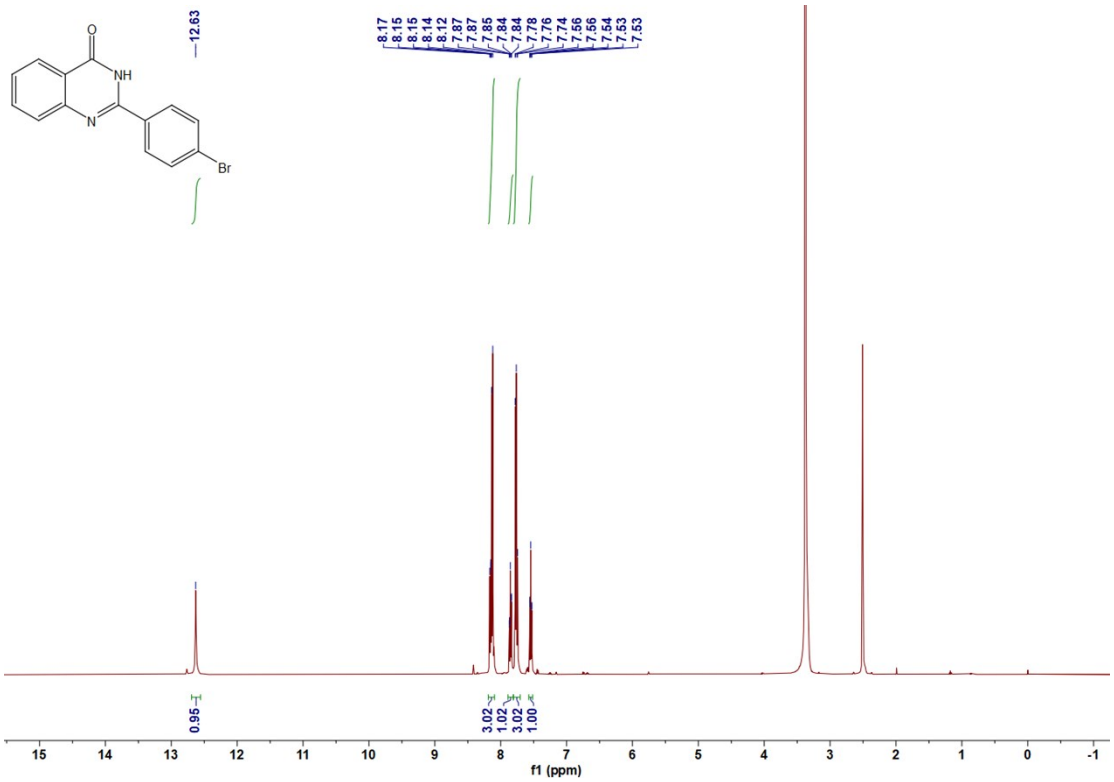


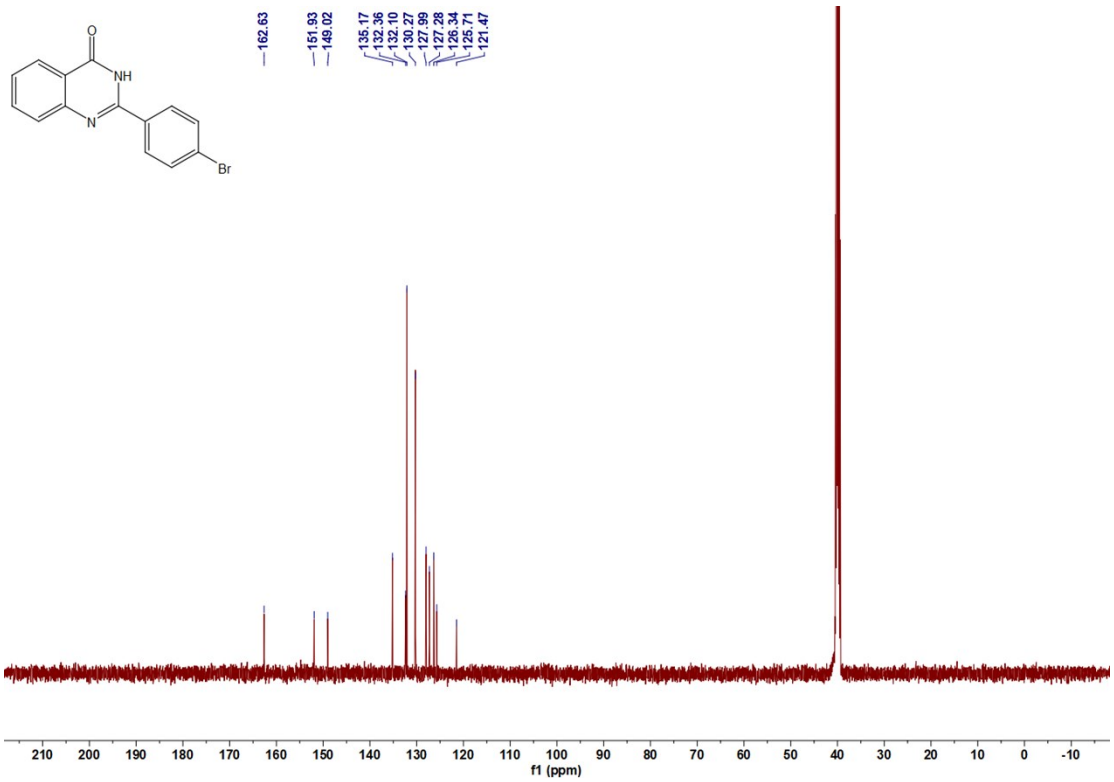



**(3ag) 2-(4-chlorophenyl)quinazolin-4(3*H*)-one**

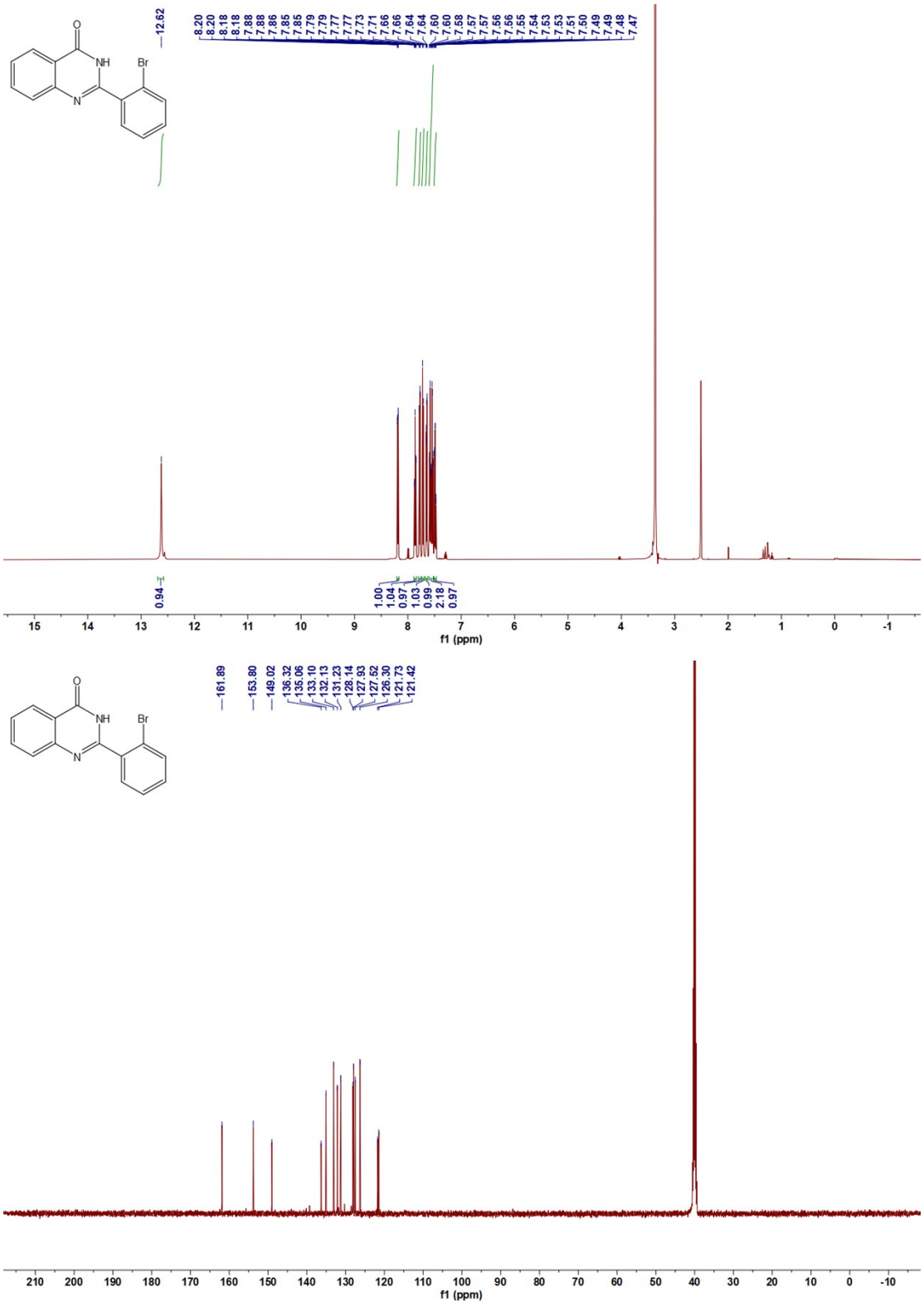


**(3ah) 2-(4-bromophenyl)quinazolin-4(3*H*)-one**

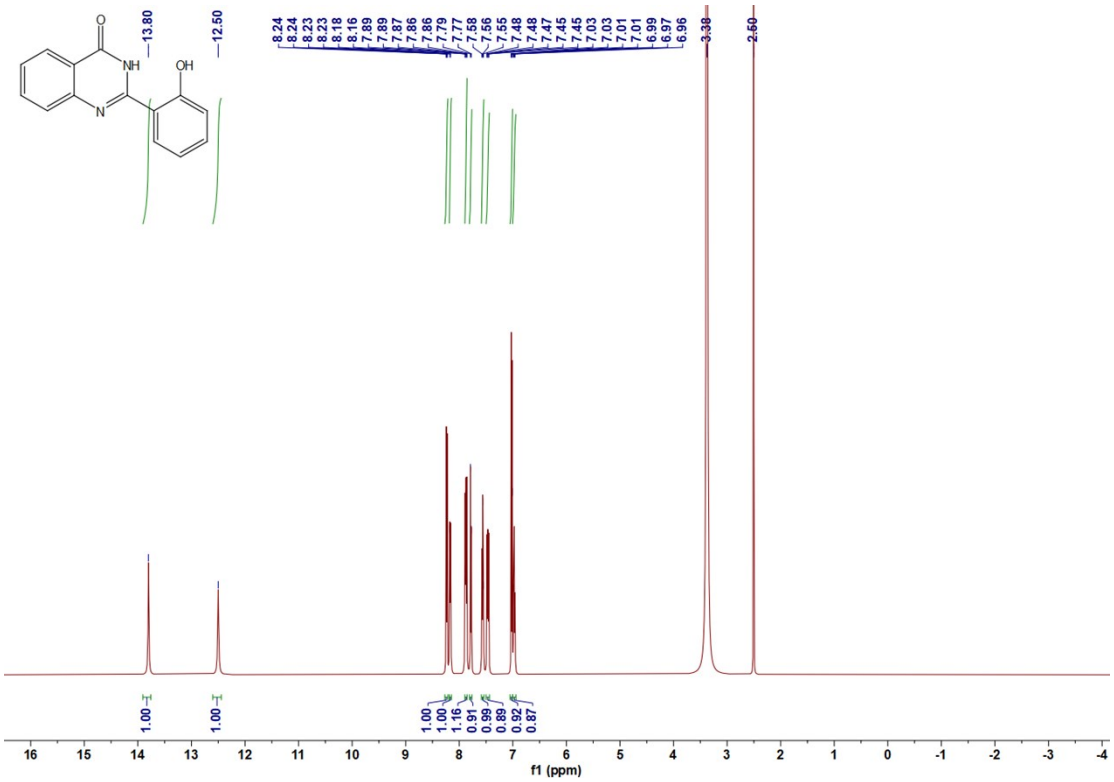


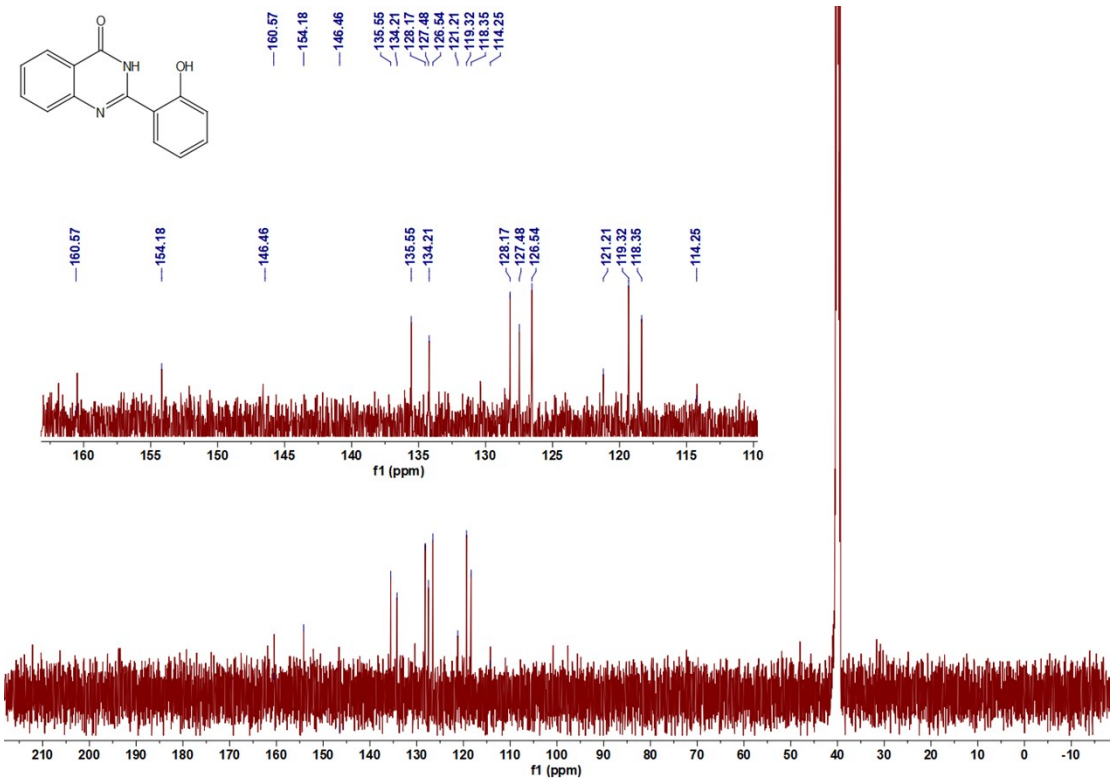



**(3ai) 2-(2-bromophenyl)quinazolin-4(3*H*)-one**

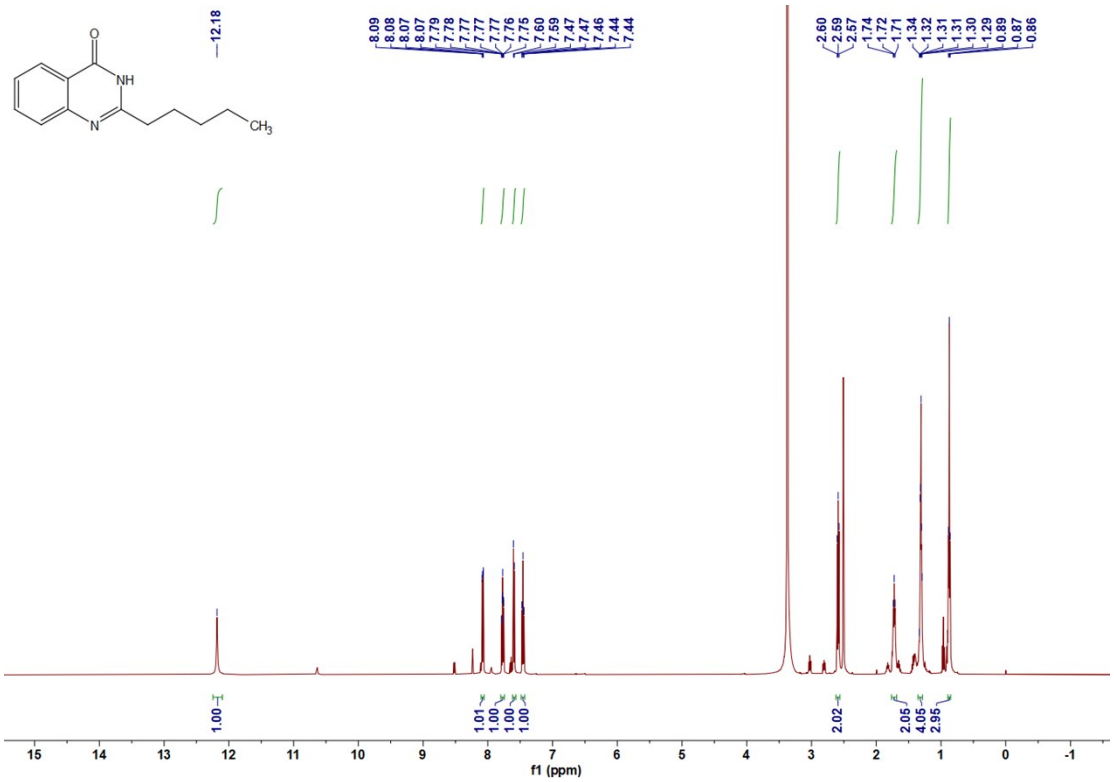


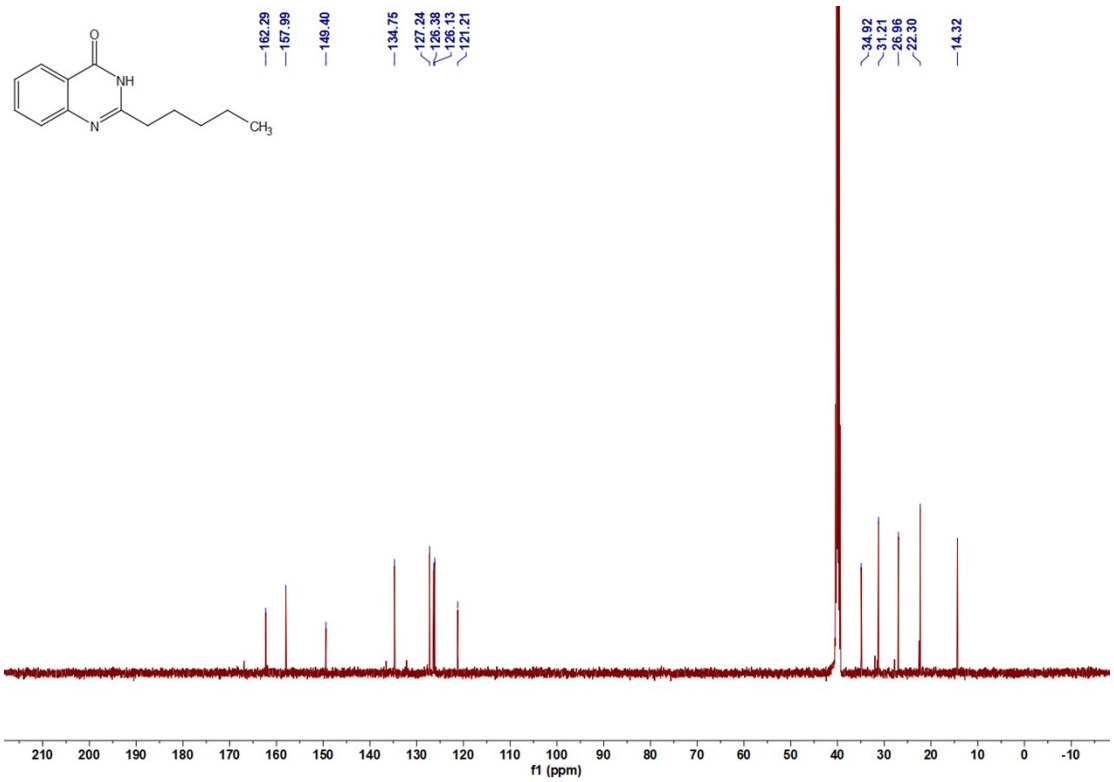
**(3aj) 2-(2-hydroxyphenyl)quinazolin-4(3*H*)-one**



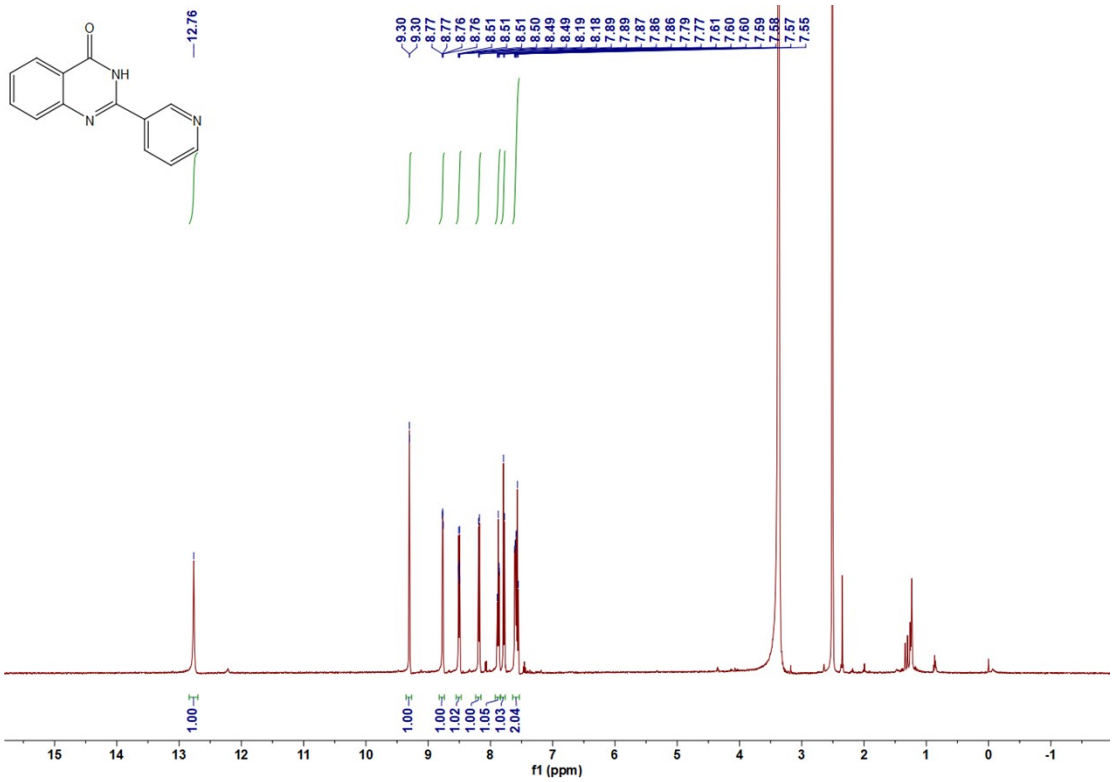



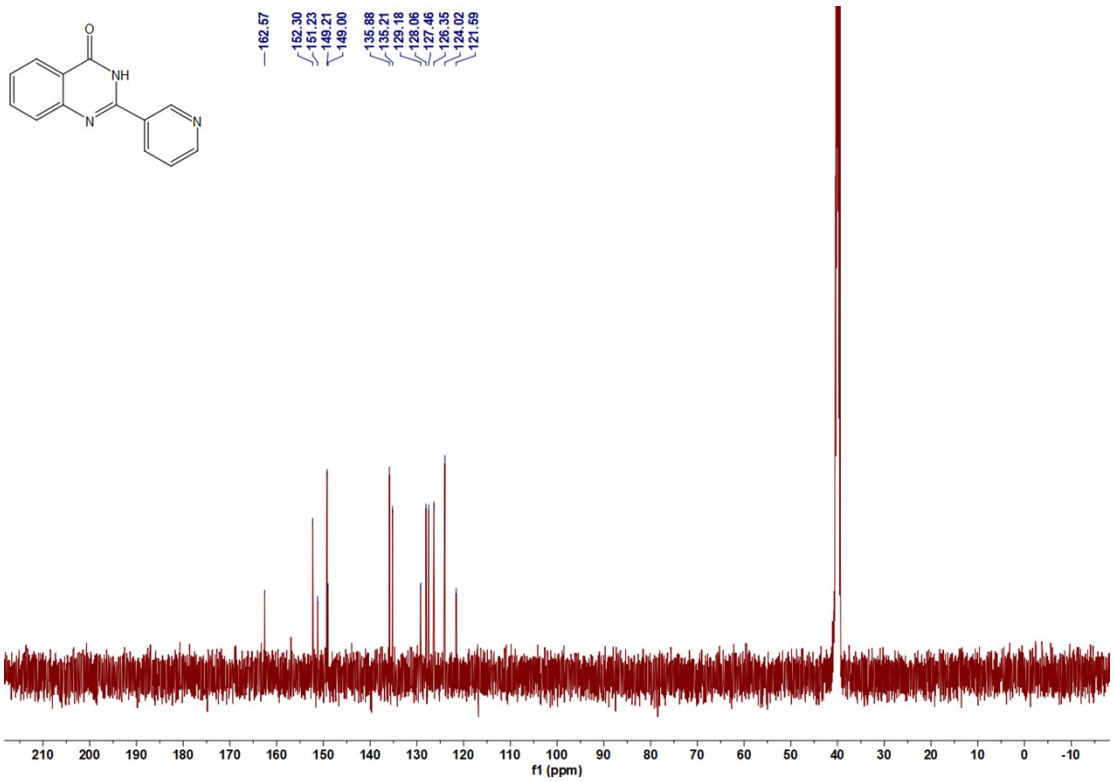
**(3ak) 2-(2-hydroxy-4-pentylphenyl)quinazolin-4(3*H*)-one**



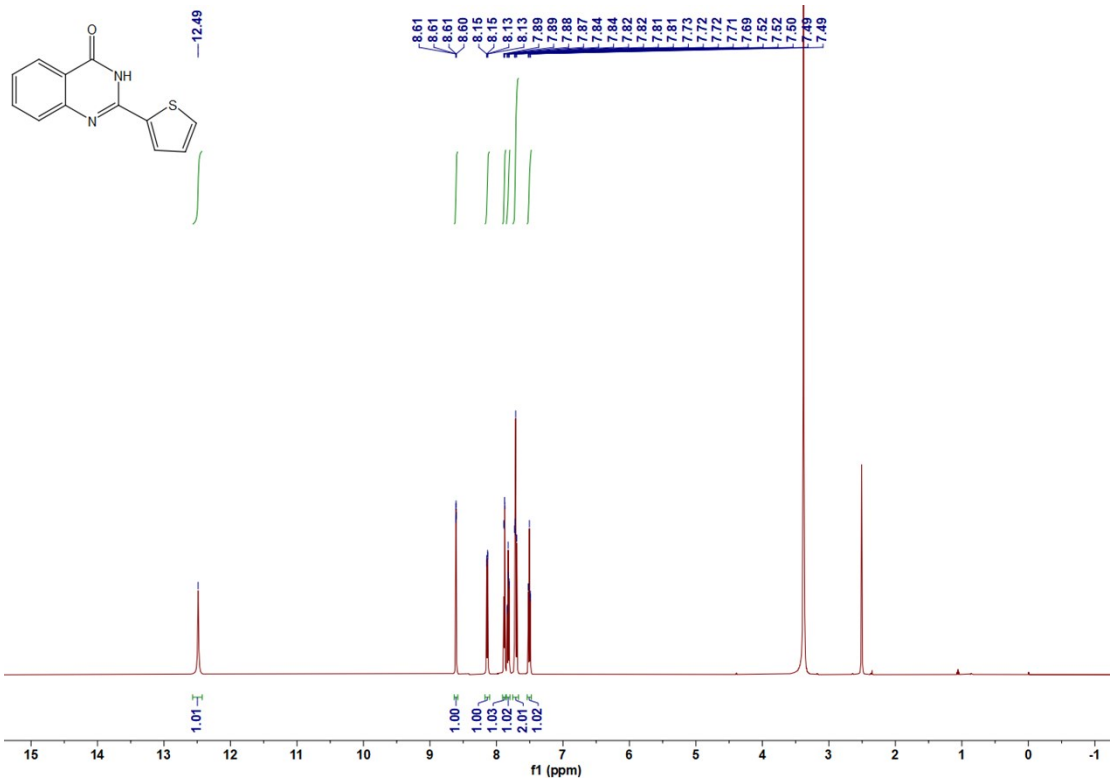



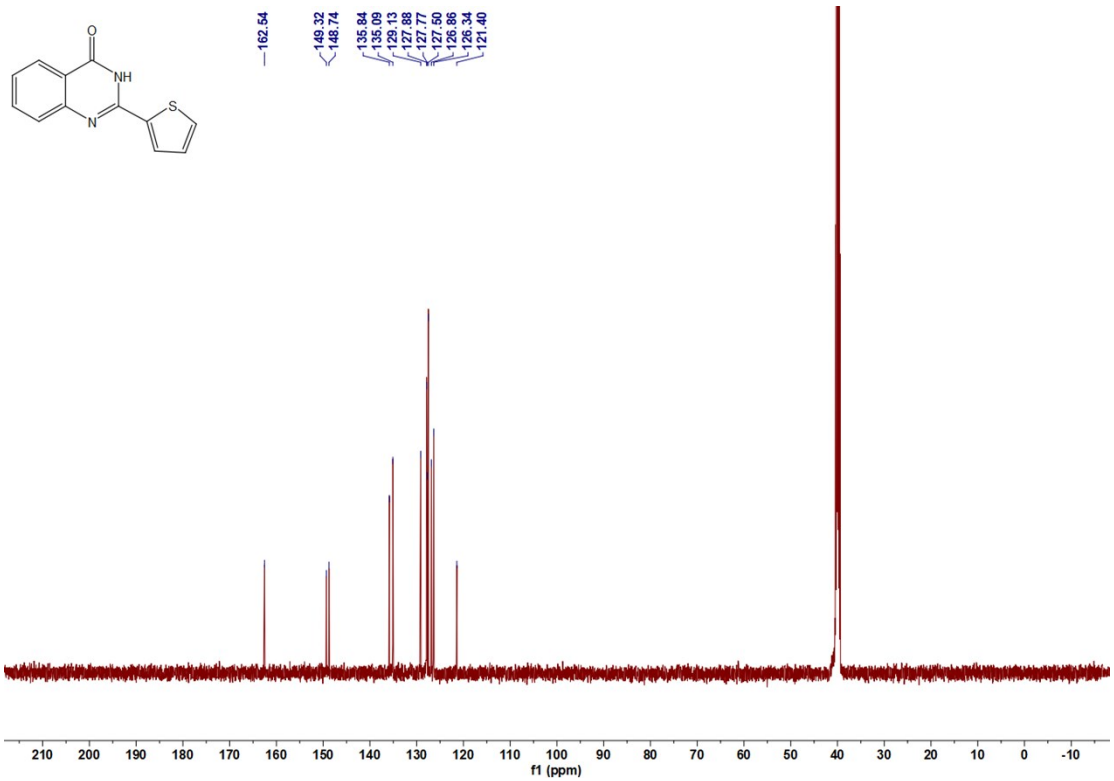
**(3al) 2-(pyridin-3-yl)quinazolin-4(3*H*)-one**



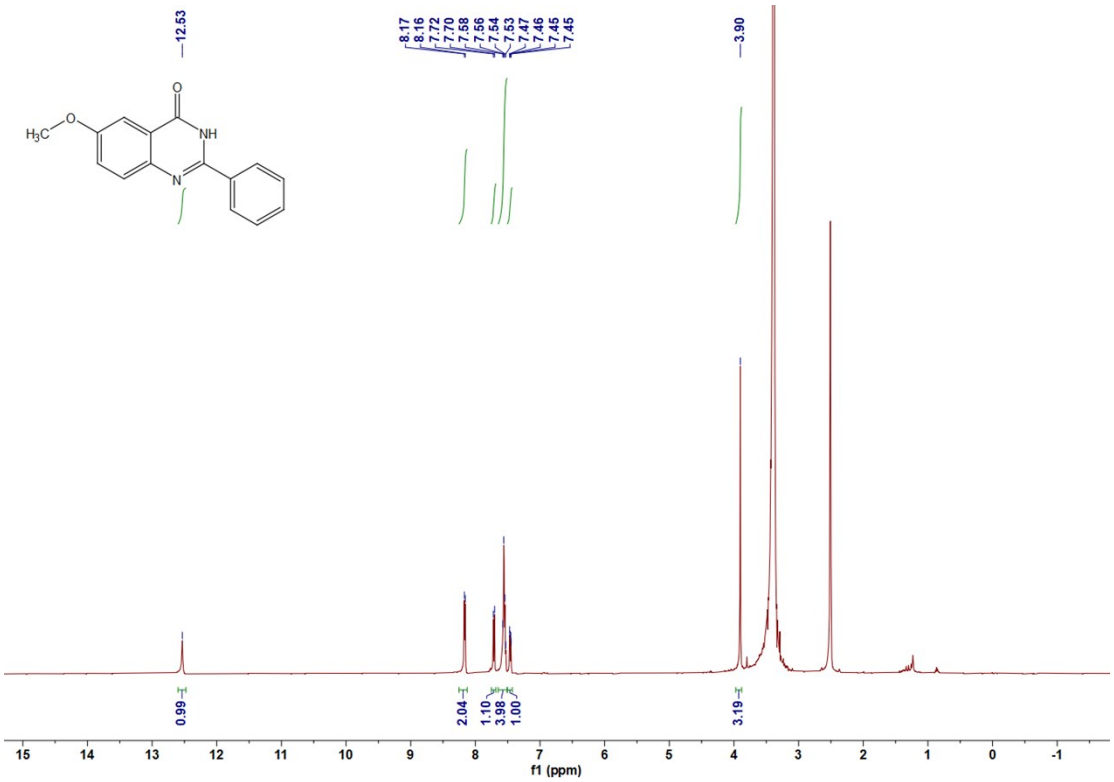



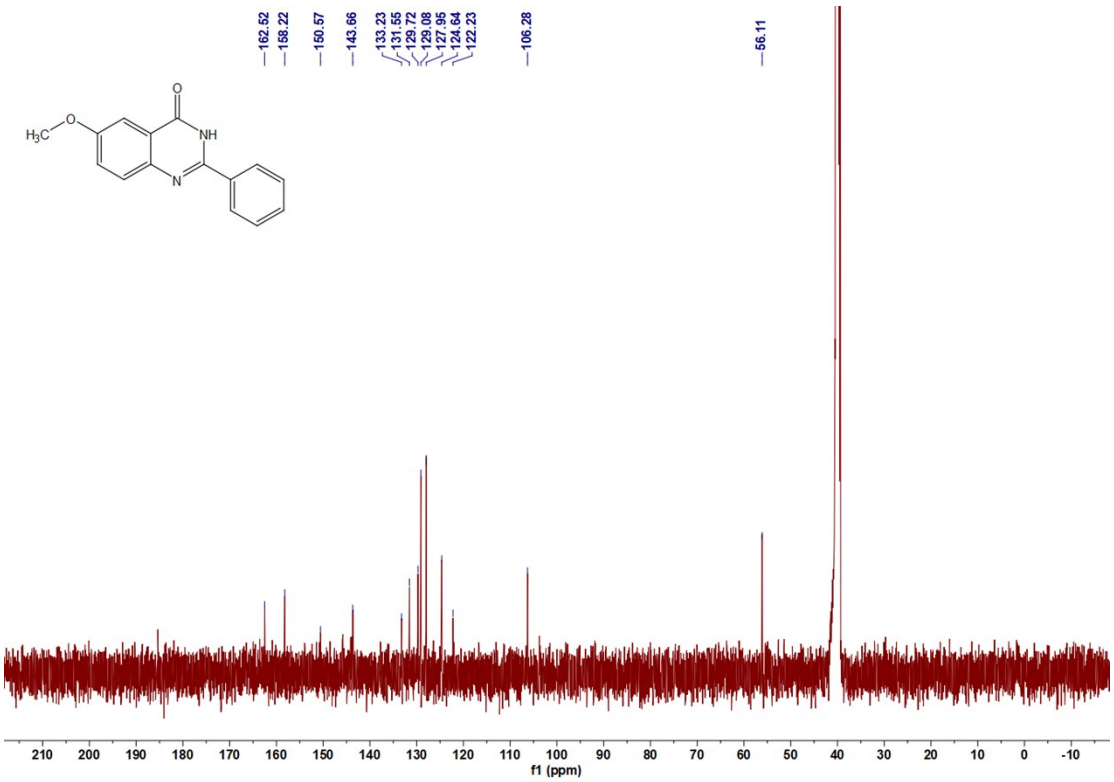
**(3am) 2-(thiophen-2-yl)quinazolin-4(3*H*)-one**



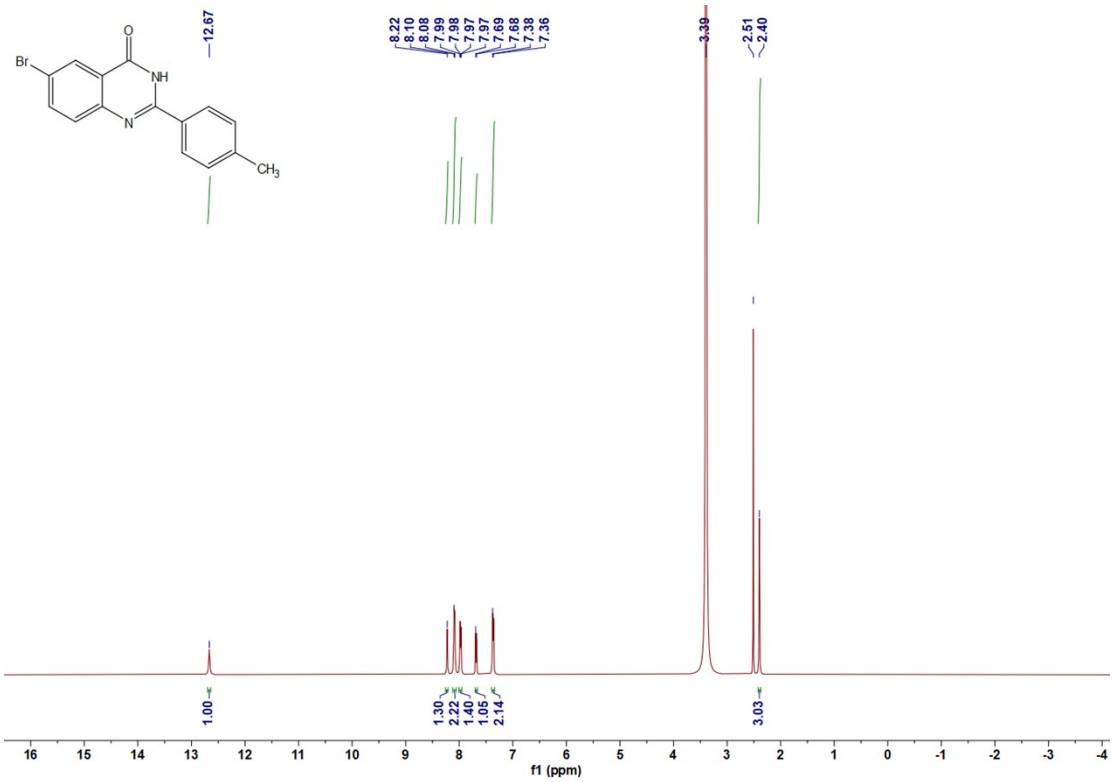



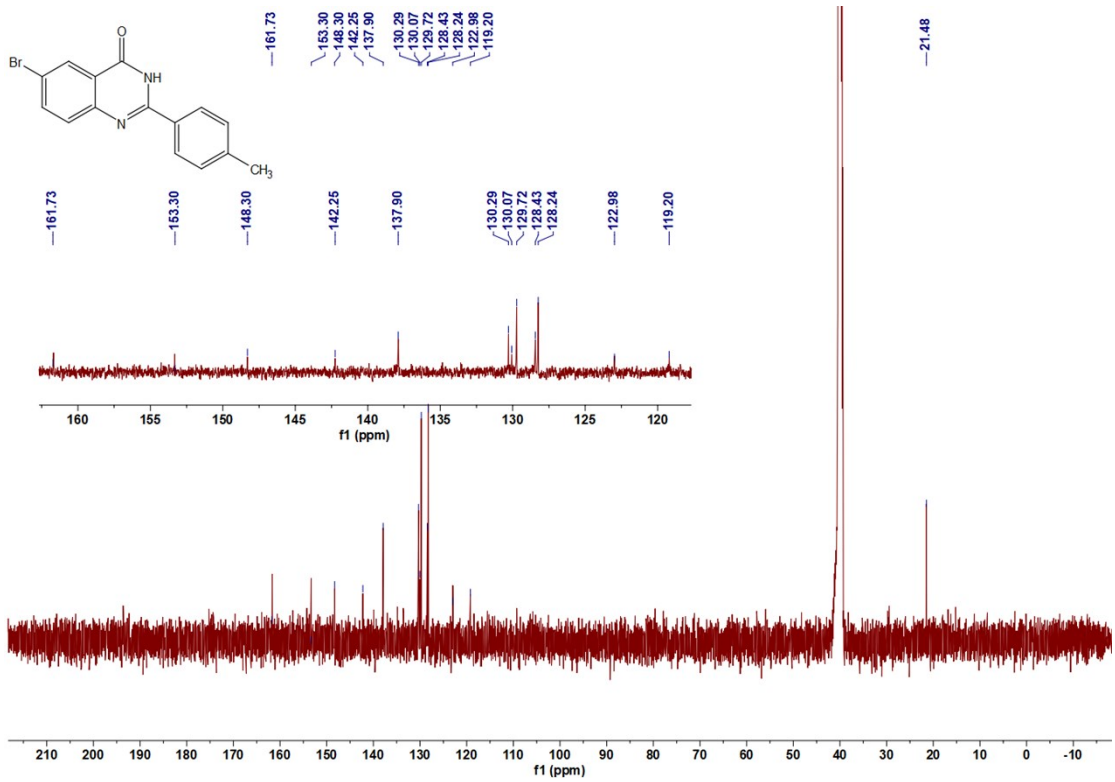
**(3an) 6-methoxy-2-phenylquinazolin-4(3*H*)-one**



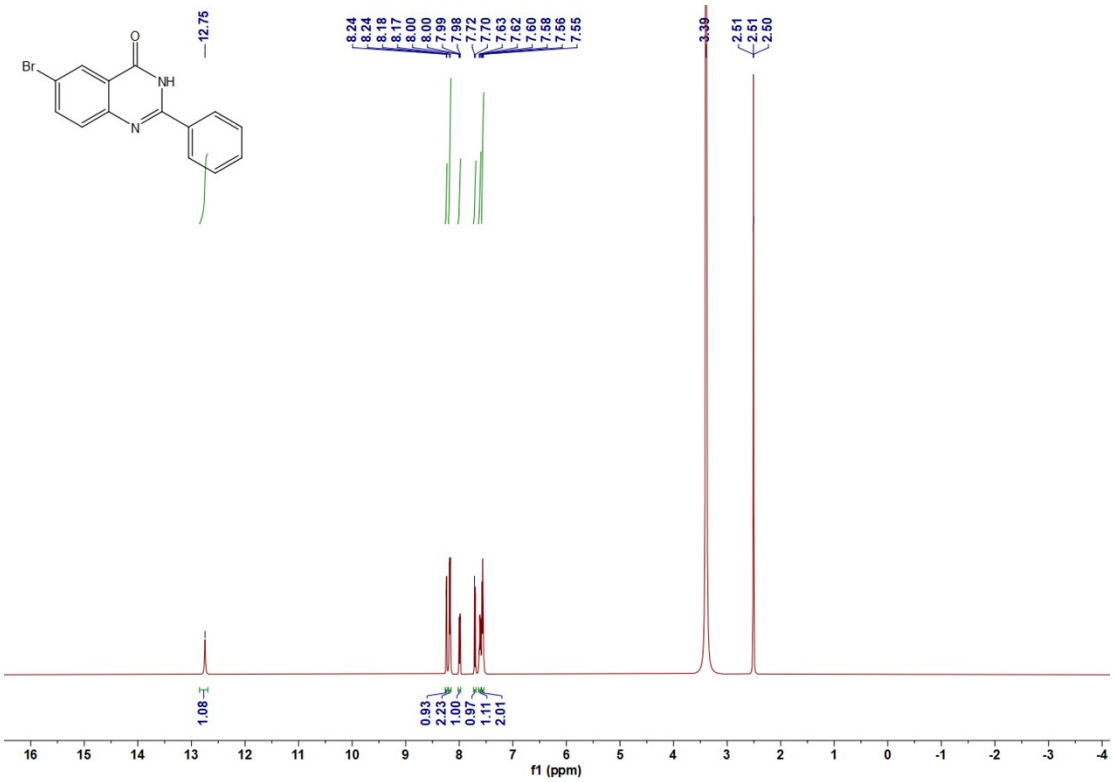



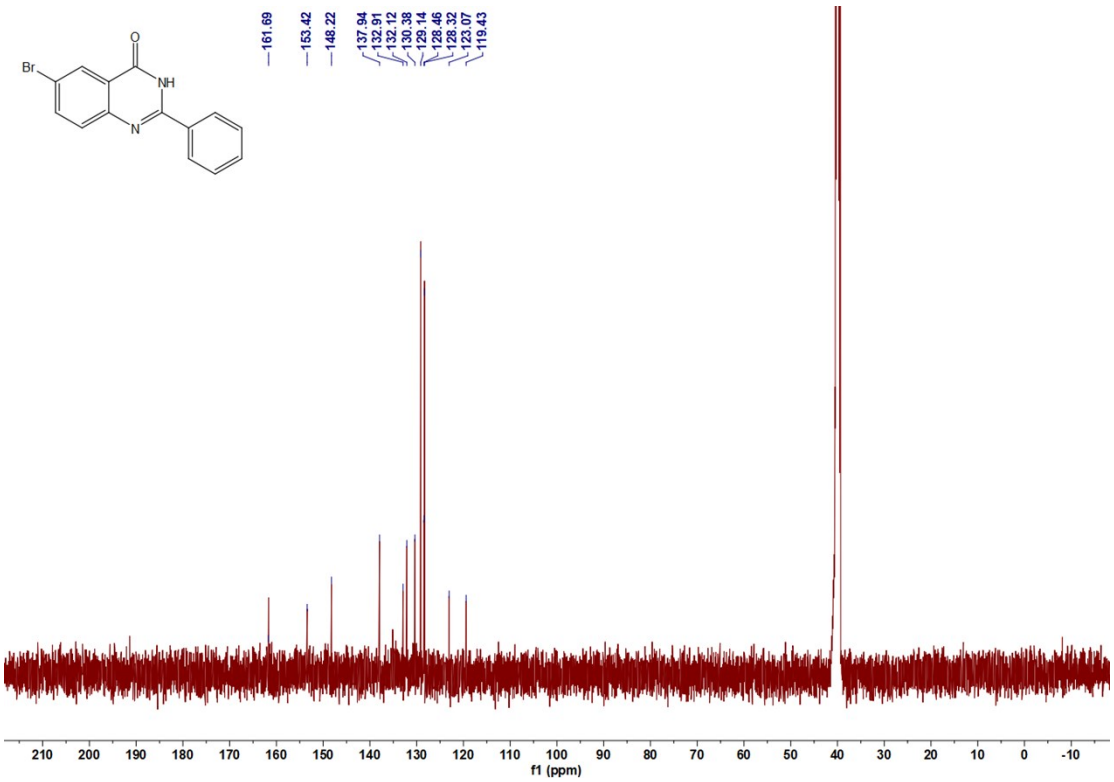
**(3ao) 6-bromo-2-(p-tolyl)quinazolin-4(3*H*)-one**



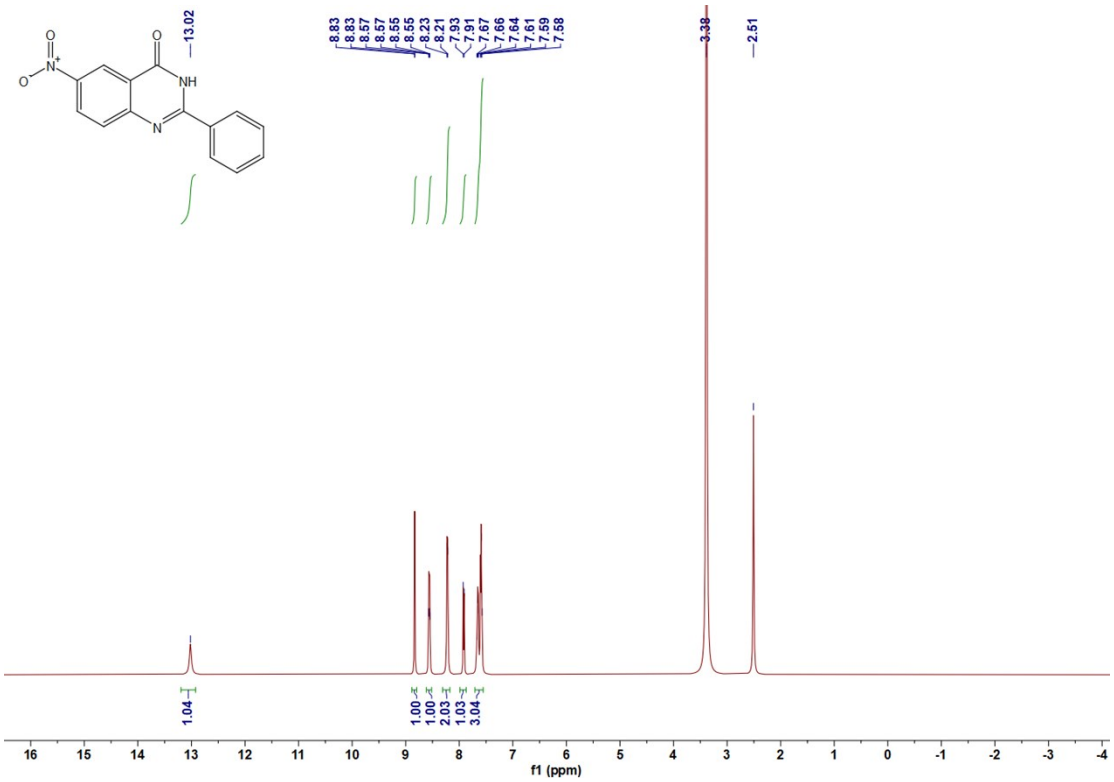



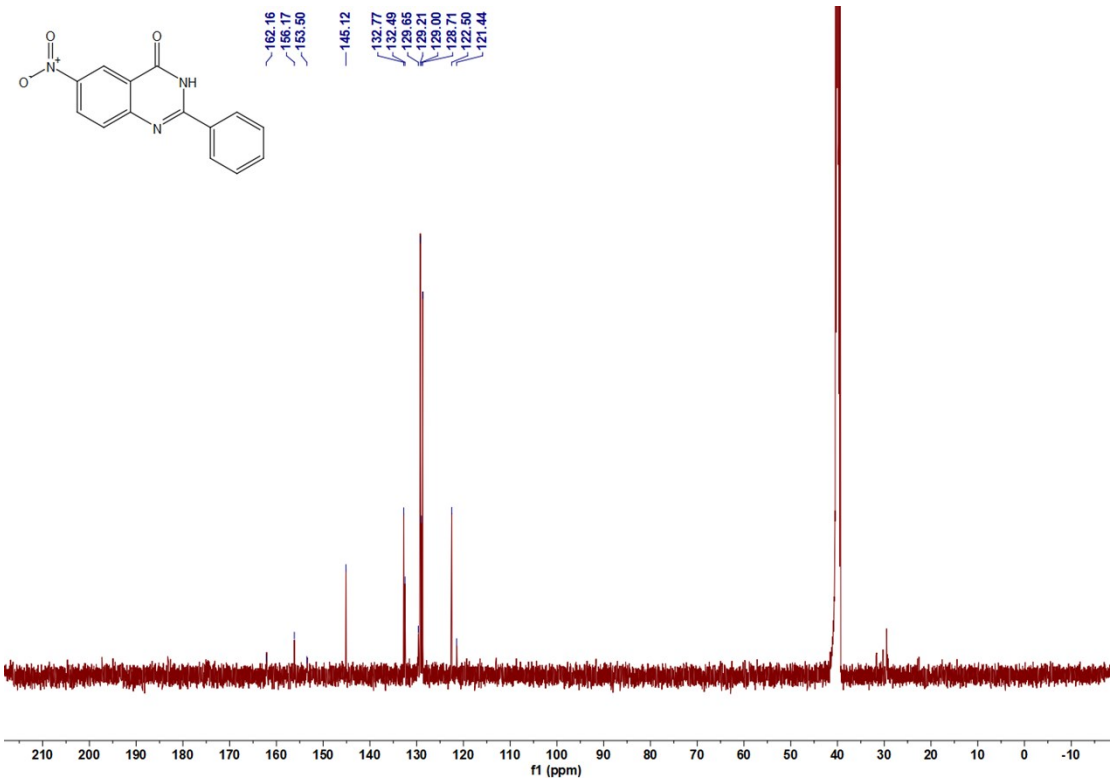
**(3ap) 6-bromo-2-phenylquinazolin-4(3*H*)-one**



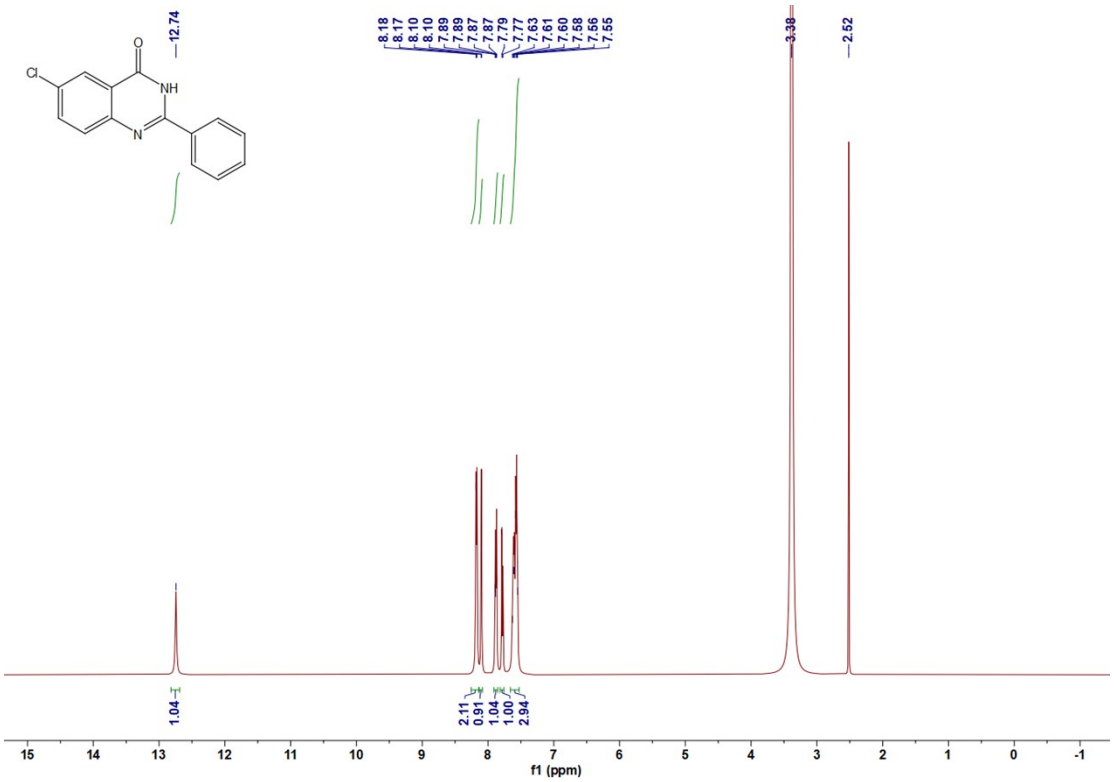



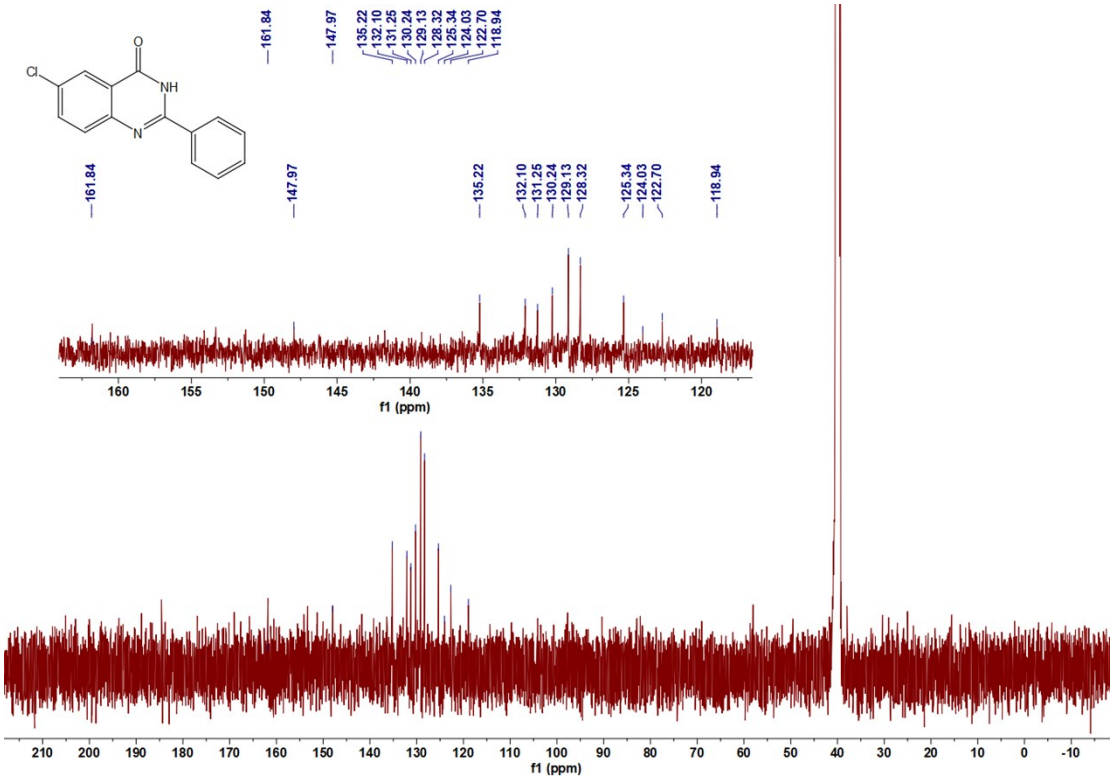
**(3aq) 6-nitro-2-phenylquinazolin-4(3*H*)-one**



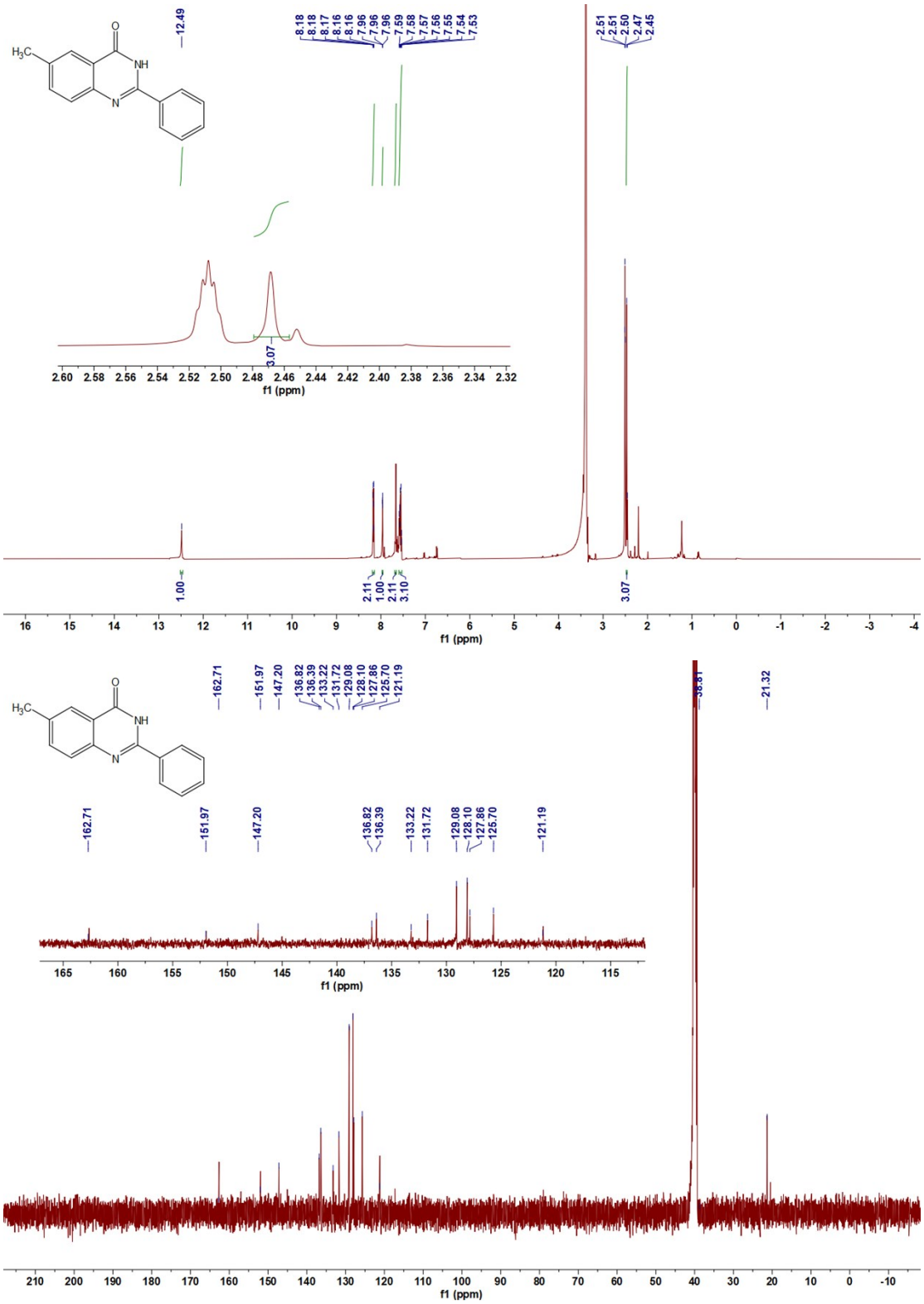



**(3ar) 6-chloro-2-phenylquinazolin-4(3*H*)-one**

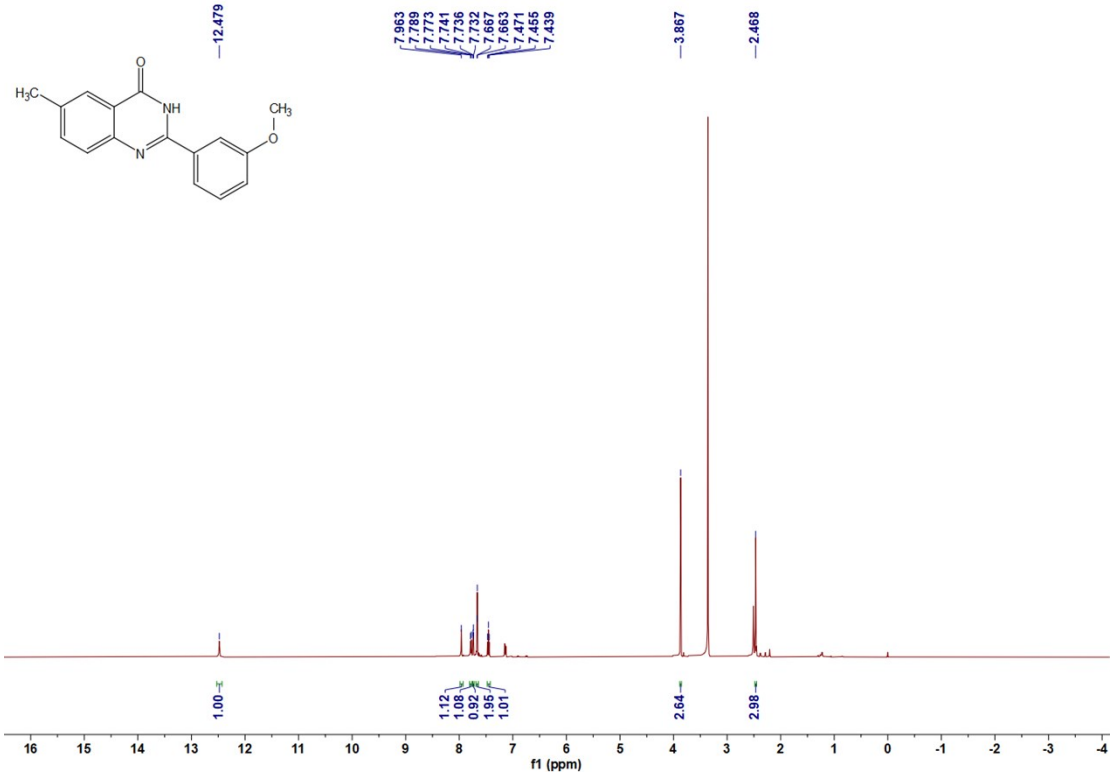


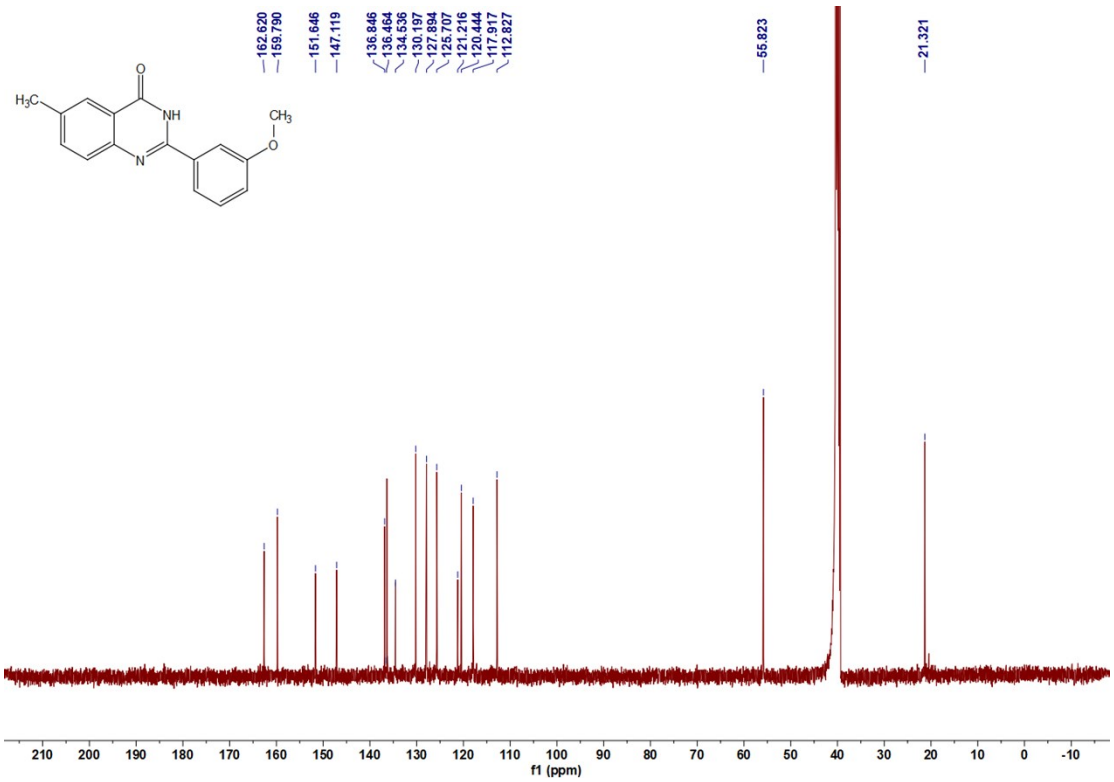



**(3as) 6-methyl-2-phenylquinazolin-4(3*H*)-one**

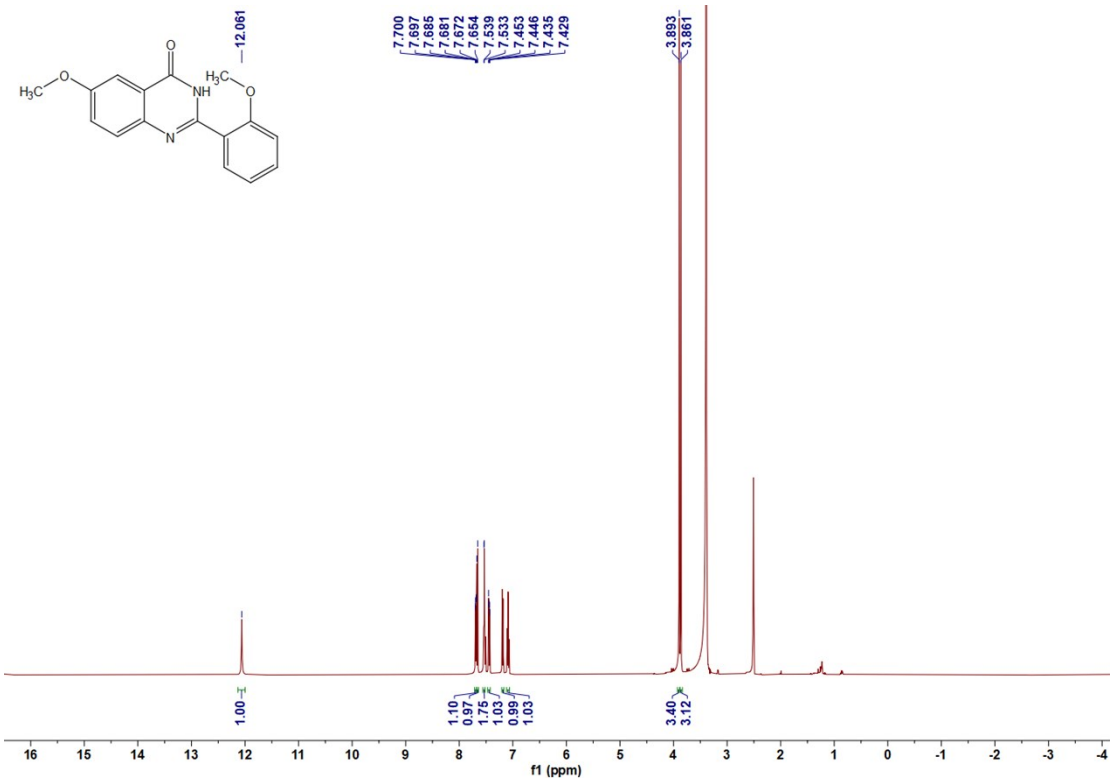


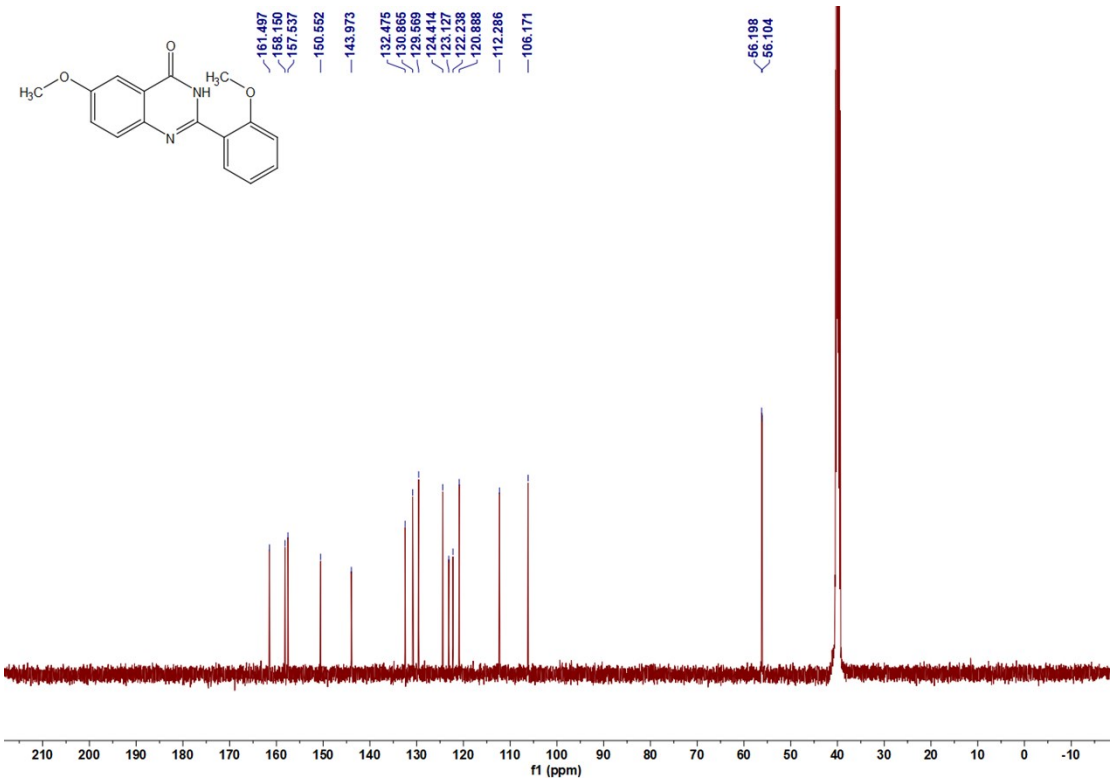
**(3at) 2-(3-methoxyphenyl)-6-methylquinazolin-4(3*H*)-one**



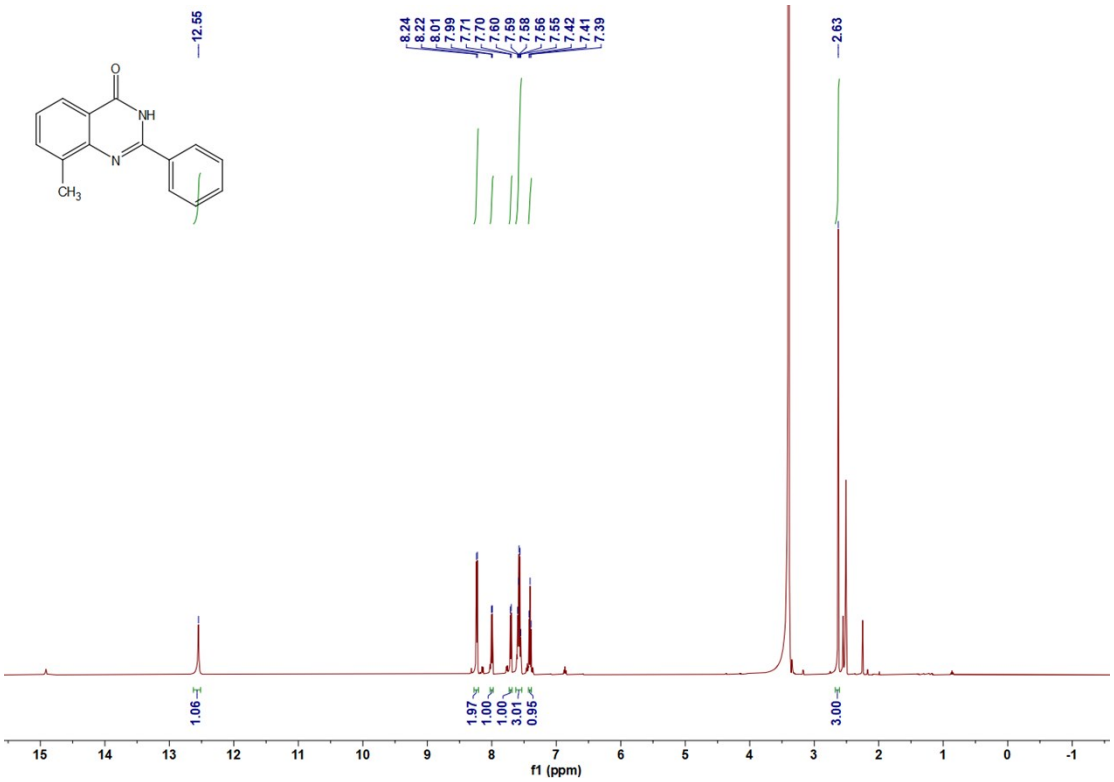



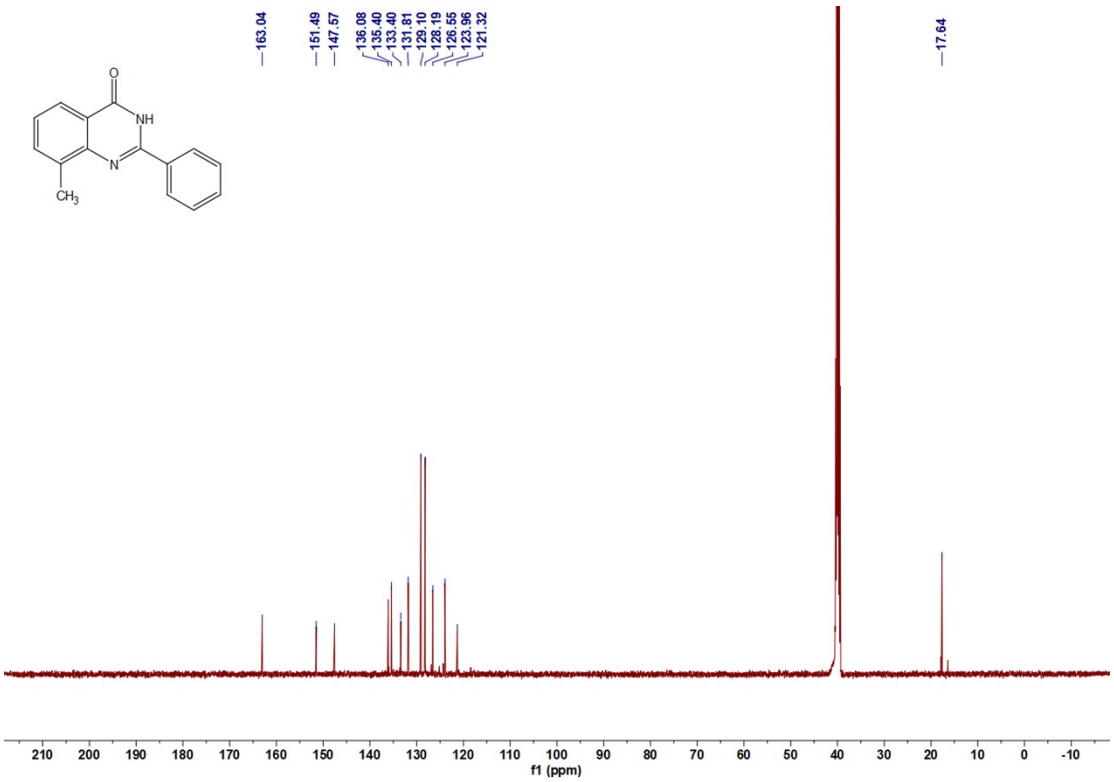
**(3au) 6-methoxy-2-(2-methoxyphenyl)quinazolin-4(3*H*)-one**



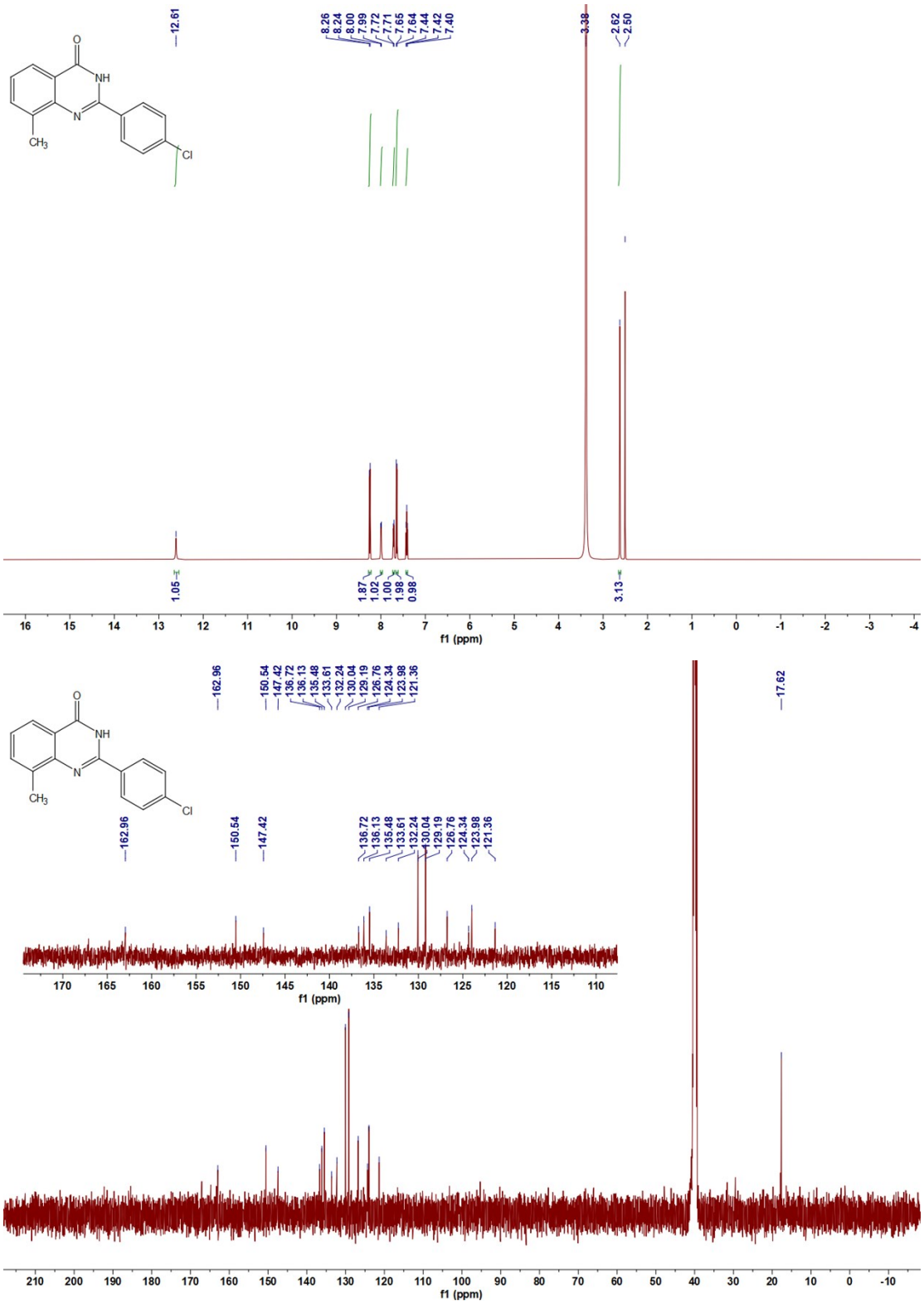



**(3av) 8-methyl-2-phenylquinazolin-4(3*H*)-one**

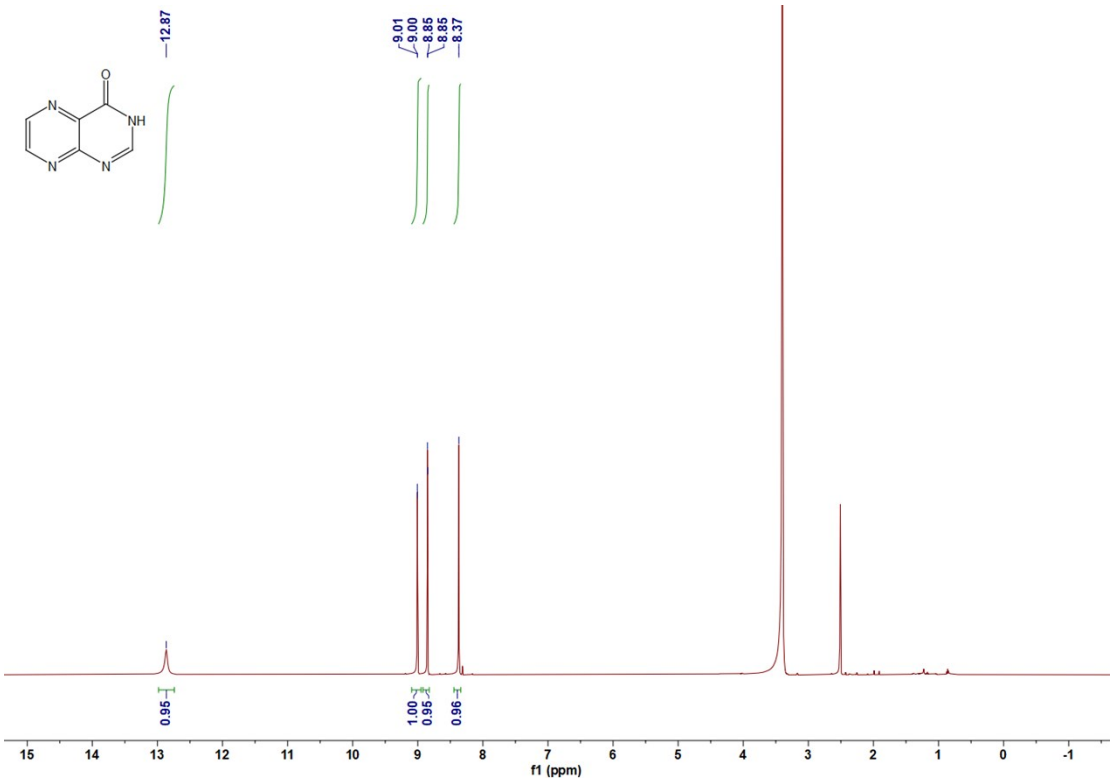


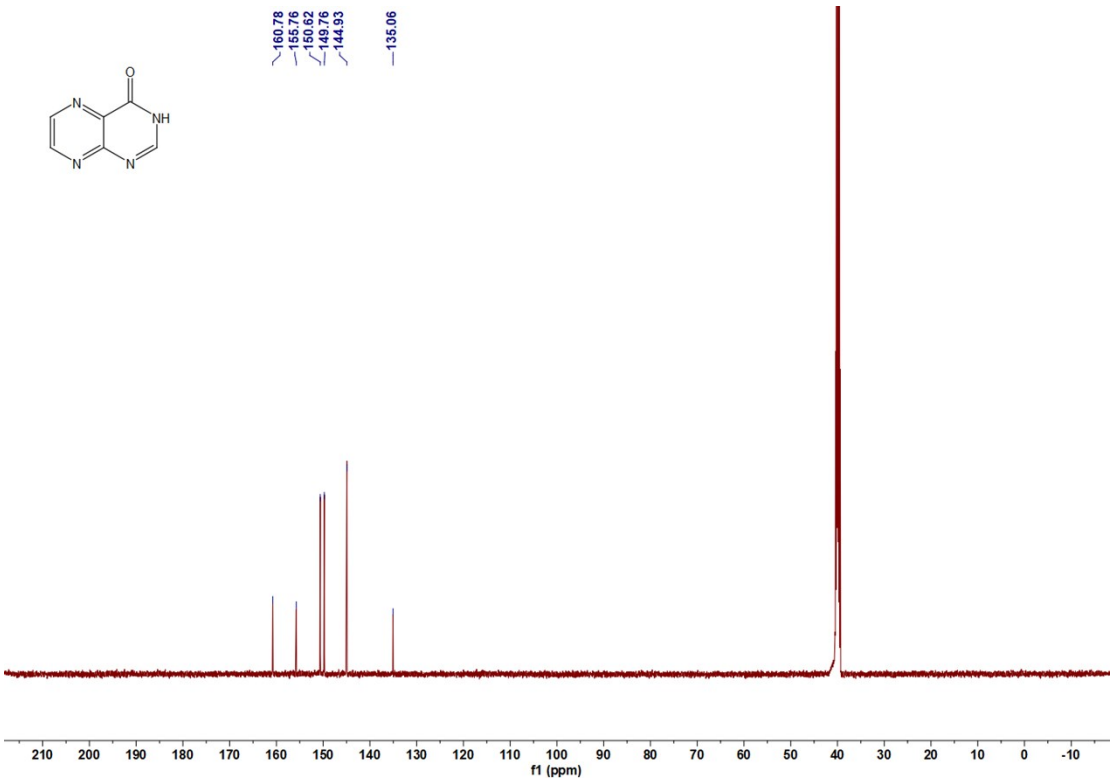



**(3aw) 2-(4-chlorophenyl)-8-methylquinazolin-4(3*H*)-one**

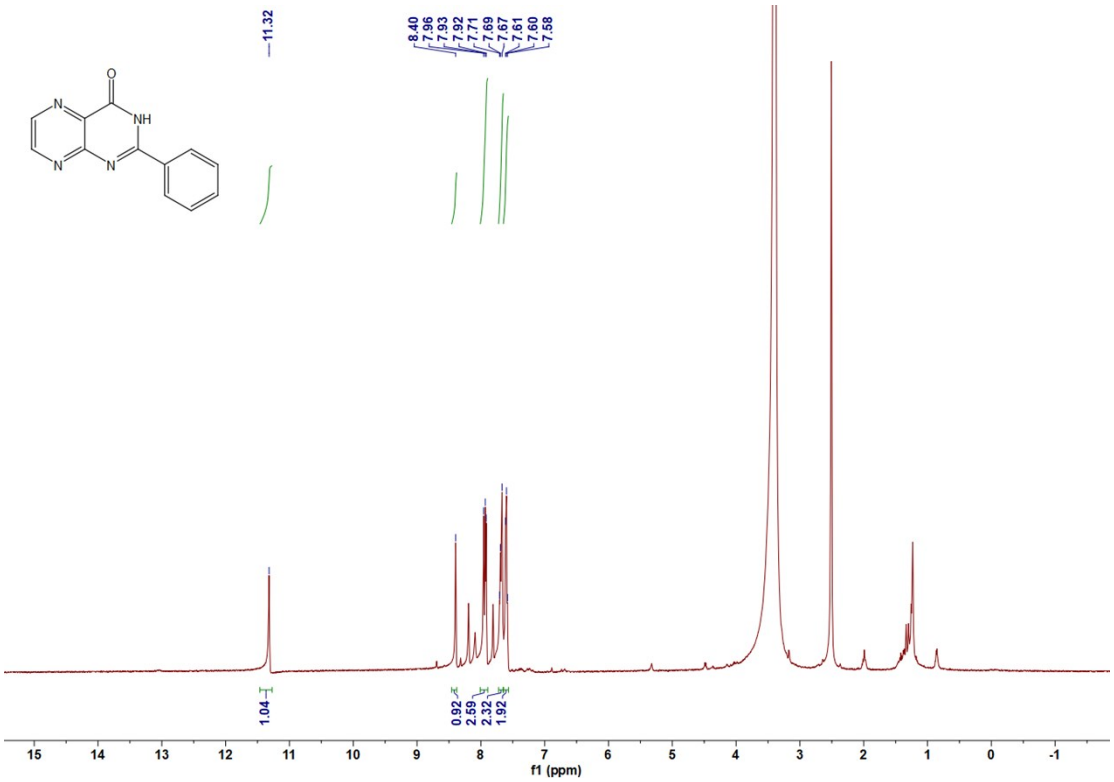


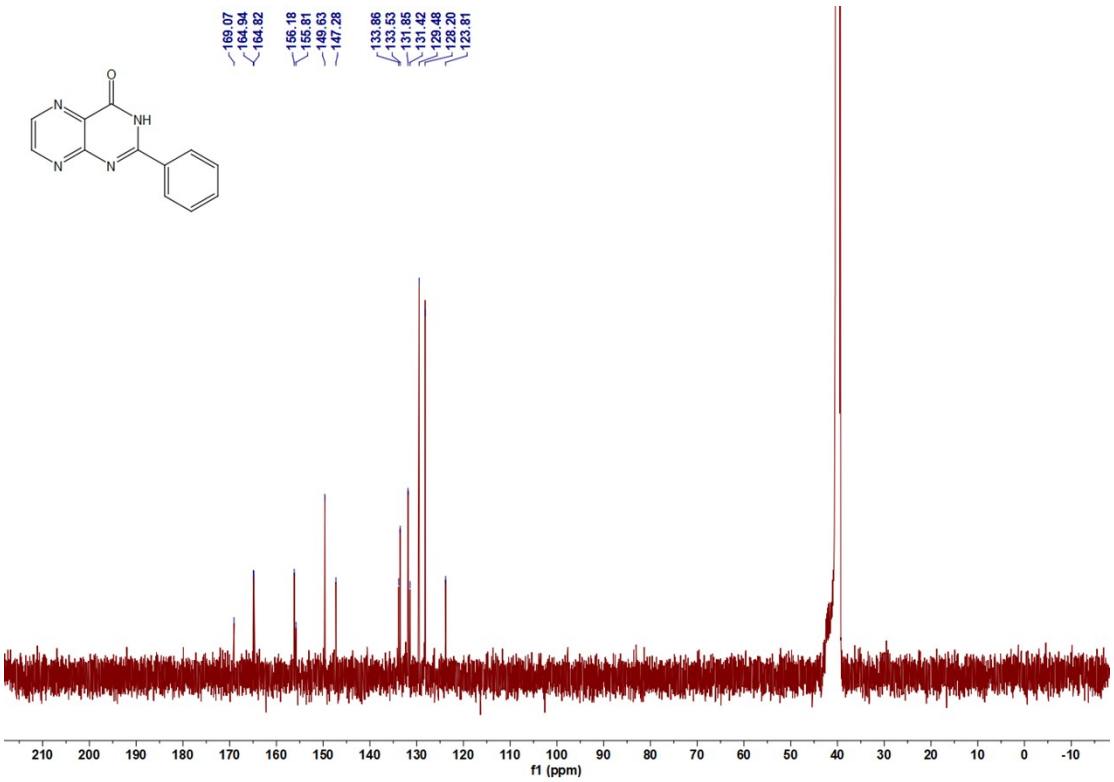
**(3ax) pteridin-4(3*H*)-one**



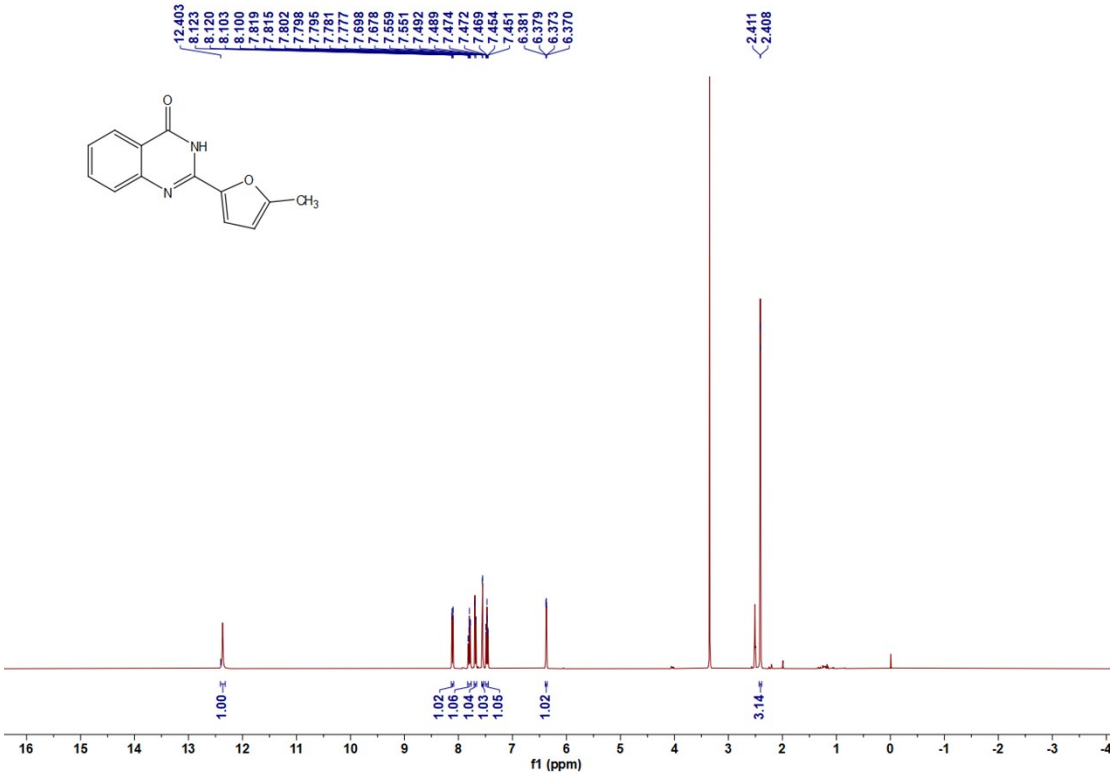



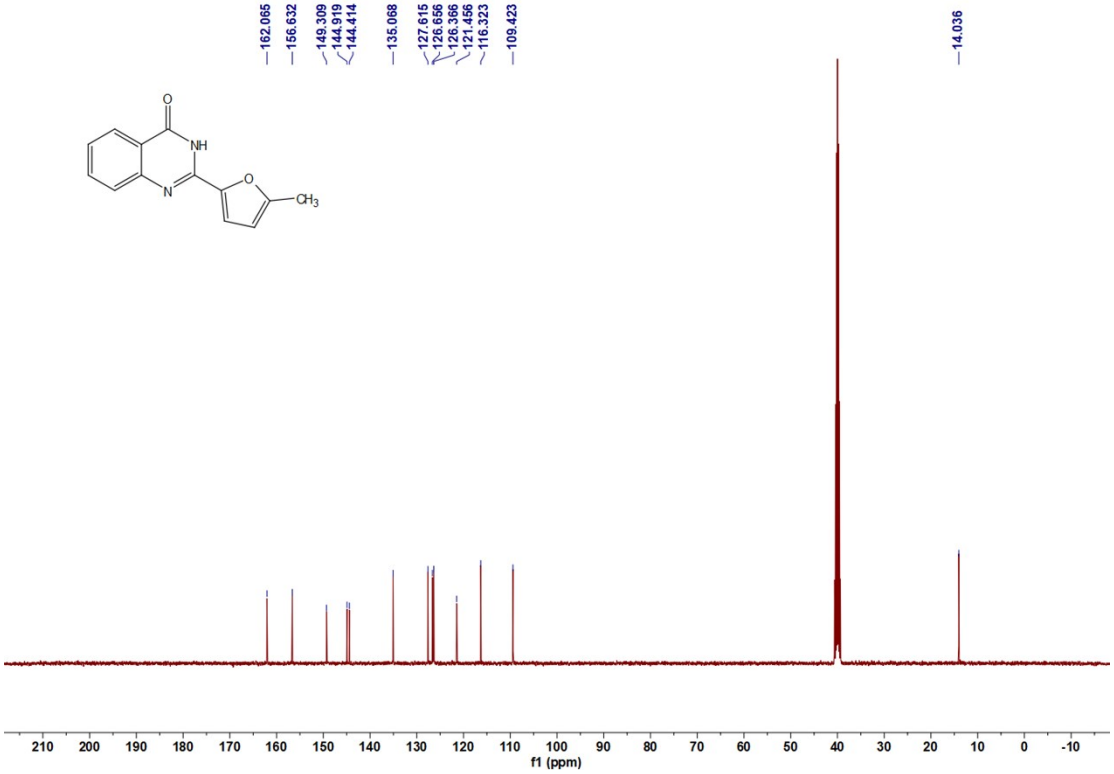
**(3ay) 2-phenylpteridin-4(3*H*)-one**



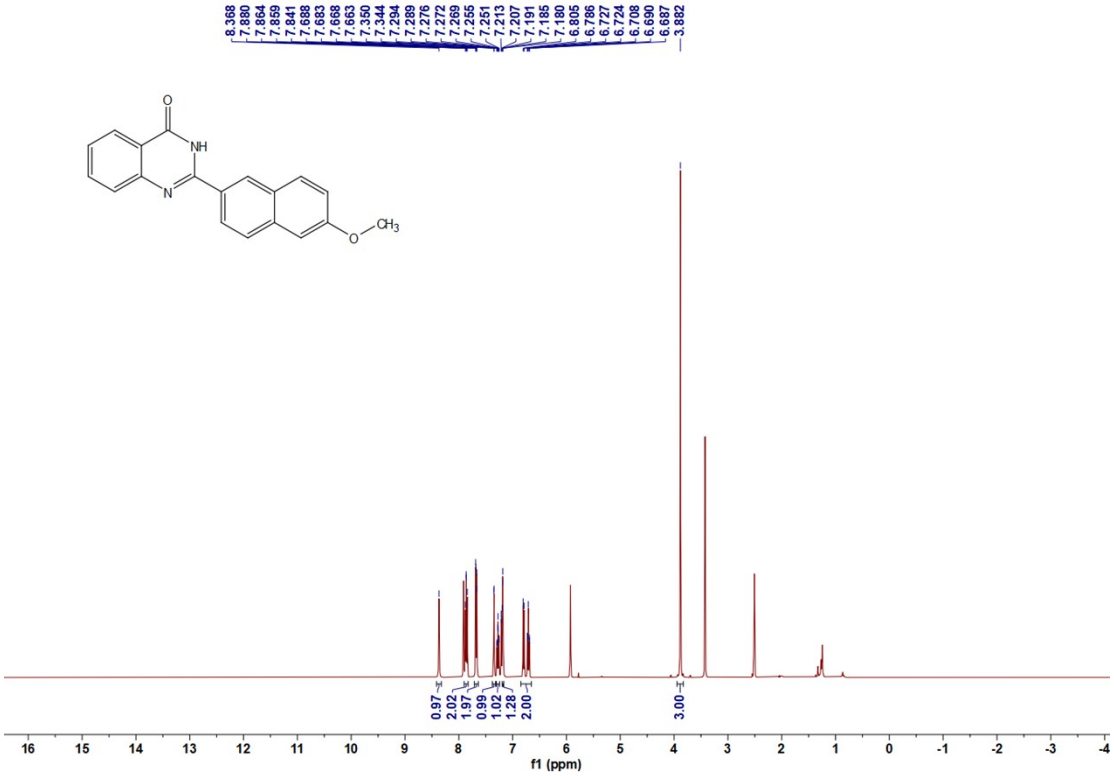



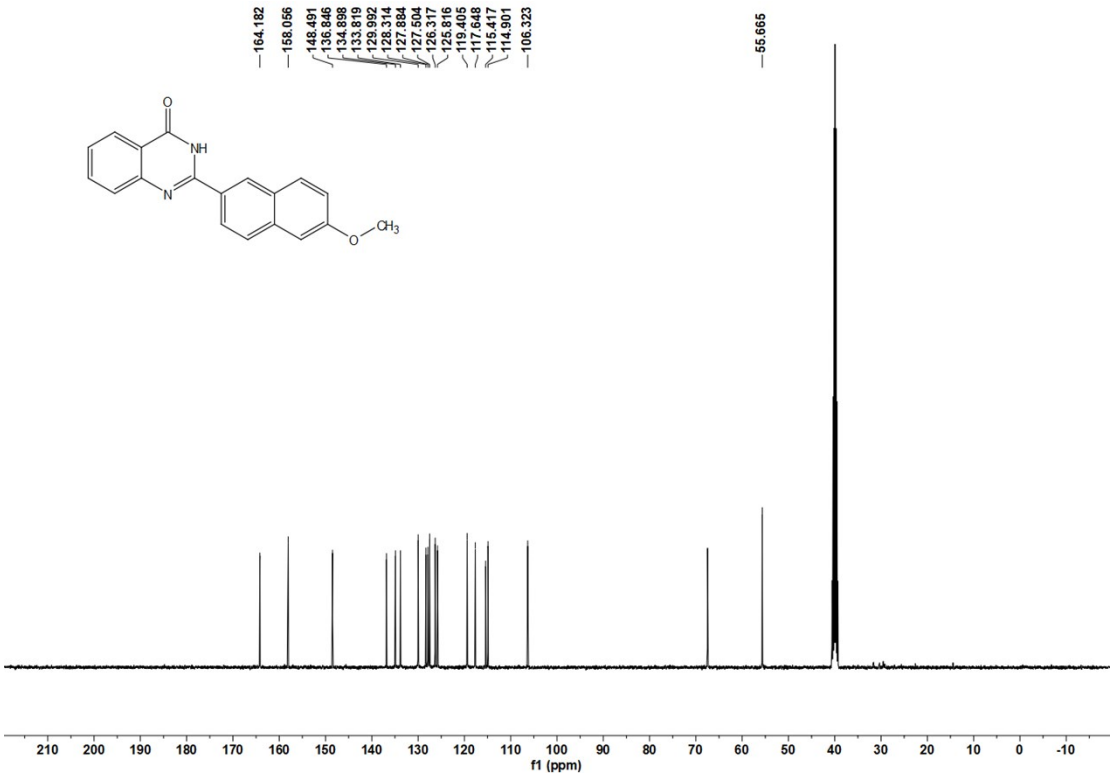
**(3az) 2-(5-methylfuran-2-yl)quinazolin-4(3*H*)-one**



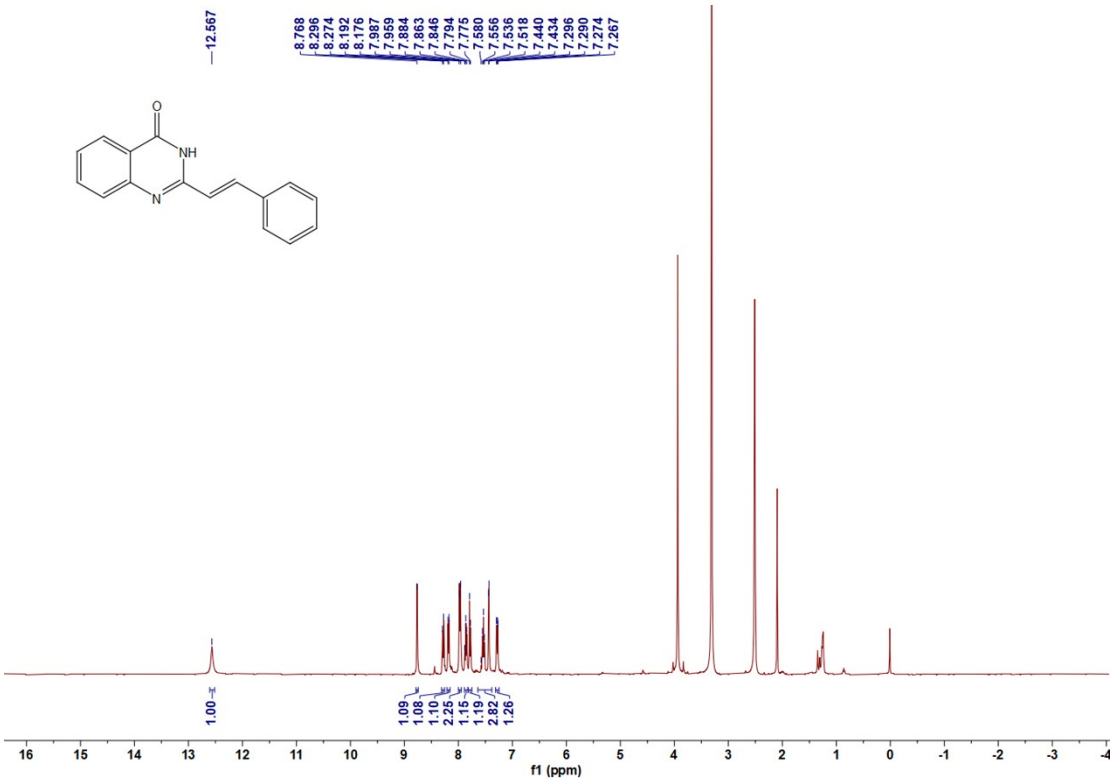



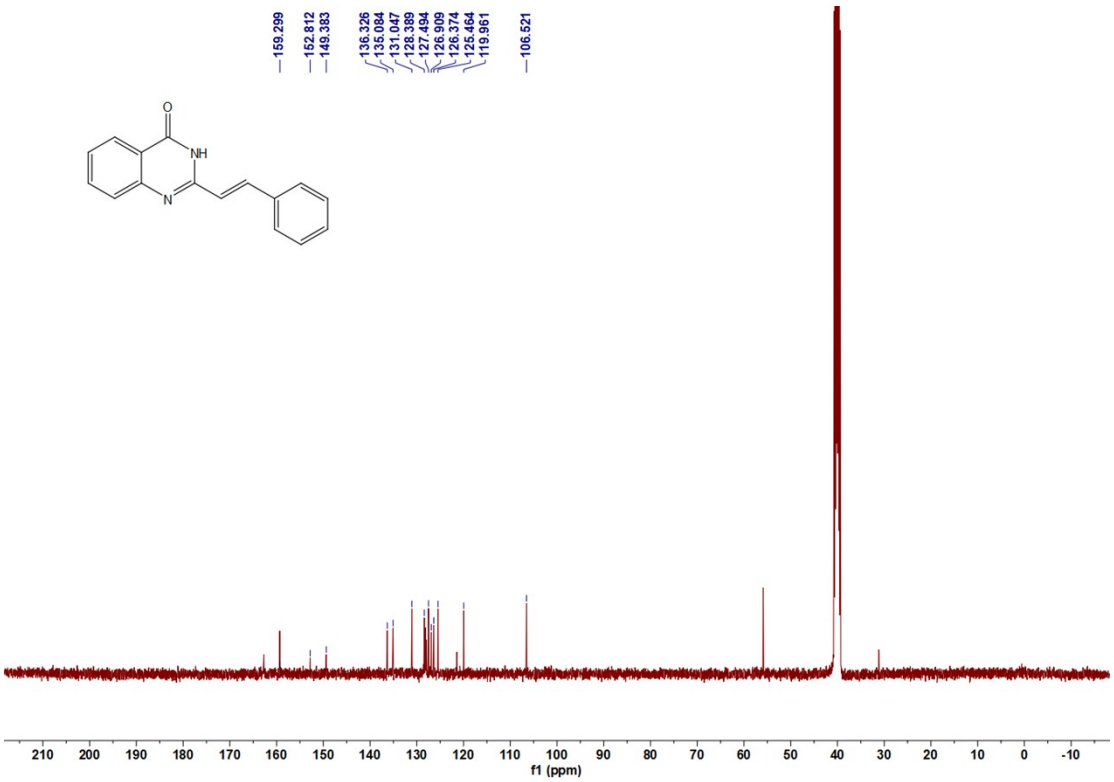
**(3ba) 2-(6-methoxynaphthalen-2-yl)quinazolin-4(3H)-one**



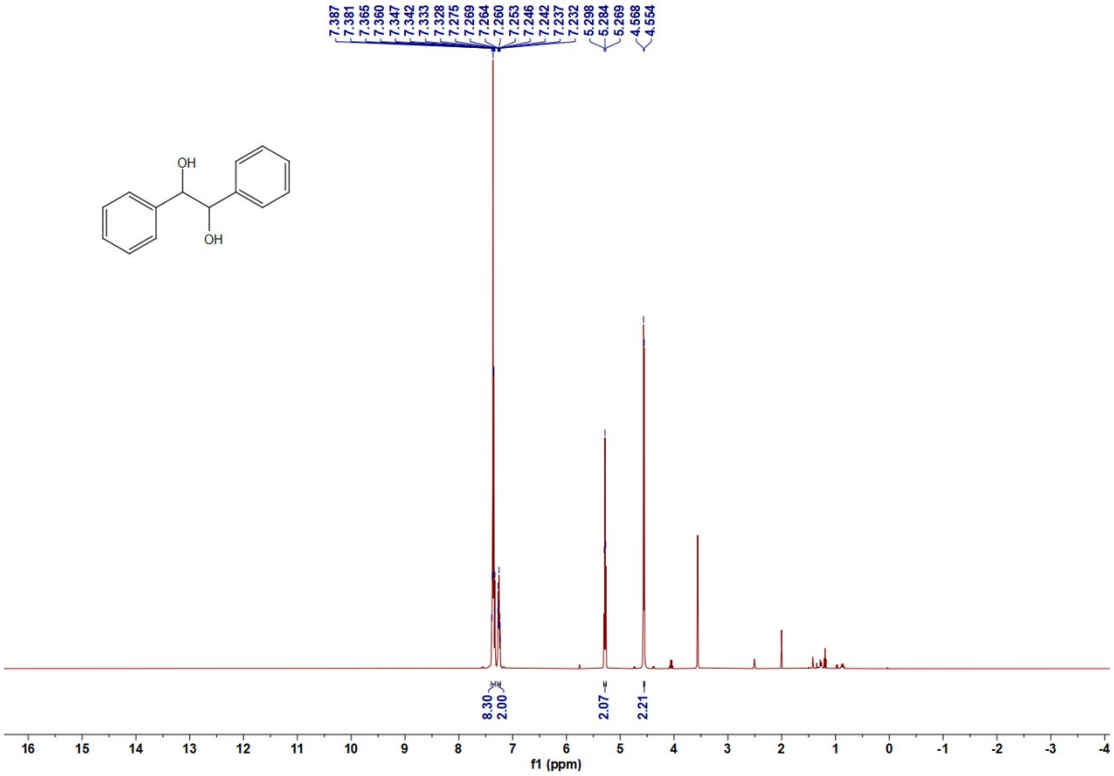



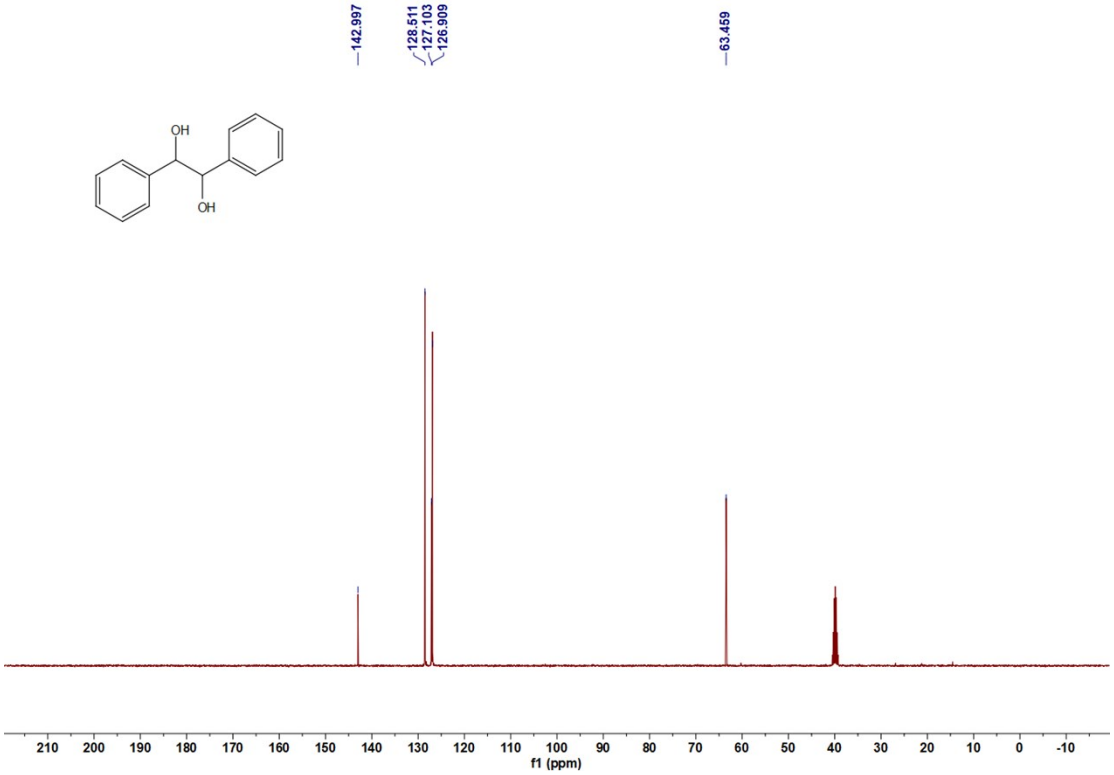
**(3bb) 2-styrylquinazolin-4(3*H*)-one**



**(5a) 1,2-diphenylethane-1,2-diol**



**(A3) *N*-(4-methoxyphenyl) -6- (2,2,2-trifluoroethoxy) pteridin -4-amine**