

Supporting Information

Iodine-Mediated Electrochemical C(sp³)-H Cyclization: Access to Quinazolinone-Fused N-Heterocycles

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General Information

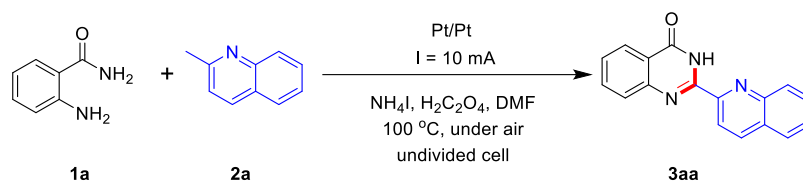
Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. NMR spectra were recorded on a Bruker AV-500 (^1H : 500 MHz, ^{13}C : 125 Hz) spectrometer using TMS as internal reference. Chemical shifts (δ) and coupling constants (J) were expressed in ppm and Hz, respectively. The following calibration was used: CDCl_3 δ = 7.26 and 77.16 ppm, DMSO δ = 2.50 and 39.70 ppm. High resolution mass spectra (HRMS) were measured using electrospray ionization (ESI) and the time-of-flight (TOF) mass analyzer. The anode electrode and cathode electrode all are Pt ($1.0 \times 1.0 \text{ cm}^2$). These electrodes are commercially available from GaossUnion, China.

Experimental Procedure

Typical Procedure A for the Electrosynthesis of 2-Quinoliny-quinazolin-4(3H)-ones: An undivided cell was equipped with a magnet stirrer, platinum plate ($1.0 \times 1.0 \text{ cm}^2$) electrode, as the working electrode and counter electrode. The substrate 2-aminobenzamide **1a** (0.3 mmol), 2-methylquinoline **2a** (0.33 mmol), $\text{H}_2\text{C}_2\text{O}_4$ (0.6 mmol), electrolyte NH_4I (0.06 mmol) and NH_4BF_4 (0.3 mmol) were added to the solvent DMF (3 mL). The electrolysis was conducted in an undivided cell at oil bath (100 °C). After the reaction was completed, the reaction system was allowed to attain room temperature and extracted with ethyl acetate ($3 \times 20 \text{ mL}$), and then the organic layer was washed with brine ($2 \times 10 \text{ mL}$) and dried with anhydrous Na_2SO_4 . Subsequently, the solvent was removed under reduced pressure and the remaining crude product was purified by column chromatography over silica gel (PE/EtOAc = 5:1) to afford the corresponding products.

Typical Procedure B for the Electrosynthesis of 2-Pyridinyl-quinazolin-4(3H)-ones: An undivided cell was equipped with a magnet stirrer, platinum plate ($1.0 \times 1.0 \text{ cm}^2$) electrode, as the working electrode and counter electrode. The substrate 2-aminobenzamide **1a** (0.3 mmol), 2-methylpyridine **2r** (0.6 mmol), $\text{Ph}_2\text{PO}_2\text{H}$ (0.6 mmol), electrolyte KI (0.3 mmol) were added to the solvent DMSO (3 mL). The electrolysis was conducted in an undivided cell at oil bath (120 °C). After the reaction was completed, the reaction system was allowed to attain room temperature and extracted with ethyl acetate ($3 \times 20 \text{ mL}$), and then the organic layer was washed with brine ($2 \times 10 \text{ mL}$) and dried with anhydrous Na_2SO_4 . Subsequently, the solvent was removed under reduced pressure and the remaining crude product was purified by column chromatography over silica gel (PE/EtOAc = 8:1) to afford the corresponding products.

Gram-scale synthesis of 3aa and 3an: An undivided cell was equipped with a magnet stirrer, platinum plate ($1.5 \times 1.5 \text{ cm}^2$) electrode, as the working electrode and counter electrode. The substrate 2-aminobenzamide **1a** (5 mmol), *N*-heteroaromatics **2** (5.5 mmol), NH_4I (1.0 mmol) and NH_4BF_4 (5 mmol) were added to the solvent DMF (50 mL). The electrolysis was electrolyzed ($J = 10 \text{ mA/cm}^2$, $I = 23 \text{ mA}$) in an undivided cell at oil bath (100 °C). After the reaction was completed (about 2 days), the reaction system was allowed to attain room temperature. Then the reaction mixture was concentrated under reduced pressure. H_2O (100 mL) was added the reaction system was extracted with ethyl acetate ($3 \times 100 \text{ mL}$). Subsequently, the organic layer was washed with brine ($2 \times 100 \text{ mL}$) and dried with anhydrous Na_2SO_4 . Finally, the solvent was removed under reduced pressure and the remaining crude product was purified by column chromatography over silica gel (PE/EtOAc = 5:1) to afford the corresponding products.

Table S1. Optimization of reaction conditions

Entry	Variations from standard conditions	Yield(%) ^b
1	None	93
2	DMA as the solvent	68
3	NMP as the solvent	trace
4	Bu ₄ NI as the electrolyte	81
5	KI as the electrolyte	76
6	NH ₄ Br, NH ₄ Cl as the electrolyte	n. d ^c
7	without acid	34
8	0.2 equivalent NH ₄ I with 1.0 equivalent NH ₄ BF ₄ instead of 1.0 equivalent NH ₄ I	95
9	0.1 equivalent NH ₄ I instead of 0.2 equivalent NH ₄ I	35
10	0.3 equivalent NH ₄ I instead of 0.2 equivalent NH ₄ I	91
11	90°C instead of 100°C	67
12	110°C instead of 100°C	86
13	5mA instead of 10mA	90
14	15mA instead of 10mA	73
15	without electricity	n.d

^a Reaction conditions: 1a (0.3 mmol), 2a (0.33 mmol), H₂C₂O₄ (0.6 mmol), NH₄I (0.3 mmol) and DMF (3 mL); the electrolysis was conducted in an undivided cell at an oil bath (T = 100 °C) for 10 h, Pt/Pt, air. ^b The isolated yields after column chromatography. ^c Not detected.

Figure S1. Cyclic Voltammetric (CV) Experiment

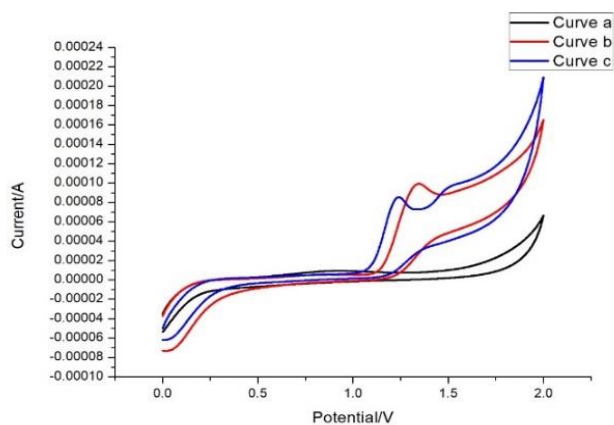
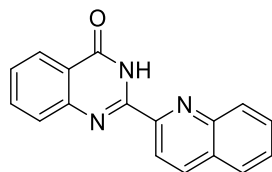


Figure S1. Cyclic voltammograms of intermediate **5** and related compounds in 0.1 M $\text{NH}_4\text{BF}_4/\text{DMF}$ using a Pt disk as the working electrode, and Pt wire and Ag/AgCl as the counter and reference electrodes, at a scan rate of 100 mV/s: background (curve a), intermediate **5** (5 mmol/L) (curve b), and intermediate **5** (5 mmol/L) and $\text{H}_2\text{C}_2\text{O}_4$ (10 mmol/L) (curve c).

Figure S1 showed that the oxidation wave of intermediate **5** was decreased in the presence of oxalic acid, indicating that the addition of oxalic acid was beneficial to the oxidation of the intermediate (curves b and c in **Figure S1**).

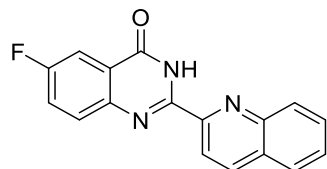
Detail descriptions for products

2-(quinolin-2-yl)quinazolin-4(3H)-one (3aa)¹:



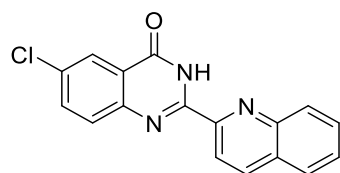
The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as white solid. 96% yield, 78.7 mg, ¹H NMR (500 MHz, CDCl₃) δ 11.20 (s, 1H), 8.64 (d, *J* = 8.5 Hz, 1H), 8.36 (dd, *J* = 13.7, 8.2 Hz, 2H), 8.15 (d, *J* = 8.4 Hz, 1H), 7.92 - 7.84 (m, 2H), 7.80 (dd, *J* = 13.6, 7.0 Hz, 2H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.53 (t, *J* = 7.5 Hz, 1H). ¹³C NMR (125 MHz, CDCl₃) δ 161.6 (s), 149.3 (s), 149.1 (s), 148.2 (s), 146.9 (s), 137.8 (s), 134.7 (s), 130.6 (s), 129.8 (s), 129.4 (s), 128.4 (s), 128.4 (s), 127.9 (s), 127.7 (s), 126.9 (s), 122.8 (s), 118.6 (s).

6-Fluoro-2-(quinolin-2-yl)quinazolin-4(3H)-one (3ba)²:



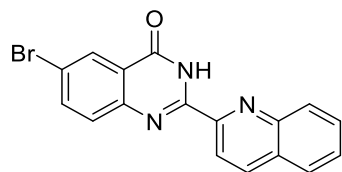
The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as yellow solid. 95% yield, 83.3 mg. ¹H NMR (500 MHz, CDCl₃) δ 11.23 (s, 1H), 8.61 (d, *J* = 8.6 Hz, 1H), 8.34 (d, *J* = 8.5 Hz, 1H), 8.14 (d, *J* = 8.3 Hz, 1H), 7.99 (dd, *J* = 8.3, 2.9 Hz, 1H), 7.92 - 7.85 (m, 2H), 7.82 - 7.78 (m, 1H), 7.67 - 7.63 (m, 1H), 7.54 - 7.49 (m, 1H). ¹³C NMR (125 MHz, CDCl₃) δ 161.5 (d, *J* = 248.4 Hz), 160.8 (d, *J* = 3.2 Hz), 148.6 (s), 147.9 (s), 146.9 (s), 145.8 (s), 137.8 (s), 130.7 (d, *J* = 5.3 Hz), 129.8 (s), 129.4 (s), 128.5 (s), 127.9 (s), 124.2 (d, *J* = 8.4 Hz), 123.2 (d, *J* = 23.9 Hz), 118.5 (s), 112.1 (d, *J* = 23.7 Hz).

6-chloro-2-(quinolin-2-yl)quinazolin-4(3H)-one (3ca)¹:



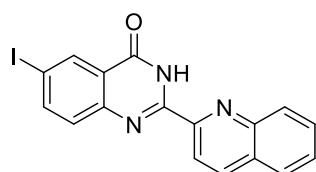
The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as yellow solid. 67% yield, 61.8 mg. ¹H NMR (500 MHz, CDCl₃) δ 11.26 (s, 1H), 8.63 (d, *J* = 8.3 Hz, 1H), 8.36 (d, *J* = 8.4 Hz, 1H), 8.34 (s, 1H), 8.16 (d, *J* = 8.3 Hz, 1H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.86 - 7.77 (m, 2H), 7.74 (d, *J* = 8.5 Hz, 1H), 7.66 (t, *J* = 7.3 Hz, 1H). ¹³C NMR (125 MHz, CDCl₃) δ 160.5 (s), 149.4 (s), 147.8 (s), 147.7 (s), 146.9 (s), 137.9 (s), 135.2 (s), 133.6 (s), 130.8 (s), 129.9 (s), 129.8 (s), 129.5 (s), 128.6 (s), 127.9 (s), 126.5 (s), 123.9 (s), 118.6 (s).

6-bromo-2-(quinolin-2-yl)quinazolin-4(3H)-one (3da):



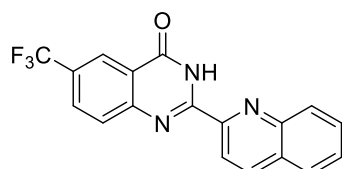
The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as white solid. 81% yield, 85.3 mg. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 11.26 (s, 1H), 8.62 (d, J = 8.6 Hz, 1H), 8.50 (s, 1H), 8.36 (d, J = 8.5 Hz, 1H), 8.15 (d, J = 8.5 Hz, 1H), 7.94 - 7.86 (m, 2H), 7.82 (t, J = 7.6 Hz, 1H), 7.74 (d, J = 8.6 Hz, 1H), 7.66 (t, J = 7.5 Hz, 1H). $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 160.4 (s), 149.5 (s), 148.1 (s), 147.8 (s), 146.9 (s), 137.9 (d, J = 3.2 Hz), 130.8 (s), 130.1 (s), 129.8 (s), 129.6 (s), 129.5 (s), 128.6 (s), 127.9 (s), 124.2 (s), 121.4 (s), 118.6 (s). HRMS calcd. $[\text{C}_{17}\text{H}_{10}\text{BrN}_3\text{O} + \text{H}]^+$: 352.0085, found: 352.0084.

6-iodo-2-(quinolin-2-yl)quinazolin-4(3H)-one (3ea)²:



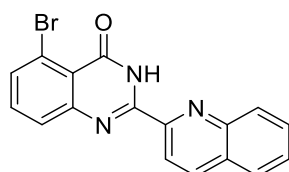
The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as yellow solid. 83% yield, 99.3 mg. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 11.26 (s, 1H), 8.70 (d, J = 2.0 Hz, 1H), 8.63 (d, J = 8.6 Hz, 1H), 8.36 (d, J = 8.5 Hz, 1H), 8.15 (d, J = 8.5 Hz, 1H), 8.06 (dd, J = 8.5, 2.1 Hz, 1H), 7.91 (d, J = 8.0 Hz, 1H), 7.84 - 7.79 (m, 1H), 7.68 - 7.63 (m, 1H), 7.60 (d, J = 8.5 Hz, 1H). $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 160.1 (s), 149.6 (s), 148.5 (s), 147.7 (s), 146.9 (s), 143.6 (s), 137.9 (s), 135.9 (s), 130.8 (s), 130.0 (s), 129.8 (s), 129.5 (s), 128.6 (s), 127.9 (s), 124.3 (s), 118.6 (s), 92.5 (s).

2-(quinolin-2-yl)-6-(trifluoromethyl)quinazolin-4(3H)-one (3fa):



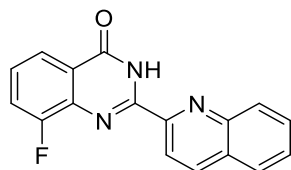
The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as yellow solid. 58% yield, 59.4 mg. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 11.36 (s, 1H), 8.69 - 8.63 (m, 2H), 8.39 (d, J = 8.5 Hz, 1H), 8.17 (d, J = 8.4 Hz, 1H), 8.03 - 7.94 (m, 2H), 7.92 (d, J = 8.1 Hz, 1H), 7.83 (t, J = 7.3 Hz, 1H), 7.67 (t, J = 7.3 Hz, 1H). $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 160.8 (s), 151.5 (s), 150.9 (s), 147.6 (s), 146.9 (s), 138.1 (s), 138.0 (s), 131.0 (q, J = 3.2 Hz), 130.9 (s), 129.9 (s), 129.7 (s), 129.5 (q, J = 33.2 Hz), 129.4 (s), 129.3 (s), 128.8 (s), 128.0 (s), 123.8 (q, J = 263.5 Hz), 118.7 (s). HRMS calcd. $[\text{C}_{18}\text{H}_{10}\text{F}_3\text{N}_3\text{O} + \text{H}]^+$: 342.0854, found: 342.0859.

5-bromo-2-(quinolin-2-yl)quinazolin-4(3H)-one (3ha):



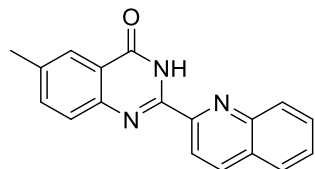
The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as white solid. 71% yield, 75.0 mg. ¹H NMR (500 MHz, CDCl₃) δ 11.08 (s, 1H), 8.61 (d, *J* = 8.4 Hz, 1H), 8.35 (d, *J* = 8.3 Hz, 1H), 8.19 (d, *J* = 8.1 Hz, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.82 (dd, *J* = 14.5, 7.7 Hz, 2H), 7.73 (d, *J* = 7.6 Hz, 1H), 7.65 (t, *J* = 7.2 Hz, 1H), 7.55 (t, *J* = 7.7 Hz, 1H). ¹³C NMR (125 MHz, CDCl₃) δ 159.7 (s), 151.4 (s), 149.4 (s), 147.5 (s), 146.9 (s), 137.9 (s), 134.4 (s), 134.2 (s), 130.8 (s), 129.9 (s), 129.5 (s), 128.6 (s), 128.3 (s), 127.9 (s), 121.8 (s), 120.9 (s), 118.6 (s). HRMS calcd. [C₁₇H₁₀BrN₃O + H]⁺: 352.0085, found: 352.0089.

8-fluoro-2-(quinolin-2-yl)quinazolin-4(3H)-one (3ia):



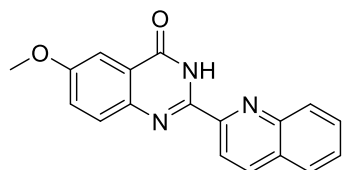
The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as yellow solid. 69% yield, 60.2 mg. ¹H NMR (500 MHz, CDCl₃) δ 11.26 (s, 1H), 8.69 (d, *J* = 8.5 Hz, 1H), 8.35 (d, *J* = 8.6 Hz, 1H), 8.14 (d, *J* = 8.1 Hz, 2H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.83 - 7.77 (m, 1H), 7.64 (t, *J* = 7.2 Hz, 1H), 7.56 - 7.50 (m, 1H), 7.50 - 7.44 (m, 1H). ¹³C NMR (125 MHz, CDCl₃) δ 160.6 (d, *J* = 3.1 Hz), 157.8 (d, *J* = 256.3 Hz), 149.4 (s), 147.8 (s), 146.8 (s), 138.7 (d, *J* = 11.7 Hz), 137.9 (s), 130.7 (s), 129.8 (s), 129.6 (s), 128.6 (s), 127.9 (s), 127.7 (d, *J* = 7.5 Hz), 124.7 (s), 122.4 (d, *J* = 4.3 Hz), 120.3 (d, *J* = 19.2 Hz), 118.8 (s). HRMS calcd. [C₁₇H₁₀FN₃O + H]⁺: 292.0886, found: 292.0887.

6-methyl-2-(quinolin-2-yl)quinazolin-4(3H)-one (3ja)¹:



The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as white solid. 90% yield, 77.8 mg. ¹H NMR (500 MHz, CDCl₃) δ 11.19 (s, 1H), 8.64 (d, *J* = 8.6 Hz, 1H), 8.35 (d, *J* = 8.6 Hz, 1H), 8.17 (s, 1H), 8.15 (d, *J* = 8.5 Hz, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.83 - 7.76 (m, 2H), 7.67 - 7.60 (m, 2H), 2.53 (s, 3H). ¹³C NMR (125 MHz, CDCl₃) δ 161.6 (s), 148.4 (s), 148.3 (s), 147.2 (s), 146.9 (s), 138.2 (s), 137.7 (s), 136.2 (s), 130.6 (s), 129.8 (s), 129.4 (s), 128.3 (s), 128.2 (s), 127.9 (s), 126.5 (s), 122.5 (s), 118.5 (s), 21.6 (s).

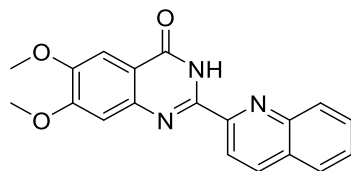
6-methoxy-2-(quinolin-2-yl)quinazolin-4(3H)-one (3ka)²:



The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as white solid. 89% yield, 80.9 mg. ¹H NMR (500 MHz, CDCl₃) δ 11.20 (s, 1H), 8.61 (d, *J* = 8.5 Hz, 1H), 8.32 (d, *J* = 8.5 Hz, 1H), 8.13

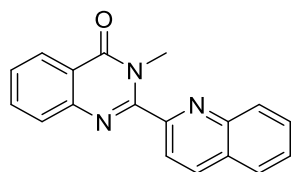
(d, $J = 8.4$ Hz, 1H), 7.87 (d, $J = 8.1$ Hz, 1H), 7.84 - 7.75 (m, 2H), 7.73 (s, 1H), 7.62 (t, $J = 7.4$ Hz, 1H), 7.39 (d, $J = 8.8$ Hz, 1H), 3.95 (s, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 161.4 (s), 159.2 (s), 148.2 (s), 147.2 (s), 146.9 (s), 143.6 (s), 137.7 (s), 130.6 (s), 129.9 (s), 129.7 (s), 129.3 (s), 128.2 (s), 127.9 (s), 124.9 (s), 123.7 (s), 118.5 (s), 106.5 (s), 56.0 (s).

7-dimethoxy-2-(quinolin-2-yl)quinazolin-4(3H)-one (3la):



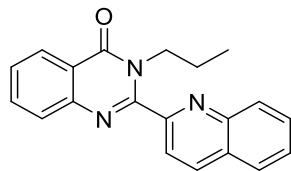
The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as white solid. 75% yield, 74.9 mg. ^1H NMR (500 MHz, CDCl_3) δ 11.17 (s, 1H), 8.59 (d, $J = 8.6$ Hz, 1H), 8.33 (d, $J = 8.6$ Hz, 1H), 8.14 (d, $J = 8.5$ Hz, 1H), 7.89 (d, $J = 8.1$ Hz, 1H), 7.80 (t, $J = 7.6$ Hz, 1H), 7.70 (s, 1H), 7.64 (t, $J = 7.4$ Hz, 1H), 7.29 (s, 1H), 4.06 (s, 3H), 4.04 (s, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 161.0 (s), 155.2 (s), 149.8 (s), 148.2 (s), 148.1 (s), 147.0 (s), 145.3 (s), 137.7 (s), 130.6 (s), 129.8 (s), 129.3 (s), 128.3 (s), 127.9 (s), 118.3 (s), 116.2 (s), 108.7 (s), 105.9 (s), 56.6 (s), 56.5 (s). HRMS calcd. $[\text{C}_{19}\text{H}_{15}\text{N}_3\text{O}_3 + \text{H}]^+$: 334.1192, found: 334.1197.

3-methyl-2-(quinolin-2-yl)quinazolin-4(3H)-one (3ma)¹:

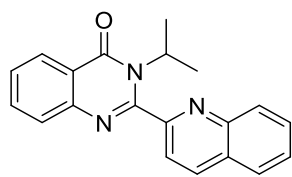


The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as white solid. 89% yield, 76.6 mg. ^1H NMR (500 MHz, CDCl_3) δ 8.43 - 8.35 (m, 2H), 8.16 (d, $J = 8.4$ Hz, 1H), 7.98 - 7.91 (m, 2H), 7.81 (t, $J = 7.7$ Hz, 1H), 7.78 (d, $J = 3.8$ Hz, 2H), 7.66 (t, $J = 7.5$ Hz, 1H), 7.51 - 7.58 (m, 1H), 3.72 (s, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 162.8 (s), 154.1 (s), 153.3 (s), 147.3 (s), 147.1 (s), 137.8 (s), 134.4 (s), 130.6 (s), 129.9 (s), 128.1 (s), 128.1 (s), 127.9 (s), 127.8 (s), 127.6 (s), 127.0 (s), 121.4 (s), 121.2 (s), 33.7 (s).

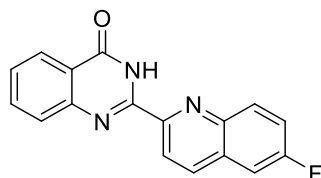
3-propyl-2-(quinolin-2-yl)quinazolin-4(3H)-one (3na)²:



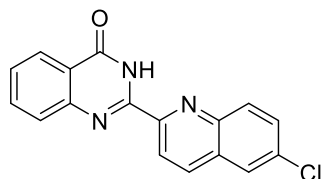
The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as white solid. 91% yield, 86.0 mg. ^1H NMR (500 MHz, CDCl_3) δ 8.38 (dd, $J = 8.1, 4.5$ Hz, 2H), 8.15 (d, $J = 8.5$ Hz, 1H), 7.93 (d, $J = 8.4$ Hz, 2H), 7.84 - 7.75 (m, 3H), 7.70 - 7.63 (m, 1H), 7.54 (ddd, $J = 8.1, 5.7, 2.6$ Hz, 1H), 4.39 - 4.11 (m, 2H), 1.90 - 1.75 (m, 2H), 0.79 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 162.4 (s), 154.2 (s), 153.4 (s), 147.1 (s), 147.0 (s), 137.7 (s), 134.4 (s), 130.6 (s), 129.9 (s), 128.1 (s), 128.1 (s), 127.9 (s), 127.6 (s), 127.5 (s), 127.1 (s), 121.7 (s), 121.4 (s), 47.2 (s), 22.5 (s), 11.4 (s).

3-isopropyl-2-(quinolin-2-yl)quinazolin-4(3H)-one (30a)²:

The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as yellow solid. 56% yield, 52.9 mg. ¹H NMR (500 MHz, CDCl₃) δ 8.38 (d, *J* = 8.4 Hz, 1H), 8.34 (d, *J* = 8.0 Hz, 1H), 8.16 (d, *J* = 8.4 Hz, 1H), 7.92 (d, *J* = 8.2 Hz, 1H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.81 (t, *J* = 7.7 Hz, 1H), 7.78 - 7.72 (m, 2H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.52 (t, *J* = 7.1 Hz, 1H), 4.43 (dt, *J* = 13.5, 6.7 Hz, 1H), 1.67 (d, *J* = 6.7 Hz, 6H). ¹³C NMR (126 MHz, CDCl₃) δ 162.6 (s), 155.0 (s), 153.8 (s), 147.3 (s), 146.5 (s), 137.8 (s), 134.3 (s), 130.6 (s), 130.0 (s), 128.0 (s), 128.0 (s), 127.5 (s), 127.3 (s), 126.7 (s), 122.5 (s), 120.9 (s), 54.6 (s), 20.0 (s).

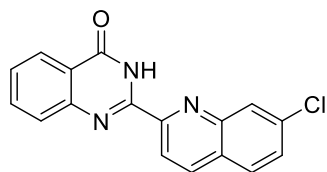
2-(6-fluoroquinolin-2-yl)quinazolin-4(3H)-one (3ab)³:

The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as white solid. 94% yield, 82.0 mg. ¹H NMR (500 MHz, CDCl₃) δ 11.08 (s, 1H), 8.64 (d, *J* = 8.4 Hz, 1H), 8.35 (d, *J* = 7.6 Hz, 1H), 8.28 (d, *J* = 8.5 Hz, 1H), 8.18 - 8.08 (m, 1H), 7.85 (d, *J* = 7.8 Hz, 1H), 7.80 (t, *J* = 7.3 Hz, 1H), 7.54 (dd, *J* = 16.7, 8.4 Hz, 2H), 7.49 (d, *J* = 8.3 Hz, 1H). ¹³C NMR (125 MHz, CDCl₃) δ 161.6 (d, *J* = 250 Hz), 161.5 (s), 149.1 (s), 148.8 (s), 147.8 (s), 144.0 (s), 137.1 (d, *J* = 5.5 Hz), 134.8 (s), 132.4 (d, *J* = 9.4 Hz), 130.2 (d, *J* = 10.3 Hz), 128.4 (s), 127.8 (s), 126.9 (s), 121.0 (d, *J* = 26.3 Hz), 120.9 (s), 119.4 (s), 111.1 (d, *J* = 21.3 Hz).

2-(6-chloroquinolin-2-yl)quinazolin-4(3H)-one (3ac)³:

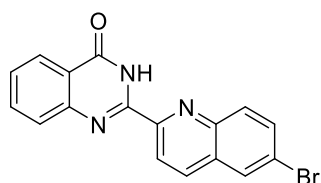
The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as white solid. 75% yield, 69.1 mg. ¹H NMR (500 MHz, CDCl₃) δ 11.09 (s, 1H), 8.67 (d, *J* = 8.6 Hz, 1H), 8.36 (dd, *J* = 7.9, 1.2 Hz, 1H), 8.26 (d, *J* = 8.6 Hz, 1H), 8.08 (d, *J* = 9.0 Hz, 1H), 7.91 - 7.85 (m, 2H), 7.84 - 7.79 (m, 1H), 7.72 (dd, *J* = 9.0, 2.3 Hz, 1H), 7.58 - 7.52 (m, 1H). ¹³C NMR (125 MHz, CDCl₃) δ 161.4 (s), 149.1 (s), 148.7 (s), 148.5 (s), 145.3 (s), 136.8 (s), 134.8 (s), 134.4 (s), 131.7 (s), 131.3 (s), 129.9 (s), 128.4 (s), 127.9 (s), 127.0 (s), 126.6 (s), 122.8 (s), 119.6 (s).

2-(7-chloroquinolin-2-yl)quinazolin-4(3H)-one (3ad)²:



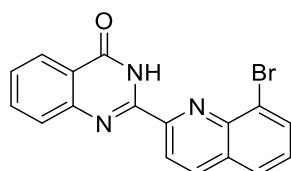
The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as white solid. 80% yield, 73.7mg. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 11.11 (s, 1H), 8.68 (d, $J = 8.4$ Hz, 1H), 8.37 (dd, $J = 14.5, 8.2$ Hz, 2H), 8.15 (s, 1H), 7.89 (d, $J = 8.0$ Hz, 1H), 7.83 (dd, $J = 16.0, 8.2$ Hz, 2H), 7.60 (d, $J = 8.6$ Hz, 1H), 7.56 (t, $J = 7.4$ Hz, 1H). $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 161.4 (s), 149.2 (s), 149.0 (s), 148.7 (s), 147.3 (s), 137.7 (s), 136.7 (s), 134.9 (s), 129.5 (s), 129.1 (s), 128.7 (s), 128.4 (s), 128.0 (s), 127.8 (s), 127.0 (s), 122.8 (s), 118.9 (s).

2-(6-bromoquinolin-2-yl)quinazolin-4(3H)-one (3ae)²:



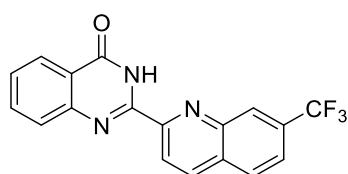
The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as yellow solid. 85% yield, 89.5 mg. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 11.08 (s, 1H), 8.67 (d, $J = 8.6$ Hz, 1H), 8.36 (d, $J = 7.9$ Hz, 1H), 8.25 (d, $J = 8.6$ Hz, 1H), 8.05 (d, $J = 2.0$ Hz, 1H), 8.01 (d, $J = 8.9$ Hz, 1H), 7.89 - 7.84 (m, 2H), 7.83 - 7.79 (m, 1H), 7.55 (t, $J = 7.5$ Hz, 1H). $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 161.4 (s), 149.1 (s), 148.7 (s), 148.6 (s), 145.5 (s), 136.7 (s), 134.8 (s), 134.2 (s), 131.4 (s), 130.4 (s), 130.0 (s), 128.4 (s), 127.9 (s), 127.0 (s), 122.8 (s), 122.6 (s), 119.6 (s).

2-(8-bromoquinolin-2-yl)quinazolin-4(3H)-one (3af):



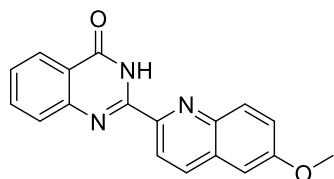
The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as yellow solid. 78% yield, 82.1 mg. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 11.07 (s, 1H), 8.60 (d, $J = 8.5$ Hz, 1H), 8.35 (d, $J = 8.5$ Hz, 1H), 8.18 (d, $J = 8.4$ Hz, 1H), 7.90 (d, $J = 8.1$ Hz, 1H), 7.85 - 7.77 (m, 2H), 7.73 (d, $J = 7.6$ Hz, 1H), 7.65 (t, $J = 7.4$ Hz, 1H), 7.55 (t, $J = 7.9$ Hz, 1H). $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 159.7 (s), 151.4 (s), 149.4 (s), 147.5 (s), 146.9 (s), 137.9 (s), 134.3 (s), 134.1 (s), 130.7 (s), 129.9 (s), 129.5 (s), 128.6 (s), 128.3 (s), 127.9 (s), 121.8 (s), 121.0 (s), 118.5 (s). HRMS calcd. $[\text{C}_{17}\text{H}_{10}\text{BrN}_3\text{O} + \text{H}]^+$: 352.0085, found: 352.0085.

2-(7-(trifluoromethyl)quinolin-2-yl)quinazolin-4(3H)-one (3ag):



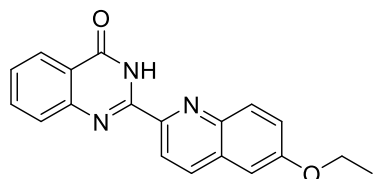
The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as yellow solid. 82% yield, 83.9 mg. ¹H NMR (500 MHz, CDCl₃) δ 11.13 (s, 1H), 8.88 (d, *J* = 8.6 Hz, 1H), 8.50 (s, 1H), 8.46 (d, *J* = 8.6 Hz, 1H), 8.40 (d, *J* = 7.8 Hz, 1H), 8.06 (d, *J* = 8.5 Hz, 1H), 7.96 (d, *J* = 8.1 Hz, 1H), 7.89 - 7.81 (m, 2H), 7.59 (t, *J* = 7.4 Hz, 1H). ¹³C NMR (125 MHz, CDCl₃) δ 161.3 (s), 149.5 (s), 148.7 (s), 148.6 (s), 146.0 (s), 137.9 (s), 135.0 (s), 132.6 (q, *J* = 32.6 Hz), 130.8 (s), 130.4 (s), 128.3 (s), 128.2 (q, *J* = 271.3 Hz), 127.6 (q, *J* = 3.8 Hz), 127.1 (s), 124.2 (s), 122.8 (s), 122.7 (s), 120.8 (s), 112.9 (s). HRMS calcd. [C₁₈H₁₀F₃N₃O + H]⁺: 342.0854, found: 342.0853.

2-(6-methoxyquinolin-2-yl)quinazolin-4(3H)-one (3ah)¹:



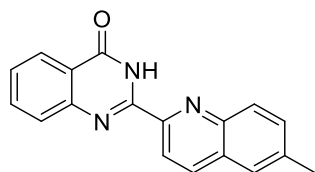
The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as white solid. 85% yield, 77.3 mg. ¹H NMR (500 MHz, CDCl₃) δ 11.16 (s, 1H), 8.62 (d, *J* = 8.6 Hz, 1H), 8.37 (d, *J* = 7.9 Hz, 1H), 8.23 (d, *J* = 8.6 Hz, 1H), 8.03 (d, *J* = 9.2 Hz, 1H), 7.88 (d, *J* = 8.1 Hz, 1H), 7.84 - 7.78 (m, 1H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.44 (dd, *J* = 9.2, 2.7 Hz, 1H), 7.13 (d, *J* = 2.6 Hz, 1H), 3.97 (s, 3H). ¹³C NMR (125 MHz, CDCl₃) δ 161.6 (s), 159.4 (s), 149.4 (s), 149.2 (s), 145.6 (s), 143.0 (s), 136.3 (s), 134.88 (s), 131.3 (s), 130.9 (s), 128.1 (s), 127.5 (s), 126.9 (s), 123.7 (s), 122.6 (s), 119.1 (s), 105.2 (s), 55.9 (s).

2-(6-ethoxyquinolin-2-yl)quinazolin-4(3H)-one (3ai):



The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as white solid. 88% yield, 83.7 mg. ¹H NMR (500 MHz, CDCl₃) δ 11.11 (s, 1H), 8.55 (d, *J* = 8.5 Hz, 1H), 8.34 (d, *J* = 7.8 Hz, 1H), 8.16 (d, *J* = 8.6 Hz, 1H), 7.98 (d, *J* = 9.2 Hz, 1H), 7.85 (d, *J* = 8.1 Hz, 1H), 7.78 (t, *J* = 7.5 Hz, 1H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.39 (dd, *J* = 9.1, 2.3 Hz, 1H), 7.06 (d, *J* = 2.2 Hz, 1H), 4.14 (q, *J* = 6.9 Hz, 2H), 1.49 (t, *J* = 6.9 Hz, 3H). ¹³C NMR (125 MHz, CDCl₃) δ 161.5 (s), 158.7 (s), 149.3 (s), 147.2 (s), 145.4 (s), 142.8 (s), 136.1 (s), 134.7 (s), 131.1 (s), 130.8 (s), 128.1 (s), 127.4 (s), 126.9 (s), 123.9 (s), 122.6 (s), 118.9 (s), 105.7 (s), 64.1 (s), 14.8 (s). HRMS calcd. [C₁₉H₁₅N₃O₂ + H]⁺: 318.1243, found: 318.1241.

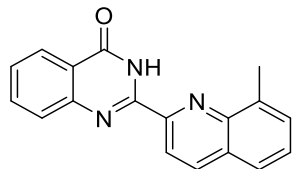
2-(6-methylquinolin-2-yl)quinazolin-4(3H)-one (3aj)²:



The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as white solid. 74% yield, 63.7 mg. ¹H NMR (500 MHz, CDCl₃) δ 11.19 (s, 1H), 8.63 (d, *J* = 8.5 Hz, 1H), 8.37 (d, *J* = 7.9 Hz, 1H),

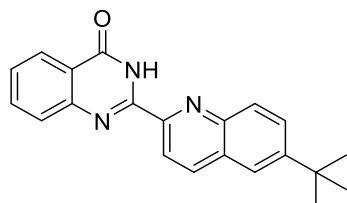
8.26 (d, $J = 8.6$ Hz, 1H), 8.04 (d, $J = 8.5$ Hz, 1H), 7.90 (d, $J = 8.1$ Hz, 1H), 7.81 (t, $J = 7.6$ Hz, 1H), 7.68 - 7.60 (m, 2H), 7.54 (t, $J = 7.5$ Hz, 1H), 2.58 (s, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 161.5 (s), 149.3 (s), 149.1 (s), 147.1 (s), 145.5 (s), 138.8 (s), 137.1 (s), 134.8 (s), 133.0 (s), 129.5 (s), 129.5 (s), 128.2 (s), 127.6 (s), 126.9 (s), 126.8 (s), 122.7 (s), 118.7 (s), 22.0 (s).

2-(8-methylquinolin-2-yl)quinazolin-4(3H)-one (3ak):



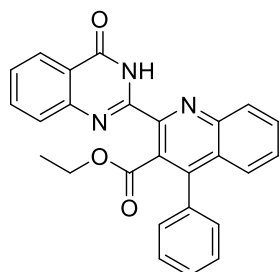
The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as yellow solid. 68% yield, 58.6 mg. ^1H NMR (500 MHz, CDCl_3) δ 11.02 (s, 1H), 8.65 (d, $J = 8.5$ Hz, 1H), 8.37 (d, $J = 7.8$ Hz, 1H), 8.31 (d, $J = 8.5$ Hz, 1H), 7.88 (d, $J = 8.0$ Hz, 1H), 7.80 (t, $J = 7.5$ Hz, 1H), 7.72 (d, $J = 8.0$ Hz, 1H), 7.62 (d, $J = 6.8$ Hz, 1H), 7.52 (dd, $J = 17.1, 7.9$ Hz, 2H), 2.89 (s, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 161.4 (s), 149.3 (s), 149.1 (s), 146.9 (s), 145.9 (s), 138.1 (s), 137.7 (s), 134.7 (s), 130.8 (s), 129.5 (s), 128.3 (s), 128.3 (s), 127.6 (s), 127.0 (s), 125.9 (s), 122.7 (s), 118.4 (s), 18.3 (s). HRMS calcd. $[\text{C}_{18}\text{H}_{13}\text{N}_3\text{O} + \text{H}]^+$: 288.1137, found: 288.1141.

2-(6-(tert-butyl)quinolin-2-yl)quinazolin-4(3H)-one (3al):



The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as white solid. 91% yield, 89.8 mg. ^1H NMR (500 MHz, CDCl_3) δ 11.23 (s, 1H), 8.62 (d, $J = 8.5$ Hz, 1H), 8.36 (d, $J = 7.8$ Hz, 1H), 8.30 (d, $J = 8.5$ Hz, 1H), 8.08 (d, $J = 8.9$ Hz, 1H), 7.92 - 7.85 (m, 2H), 7.83 - 7.75 (m, 2H), 7.52 (t, $J = 7.4$ Hz, 1H), 1.45 (s, 9H). ^{13}C NMR (125 MHz, CDCl_3) δ 161.6 (s), 151.6 (s), 149.3 (s), 149.2 (s), 147.4 (s), 145.5 (s), 137.7 (s), 134.7 (s), 129.7 (s), 129.3 (s), 129.3 (s), 128.2 (s), 127.6 (s), 126.9 (s), 122.8 (s), 122.7 (s), 118.5 (s), 35.3 (s), 31.2 (s). HRMS calcd. $[\text{C}_{21}\text{H}_{19}\text{N}_3\text{O} + \text{H}]^+$: 330.1606, found: 330.1606.

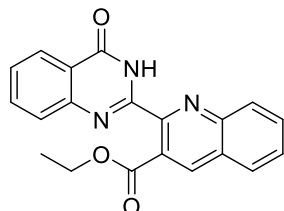
ethyl 2-(4-oxo-3,4-dihydroquinazolin-2-yl)-4-phenylquinoline-3-carboxylate (3an):



The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as yellow solid. 68% yield, 85.9 mg. ^1H NMR (500 MHz, CDCl_3) δ 11.19 (s, 1H), 8.38 (d, $J = 7.8$ Hz, 1H), 8.23 (d, $J = 8.4$ Hz, 1H), 7.85 (t, $J = 7.4$ Hz, 1H), 7.77 (t, $J = 7.6$ Hz, 1H), 7.69 (d, $J = 8.0$ Hz, 1H), 7.64 - 7.50 (m, 6H), 7.44 -

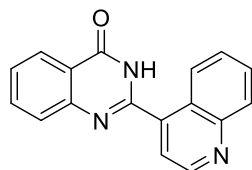
7.39 (m, 2H), 4.26 (q, $J = 7.1$ Hz, 2H), 1.06 (t, $J = 7.1$ Hz, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 167.3 (s), 161.5 (s), 148.6 (s), 148.5 (s), 148.0 (s), 146.4 (s), 143.6 (s), 134.7 (s), 134.5 (s), 131.3 (s), 129.9 (s), 129.7 (s), 129.1 (s), 129.0 (s), 128.3 (s), 128.3 (s), 128.0 (s), 127.9 (s), 126.9 (s), 126.9 (s), 126.4 (s), 122.8 (s), 61.5 (s), 13.9 (s). HRMS calcd. $[\text{C}_{26}\text{H}_{19}\text{N}_3\text{O}_3 + \text{H}]^+$: 422.1505, found: 422.1513.

ethyl 2-(4-oxo-3,4-dihydroquinazolin-2-yl)quinoline-3-carboxylate (3ao)⁴:



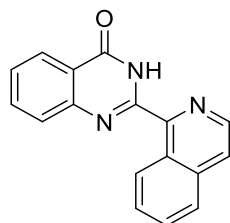
The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as yellow solid. 83% yield, 85.9 mg. ^1H NMR (500 MHz, CDCl_3) δ 11.03 (s, 1H), 8.45 - 8.33 (m, 2H), 8.16 (d, $J = 8.3$ Hz, 1H), 7.91 (d, $J = 8.0$ Hz, 1H), 7.84 (t, $J = 7.5$ Hz, 1H), 7.81 - 7.77 (m, 1H), 7.74 (d, $J = 7.8$ Hz, 1H), 7.67 (t, $J = 7.3$ Hz, 1H), 7.54 (t, $J = 7.1$ Hz, 1H), 4.53 (q, $J = 6.7$ Hz, 2H), 1.35 (t, $J = 7.0$ Hz, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 168.5 (s), 161.4 (s), 148.4 (s), 148.1 (s), 146.7 (s), 145.0 (s), 137.3 (s), 134.8 (s), 131.9 (s), 129.7 (s), 129.3 (s), 128.1 (s), 128.1 (s), 128.0 (s), 127.8 (s), 127.1 (s), 127.0 (s), 122.6 (s), 62.3 (s), 14.3 (s).

2-(quinolin-4-yl)quinazolin-4(3H)-one (3ap)³:



The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as white solid. 65% yield, 53.5 mg. ^1H NMR (500 MHz, DMSO) δ 12.84 (s, 1H), 9.08 (d, $J = 4.3$ Hz, 1H), 8.29 - 8.19 (m, 2H), 8.16 (d, $J = 5.0$ Hz, 1H), 7.92 - 7.84 (m, 2H), 7.81 (d, $J = 4.3$ Hz, 1H), 7.77 (d, $J = 8.0$ Hz, 1H), 7.68 (t, $J = 7.8$ Hz, 1H), 7.62 (t, $J = 7.3$ Hz, 1H). ^{13}C NMR (125 MHz, DMSO) δ 161.9 (s), 151.9 (s), 150.3 (s), 148.1 (s), 145.7 (s), 139.4 (s), 134.9 (s), 134.6 (s), 130.2 (s), 129.6 (s), 127.9 (s), 127.5 (s), 127.0 (s), 126.1 (s), 125.8 (s), 124.9 (s), 121.7 (s).

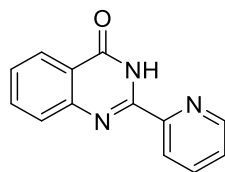
2-(isoquinolin-1-yl)quinazolin-4(3H)-one (3aq)²:



The title compound was prepared according to the general working procedure A and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as white solid. 84% yield, 69.0 mg. ^1H NMR (500 MHz, CDCl_3) δ 11.36 (s, 1H), 10.15 (d, $J = 7.6$ Hz, 1H), 8.58 (d, $J = 4.9$ Hz, 1H), 8.38 (d, $J = 7.7$ Hz, 1H), 7.96 (d, $J = 8.0$ Hz, 1H), 7.90 (d, $J = 5.2$ Hz, 1H), 7.87 - 7.81 (m, 2H), 7.80 - 7.76 (m, 2H), 7.55 (t, $J = 7.3$ Hz, 1H). ^{13}C NMR (125 MHz, CDCl_3) δ 161.6 (s), 150.3 (s), 149.0 (s),

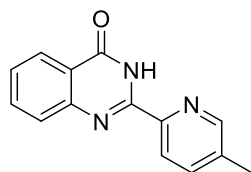
145.8 (s), 140.6 (s), 137.8 (s), 134.6 (s), 130.8 (s), 129.2 (s), 128.6 (s), 128.3 (s), 127.8 (s), 127.4 (s), 127.4 (s), 126.7 (s), 124.8 (s), 122.5 (s).

2-(pyridin-2-yl)quinazolin-4(3H)-one (3ar)¹:



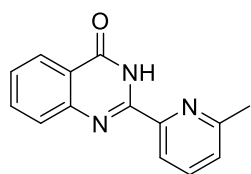
The title compound was prepared according to the general working procedure B and purified by column chromatography (petroleum ether/ethyl acetate = 8/1) to give the product as white solid. 73% yield, 48.8 mg. ¹H NMR (500 MHz, CDCl₃) δ 10.98 (s, 1H), 8.67 (d, *J* = 4.4 Hz, 1H), 8.63 (d, *J* = 7.9 Hz, 1H), 8.35 (d, *J* = 7.9 Hz, 1H), 7.93 (t, *J* = 7.7 Hz, 1H), 7.87 (d, *J* = 8.1 Hz, 1H), 7.80 (t, *J* = 7.6 Hz, 1H), 7.55 - 7.45 (m, 2H). ¹³C NMR (125 MHz, CDCl₃) δ 161.5 (s), 149.1 (s), 149.1 (s), 148.9 (s), 148.4 (s), 137.7 (s), 134.8 (s), 128.1 (s), 127.5 (s), 126.9 (s), 126.5 (s), 122.6 (s), 122.2 (s).

2-(5-methylpyridin-2-yl)quinazolin-4(3H)-one (3as):



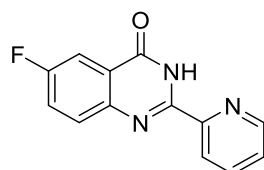
The title compound was prepared according to the general working procedure B and purified by column chromatography (petroleum ether/ethyl acetate = 8/1) to give the product as white solid. 63% yield, 44.8 mg. ¹H NMR (500 MHz, CDCl₃) δ 10.94 (s, 1H), 8.48 (s, 1H), 8.46 (d, *J* = 8.1 Hz, 1H), 8.34 (d, *J* = 7.9 Hz, 1H), 7.80 (t, *J* = 8.9 Hz, 2H), 7.71 (d, *J* = 7.2 Hz, 1H), 7.50 (t, *J* = 7.2 Hz, 1H), 2.44 (s, 3H). ¹³C NMR (125 MHz, CDCl₃) δ 161.6 (s), 149.3 (s), 149.3 (s), 146.0 (s), 138.1 (s), 136.8 (s), 135.8 (s), 134.7 (s), 128.0 (s), 127.2 (s), 126.9 (s), 122.5 (s), 121.7 (s), 18.8 (s). HRMS calcd. [C₁₄H₁₁N₃O + H]⁺: 238.0980, found: 238.0984.

2-(6-methylpyridin-2-yl)quinazolin-4(3H)-one (3at)¹:



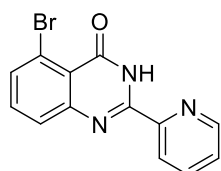
The title compound was prepared according to the general working procedure B and purified by column chromatography (petroleum ether/ethyl acetate = 8/1) to give the product as white solid. 71% yield, 50.5 mg. ¹H NMR (500 MHz, CDCl₃) δ 11.08 (s, 1H), 8.40 (d, *J* = 7.7 Hz, 1H), 8.34 (d, *J* = 7.8 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.81 - 7.75 (m, 2H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.32 (d, *J* = 7.6 Hz, 1H), 2.63 (s, 3H). ¹³C NMR (125 MHz, CDCl₃) δ 161.6 (s), 158.1 (s), 149.3 (s), 149.2 (s), 147.5 (s), 137.9 (s), 134.7 (s), 128.0 (s), 127.4 (s), 126.9 (s), 126.2 (s), 122.5 (s), 119.3 (s), 24.4 (s).

6-fluoro-2-(pyridin-2-yl)quinazolin-4(3H)-one (3br):



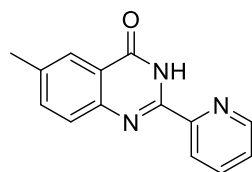
The title compound was prepared according to the general working procedure B and purified by column chromatography (petroleum ether/ethyl acetate = 8/1) to give the product as white solid. 66% yield, 47.7 mg. ¹H NMR (500 MHz, CDCl₃) δ 10.99 (s, 1H), 8.67 (d, *J* = 4.4 Hz, 1H), 8.56 (d, *J* = 7.9 Hz, 1H), 7.97 (dd, *J* = 8.3, 2.8 Hz, 1H), 7.92 (t, *J* = 7.7 Hz, 1H), 7.84 (dd, *J* = 8.9, 4.9 Hz, 1H), 7.58 - 7.44 (m, 2H). ¹³C NMR (125 MHz, CDCl₃) δ 161.3 (d, *J* = 247.5 Hz), 160.8 (s), 148.9 (s), 148.5 (s), 148.2 (s), 145.8 (s), 137.7 (s), 130.5 (d, *J* = 8.2 Hz), 126.5 (s), 123.9 (d, *J* = 8.6 Hz), 123.2 (d, *J* = 23.8 Hz), 122.1 (s), 112.0 (d, *J* = 23.8 Hz). HRMS calcd. [C₁₃H₈FN₃O + H]⁺: 242.0730, found: 242.0735.

5-bromo-2-(pyridin-2-yl) quinazolin-4(3H)-one (3hr):



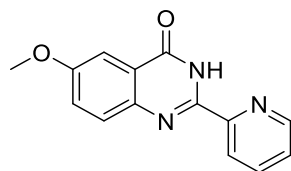
The title compound was prepared according to the general working procedure B and purified by column chromatography (petroleum ether/ethyl acetate = 8/1) to give the product as white solid. 41% yield, 37.0 mg. ¹H NMR (500 MHz, CDCl₃) δ 10.84 (s, 1H), 8.67 (d, *J* = 4.3 Hz, 1H), 8.54 (d, *J* = 7.9 Hz, 1H), 7.91 (t, *J* = 7.7 Hz, 1H), 7.76 (d, *J* = 8.1 Hz, 1H), 7.71 (d, *J* = 7.7 Hz, 1H), 7.55 - 7.46 (m, 2H). ¹³C NMR (125 MHz, CDCl₃) δ 159.7 (s), 151.5 (s), 149.4 (s), 149.0 (s), 147.9 (s), 137.7 (s), 134.3 (s), 133.9 (s), 128.1 (s), 126.7 (s), 122.2 (s), 121.8 (s), 120.8 (s). HRMS calcd. [C₁₃H₈BrN₃O + H]⁺: 301.9929, found: 301.9926.

6-methyl-2-(pyridin-2-yl) quinazolin-4(3H)-one :



The title compound was prepared according to the general working procedure B and purified by column chromatography (petroleum ether/ethyl acetate = 8/1) to give the product as white solid. 68% yield, 48.3 mg. ¹H NMR (500 MHz, CDCl₃) δ 10.91 (s, 1H), 8.67 - 8.57 (m, 1H), 8.52 (d, *J* = 7.7 Hz, 1H), 8.11 (s, 1H), 7.87 (t, *J* = 7.5 Hz, 1H), 7.69 (d, *J* = 8.2 Hz, 1H), 7.57 (d, *J* = 8.0 Hz, 1H), 7.48 - 7.39 (m, 1H), 2.48 (s, 3H). ¹³C NMR (125 MHz, CDCl₃) δ 161.5 (s), 148.8 (s), 148.6 (s), 148.3 (s), 147.2 (s), 137.7 (s), 137.5 (s), 136.1 (s), 127.9 (s), 126.3 (s), 126.1 (s), 122.2 (s), 121.9 (s), 21.5 (s). HRMS calcd. [C₁₄H₁₁N₃O + H]⁺: 238.0980, found: 238.0988.

6-methoxy-2-(pyridin-2-yl) quinazolin-4(3H)-one (3kr):

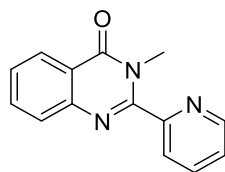


The title compound was prepared according to the general working procedure B and purified by column chromatography (petroleum ether/ethyl acetate = 5/1) to give the product as white solid. 56% yield, 42.5 mg. ¹H NMR (500 MHz, CDCl₃) δ 10.91 (s, 1H), 8.58 (d, *J* = 4.6 Hz, 1H), 8.46 (d, *J* = 7.9 Hz, 1H), 7.83 (t, *J* = 7.7 Hz, 1H), 7.69 (d, *J* = 8.9 Hz, 1H), 7.66 (d, *J* = 2.8 Hz, 1H), 7.42 - 7.35 (m, 1H), 7.32 (dd, *J* = 8.9, 2.8 Hz, 1H), 3.89 (s, 3H). ¹³C NMR (125 MHz, CDCl₃) δ 161.3 (s), 158.9 (s), 148.7 (s), 148.6

(s), 146.9 (s), 143.6 (s), 137.5 (s), 129.6 (s), 125.9 (s), 124.8 (s), 123.3 (s), 121.6 (s), 106.3 (s), 55.9 (s).

HRMS calcd. $[\text{C}_{14}\text{H}_{11}\text{N}_3\text{O}_2 + \text{H}]^+$: 254.0930, found: 254.0928.

3-methyl-2-(pyridin-2-yl)quinazolin-4(3H)-one (3mr)¹:



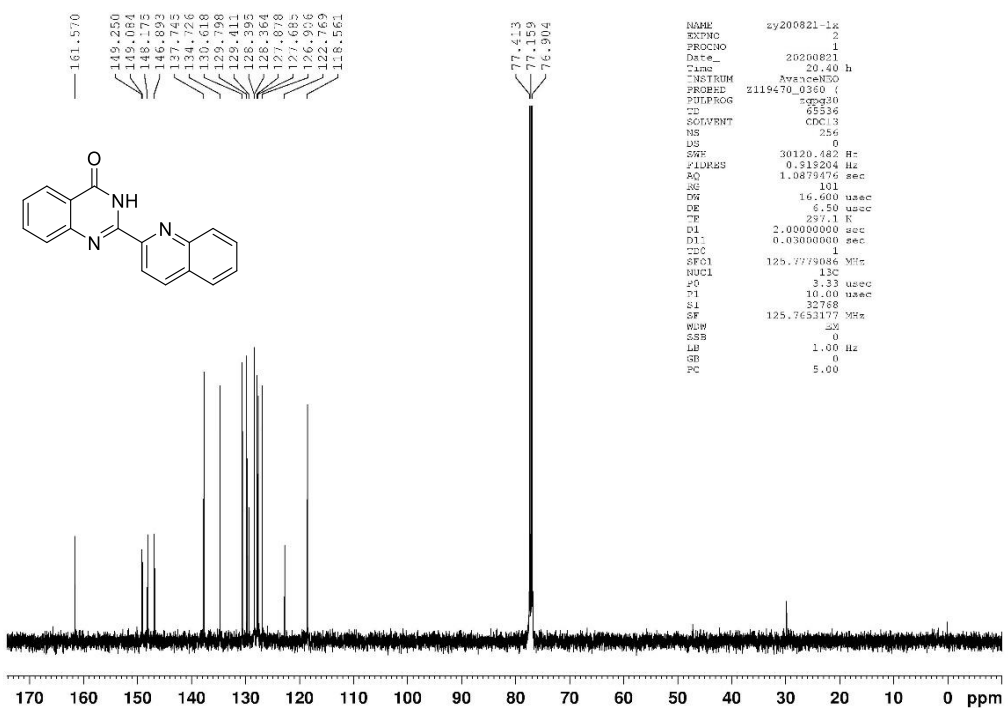
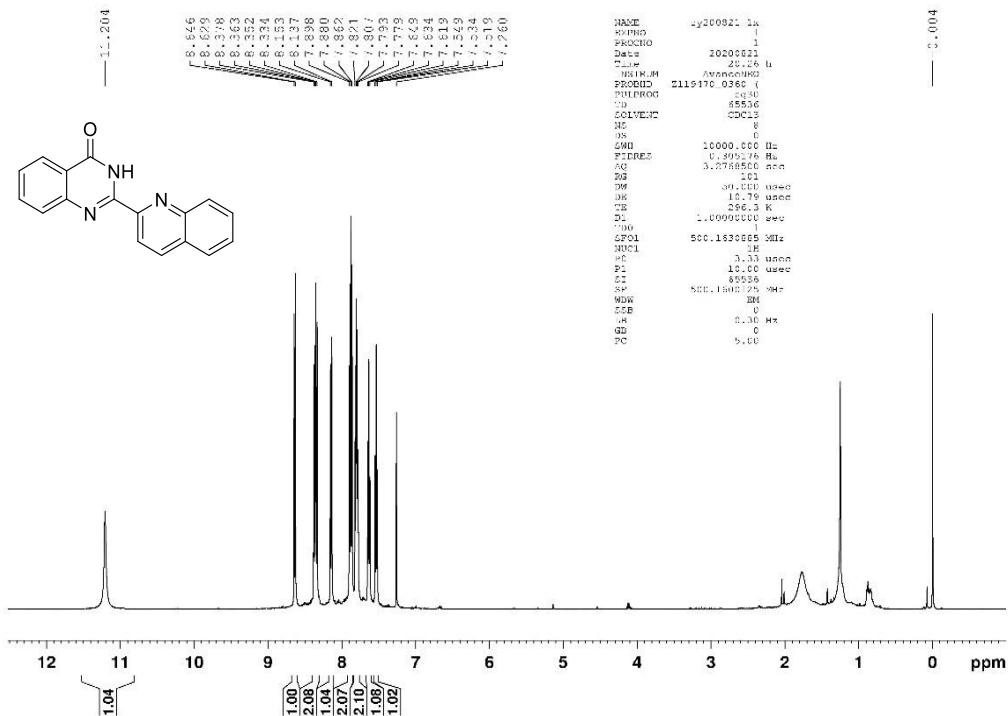
The title compound was prepared according to the general working procedure B and purified by column chromatography (petroleum ether/ethyl acetate = 10/1) to give the product as white solid. 74% yield, 52.6 mg. ¹H NMR (500 MHz, CDCl₃) δ 8.71 (d, *J* = 4.4 Hz, 1H), 8.33 (d, *J* = 8.0 Hz, 1H), 7.90 (t, *J* = 7.3 Hz, 1H), 7.83 (d, *J* = 7.7 Hz, 1H), 7.74 (d, *J* = 3.8 Hz, 2H), 7.50 (dt, *J* = 8.1, 4.1 Hz, 1H), 7.47 - 7.40 (m, 1H), 3.59 (s, 3H). ¹³C NMR (125 MHz, CDCl₃) δ 162.6 (s), 154.0 (s), 153.5 (s), 149.0 (s), 147.0 (s), 137.6 (s), 134.4 (s), 127.5 (s), 127.5 (s), 126.9 (s), 124.9 (s), 124.5 (s), 121.0 (s), 33.6 (s).

References

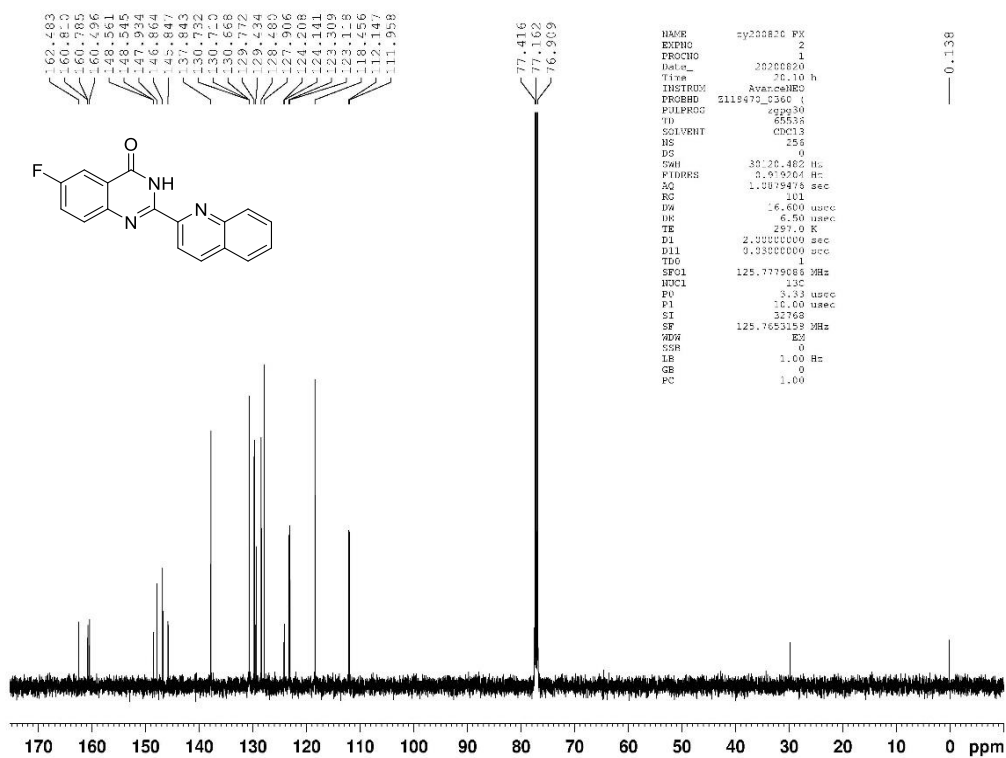
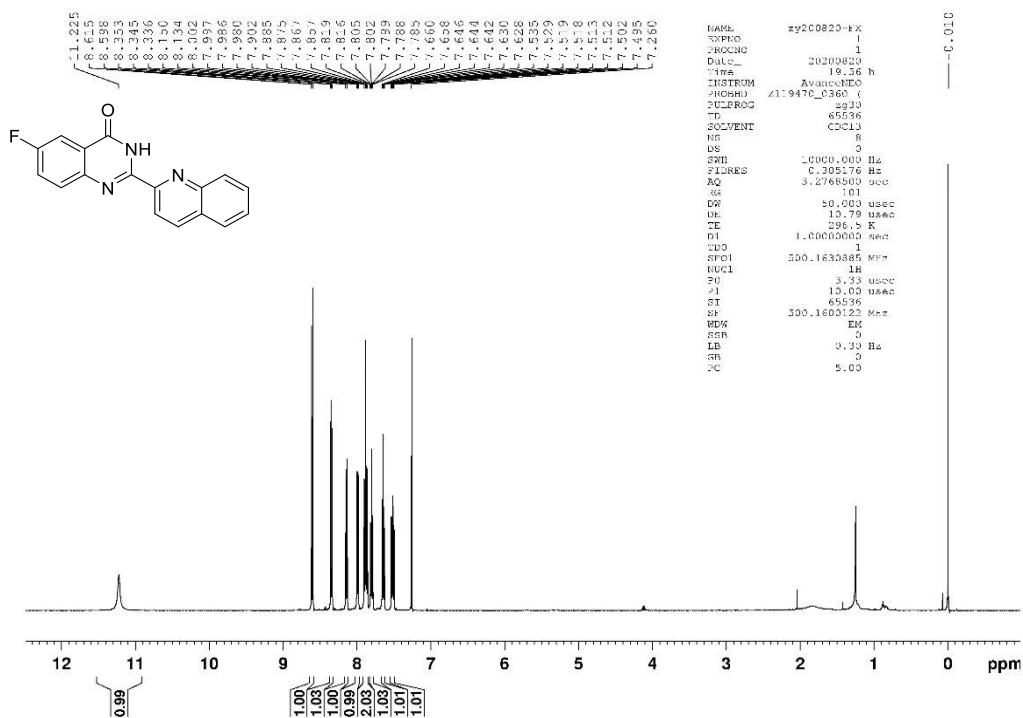
- (1) Li, Q.; Huang, Y.; Chen, T. Q.; Zhou, Y. B.; Xu, Q.; Yin, S. F.; Han, L. B. *Org. Lett.* 2014, 16, 3672-3675.
- (2) Liu, H. H.; Zhai, T. R.; Ding, S. T.; Hou, Y. L.; Zhang, X. Y.; Feng, L.; Ma, C. *Org. Chem. Front.* 2016, 3, 1096-1099.
- (3) Yang, L.; Shi, X.; Hu, B. Q.; Wang, L. X. *Asian J. Org. Chem.* 2016, 5, 494-498.
- (4) Lingaiah, N.; Hanmant, K. G., Rajashaker B. *Synlett.* 2012, 23, 12, 1775-1778.

Copies of product NMR spectra

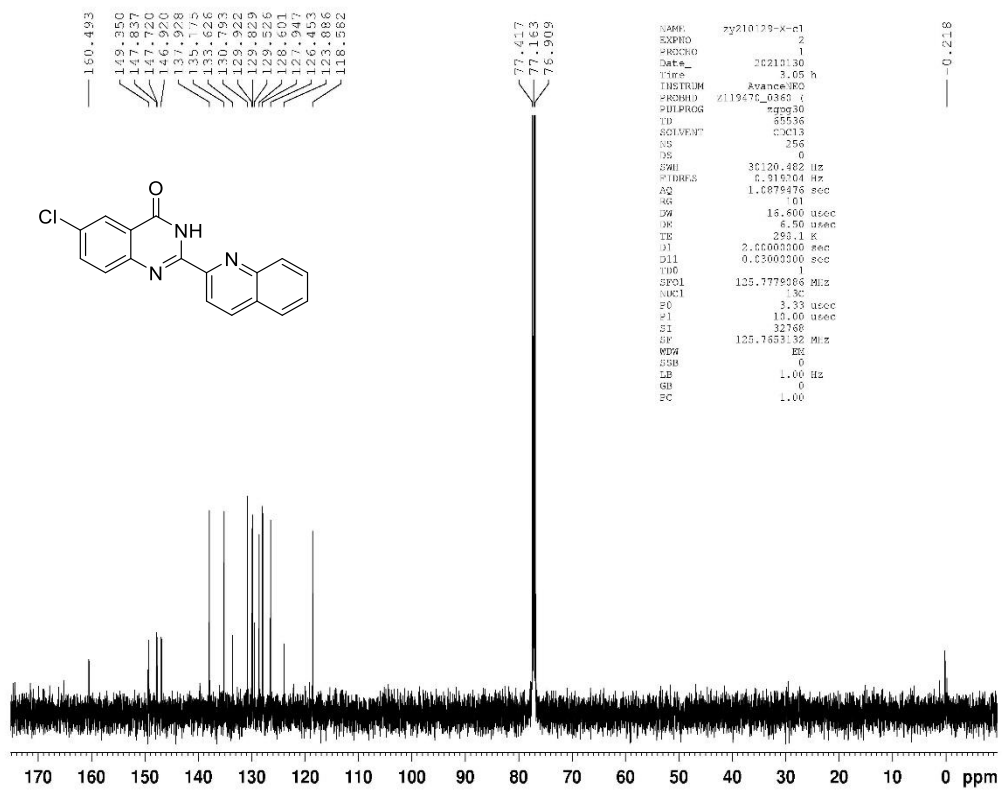
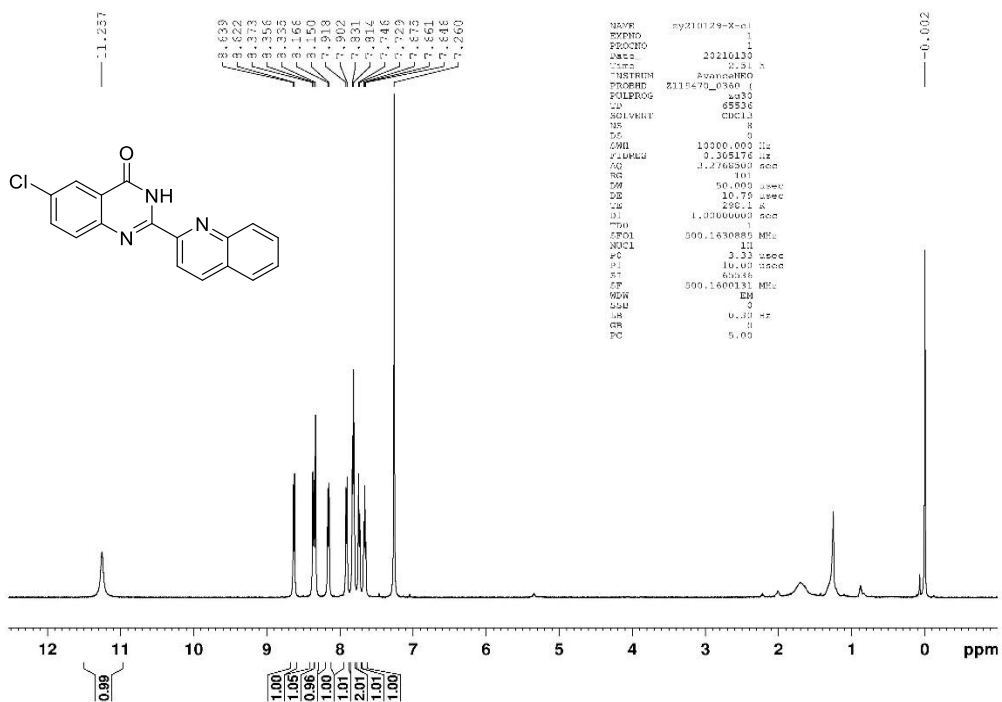
2-(quinolin-2-yl)quinazolin-4(3H)-one (3aa):



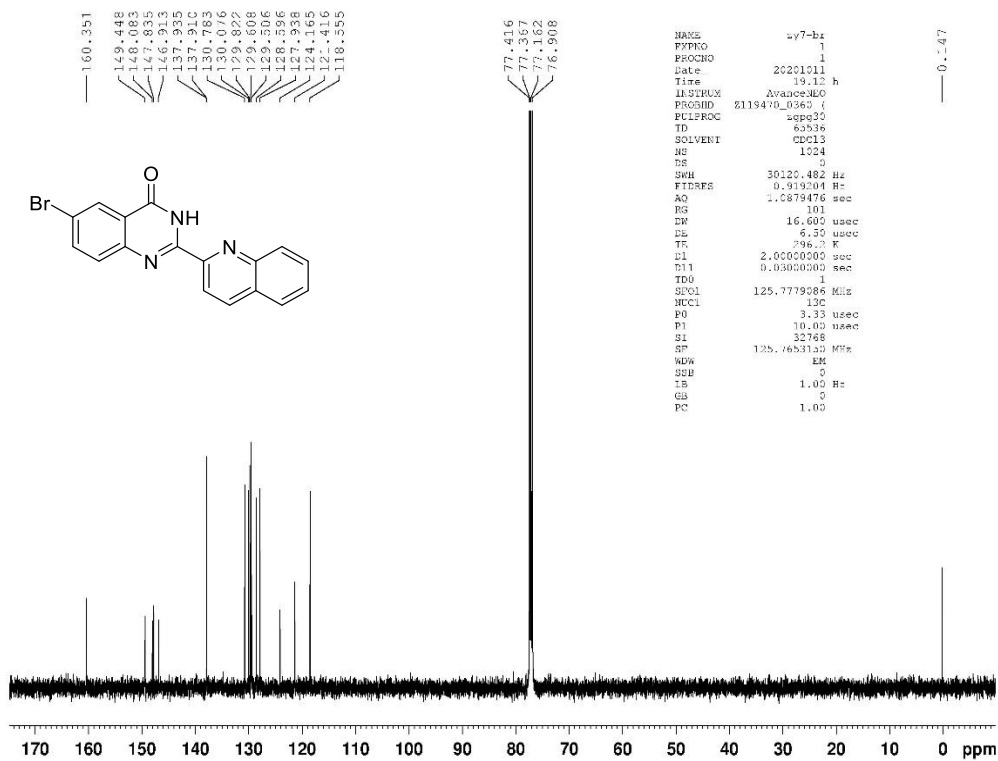
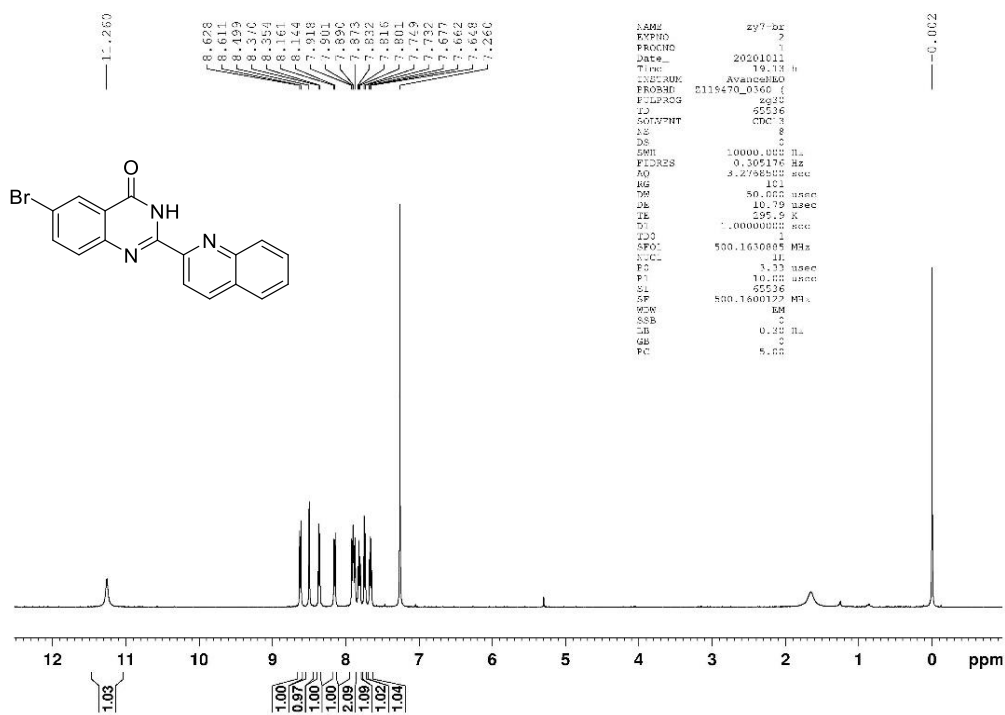
6-Fluoro-2-(quinolin-2-yl)quinazolin-4(3H)-one (3ba):



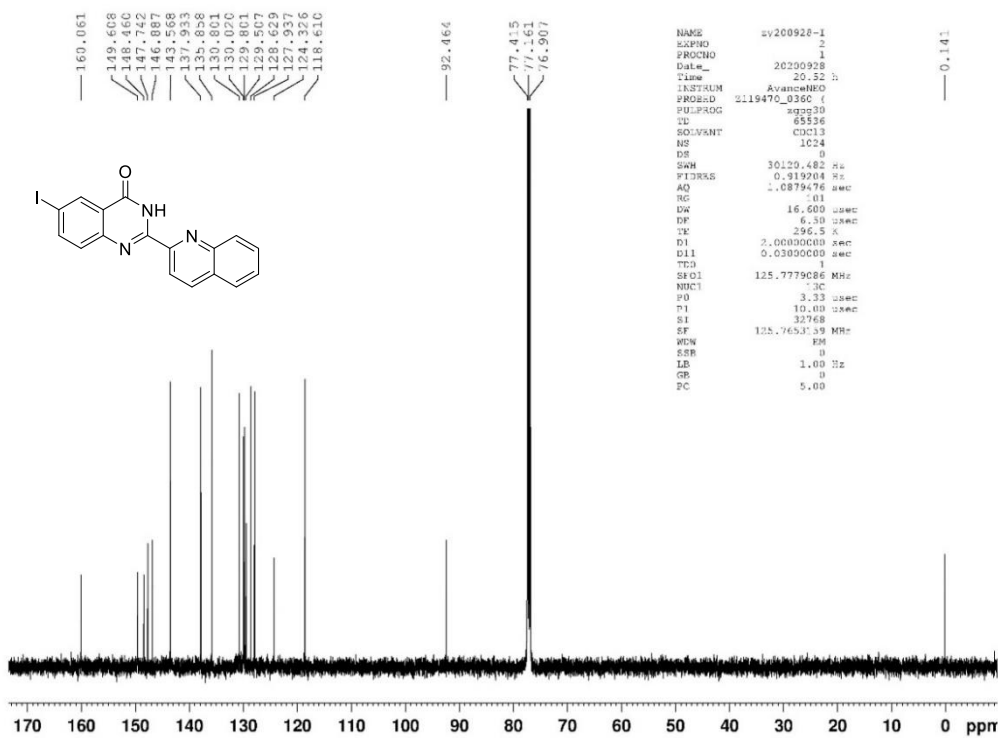
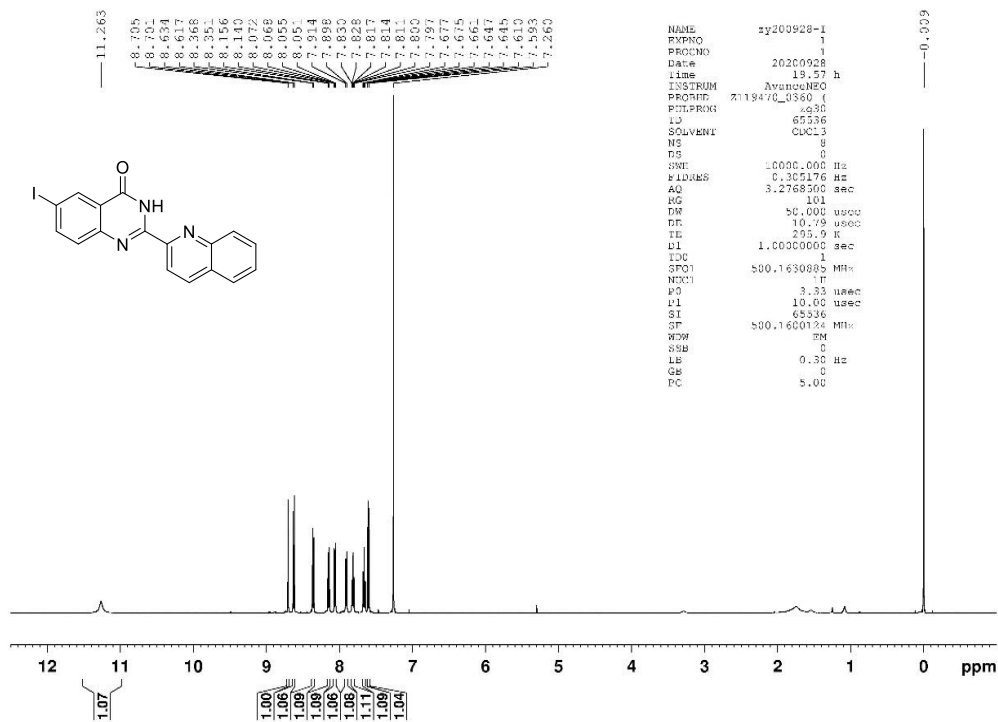
6-chloro-2-(quinolin-2-yl)quinazolin-4(3H)-one (3ca):



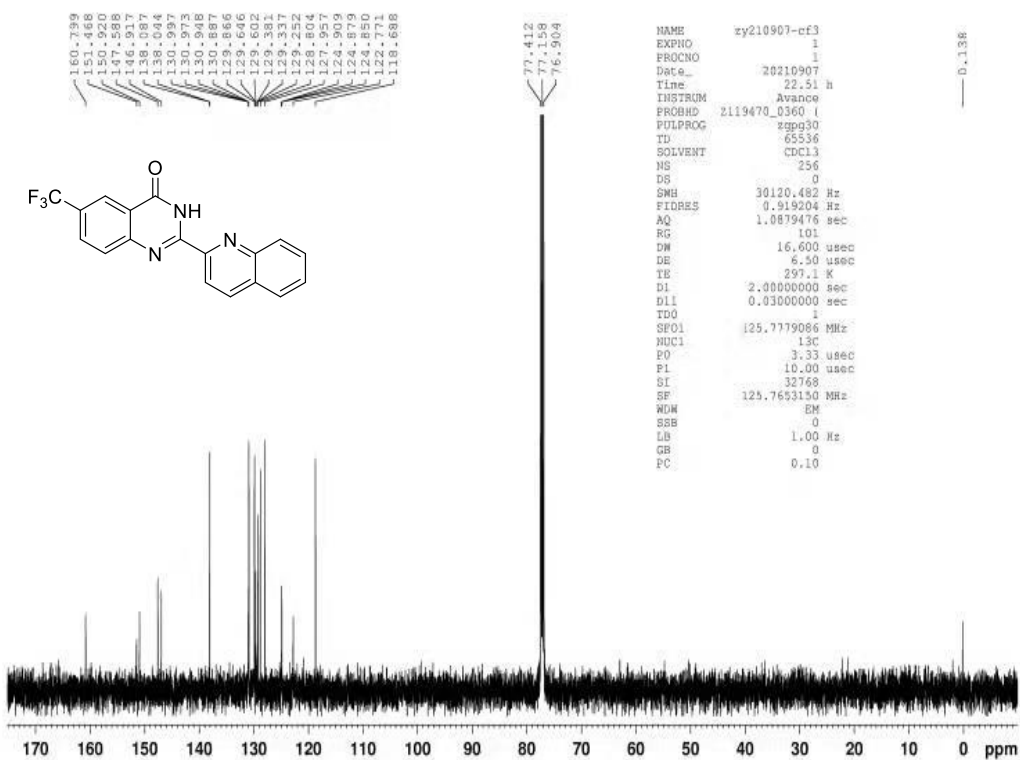
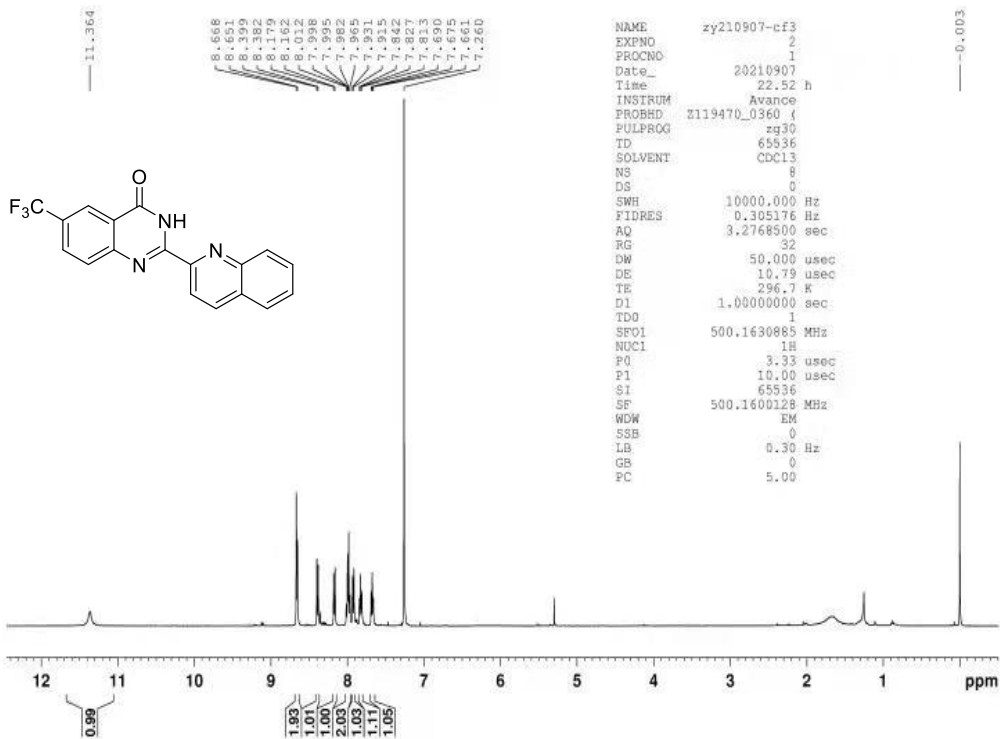
6-bromo-2-(quinolin-2-yl)quinazolin-4(3H)-one (3da):



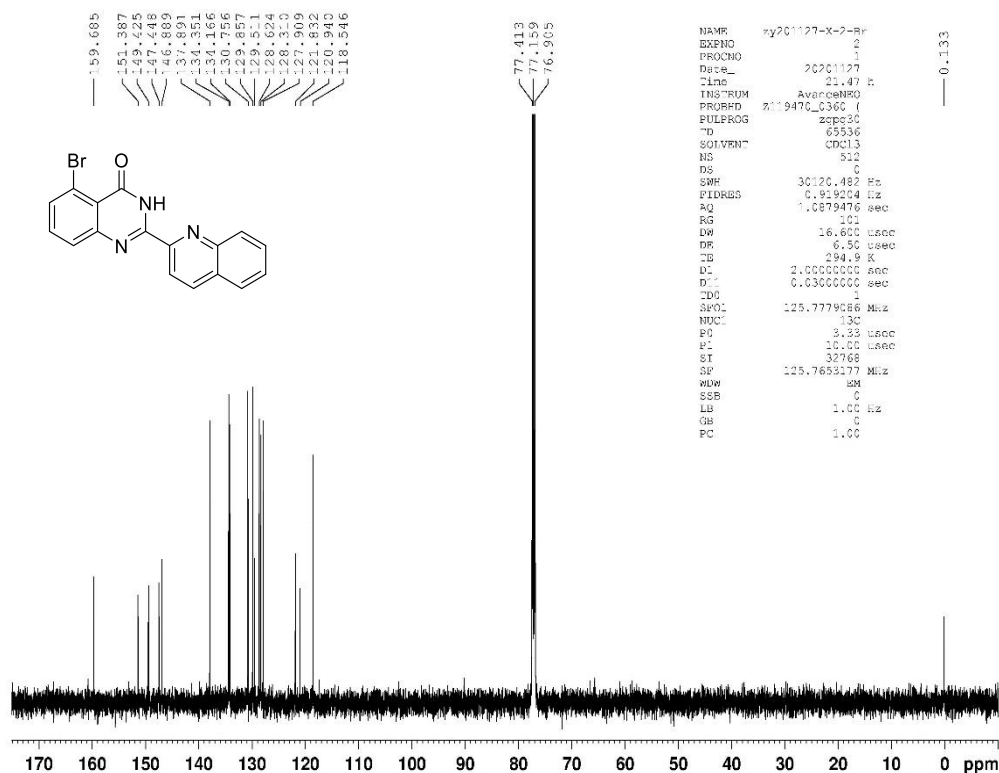
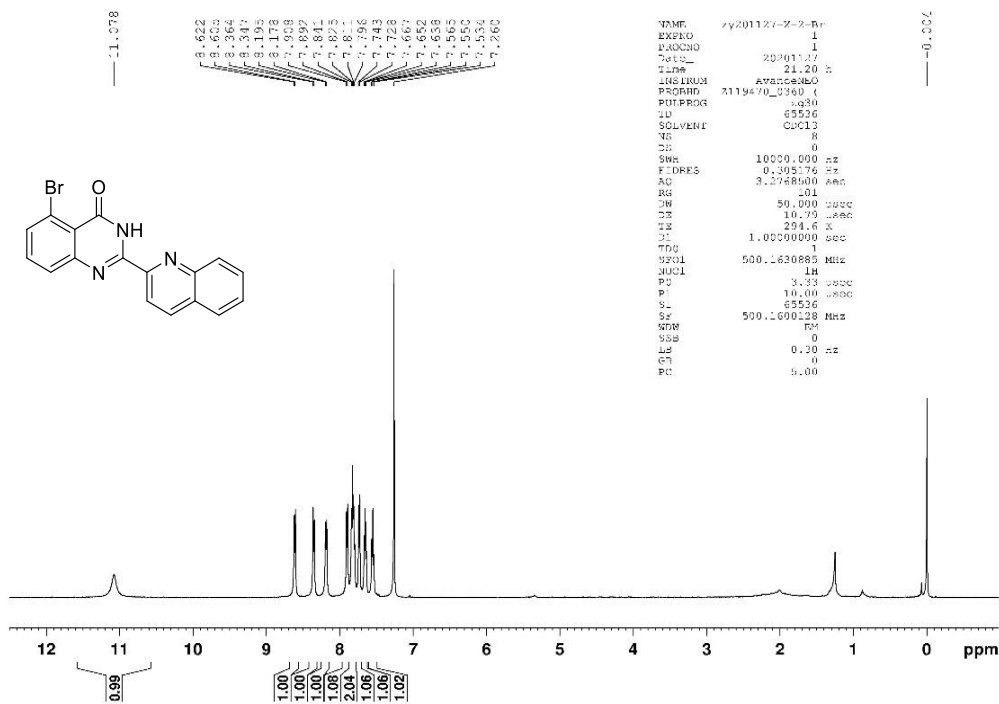
6-iodo-2-(quinolin-2-yl)quinazolin-4(3H)-one (3ea):



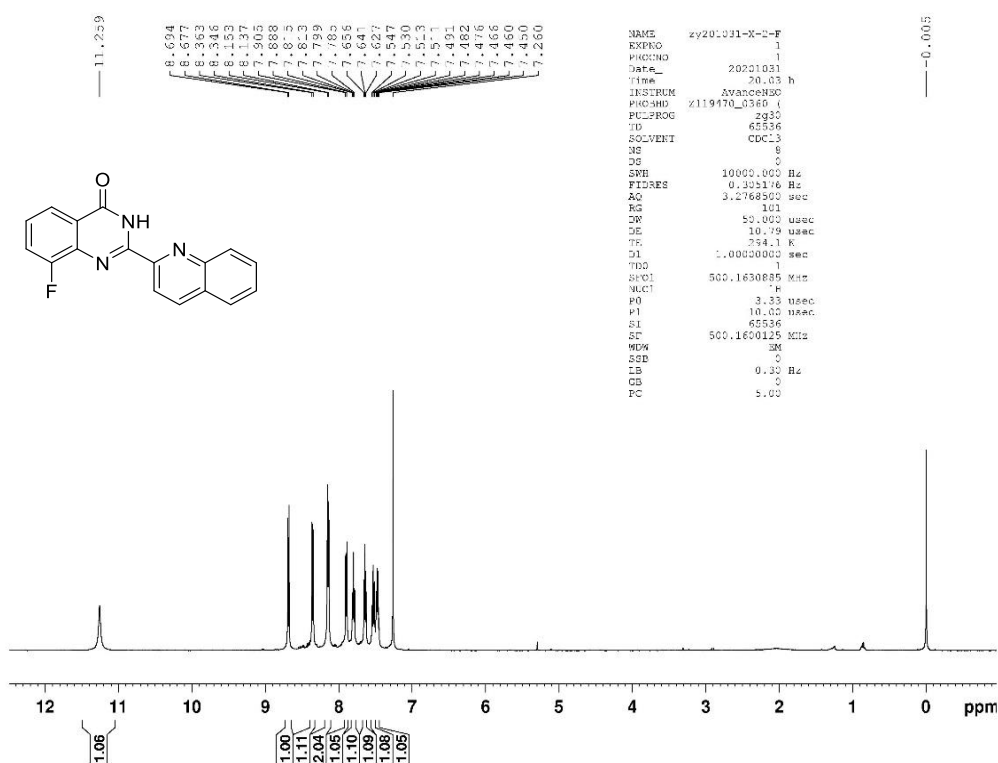
2-(quinolin-2-yl)-6-(trifluoromethyl)quinazolin-4(3H)-one (3fa):



5-bromo-2-(quinolin-2-yl)quinazolin-4(3H)-one (3ha):

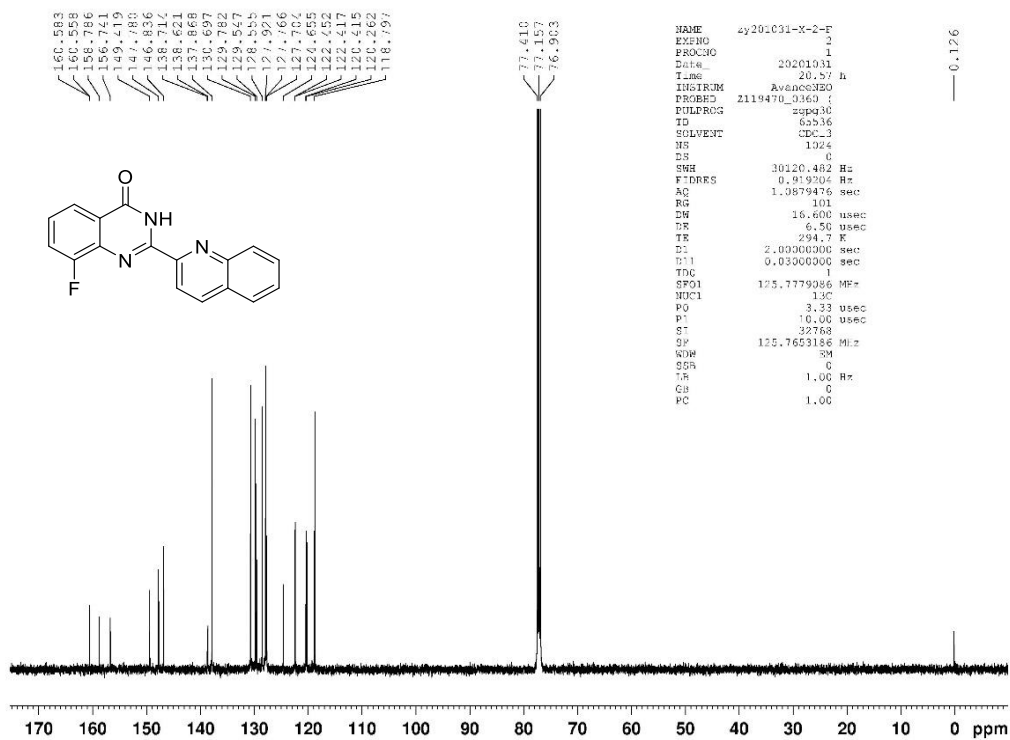


8-fluoro-2-(quinolin-2-yl)quinazolin-4(3H)-one (3ia):



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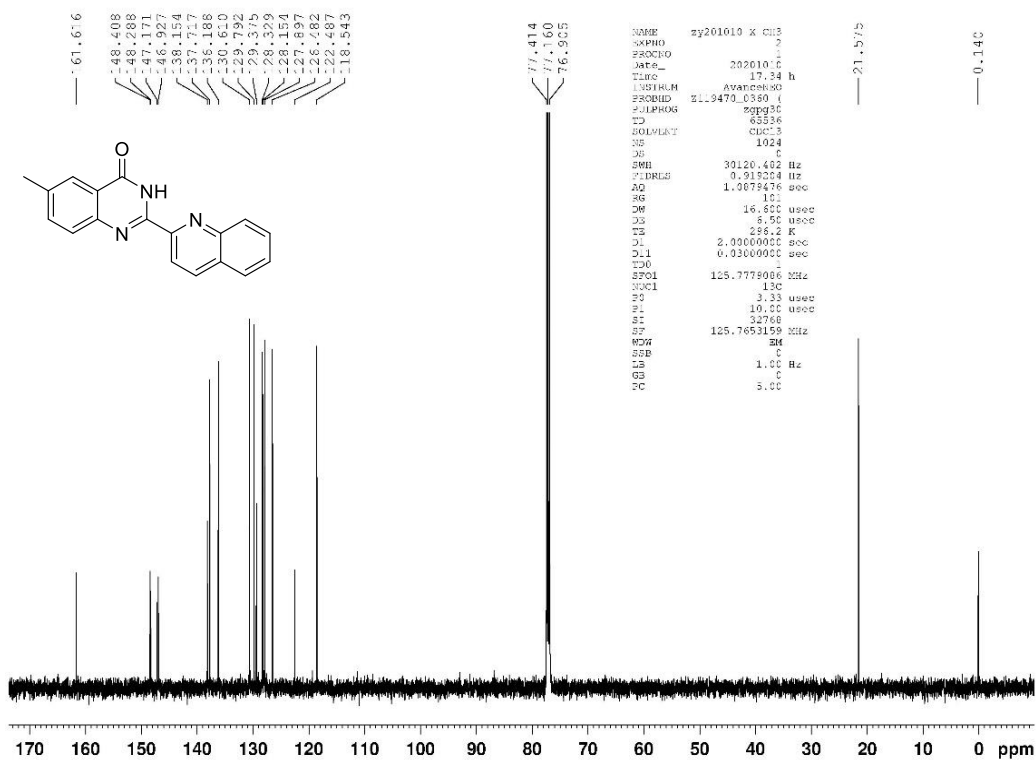
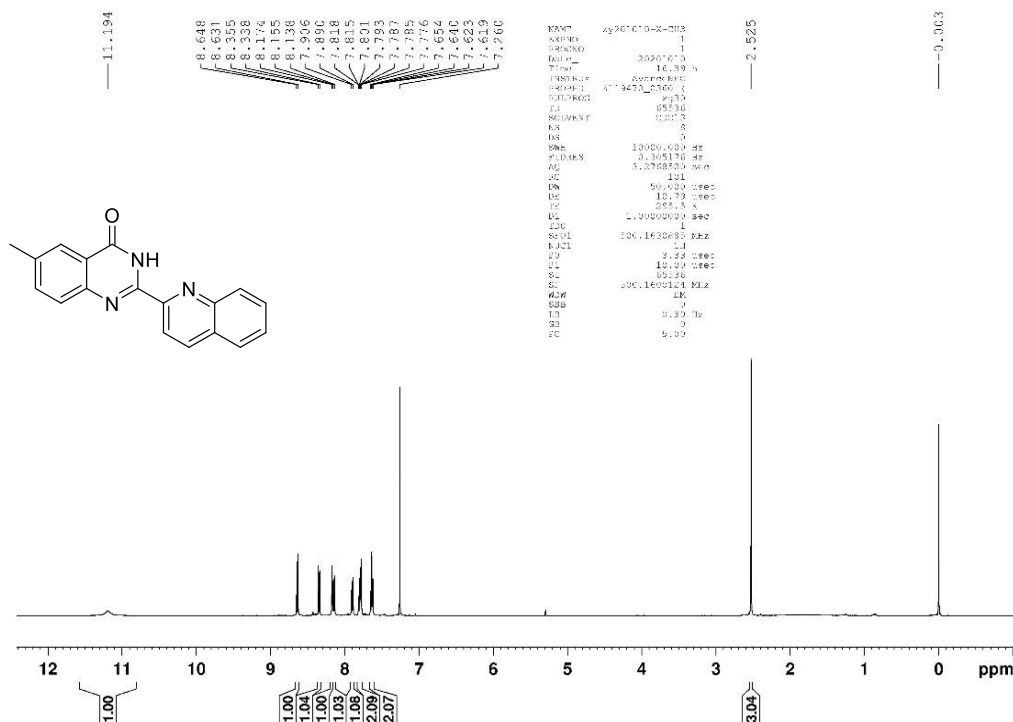
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RG       101
CW       50.000 ussec
DE       10.79 ussec
TE       294.1 K
D1       1.00000000 sec
SI       1
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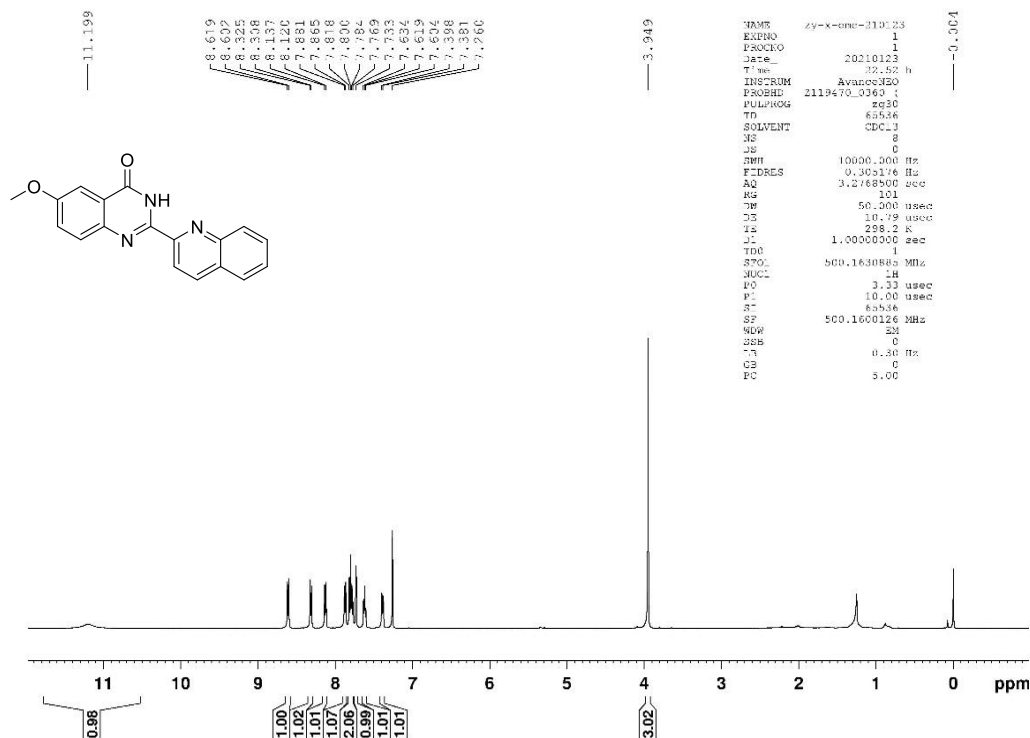
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6-methyl-2-(quinolin-2-yl)quinazolin-4(3H)-one (3ja)

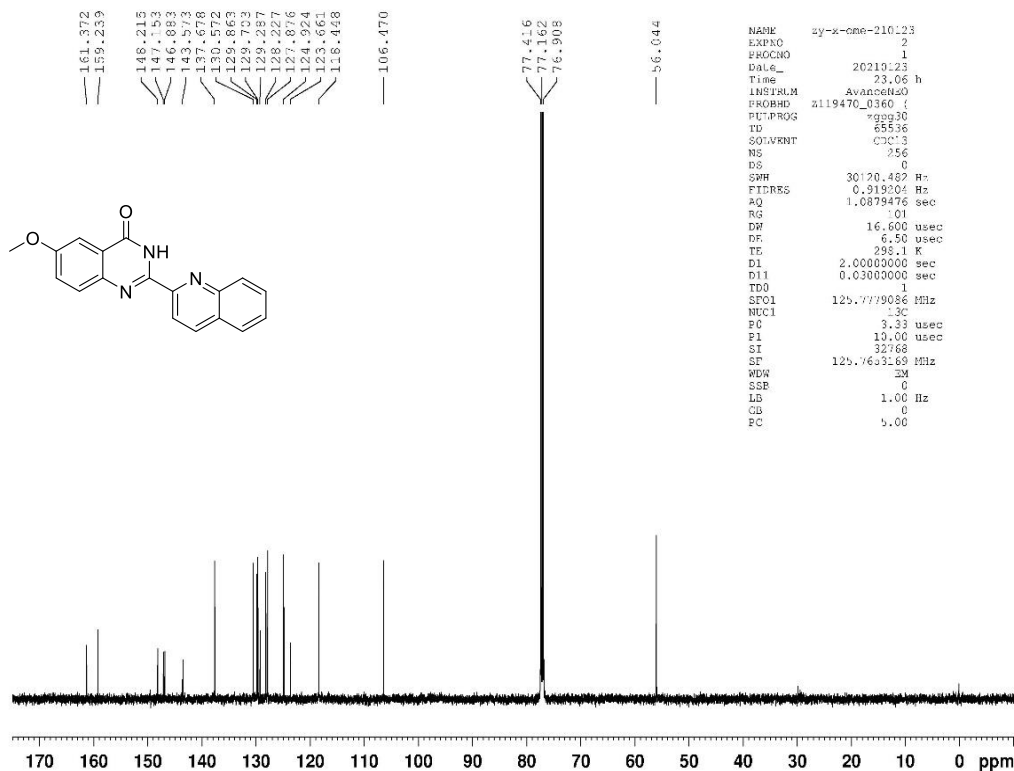


6-methoxy-2-(quinolin-2-yl)quinazolin-4(3H)-one (3ka):



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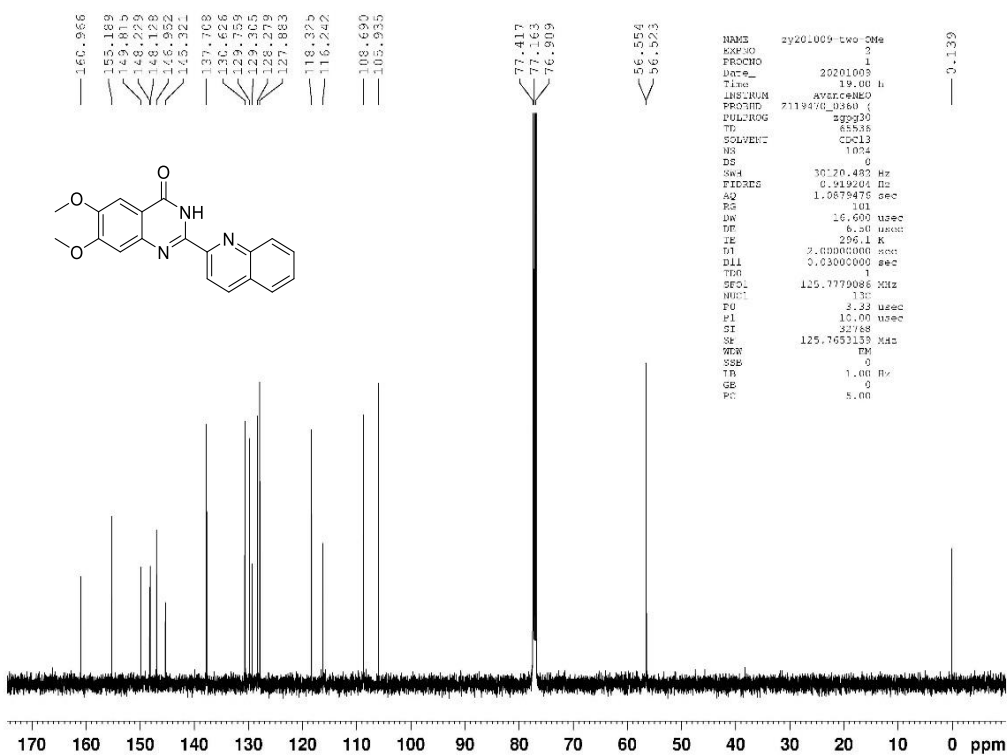
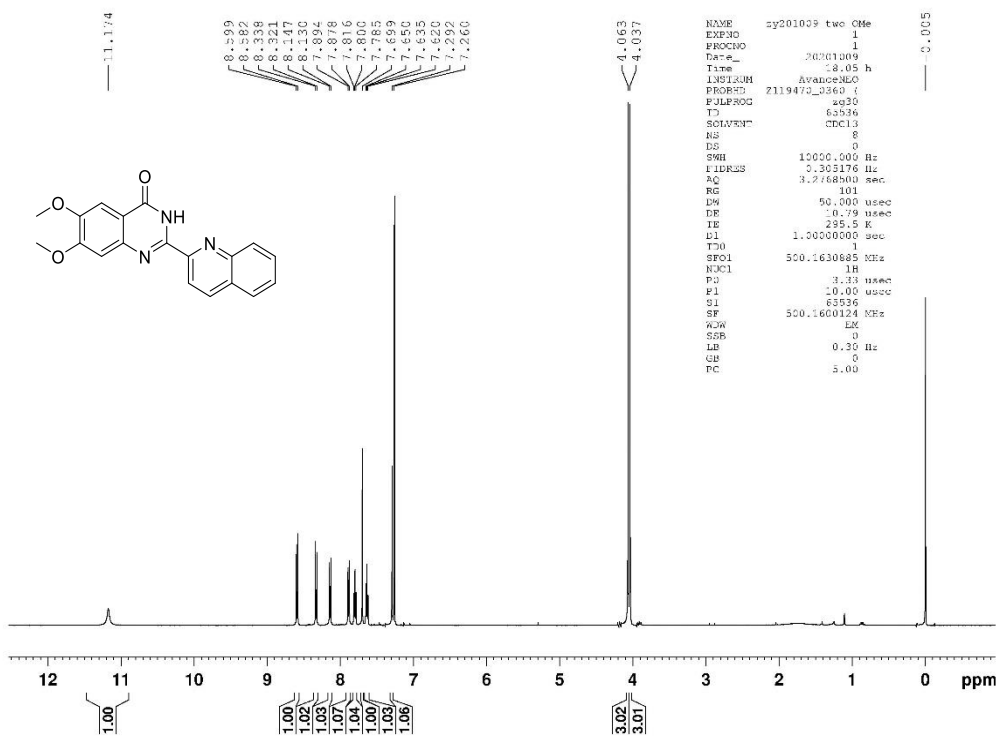
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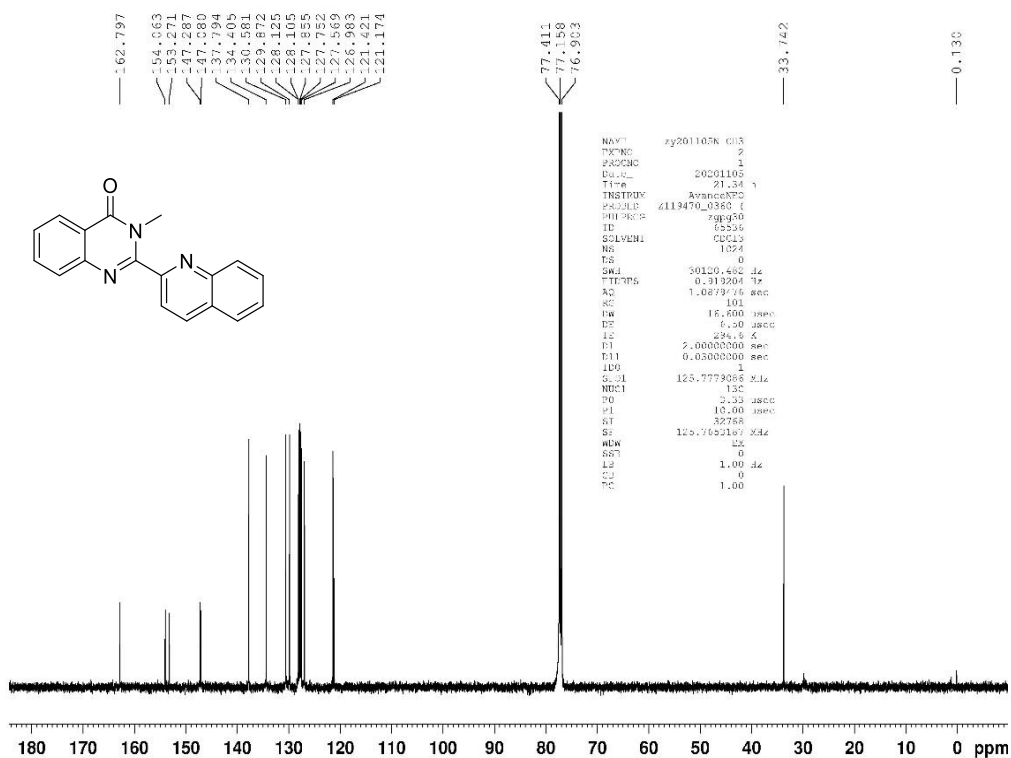
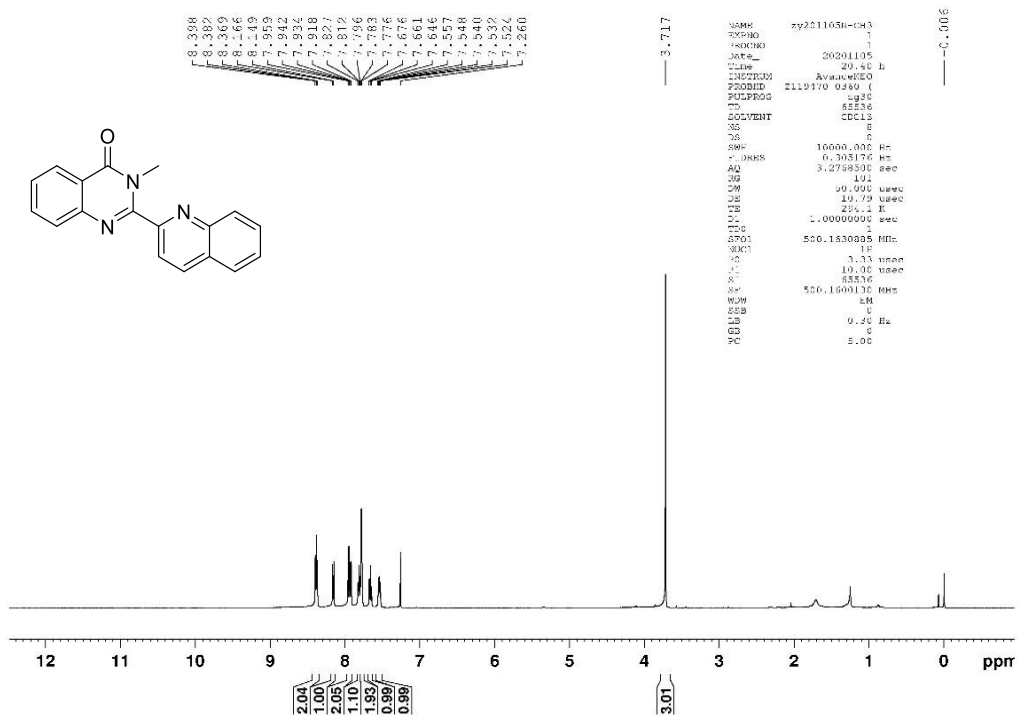
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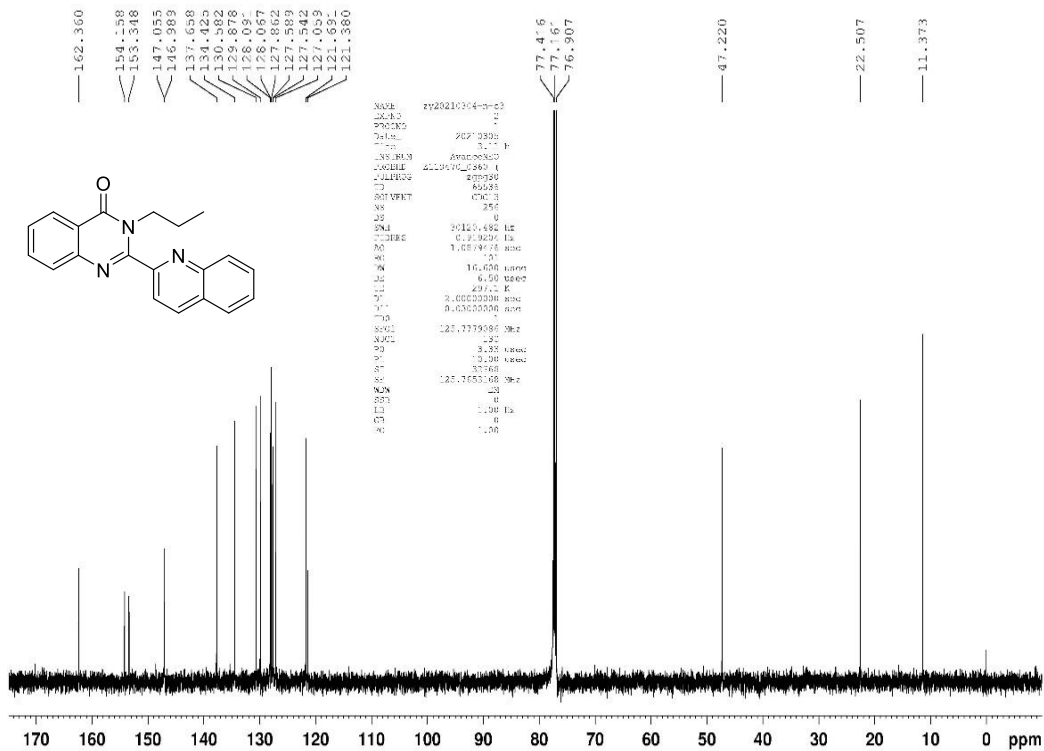
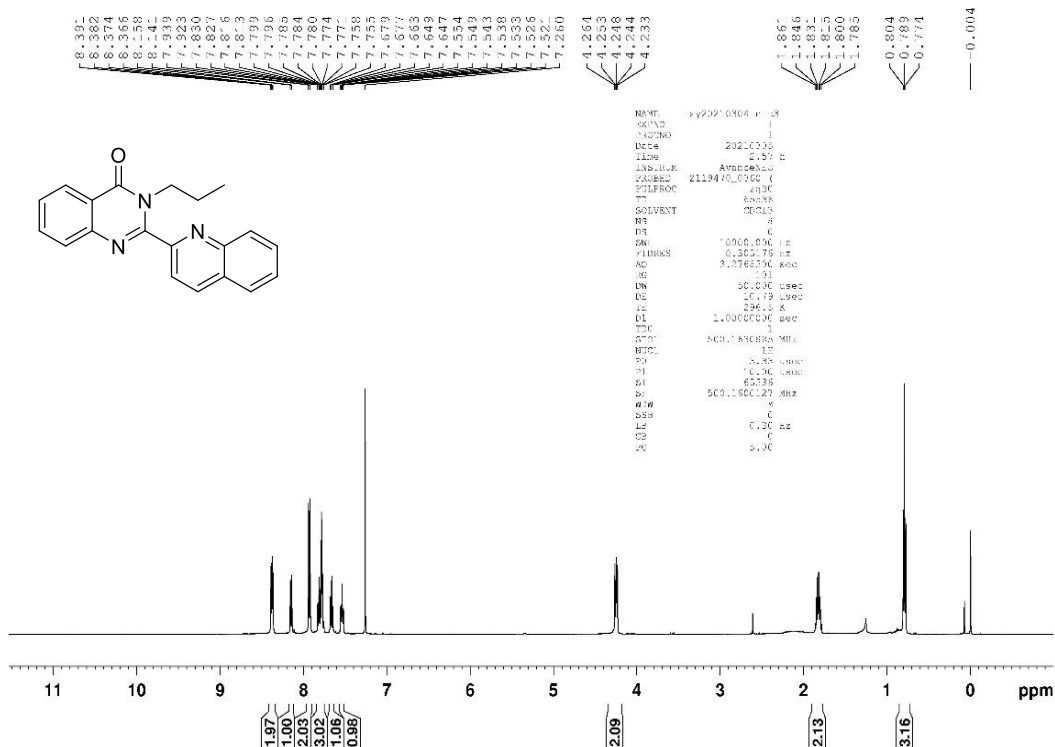
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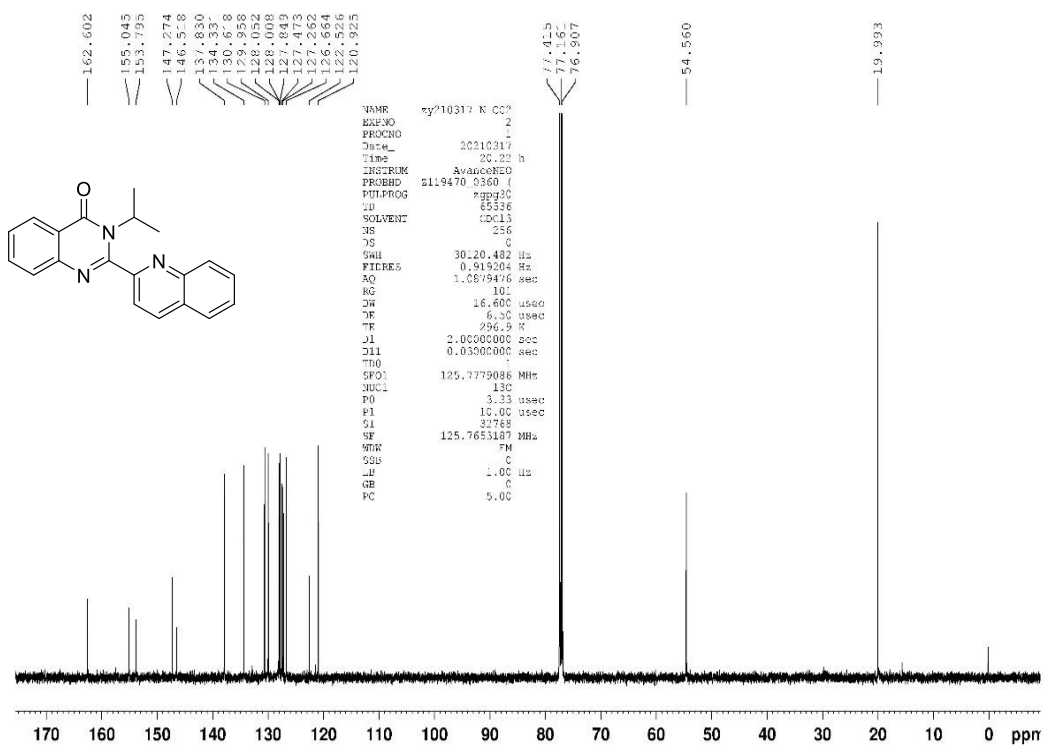
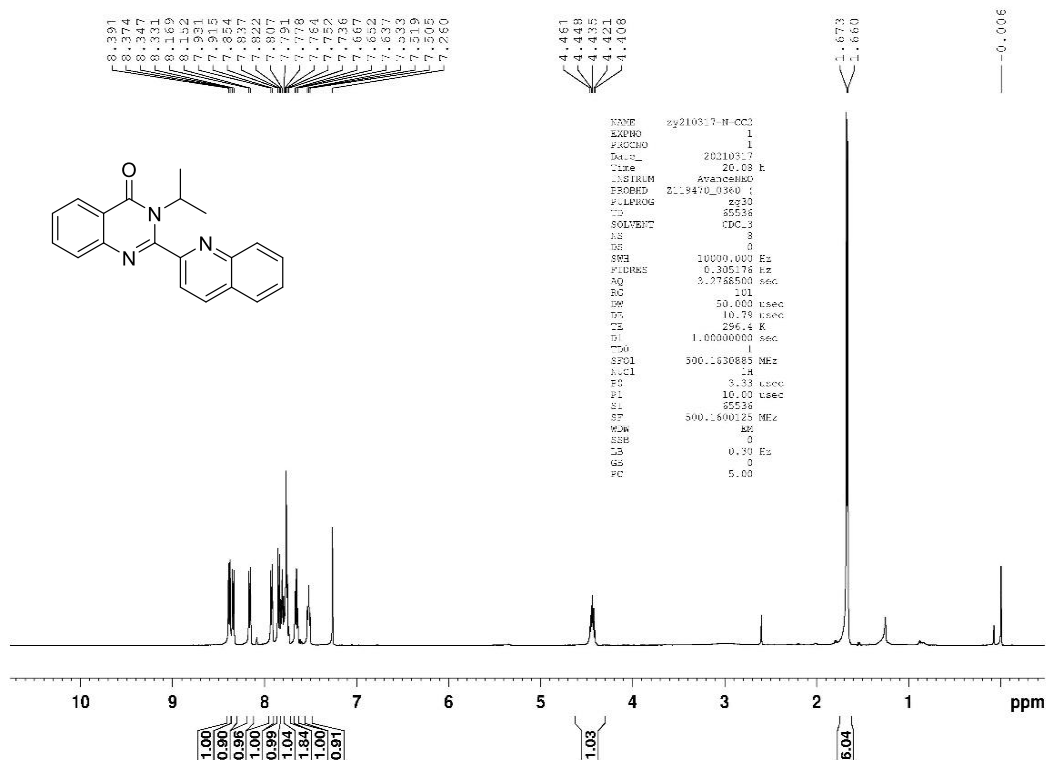
3-methyl-2-(quinolin-2-yl)quinazolin-4(3H)-one (3ma):



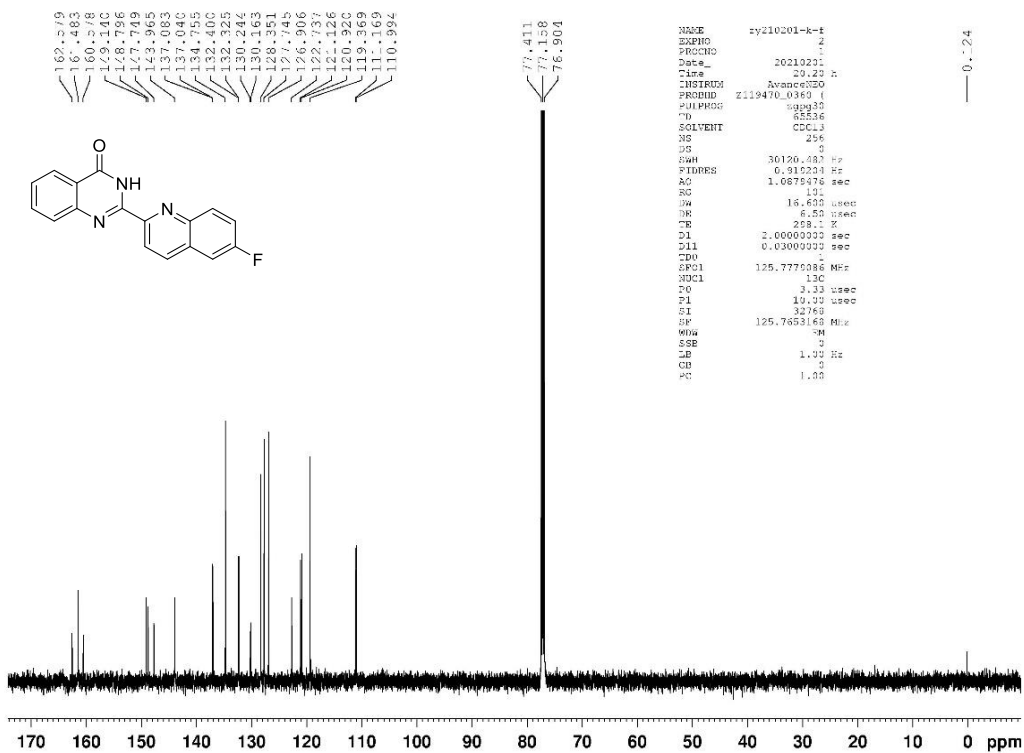
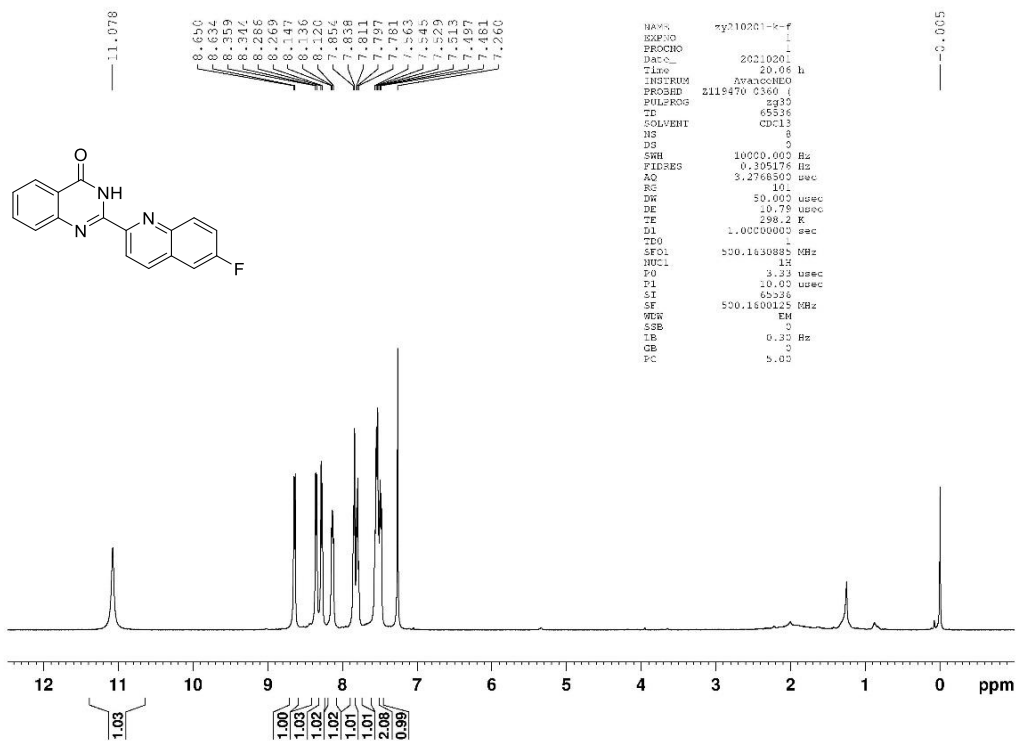
3-propyl-2-(quinolin-2-yl)quinazolin-4(3H)-one (3na):



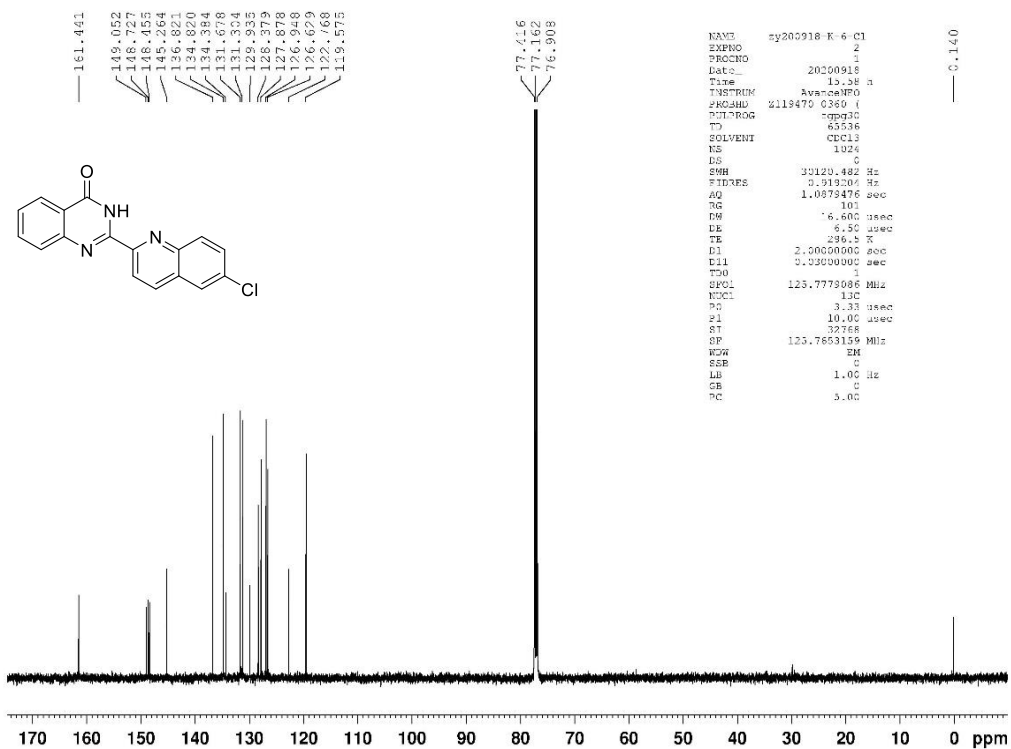
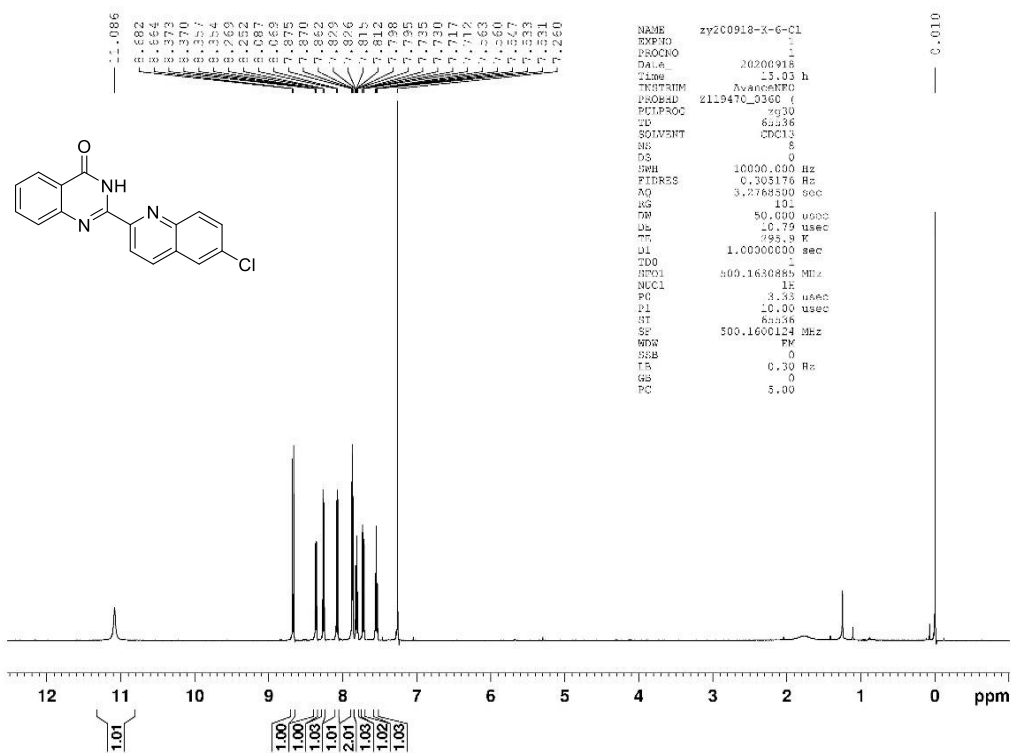
3-isopropyl-2-(quinolin-2-yl)quinazolin-4(3H)-one (30a):



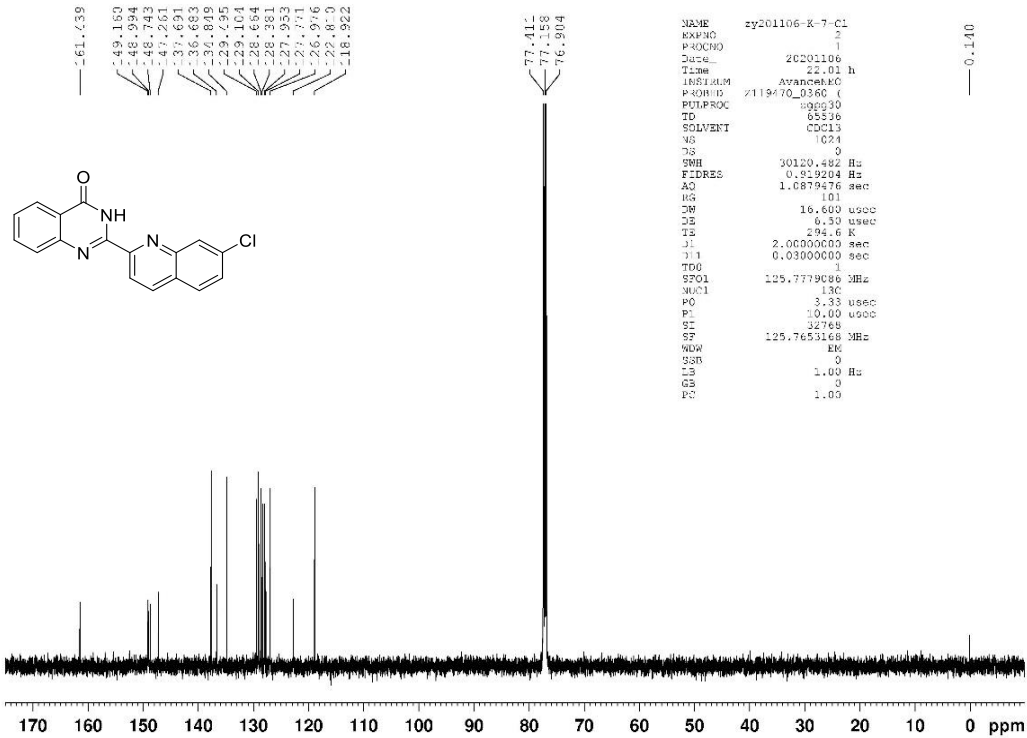
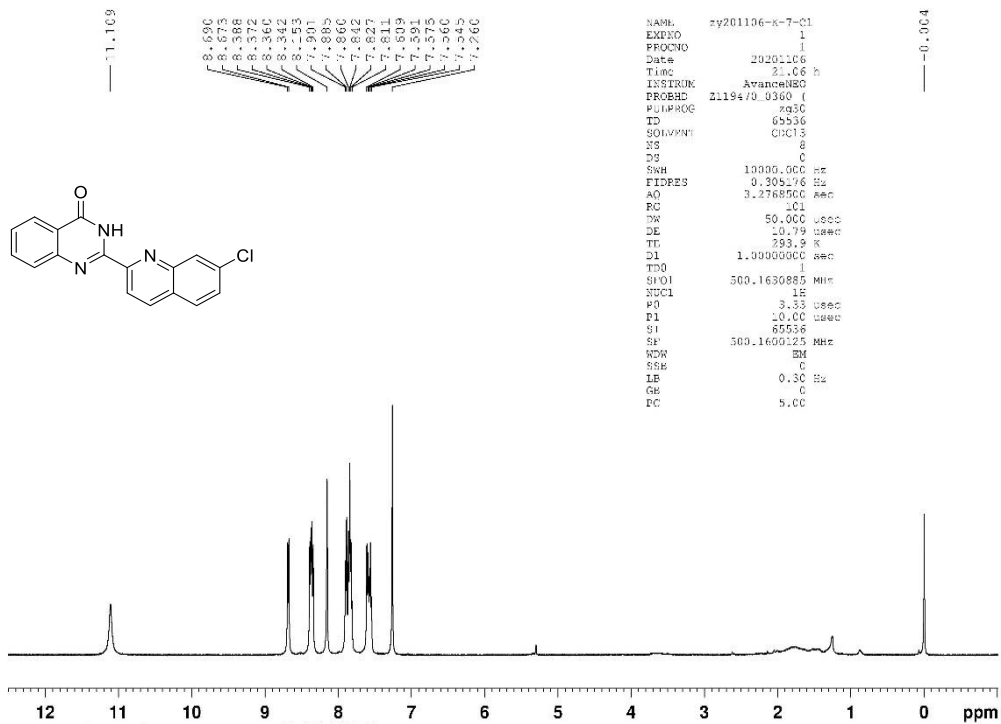
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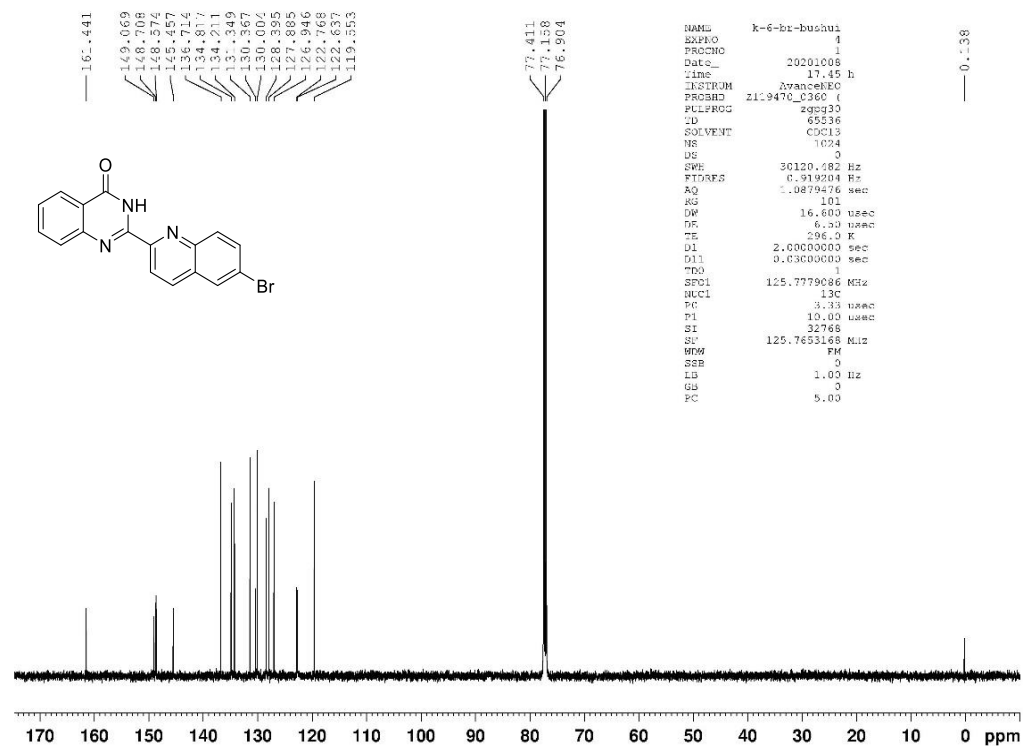
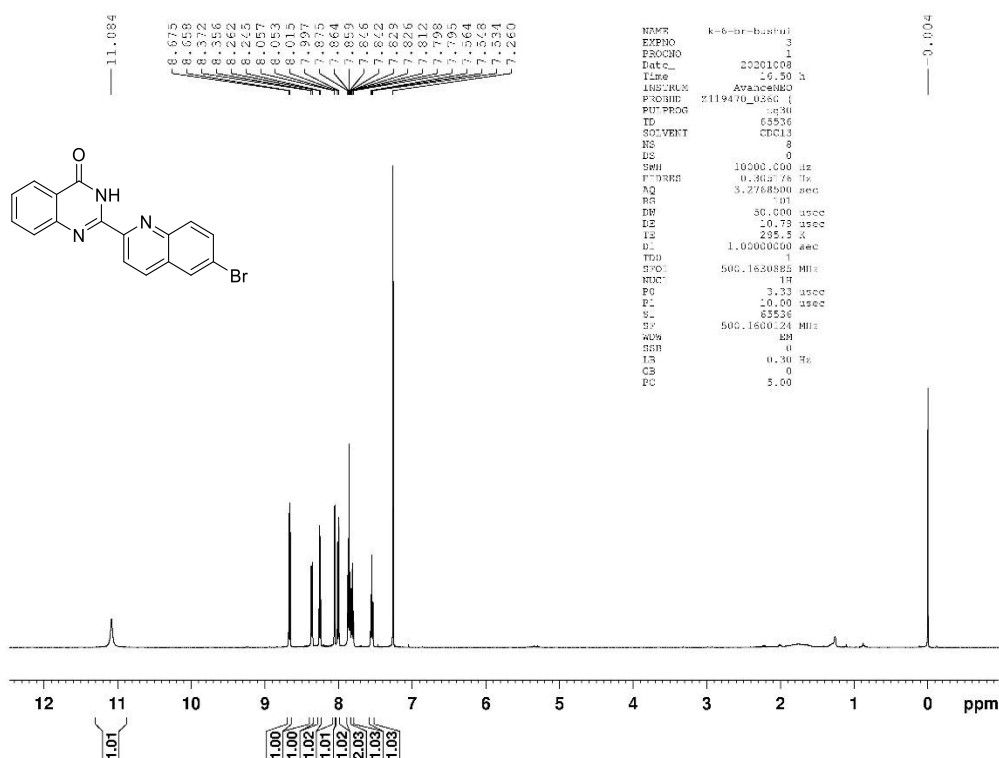
2-(6-chloroquinolin-2-yl)quinazolin-4(3H)-one (3ac):



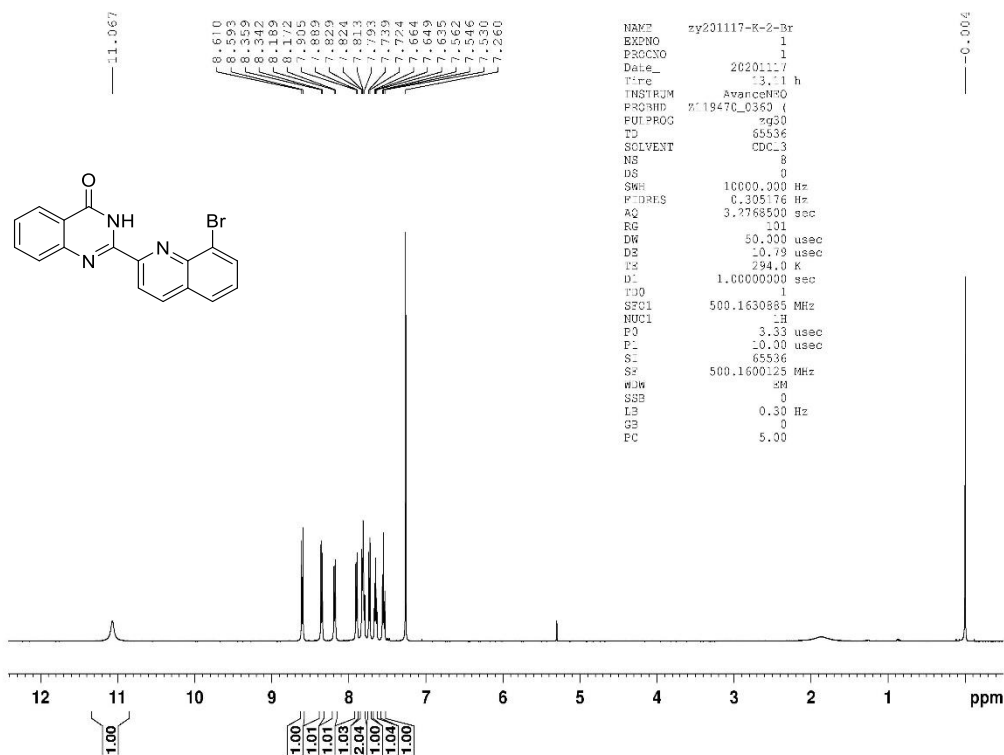
2-(7-chloroquinolin-2-yl)quinazolin-4(3H)-one (3ad):



2-(6-bromoquinolin-2-yl)quinazolin-4(3H)-one (3ae):

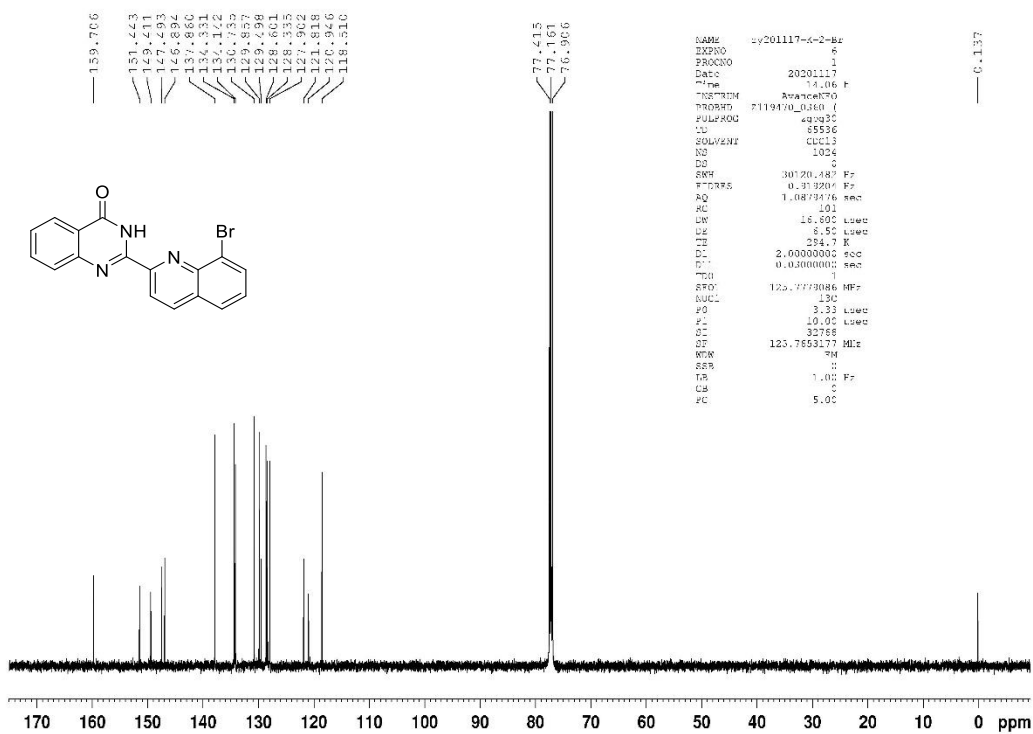


2-(8-bromoquinolin-2-yl)quinazolin-4(3H)-one (3af):



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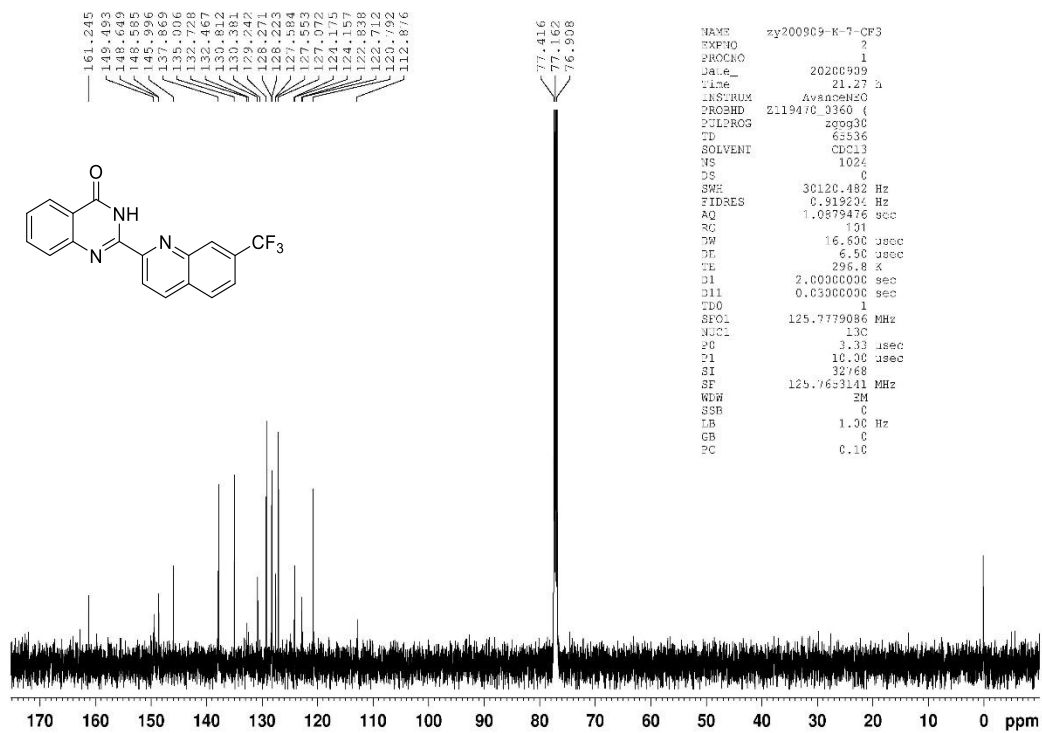
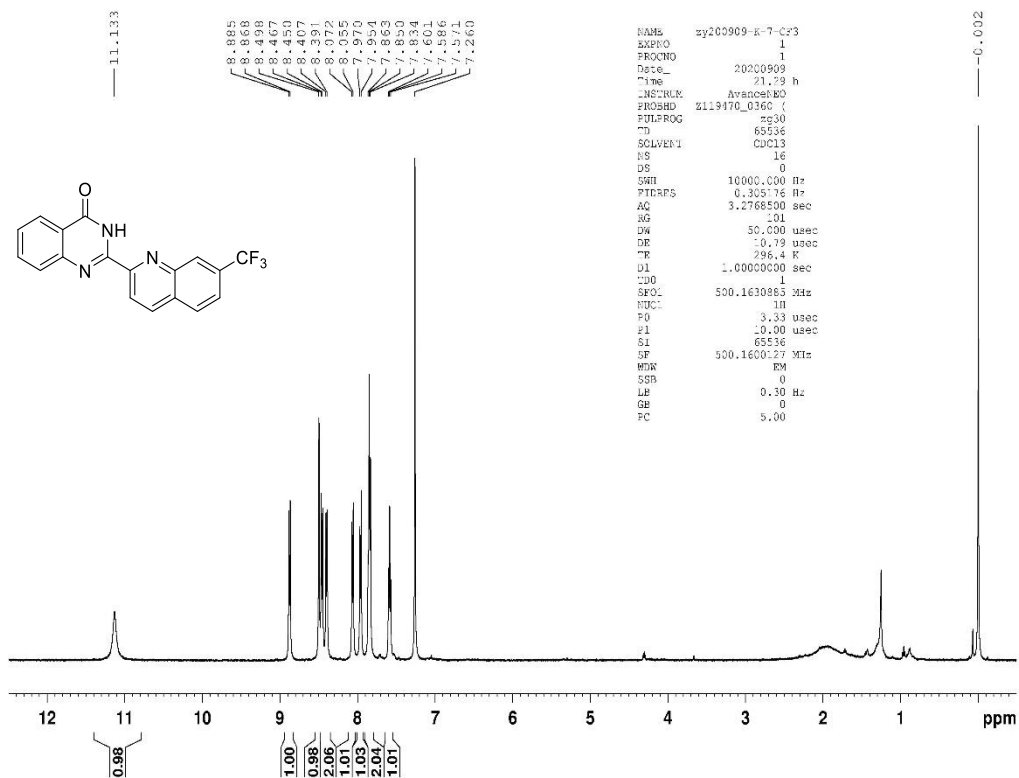
NAME      zy201117-K-2-Br
EXPNO     1
PROCNO    1
Date_     20201117
Time      3.11 h
INSTRUM   Avance600
PROBHD    Z119470_0380 (
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         0
SWH        10000.000 Hz
F2DRFS     0.305176 Hz
AQ         3.2768500 sec
RG         101
DW         50.300 usec
DE         10.79 usec
TE         294.0 K
D1         1.00000000 sec
TJ0        1
SFO1       500.1630885 MHz
NUC1       13
P0         3.33 usec
P1         10.00 usec
S1         65536
S2         500.1600125 MHz
wJH        3M
SES        0
LB         0.30 Hz
GB         0
PC         5.00
    
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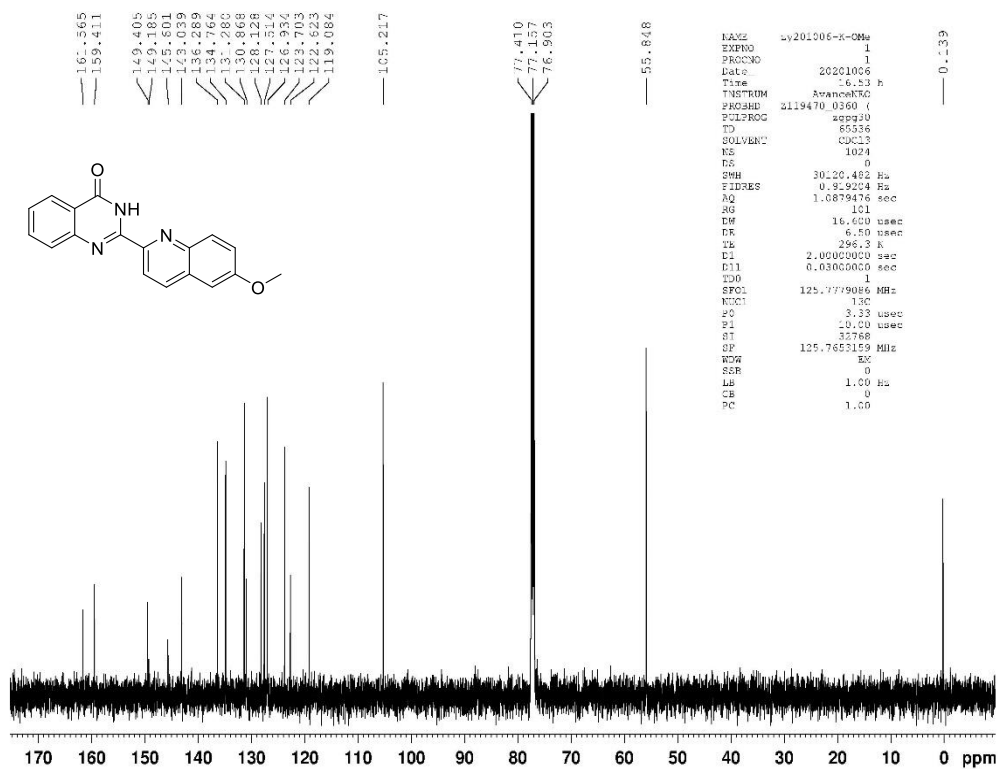
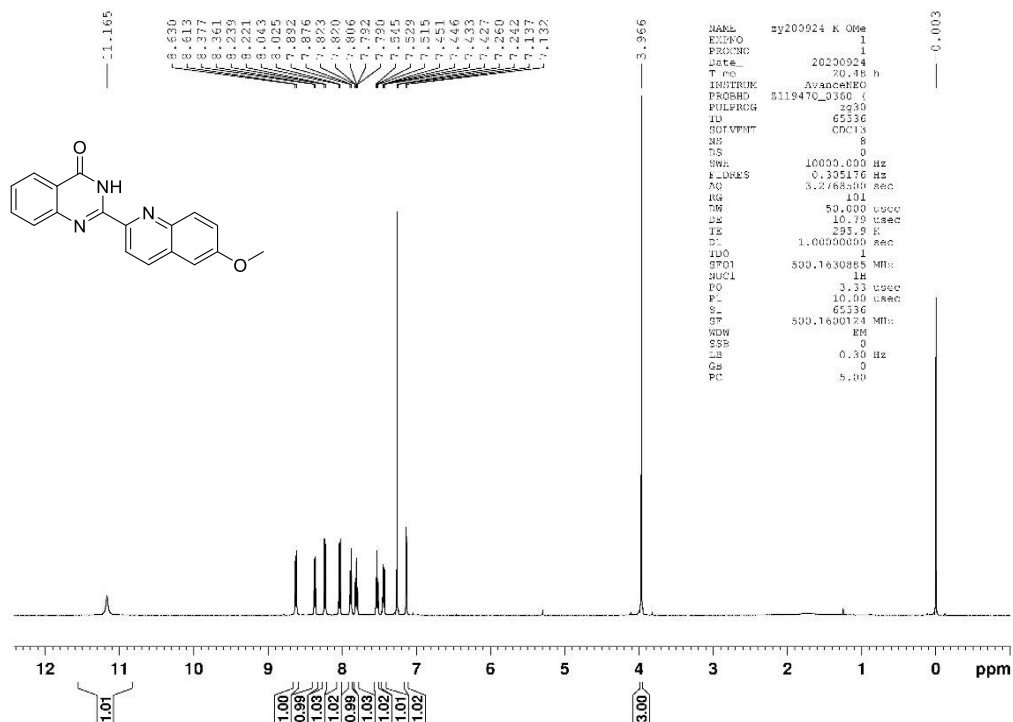
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NAME      zy201117-K-2-Br
EXPNO     5
PROCNO    1
Date_     20201117
Time      14.06 h
INSTRUM   Avance600
PROBHD    Z119470_0380 (
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         0
SWH        30120.487 Hz
F2DRFS     0.313204 Hz
AQ         1.0879746 sec
RG         101
DW         16.600 usec
DE         6.50 usec
TE         294.2 K
D1         2.00000000 sec
TJ0        1
SFO1       125.7773086 MHz
NUC1       13
P0         3.33 usec
P1         10.00 usec
S1         32768
S2         125.7653177 MHz
wJH        3M
SES        0
LB         1.00 Hz
GB         0
PC         5.00
    
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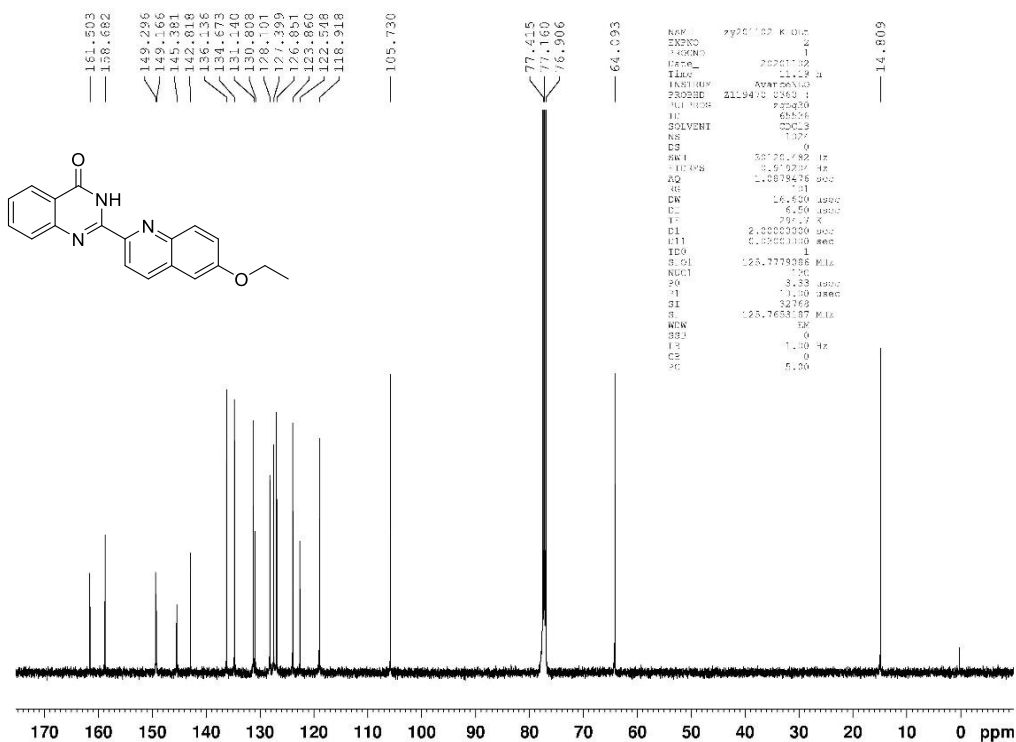
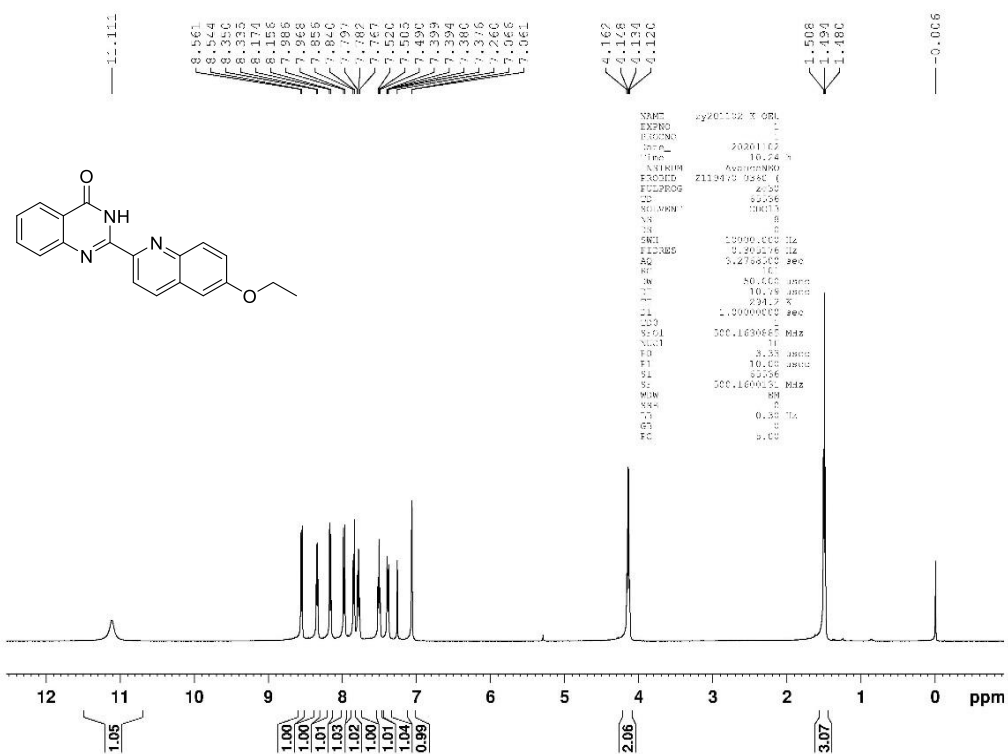
2-(7-(trifluoromethyl)quinolin-2-yl)quinazolin-4(3H)-one (3ag):



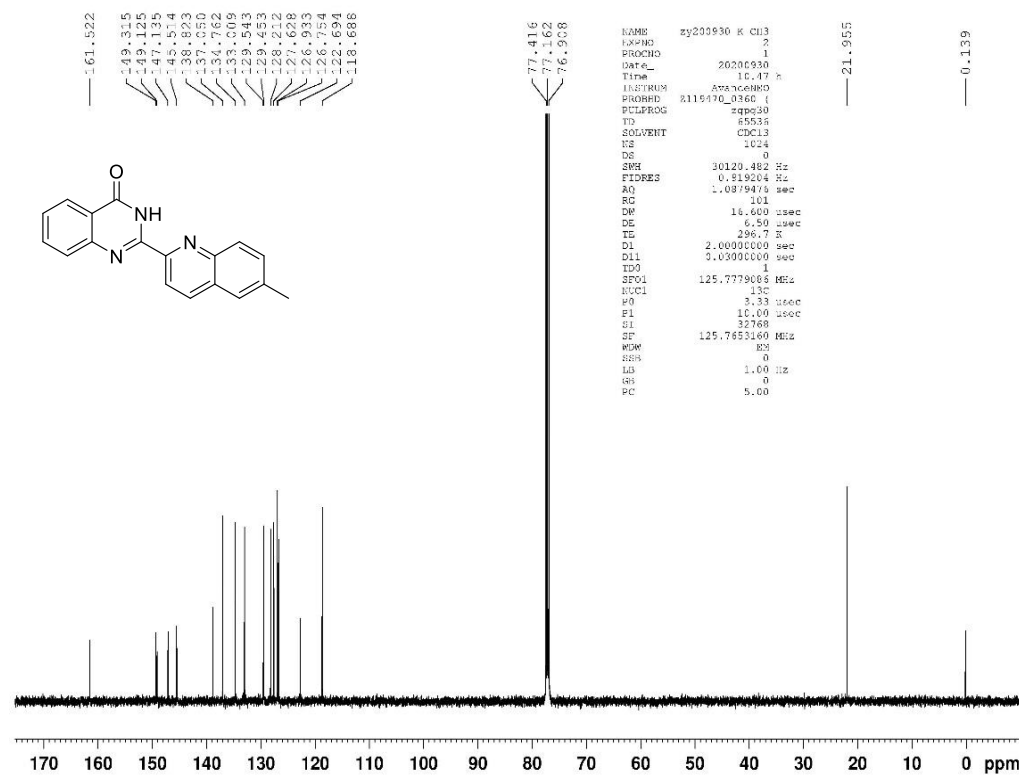
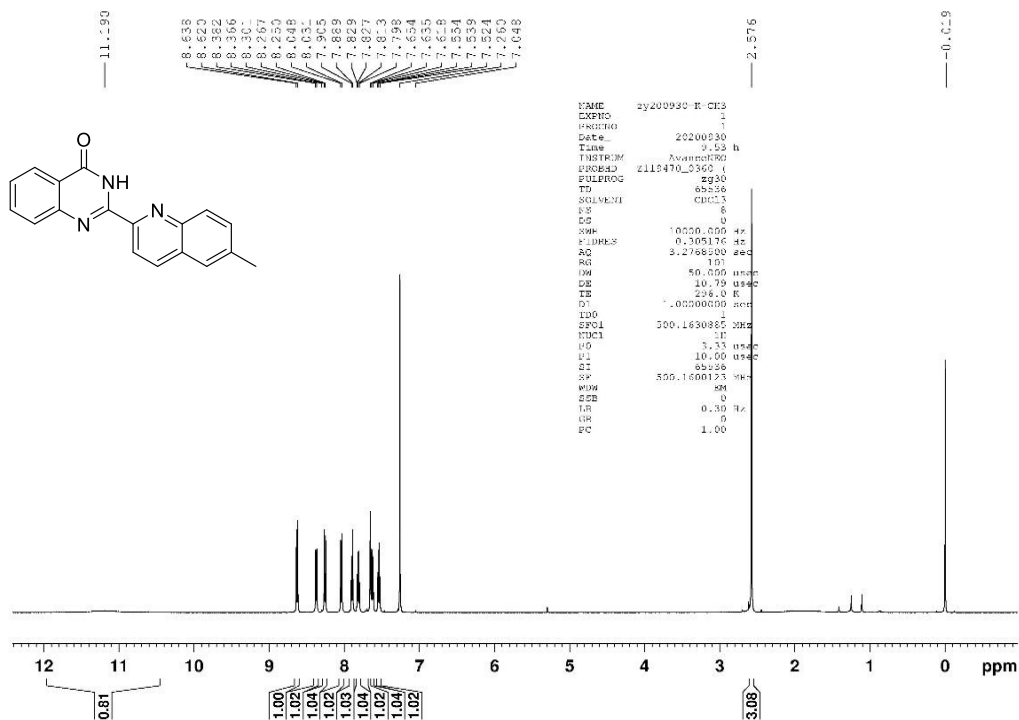
2-(6-methoxyquinolin-2-yl)quinazolin-4(3H)-one (3ah):



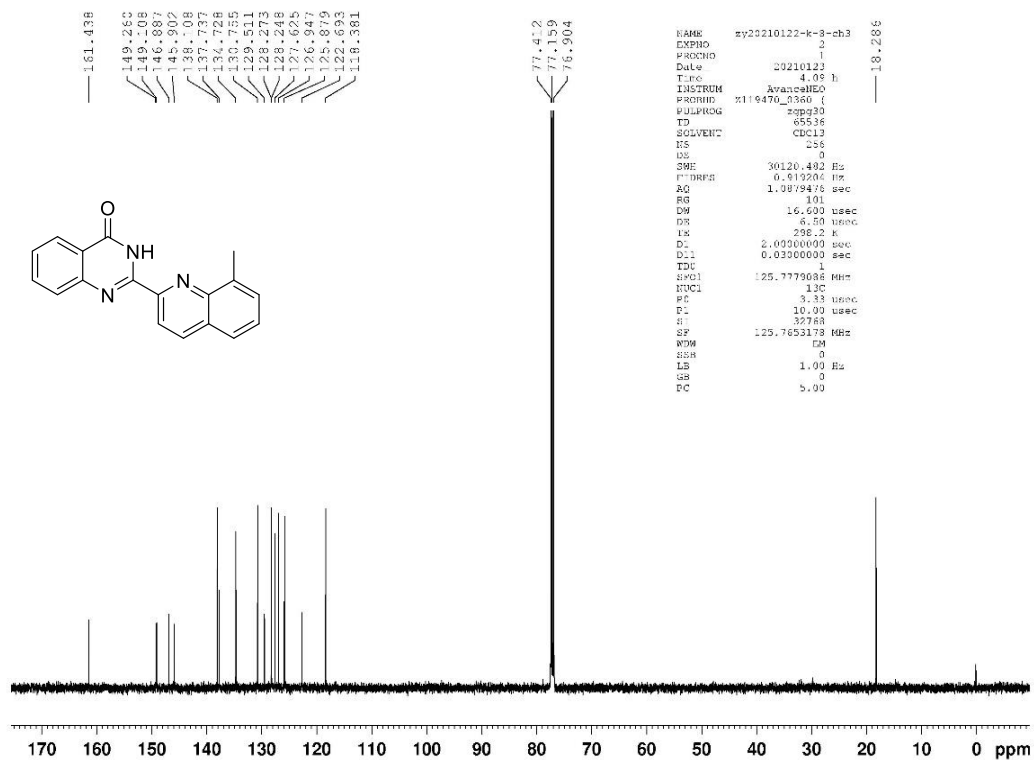
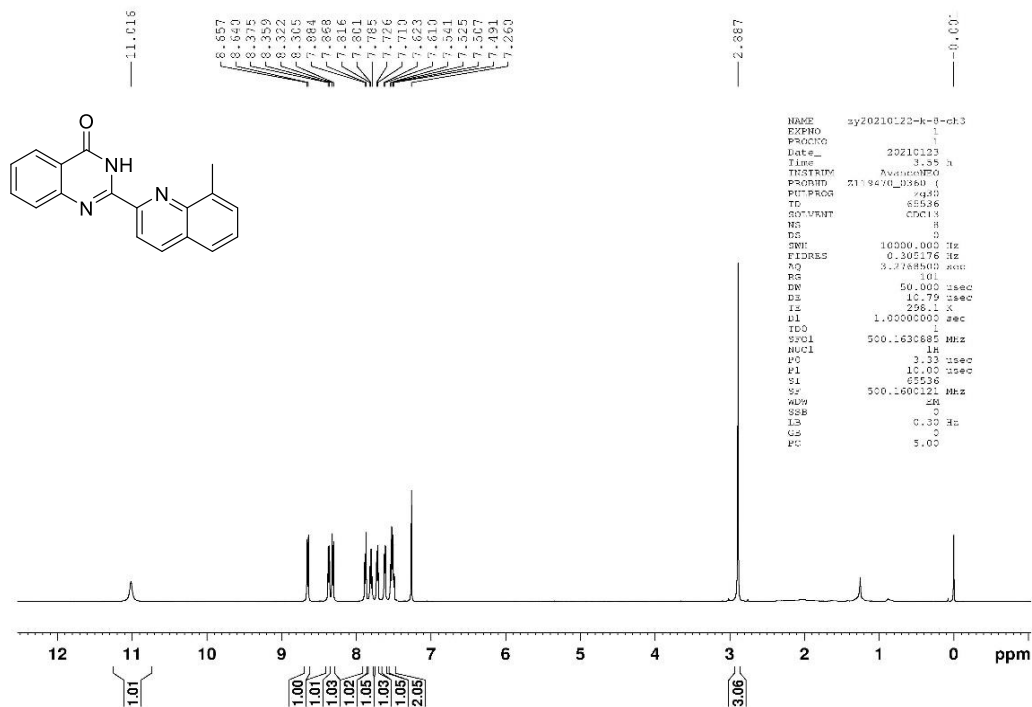
2-(6-ethoxyquinolin-2-yl)quinazolin-4(3H)-one (3ai):



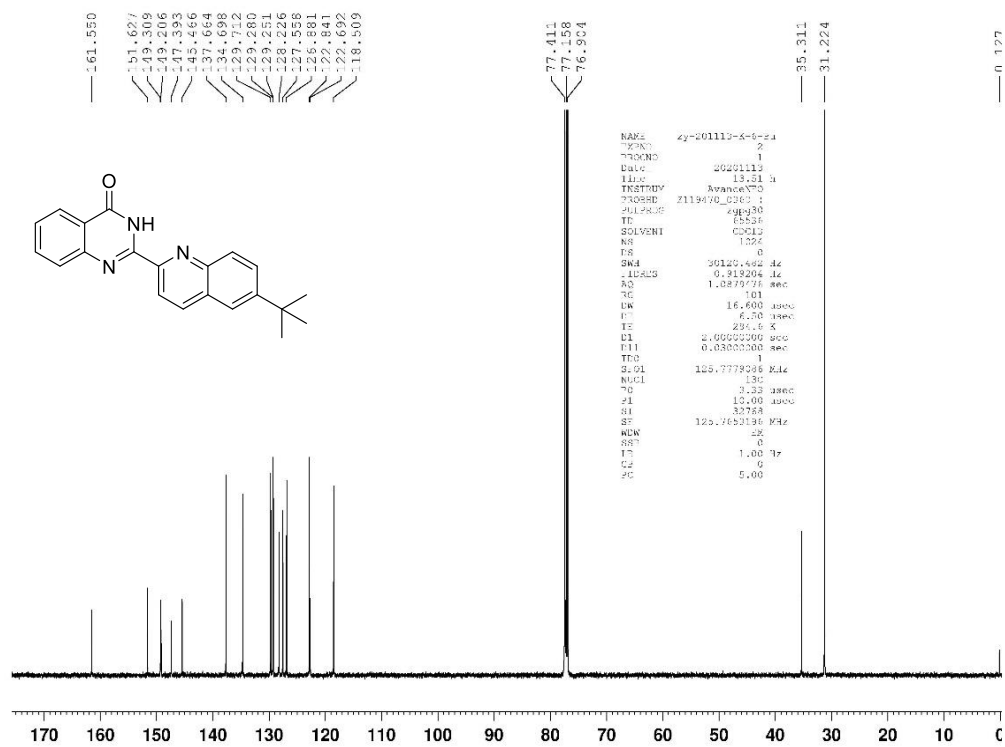
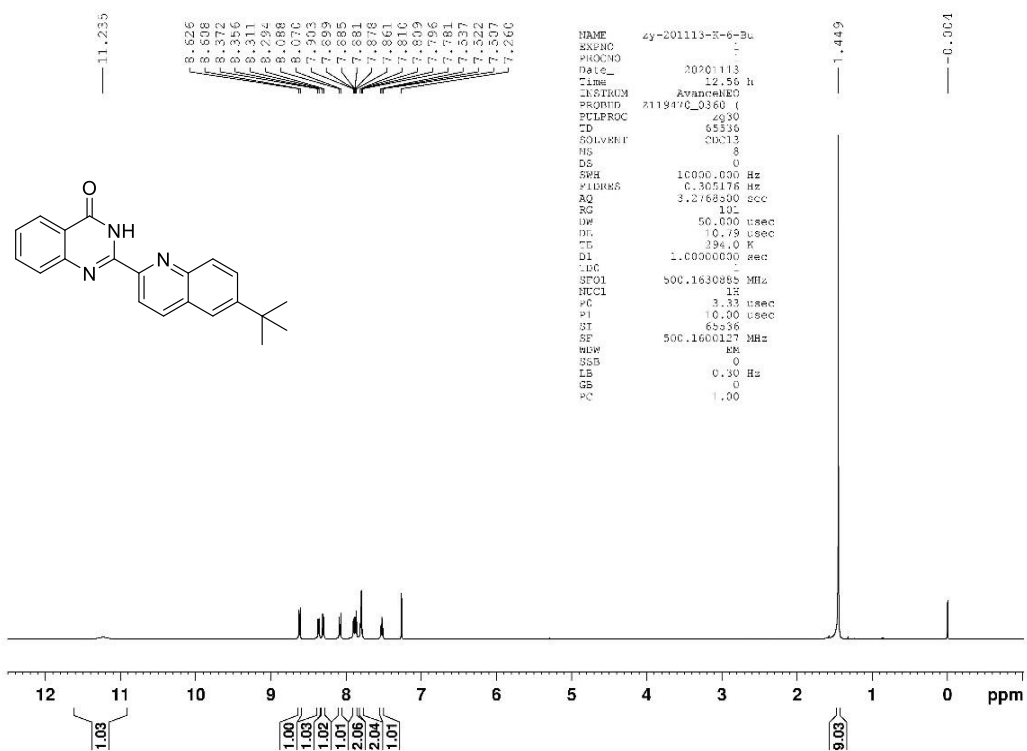
2-(6-methylquinolin-2-yl)quinazolin-4(3H)-one (3aj):



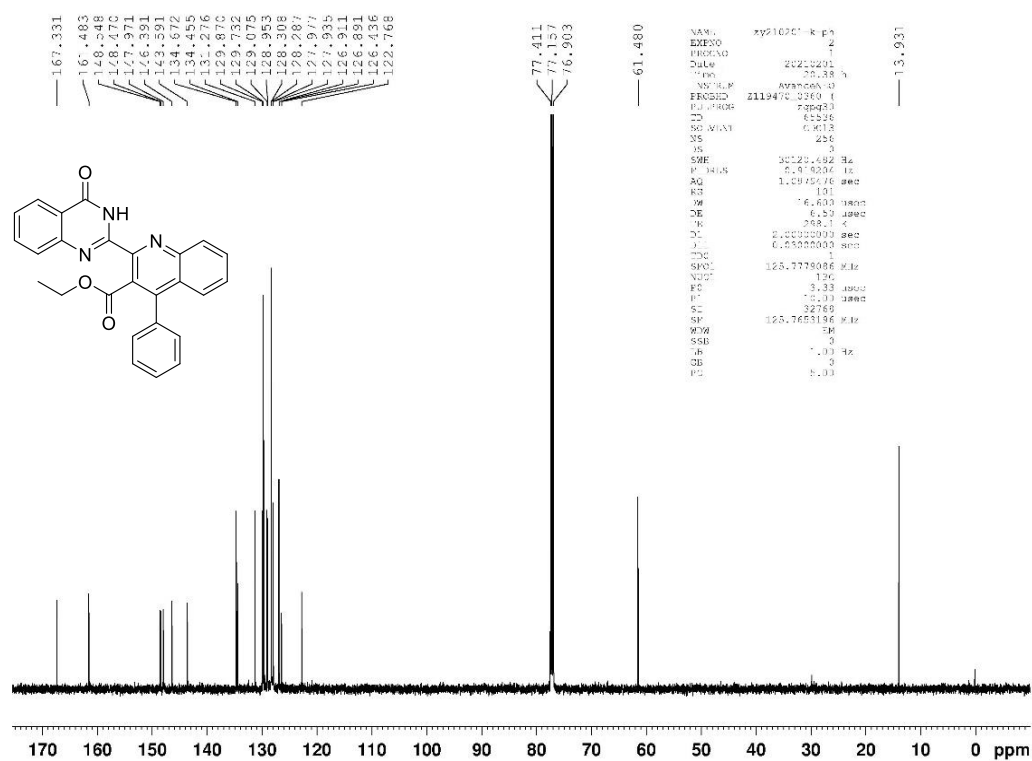
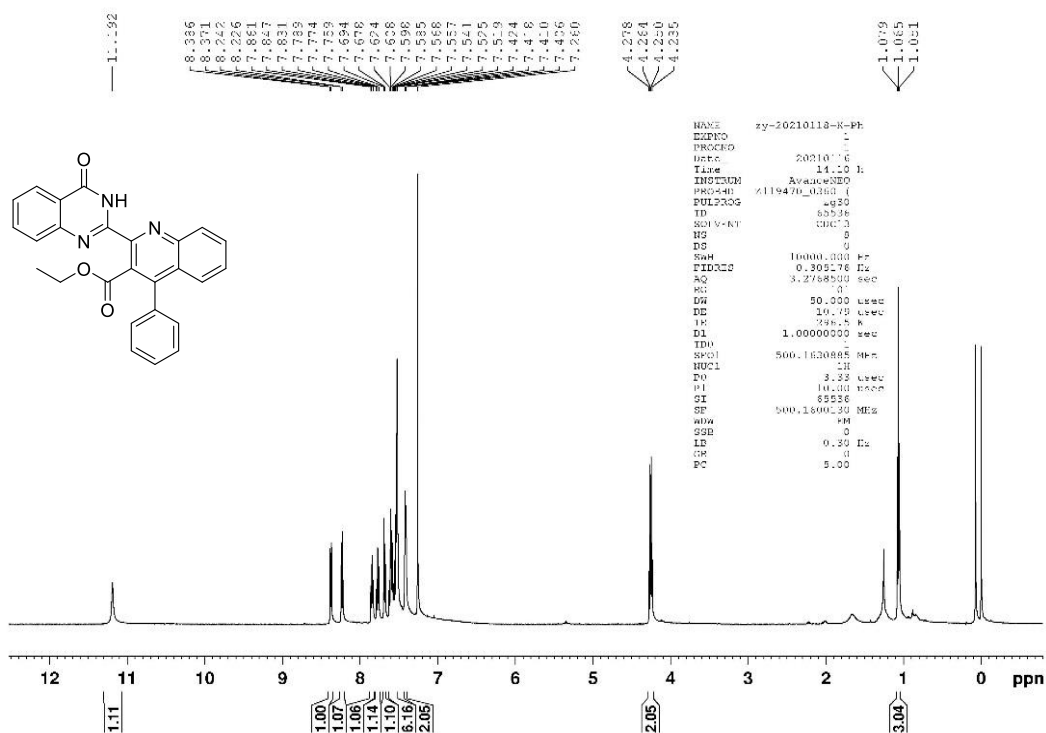
2-(6-methylquinolin-2-yl)quinazolin-4(3H)-one (3aj):



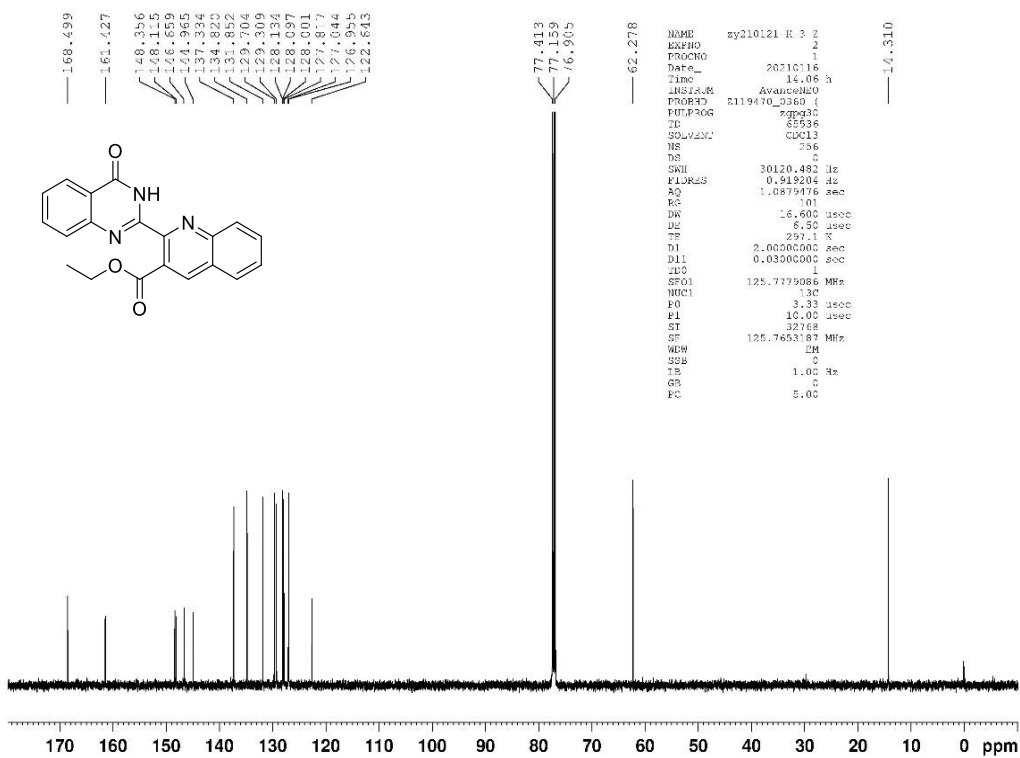
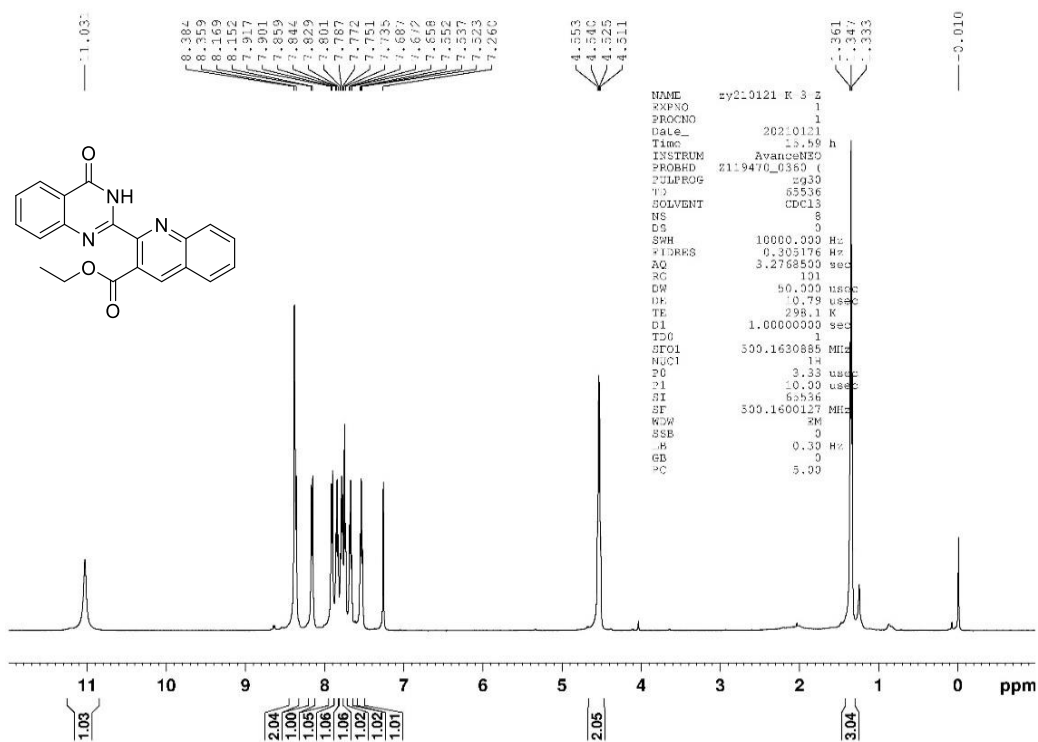
2-(6-(tert-butyl)quinolin-2-yl)quinazolin-4(3H)-one (3al):



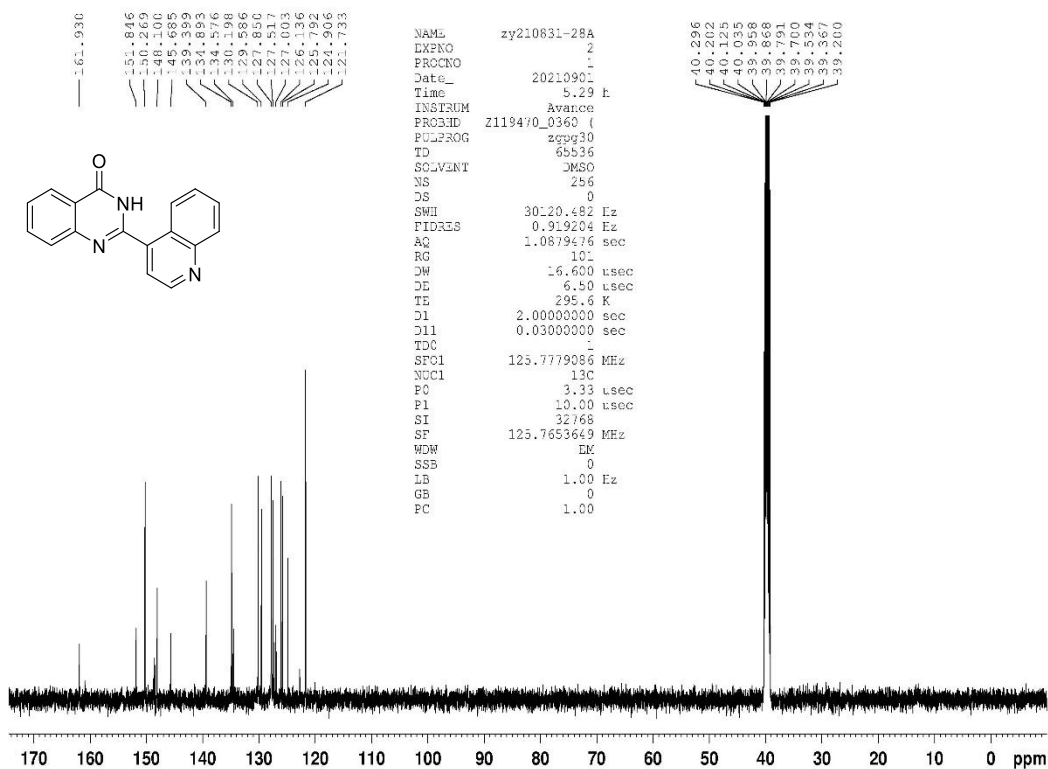
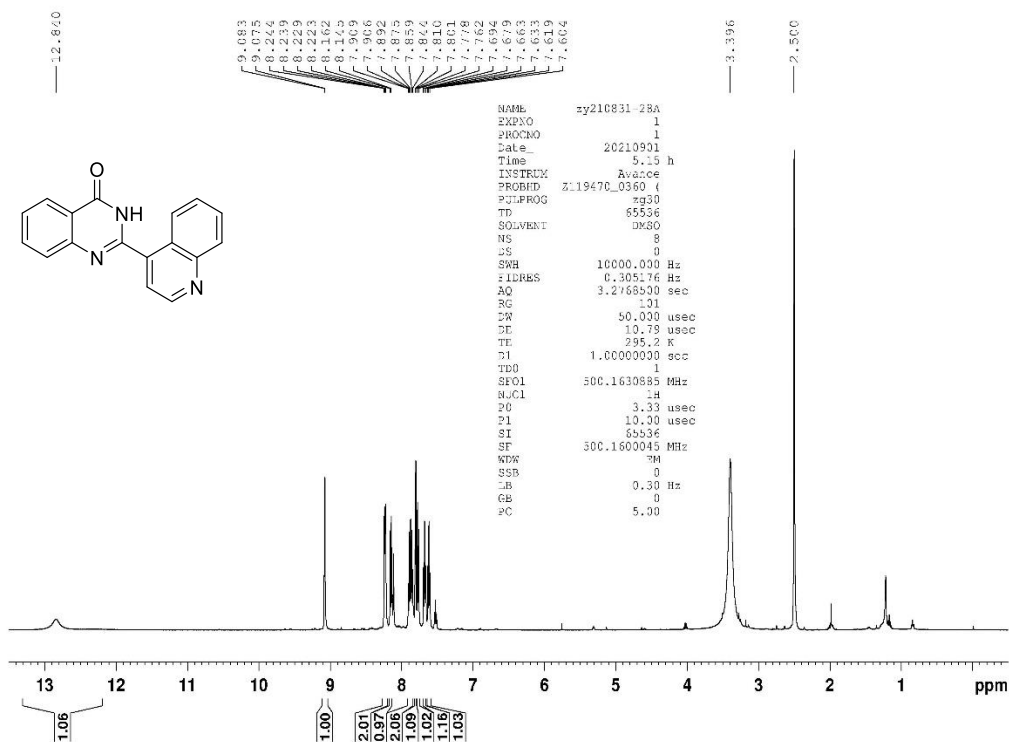
ethyl 2-(4-oxo-3,4-dihydroquinazolin-2-yl)-4-phenylquinoline-3-carboxylate (3an):



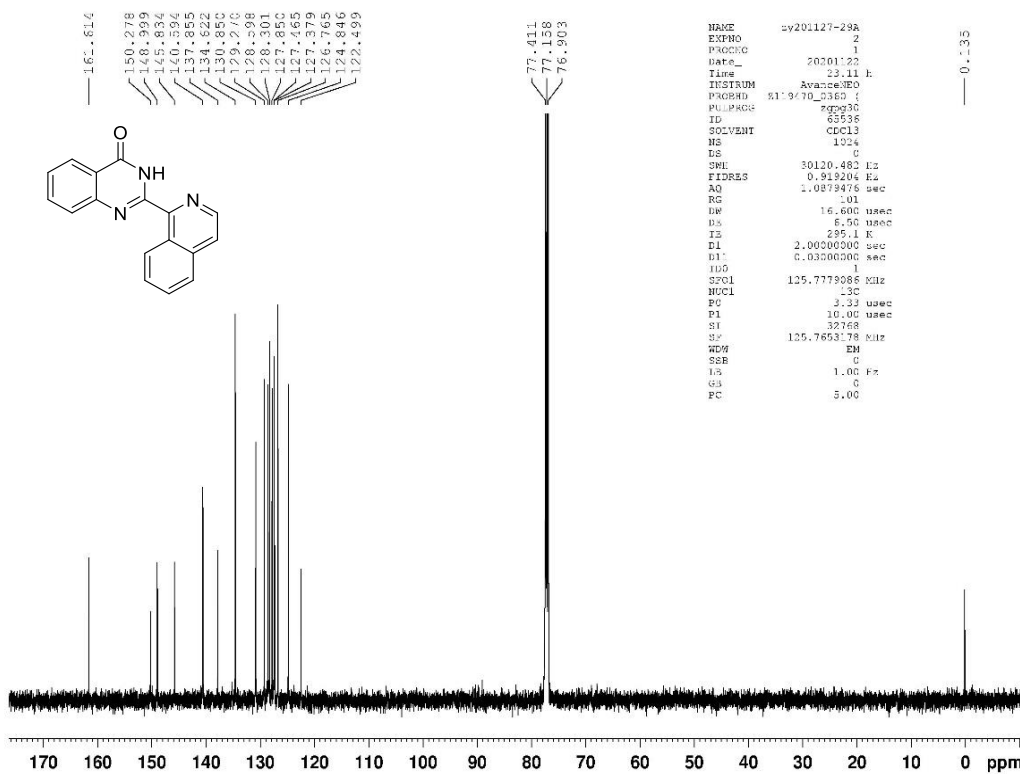
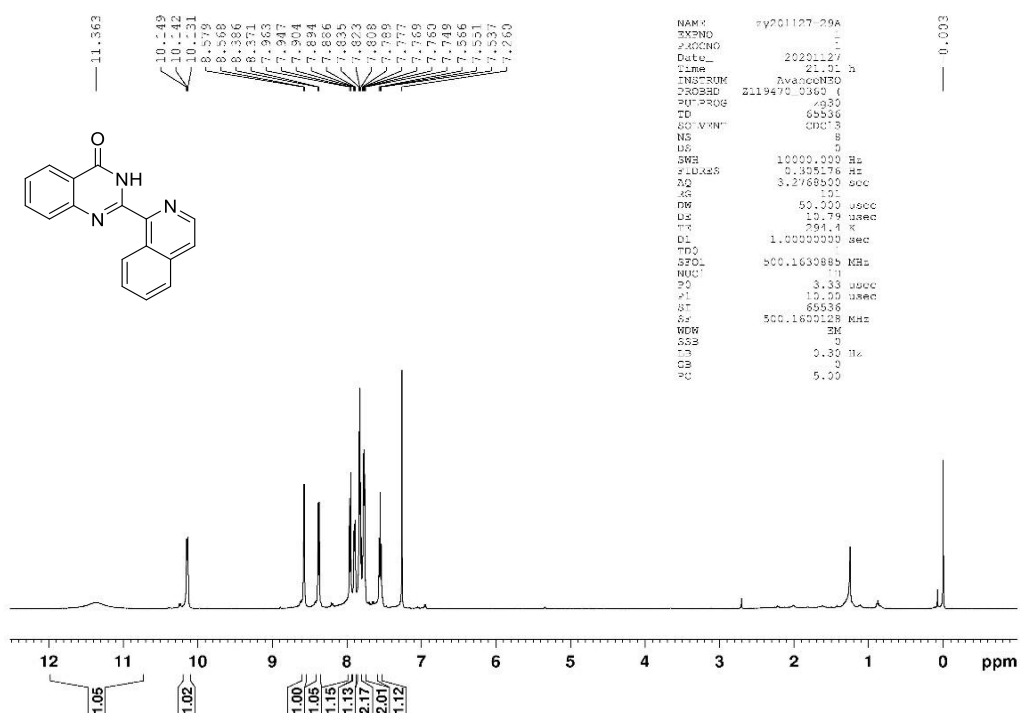
ethyl 2-(4-oxo-3,4-dihydroquinazolin-2-yl)quinoline-3-carboxylate (3ao):



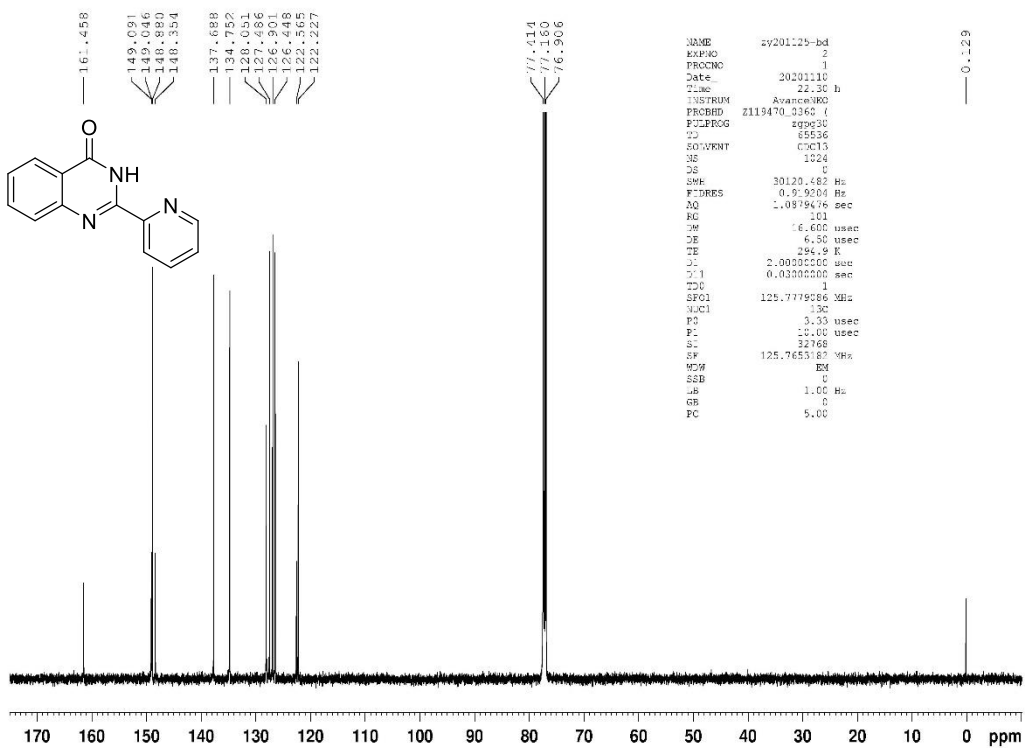
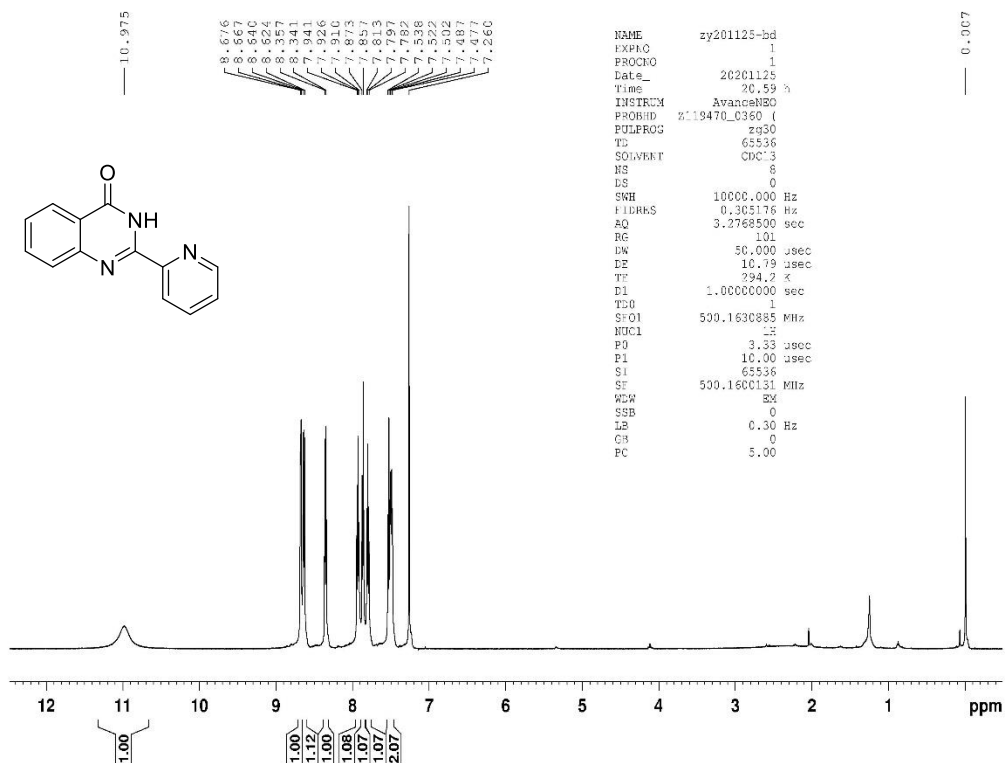
2-(quinolin-4-yl)quinazolin-4(3H)-one (3ap):



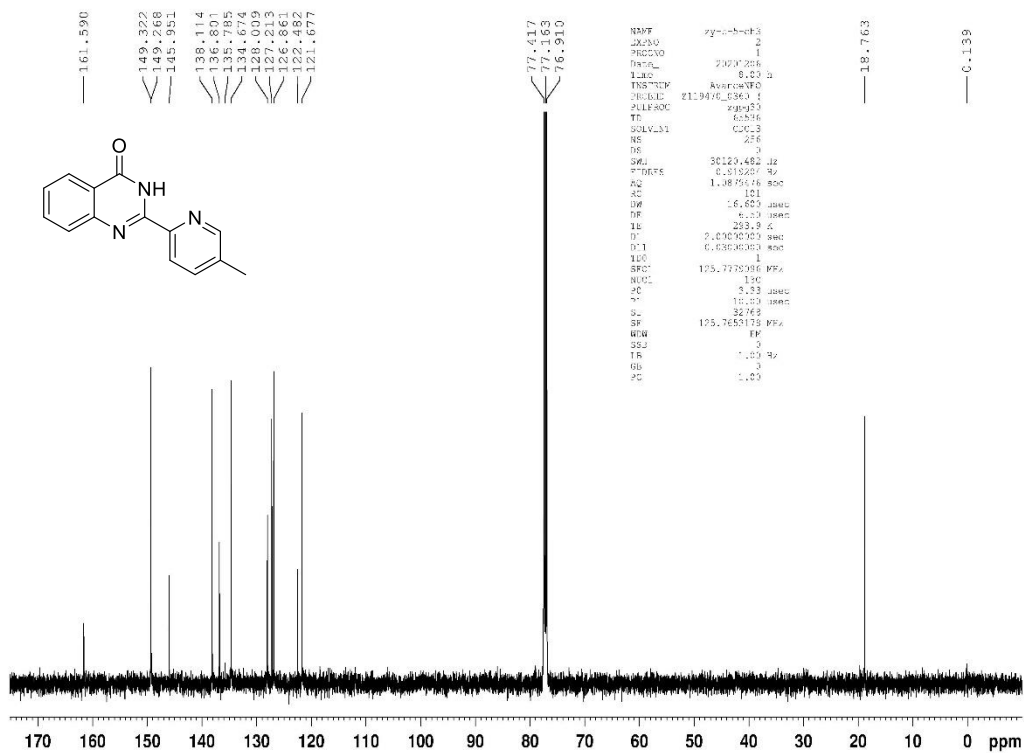
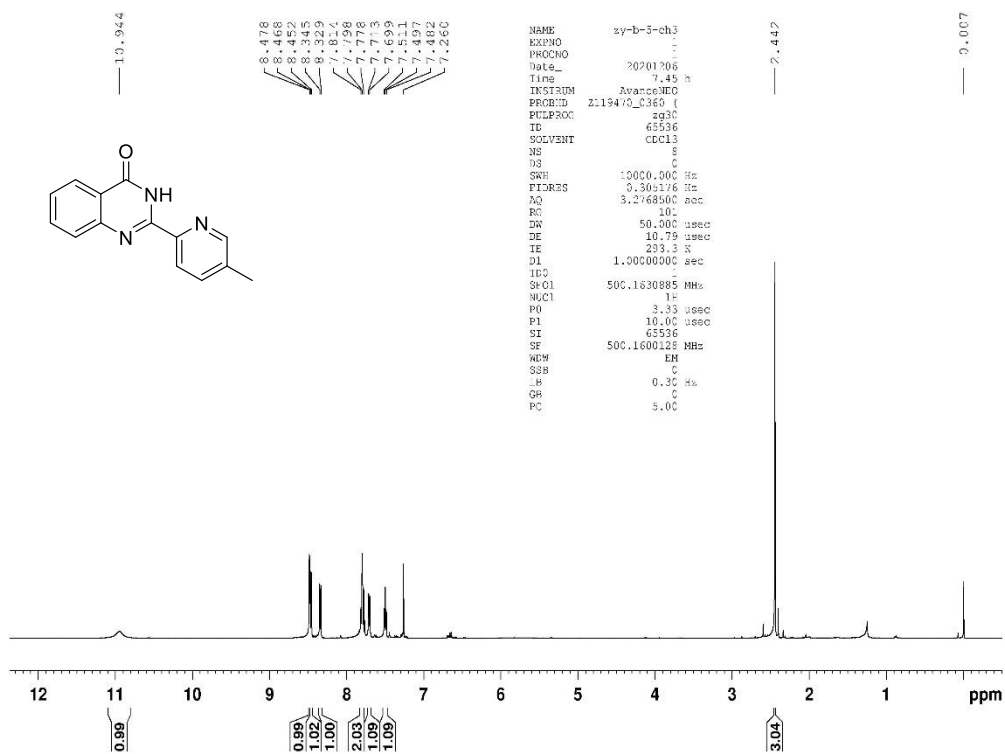
2-(isoquinolin-1-yl)quinazolin-4(3H)-one (3aq):



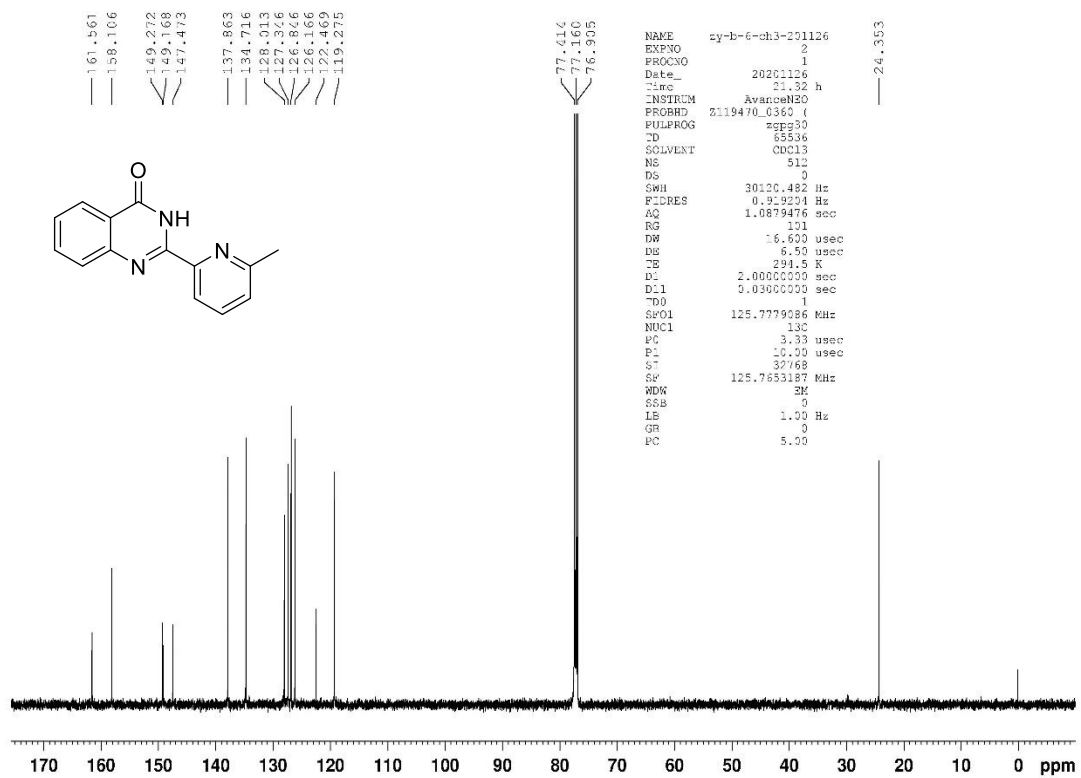
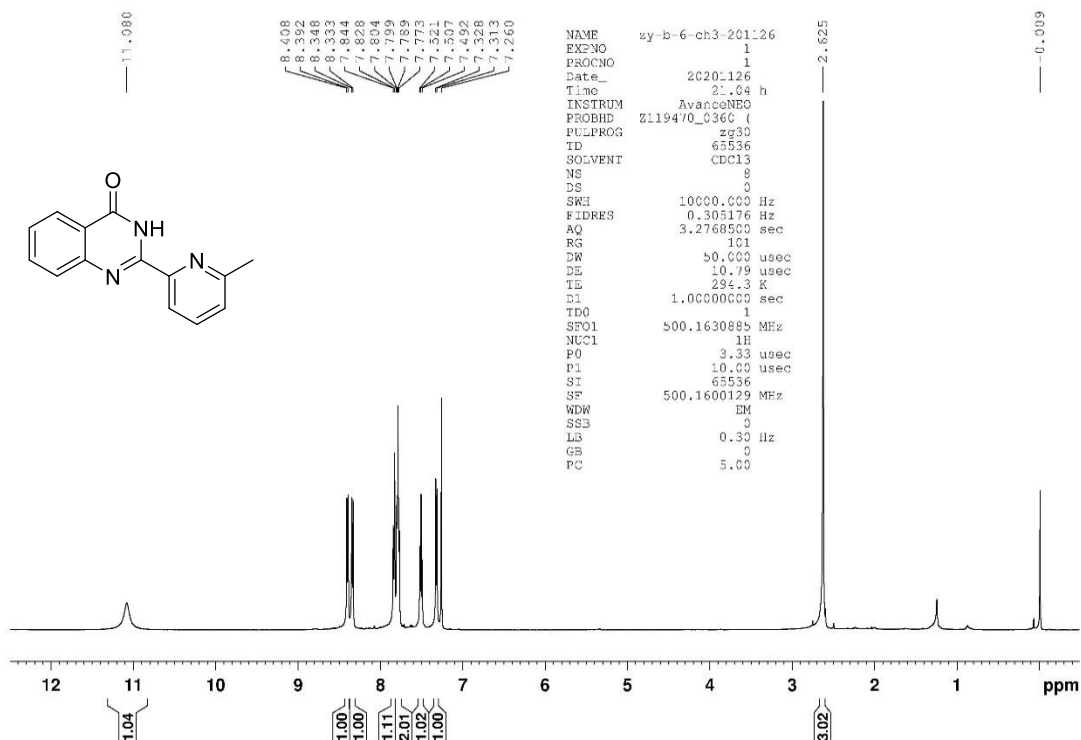
2-(pyridin-2-yl)quinazolin-4(3H)-one (3ar):



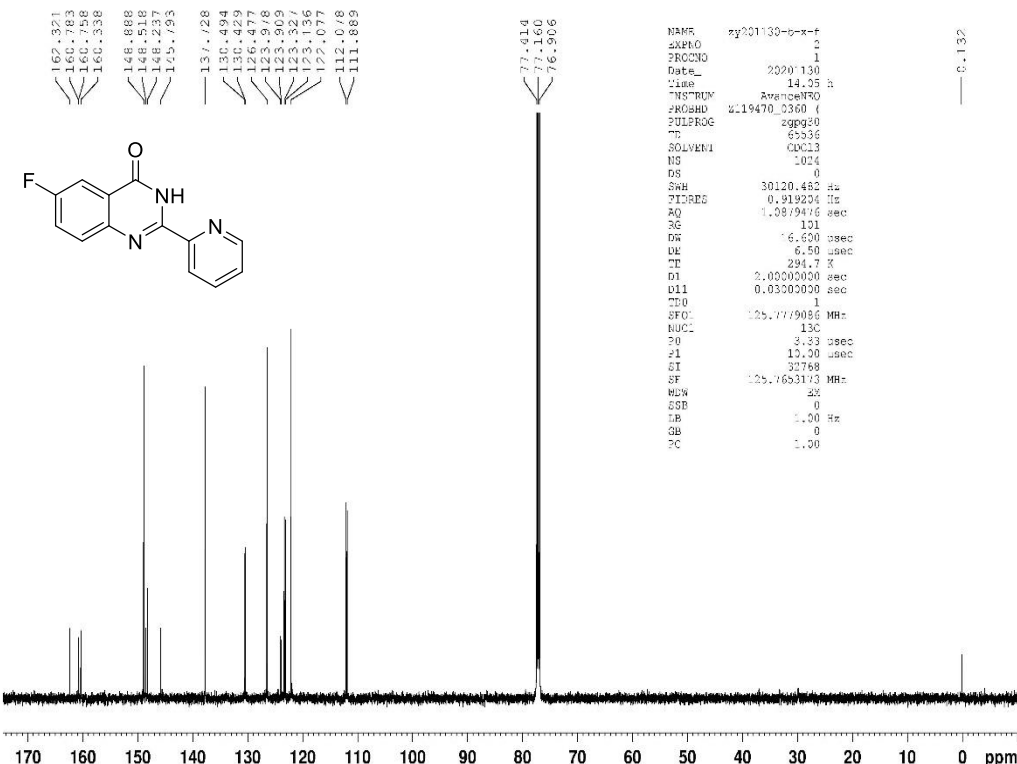
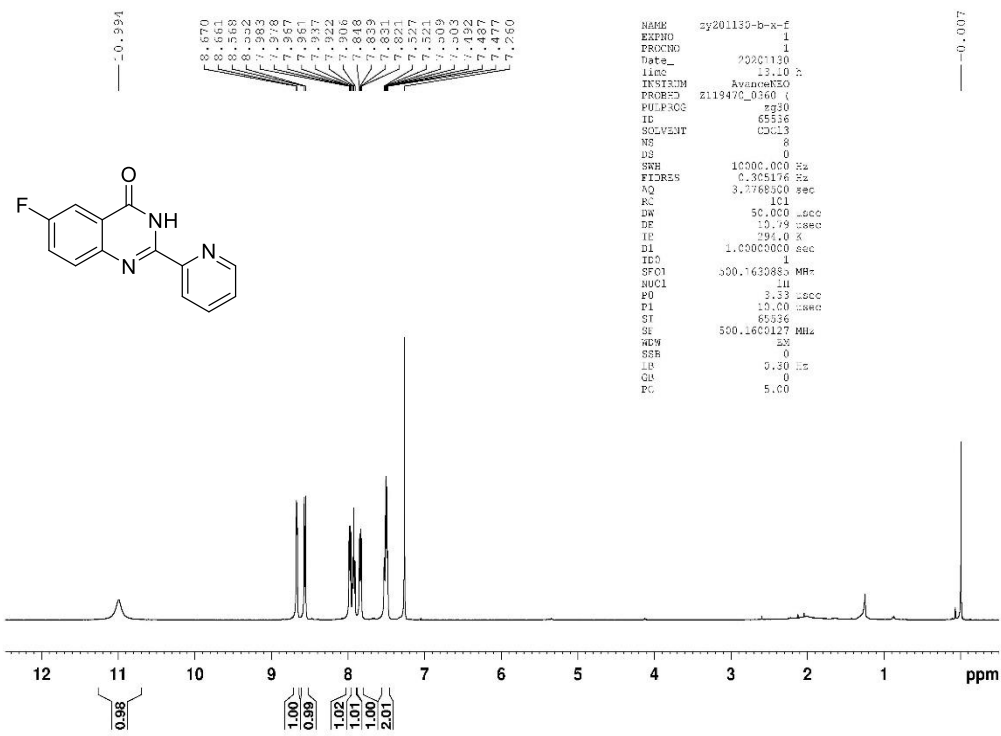
2-(5-methylpyridin-2-yl)quinazolin-4(3H)-one (3as):



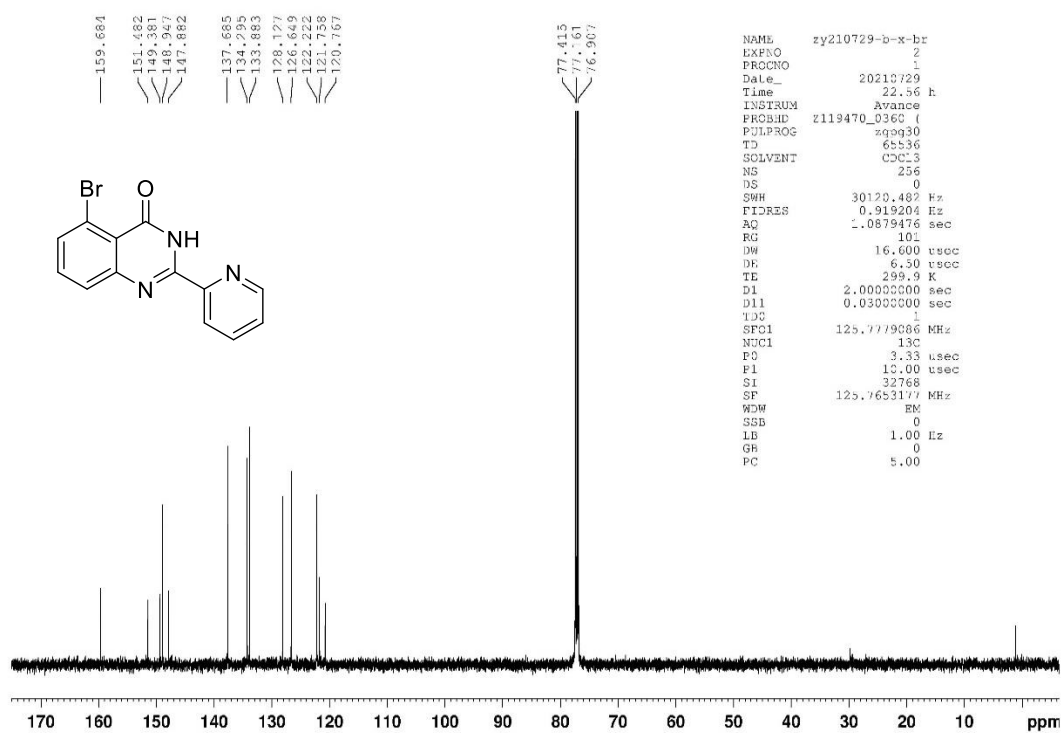
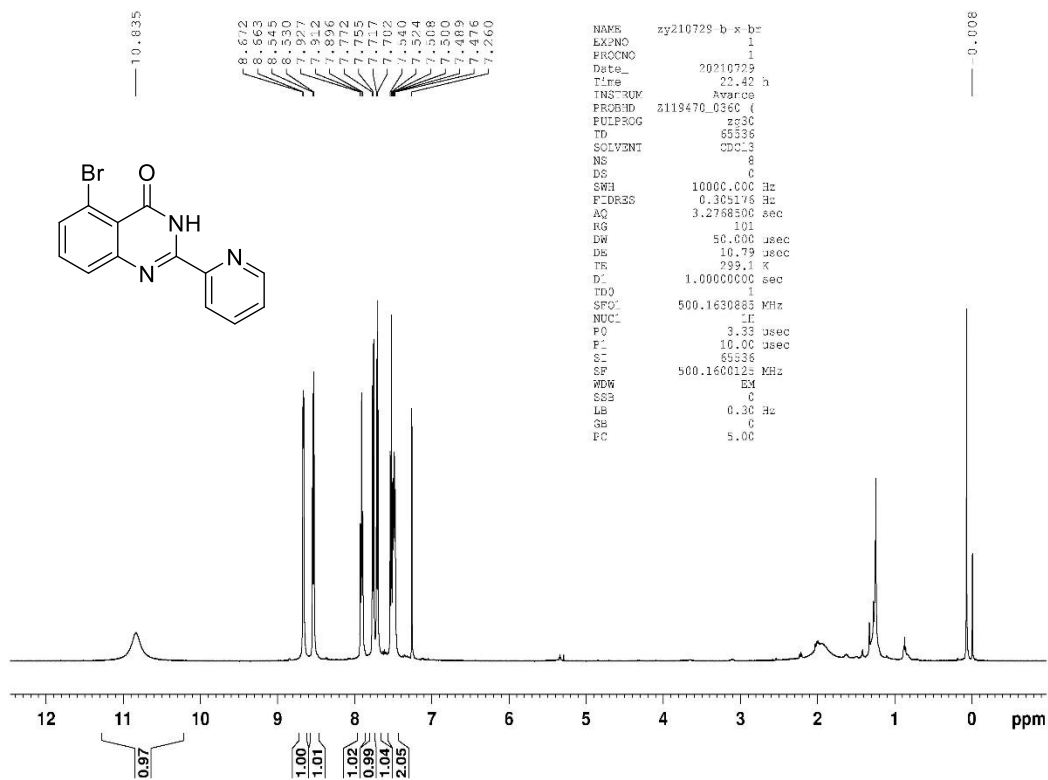
2-(6-methylpyridin-2-yl)quinazolin-4(3H)-one (3at):



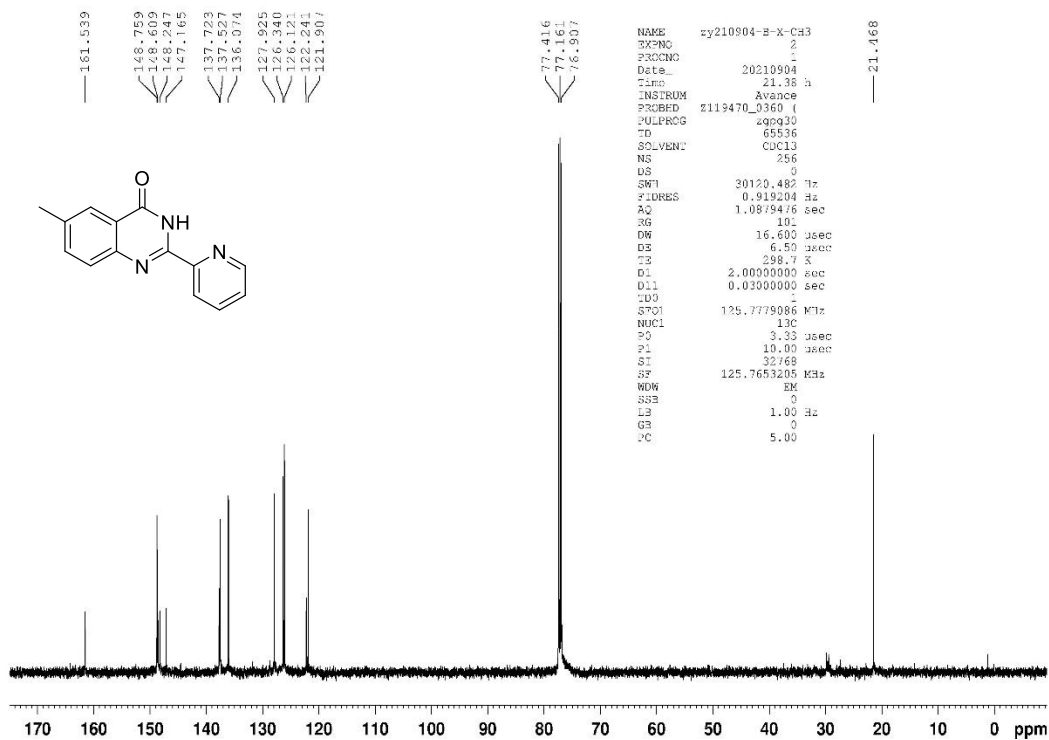
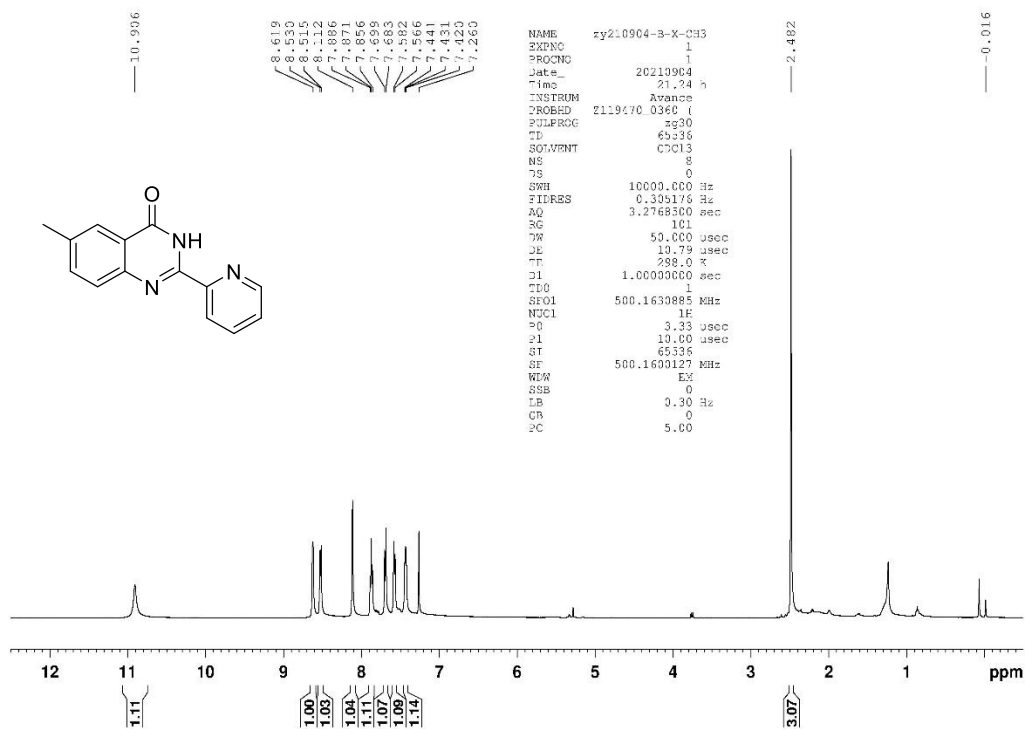
6-fluoro-2-(pyridin-2-yl)quinazolin-4(3H)-one (3br):



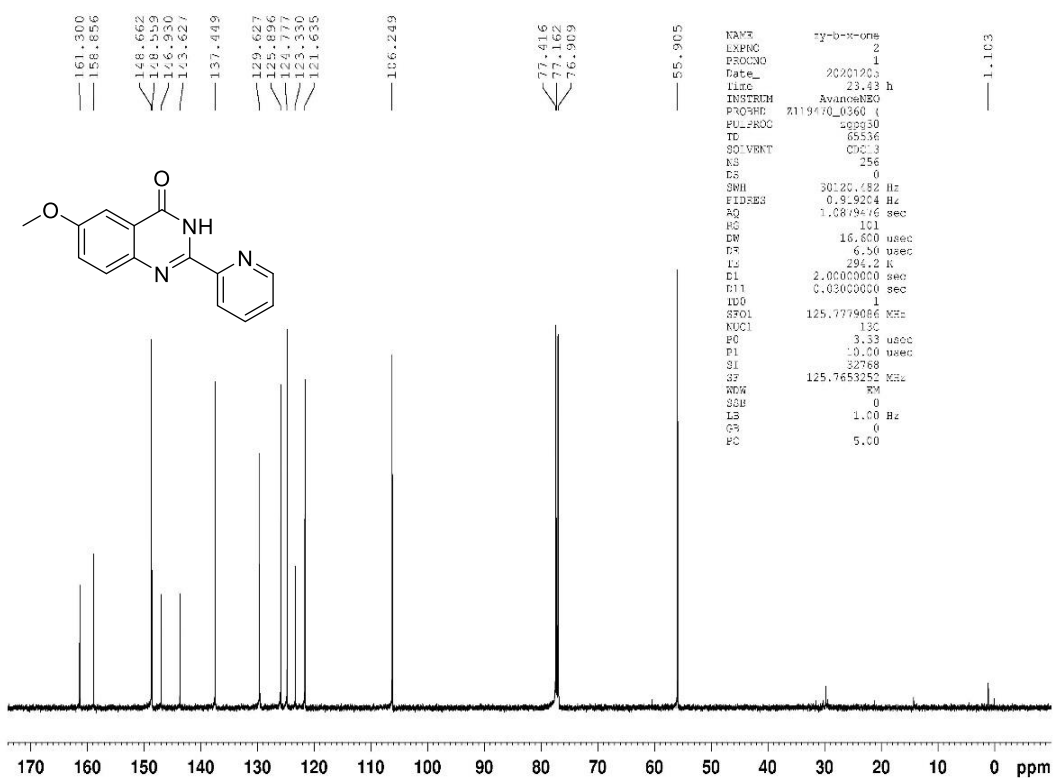
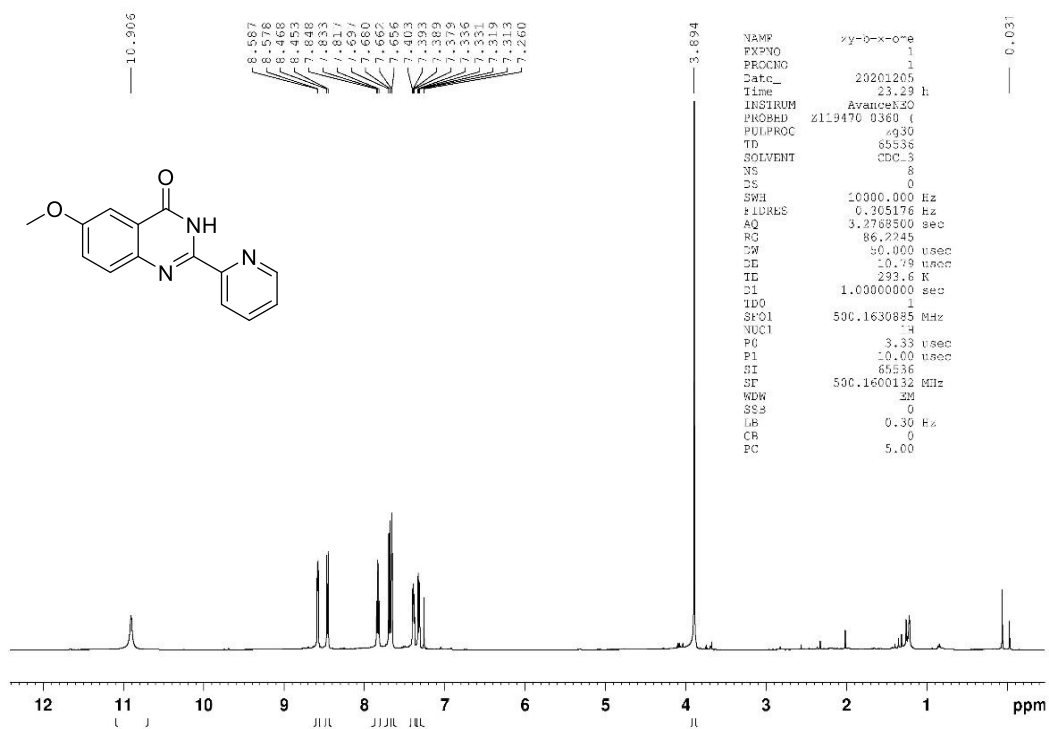
5-bromo-2-(pyridin-2-yl)quinazolin-4(3H)-one (3hr):



6-methyl-2-(pyridin-2-yl)quinazolin-4(3H)-one (3jr):



6-methoxy-2-(pyridin-2-yl)quinazolin-4(3H)-one (3kr):



3-methyl-2-(pyridin-2-yl)quinazolin-4(3H)-one (3mr):

