SUPPORTING INFORMATION

Iodine - Promoted Amide Formation via Oxidative Cleavage of Indoles: Novel Quinazoline-4(3H)-ones and Tryptanthrins Synthesis

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Section S1. *General Information*

Chemicals used in this work: All starting reagents, materials and solvents were obtained commercially from Sigma-Aldrich, Acros, Fisher and were used as received without any further purification unless otherwise noted.

Analytical techniques:

Gas chromatographic (GC) analyses were performed using a Shimadzu GC 2010-Plus equipped with a flame ionization detector (FID) and a SPB-5 column (length = 30 m, inner diameter = 0.25 mm, and film thickness = 0.25 μm). The temperature program for GC analysis heated samples at 100 ^{o}C and held for 1 min, then heated them from 100 ^{o}C to 280 ^{o}C at 40 ^{o}C/min. Finally, the samples were heated up to 280 ^{o}C and were hold for 4.5 min. Diphenyl ether was used as an internal standard to calculate reaction yields.

GC-MS analyses were analyzed on a Shimadzu GCMS-QP2010Ultra with a ZB-5MS column (length = 30 m, inner diameter = 0.25 mm, and film thickness = 0.25 μm). The temperature program for GC-MS analysis held samples at 100 ^{o}C for 2 min; heated samples from 100 to 280 ^{o}C at 4.5 ^{o}C/min and held them at 280 ^{o}C for 10 min. Inlet temperature was set constant at 280 ^{o}C. MS spectra were compared with the spectra gathered in the NIST library.

Analytical thin layer chromatography (TLC) was purchased from Merck KGaA (silica gel 60 F254). Visualization of the chromatogram was performed by UV light (254 nm or 365 nm) or Dragendorff's stain.

Column chromatography was carried out using silica gel (230 - 400 mesh) purchased from Himedia, India.

^{1}H and ^{13}C-NMR spectra were recorded on a Bruker AV 500 MHz spectrometer operating at 500 MHz for ^{1}H and 125 MHz for ^{13}C respectively. NMR chemical shifts (δ) were reported in ppm relative to tetramethylsilane (TMS) with the residual solvent as internal reference. Data was reported as follows: chemical shift, multiplicity (*s* = singlet, *d* = doublet, *t* = triplet, *q* = quartet, *m* = multiplet), coupling constants (Hz) and integration.

Single crystals suitable for X-ray analysis were obtained by re-crystallization from methanol. The single crystal data for a colorless plate-shaped crystal (0.25 × 0.25 × 0.012 mm^{3}) was collected on a Bruker D8 QUEST diffractometer at 100 K with Mo Kα radiation (λ = 0.71076 Å) using a TRIUMP monochromator, operated at 50 kV and 30.0 mA. The raw data was processed with the Bruker APEX3 software package[1] and then integrated with the Bruker SAINT package[2] using a

narrow-frame algorithm – corrected for absorption using the SADABS procedure.[3] The structures were solved by intrinsic phasing methods. The refinement was performed by full-matrix least squares on F^2 (SHELXL-2014)[4] using the Olex2 software package.[5]

Electron paramagnetic resonance (EPR) measurements were performed on a Bruker EMX-Micro-EPR spectrometer, with a continuous wave X-band. EPR spectra were recorded at room temperature. Typical spectrometer parameters are scan range, 150 G; field set, 3360 G; time constant, 0.03s; scan time, 60s; modulation amplitude 2.0 G; modulation frequency 100 kHz; and microwave power, 0.998 mW. Platforms MatLab (R2018b) and EPR simulator (Isotropic EPR spectra X-band, 9.5 GHz) were employed for simulations.

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Section S2. *Reaction Conditions*

Procedure for synthesis of 2-phenylquinazolin-4(3*H*)-one

In a typical procedure, 2-phenylindole (28.8 mg, 0.15 mmol), K_2CO_3 (41.5 mg, 0.3 mmol) and ammonium hydrocarbonate (17.8 mg, 0.225 mmol) as nitrogen donor were put in an orderly fashion into an 8 mL screw-capped vial, which was subsequently filled with ethyl acetate (2 mL) before adding iodine (45.7 mg, 0.18 mmol). The vial was then purged with oxygen (1 atm) before capping and was vigorously stirred on a magnetic hot plate at 80 ^oC in 4 hours. After cooling down to room temperature, diphenyl ether (27 μL, 0.15 mmol) was added as internal standard for GC yield determination. About one milliliter of DMSO could also be added to this vial to dissolve the components completely, and the resulting aliquot was subsequently extracted with 3 mL of ethyl acetate and 1 mL of distilled water. After withdrawing the organic phase and dried over anhydrous Na_2SO_4, the product formation was monitored by gas chromatography (GC) and the GC yield was calculated based on the calibration curve.

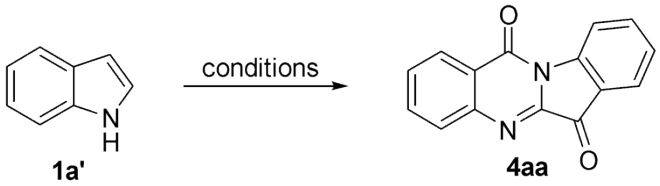
This procedure was also applied for synthesis of 2,3-disubstituted quinazolinones derived from anilines as other nitrogen sources, however, with the addition of H_2O_2 (65 μL, 0.6 mmol) right after iodine being added.

For the isolation of the typical product, namely 2-phenylquinazolin-4(*3H*)-one, resulting solution was quenched with 10 mL of $Na_2S_2O_3$ solution (20% in water), extracted with ethyl acetate (15 mL), dried over anhydrous Na_2SO_4 prior to the removal of solvent under vacuum. The crude product was purified by silica gel column chromatography (using *n*-hexane: ethyl acetate = 7: 3 as eluent) or by recrystallizing in methanol prior to washing obtained crystals two times with cold ethyl acetate. ^1H and ^{13}C-NMR analyses were used to confirm the product structure.

Procedure for synthesis of tryptanthrin and analogues

Tryptanthrin and its structural analogues were synthesized by using indole derivatives as a starting material, which was carried out under an oxygen atmosphere in presence of K_2CO_3, $TBHP_{aq}$, I_2, and CH_3CN as solvent for the reaction.

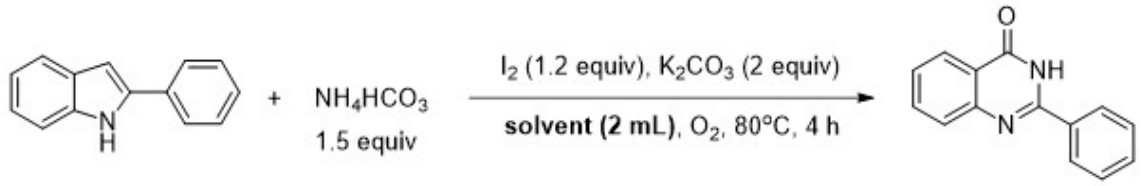
Table S1. Optimization of reaction conditions for synthesis of tryptanthrin derivatives[a]

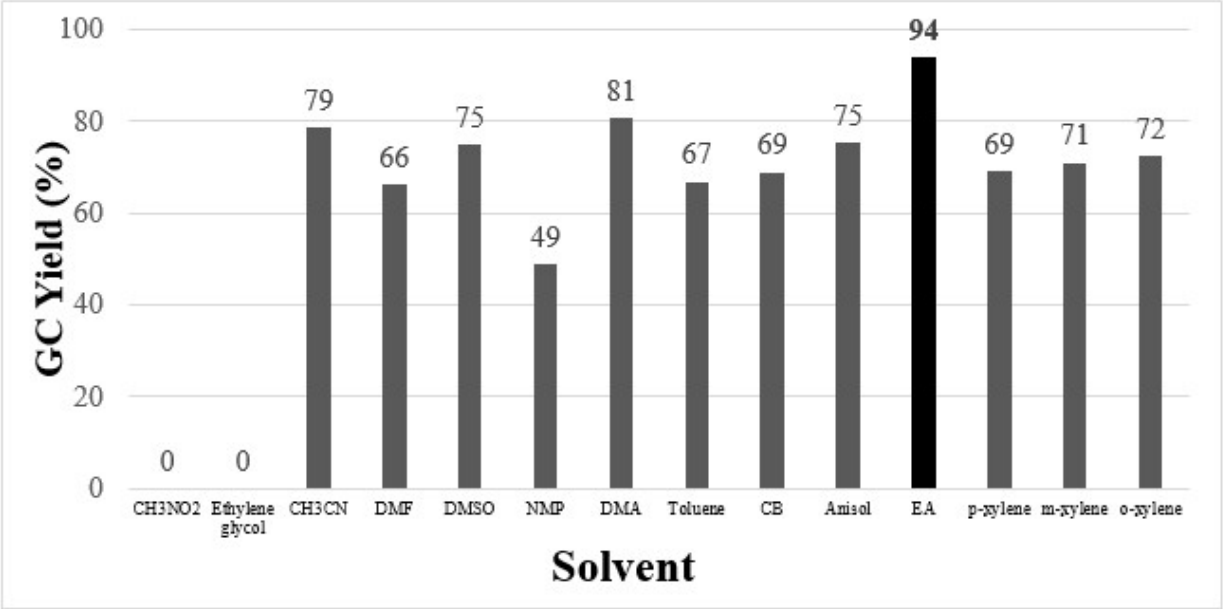


entry	catalyst	additive	base	solvent	yield[b] (%)
1	oxone	_	K_2CO_3	DMSO	_
2	I_2O_5	_	K_2CO_3	DMSO	_
3	KI	TBHP	K_2CO_3	DMSO	20
4	I_2	TBHP	K_2CO_3	DMSO	50
5	I_2	TBHP	K_2CO_3	DMF	12
6	I_2	TBHP	K_2CO_3	toluene	39
7	**I_2**	**TBHP**	**K_2CO_3**	**CH_3CN**	**86**
8[c]	I_2	TBHP	K_2CO_3	CH_3CN	80
9	I_2	TBHP	Cs_2CO_3	CH_3CN	65

10	I_2	TBHP	KOAc	CH_3CN	72
11	I_2	H_2O_2	K_2CO_3	CH_3CN	46
12	I_2	DTBP	K_2CO_3	CH_3CN	24
13[d]	I_2	TBHP	K_2CO_3	CH_3CN	41
14[e]	I_2	TBHP	K_2CO_3	CH_3CN	23
15[f]	I_2	TBHP	K_2CO_3	CH_3CN	85

[a]Reaction condition: **1a´** (0.25 mmol), catalyst (50 mol %), additive (3 equiv), base (2 equiv) in solvent (3 mL) for 2 h under O_2 atmosphere. [b]All yields were isolated yield. [c]The reaction was run at 100°C. [d]Under air. [e]The reaction was tested in N_2 atmosphere. [f]Used 1.2 equiv. of I_2.



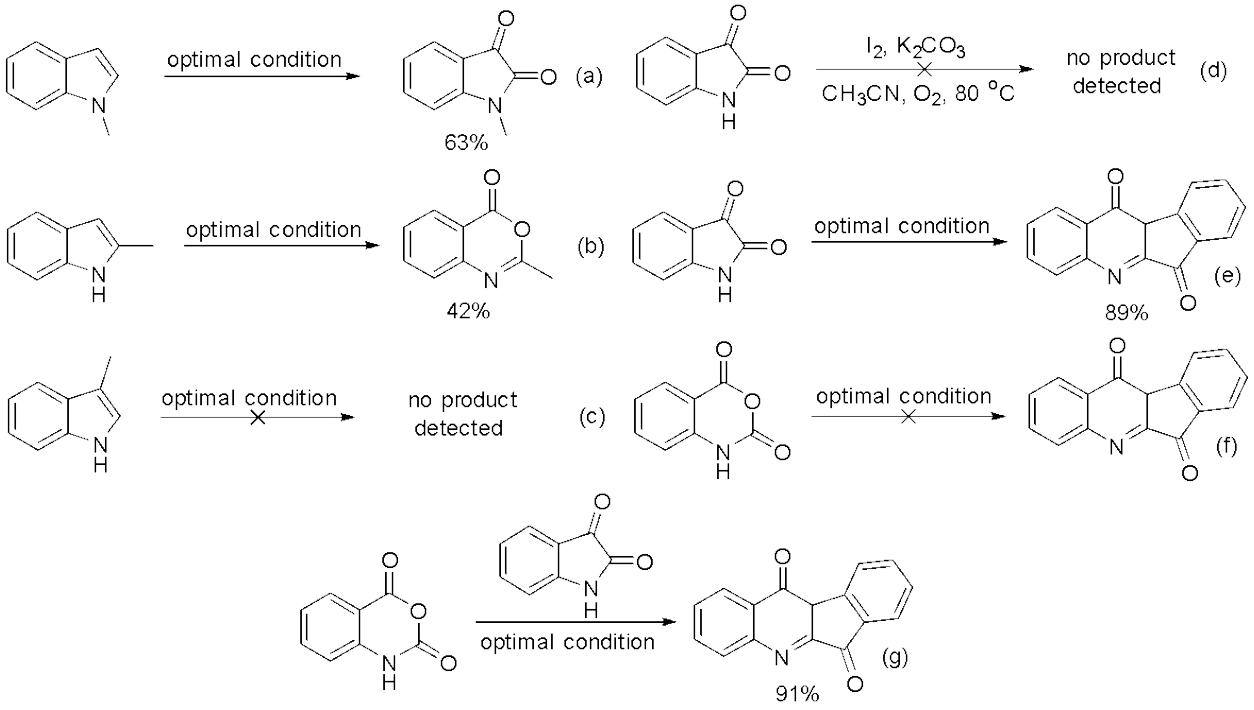


Scheme S1. Column chart illustrating effect of solvent on the reaction

In a typical experiment, a mixture of indole (0.25 mmol, 29.28 mg) and potassium carbonate (2 equiv., 69 mg) were added to a 8 mL pressurized vial. The oxidation reagent $TBHP_{aq}$ (166 µl) was then introduced to the mixture, followed by addition of CH_3CN (3 mL) as reaction solvent. Next, iodine (50 mol %, 31.7 mg) was carefully put into the vial. Finally, the vial was filled completely

with O_2 atmosphere and the reaction mixture was magnetically stirred at 80^{o}C for 2 h. Samples were withdrawn after the reaction and quenched with water under room temperature. Ethyl acetate with 10% $Na_2S_2O_3$ was used to extract organic components, and the obtained solution was dried utilizing anhydrous Na_2SO_4. The product yield was determined by GC analysis. Tryptanthrin was isolated on silicagel by column chromatography using solvent system hexane-ethyl acetate 7:3 (v:v) and was authenticated by ^{1}H NMR, ^{13}C NMR and GC-MS.

Section S3. *Mechanistic studies*



Scheme S2. Different control experiments on synthesis of tryptanthrins

Electron paramagnetic resonance (EPR) measurements

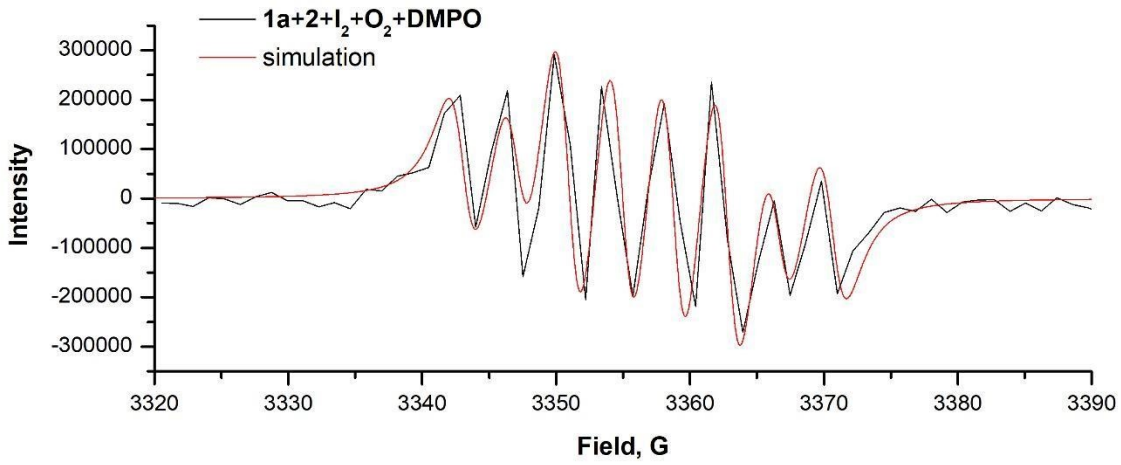


Figure S1. 1a and 2 under standard reaction condition

2-phenylindole **1a** (28.8 mg, 0.15 mmol), NH_4HCO_3 (**2**, 17.8 mg, 1.5 eq.) and K_2CO_3 (41.5 mg, 0.3 mmol) were added into a vial, followed by introduction of ethyl acetate (2 mL) and iodine

(45.7 mg, 0.18 mmol). The mixture was then stirred at 80 °C under oxygen atmosphere in 15 minutes. Next, to 70 uL of the obtained reaction solution was added 70 uL of 200 mM DMPO solution in dimethyl sulfoxide and EPR measurements were performed finally.

Parameters observed for the spin adduct are g = 2.0220, $\alpha_{N1} = \alpha_{H1}$ = 7.85 G, and α_{H2} = 4.00 G.

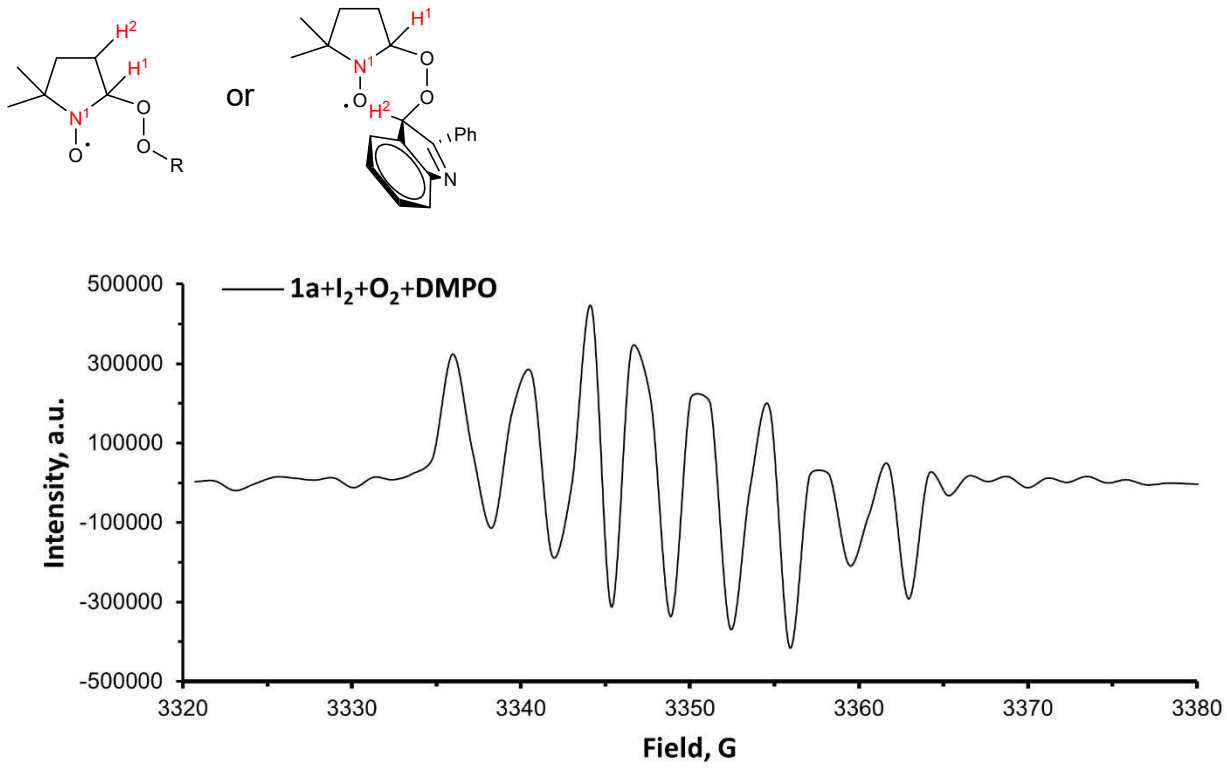
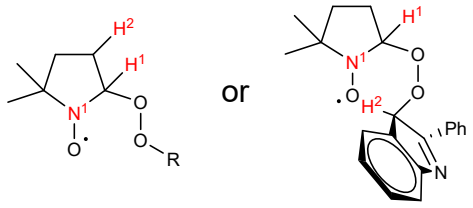


Figure S2. 1a in O_2 atmosphere

2-phenylindole **1a** (28.8 mg, 0.15 mmol) and K_2CO_3 (41.5 mg, 0.3 mmol) were added into a vial, followed by introduction of ethyl acetate (2 mL) and iodine (45.7 mg, 0.18 mmol). The mixture was then stirred at 80 °C under oxygen atmosphere in 15 minutes. Next, to 70 uL of the obtained reaction solution was added 70 uL of 200 mM DMPO solution in dimethyl sulfoxide and EPR measurements were performed finally.

Parameters observed for the spin adduct are g = 2.0220, $\alpha_{N1} = \alpha_{H1}$ = 7.85 G, and α_{H2} = 4.00 G.



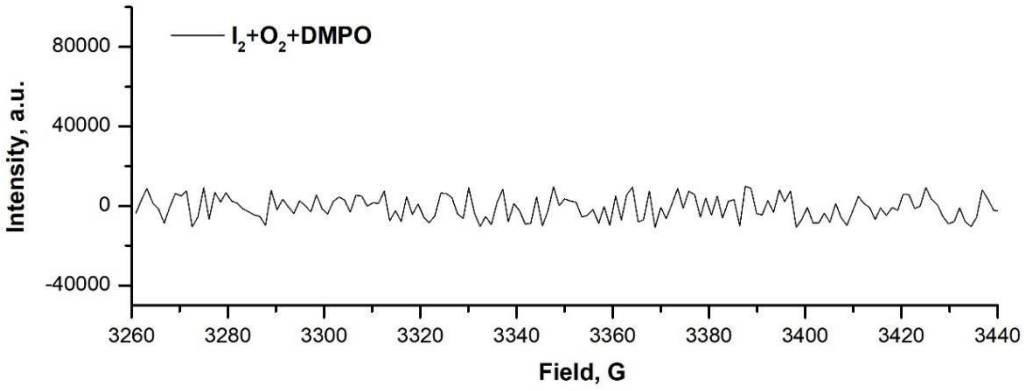


Figure S3. I_2 + O_2 without 1a and 2

K_2CO_3 (41.5 mg, 0.3 mmol) and iodine (45.7 mg, 0.18 mmol) were added into a vial, followed by introduction of ethyl acetate (2 mL). The mixture was then stirred at 80 °C under oxygen atmosphere in 15 minutes. Next, to 70 uL of the obtained reaction solution was added 70 uL of 200 mM DMPO solution in dimethyl sulfoxide and EPR measurements were performed finally.

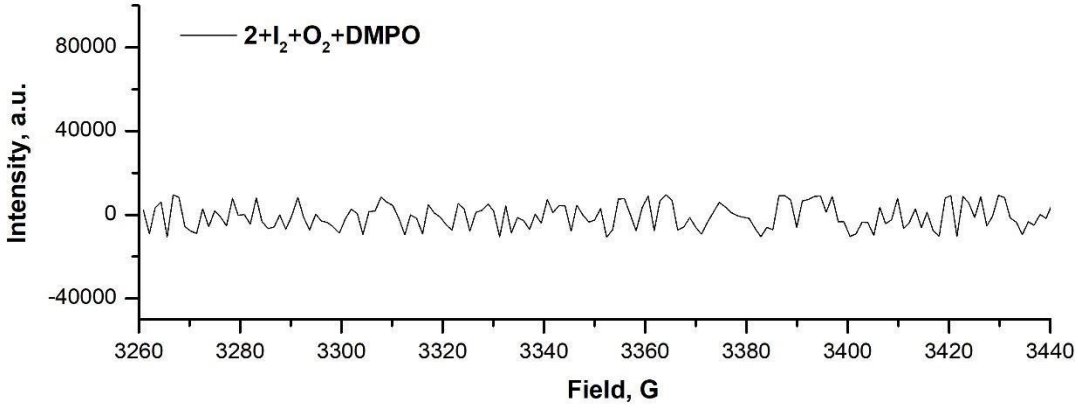


Figure S4. 2 in presence of iodine

NH_4HCO_3 (**2**, 17.8 mg, 1.5 eq.) and K_2CO_3 (41.5 mg, 0.3 mmol) were added into a vial, followed by introduction of ethyl acetate (2 mL). The mixture was then stirred at 80 °C under oxygen atmosphere in 15 minutes. Next, to 70 uL of the obtained reaction solution was added 70 uL of 200 mM DMPO solution in dimethyl sulfoxide and EPR measurements were performed finally.

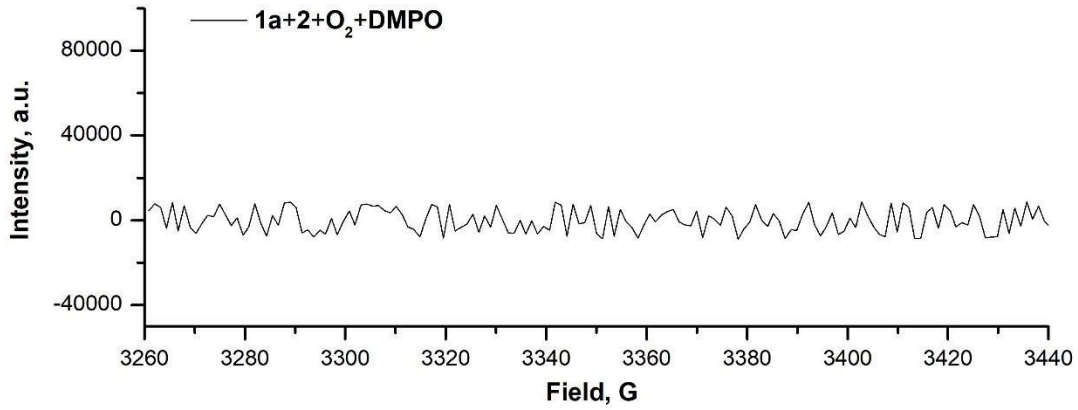


Figure S5. 1a and 2 in absence of iodine

2-phenylindole **1a** (28.8 mg, 0.15 mmol), NH_4HCO_3 (**2**, 17.8 mg, 1.5 eq.) and K_2CO_3 (41.5 mg, 0.3 mmol) were added into a vial, followed by introduction of ethyl acetate (2 mL). The mixture was then stirred at 80 °C under oxygen atmosphere in 15 minutes. Next, to 70 uL of the obtained reaction solution was added 70 uL of 200 mM DMPO solution in dimethyl sulfoxide and EPR measurements were performed finally.

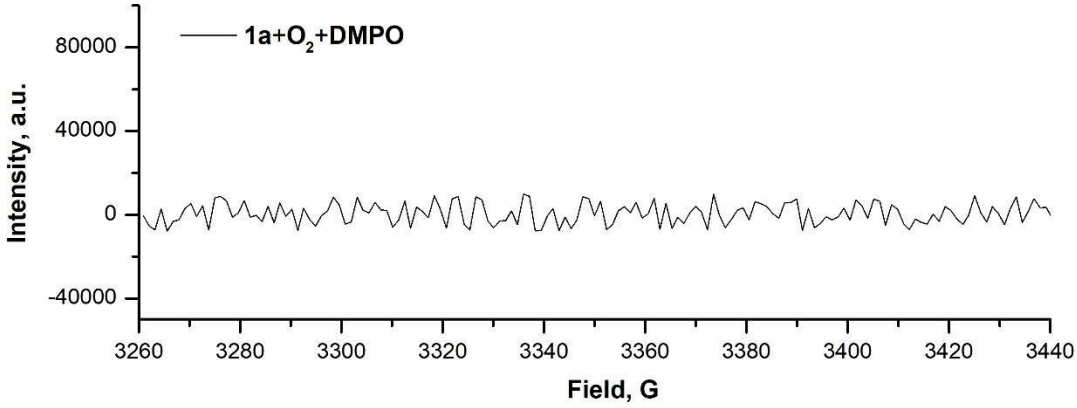


Figure S6. 1a in oxygen atmosphere without iodine

2-phenylindole **1a** (28.8 mg, 0.15 mmol) and K_2CO_3 (41.5 mg, 0.3 mmol) were added into a vial, followed by introduction of ethyl acetate (2 mL). The mixture was then stirred at 80 °C under oxygen atmosphere in 15 minutes. Next, to 70 uL of the obtained reaction solution was added 70 uL of 200 mM DMPO solution in dimethyl sulfoxide and EPR measurements were performed finally.

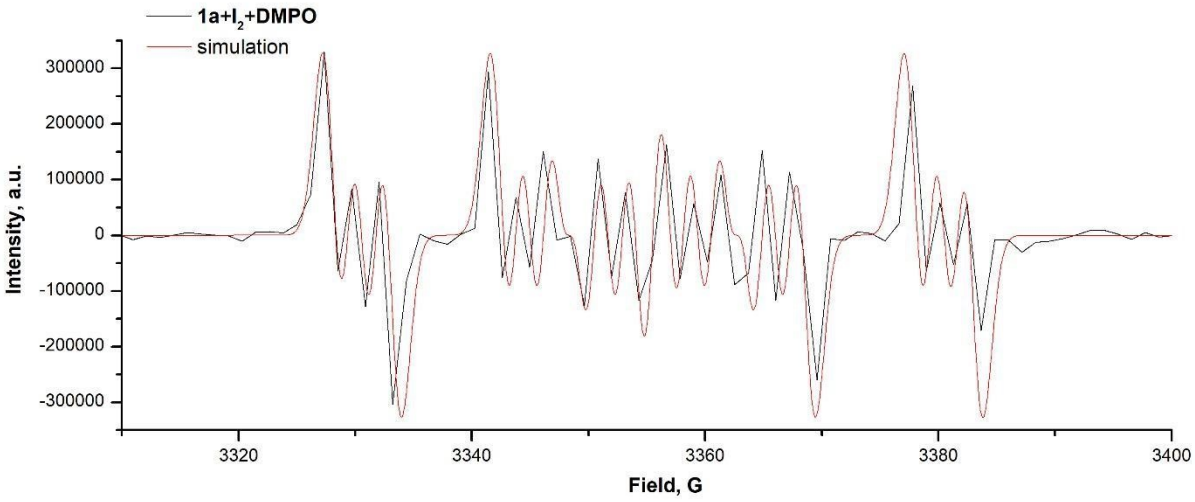
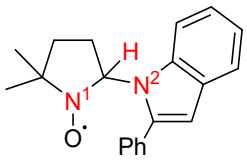


Figure S7. 1a in inert gas atmosphere (N_2 or Ar)

2-phenylindole **1a** (28.8 mg, 0.15 mmol) and K_2CO_3 (41.5 mg, 0.3 mmol) were added into a vial, followed by introduction of ethyl acetate (2 mL) and iodine (45.7 mg, 0.18 mmol). The mixture was then stirred at 80 °C under an inert gas atmosphere in 15 minutes. Next, to 70 uL of the obtained reaction solution was added 70 uL of 200 mM DMPO solution in dimethyl sulfoxide and EPR measurements were performed finally.

Parameters observed for the spin adduct are g = 2.0228, α_{N1} = 14.38 G, α_{N2} = 2.40 G, and α_H = 21.12 G.



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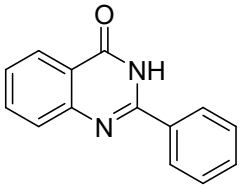
Section S4. ***Structural data of Products***

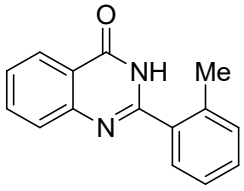
2-Phenylquinazolin-4(*3H*)-one (3aa)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 11.22 (br, 1H), 8.34 (dd, J = 8.0, 1.0 Hz, 1H), 8.23-8.21 (m, 2H), 7.85- 7.80 (m, 2H), 7.61- 7.59 (m, 3H), 7.53- 7.50 (m, 1H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 163.7 (C), 151.8 (C), 149.6 (C), 135.1 (CH), 133.0 (C), 131.8 (CH), 129.3 (2 x CH), 128.2 (CH), 127.4 (2 x CH), 127.0 (CH), 126.6 (CH), 121.1 (C).

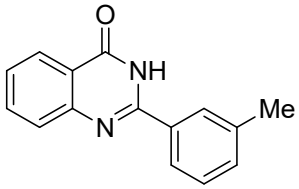
2-(2-Methylphenyl)quinazolin-4(3*H*)-one (3ba)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 12.44 (s, 1H), 8.17 (d, J = 8.0 Hz, 1H), 7.84 (t, J= 7.5 Hz, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.56- 7.50 (m, 2H), 7.43 (t, J = 7.5, 1H), 7.36- 7.31 (m, 2H), 2.38 (s, 3H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 161.8 (C), 154.4 (C), 148.7 (C), 136.1 (C), 134.4 (CH), 134.2 (C), 130.5 (CH), 129.9 (CH), 129.1 (CH), 127.4 (CH), 126.6 (CH), 125.8 (CH), 125.7 (CH), 121.0 (C), 19.5 (CH_3).

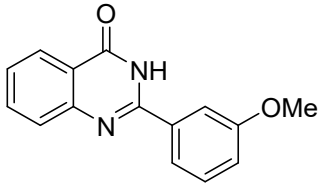
2-(3-Methylphenyl)quinazolin-4(3*H*)-one (3ca)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 12.47 (s, 1H), 8.15 (d, J = 7.5 Hz, 1H), 8.03 (s, 1H), 7.97 (d, J = 7.5 Hz, 1H), 7.84 (t, J = 8.0 Hz, 1H), 7.74 (d, J= 8.0 Hz, 1H), 7.52 (t, J = 7.5, 1H), 7.45-7.40 (m, 2H), 2.41 (s, 3H).

^{13}C NMR (CDCl3, 125 MHz, ppm): δ_C 162.2 (C), 152.4 (C), 148.8 (C), 137.9 (C), 134.6 (CH), 132.6 (C), 132.0 (CH), 128.5 (CH), 128.3 (CH), 127.5 (CH), 126.5 (C), 125.8 (CH), 124.9 (CH), 121.0 (C), 20.9 (CH_3).

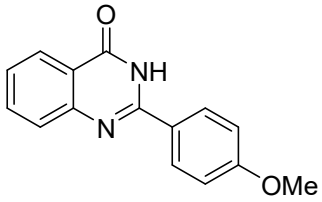
2-(3-Methoxyphenyl)quinazolin-4(*3H*)-one (3da)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 12.54 (s, 1H), 8.16 (dd, J = 8.0, 1.0 Hz, 2H), 7.86- 7.83 (m, 1H), 7.79 (d, J = 8.0 Hz, 1H), 7.75 (dd, J = 5.0, 2.5 Hz, 2H), 7.54- 7.51 (m, 1H), 7.46 (t, J = 8.0 Hz, 1H), 7.15 (dd, J = 8.0, 2.0 Hz, 1H) 3.87 (s, 3H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 162.2 (C), 159.3 (C), 152.0 (C), 148.7 (C), 134.6 (CH), 134.0 (C), 129.7 (CH), 127.5 (CH), 126.6 (CH), 125.8 (CH), 121.0 (C), 120.1 (CH), 117.6 (CH), 112.5 (CH), 55.4 (CH_3).

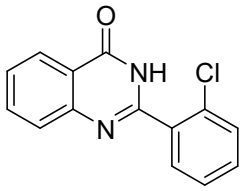
2-(4-Methoxyphenyl)quinazolin-4(*3H*)-one (3ea)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 12.41 (s, 1H), 8.19 (d, J = 9.0 Hz, 2H), 8.13 (dd, J = 8.0, 1.0 Hz, 1H), 7.82- 7.80 (m, 1H), 7.70 (d, J = 8.0 Hz, 1H), 7.48 (t, J = 7.5 Hz, 1H), 7.09 (d, J = 9.0 Hz, 2H), 3.85 (s, 3H).

^{13}C NMR (CDCl3, 125 MHz, ppm): δ_C 162.3 (C), 161.9 (C), 151.9 (C), 148.9 (C), 135.5 (CH), 129.4 (2 x CH), 127.3 (CH), 126.1 (CH), 125.8 (CH), 124.8 (CH), 120.7 (CH), 114.0 (2 x CH), 55.4 (CH_3).

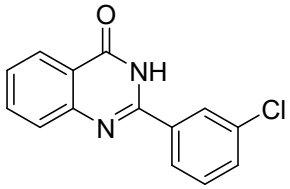
2-(2-Chlorophenyl)quinazolin-4(*3H*)-one (3fa)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 12.64 (s, 1H), 8.18 (dd, J = 8.0, 1.0 Hz, 1H), 7.89- 7.83 (m, 1H), 7.71 (d, J = 8.0 Hz, 1H), 7.67 (dd, J = 7.5, 1.5 Hz, 1H), 7.62 (d, J = 8.0 Hz, 1H), 7.58-7.55 (m, 2H), 7.50 (td, J= 7.5, 1.0 Hz, 1H).

^{13}C NMR (CDCl3, 125 MHz, ppm): δ_C 161.4 (C), 152.2 (CH), 148.6 (C), 134.6 (C), 133.8 (C), 131.6 (CH), 131.5 (C), 130.9 (CH), 129.6 (CH), 127.5 (CH), 127.2 (CH), 127.0 (CH), 125.8 (CH), 121.3 (C).

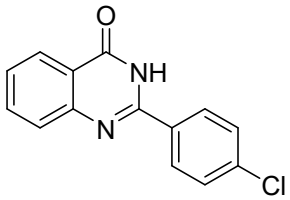
2-(3-Chlorophenyl)quinazolin-4(*3H*)-one (3ga)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 12.63 (s, 1H), 8.25 (t, *J* = 1.5 Hz, 1H), 8.17- 8.15 (m, 2H), 7.88- 7.84 (m, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.67 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.59 (t, *J* = 8.0 Hz, 1H), 7.56- 7.53 (m, 1H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 162.1 (C), 152.5 (C), 148.5 (C), 134.7 (C), 134.6 (CH), 133.4 (CH), 131.1 (CH), 130.5 (CH), 127.6 (C), 127.5 (CH), 126.9 (CH), 126.4 (CH), 125.9 (CH), 121.1 (C).

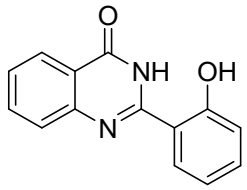
2-(4-Chlorophenyl)quinazolin-4(*3H*)-one (3ha)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 12.61 (s, 1H), 8.20 (d, *J* = 8.5 Hz, 2H), 8.15 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.85 (dd, *J* = 7.0, 1.5 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.63 (d, *J* = 8.5 Hz, 2H), 7.54 (dd, *J* = 7.0, 1.0 Hz, 1H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 162.1 (C), 151.3 (C), 148.6 (C), 136.3 (C), 134.7 (CH), 131.5 (C), 129.6 (2 x CH), 128.7 (2 x CH), 127.5 (CH), 126.8 (CH), 125.9 (CH), 121.0 (C).

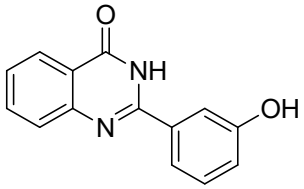
2-(2-Hydroxyphenyl)quinazolin-4(3*H*)-one (3ia)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 13.78 (s, 1H), 12.47 (s, 1H), 8.23 (d, *J* = 8.0 Hz, 1H), 8.16 (d, *J* = 8.0 Hz, 1H), 7.87- 7.84 (m, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.54 (t, *J* = 7.5, 1H), 7.45 (t, *J* = 7.5, 1H), 7.01 (d, *J* = 8.0 Hz, 1H), 6.96 (t, *J*= 7.5 Hz, 1H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 161.4 (C), 160.0 (C), 153.7 (C), 146.1 (C), 135.0 (CH), 133.7 (CH), 127.7 (CH), 126.9 (CH), 126.0 (CH), 120.3 (C), 118.8 (2 x CH), 117.9 (CH), 113.7 (C).

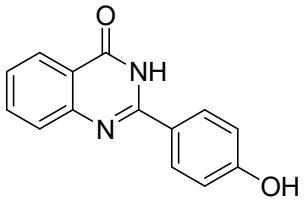
2-(3-Hydroxyphenyl)quinazolin-4(3*H*)-one (3ja)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 12.43 (s, 1H), 9.76 (s 1H), 8.15 (d, J = 8.0 Hz, 1H), 7.83 (t, J = 7.0 Hz, 1H), 7.72 (d, J = 8.5 Hz, 1H), 7.60- 7.59 (m, 2H), 7.52 (t, J = 7.5, 1H), 7.33 (t, J = 8.0 Hz, 1H), 6.98 (d, J = 7.5, 1H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 162.2 (C), 157.5 (C), 152.3 (C), 148.7 (C), 134.6 (CH), 134.0 (C), 129.6 (CH), 127.5 (CH), 126.5 (CH), 125.8 (CH), 121.0 (C), 118.5 (CH), 118.3 (CH), 114.6 (CH).

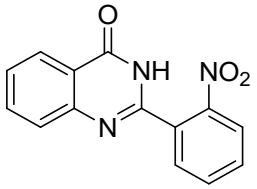
2-(4-Hydroxyphenyl)quinazolin-4(3*H*)-one (3ka)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 12.30 (s, 1H), 10.16 (s, 1H), 8.12 (d, J = 7.5 Hz, 1H), 8.08 (d, J = 9.0 Hz, 2H), 7.81- 7.78 (m, 1H), 7.68 (d, J = 8.0 Hz, 1H), 7.46 (t, J = 7.5, 1H), 6.89 (d, J = 7.5, 2H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 162.3 (C), 160.5 (C), 152.1 (C), 149.1 (C), 134.5 (CH), 129.6 (2 x CH), 127.2 (CH), 125.9 (CH), 125.8 (CH), 123.2 (C), 120.6 (C), 115.4 (2 x CH).

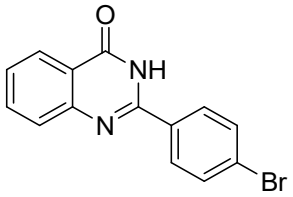
2-(2-Nitrophenyl)quinazolin-4(3*H*)-one (3la)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 12.83 (s, 1H), 8.40 (q, J = 9.0 Hz, 4H), 8.18 (d, J= 8.0 Hz, 1H), 7.88 (t, J = 8.5 Hz, 1H), 7.80 (d, J= 8.0 Hz, 1H), 7.58 (t, J = 8.0 Hz, 1H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 162.0 (C), 150.7 (C), 149.0 (C), 148.3 (C), 138.5 (C), 134.8 (CH), 129.3 (2 x CH), 127.8 (CH), 127.4 (CH), 125.9 (CH), 123.6 (2 x CH), 121.3 (C).

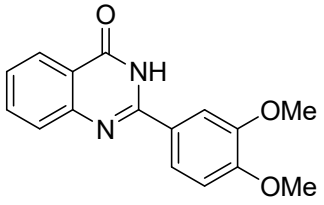
2-(4-Bromophenyl)quinazolin-4(3*H*)-one (3ma)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 12.61 (s, 1H), 8.15 (d, J = 8.0 Hz, 1H), 8.13 (d, J= 8.5 Hz, 2H), 7.85 (t, J= 8.0 Hz, 1H), 7.77 (d, J= 8.5 Hz, 1H), 7.75 (d, J= 8.5 Hz, 1H), 7.54 (t, J= 7.5 Hz, 1H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 162.2 (C), 151.4 (C), 134.7 (CH), 131.9 (C), 131.6 (2 x CH), 129.8 (2 x CH), 127.5 (C), 126.8 (C), 125.9 (CH), 125.2 (C), 121.0 (C).

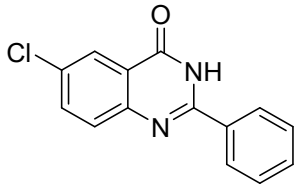
2-(3,4-Dimethoxyphenyl)quinazolin-4(3*H*)-one (3na)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 12.43 (s, 1H), 8.13 (d, J = 8.0 Hz, 1H), 7.87 (dd, J = 8.5, 2.0 Hz, 1H), 7.83- 7.80 (m, 2H), 7.71 (d, J = 8.0 Hz, 1H), 7.49 (t, J = 7.5 Hz, 1H), 7.12 (d, J = 8.5, 1H), 3.88 (s, 3H), 3.85 (s, 3H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 162.3 (C), 151.8 (C), 151.6 (C), 148.9 (C), 148.5 (C), 134.6 (CH), 127.3 (CH), 126.1 (CH), 125.8 (CH), 124.7 (C), 121.1 (CH), 120.7 (C), 111.4 (CH), 110.7 (CH), 55.7 (2 x CH_3).

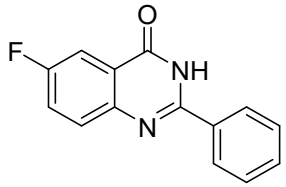
6-Chloro-2-phenylquinazolin-4(3*H*)-one (3oa)



^{1}H NMR (DMSO-d_6, 500 MHz, ppm): δ_H 12.72 (br, 1H), 8.18 (d, J = 8.0 Hz, 2H), 8.10 (d, J = 1.0 Hz, 1H), 7.89 (dd, J = 8.0, 1.0 Hz, 1H), 7.77 (d, J = 8.0 Hz, 1H), 7.63- 7.55 (m, 3H)

^{13}C NMR (DMSO-d_6, 125 MHz, ppm): δ_C 161.9 (C), 153.6 (C), 147.9 (C), 135.1 (CH), 133.0 (C), 132.1 (CH), 131.2 (CH), 130.2 (C), 129.1 (2xCH), 128.3 (2xCH), 125.3 (CH), 122.7 (C).

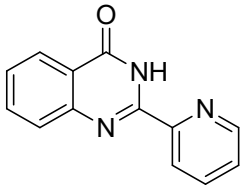
6-Fluoro-2-phenylquinazolin-4(3*H*)-one (3pa)



^{1}H NMR (DMSO-d_6, 500 MHz, ppm): δ_H 12.68 (br, 1H), 8.18 (d, J = 8.0 Hz, 2H), 7.86–7.82 (m, 2H), 7.74 (td, J = 8.0, 2.5 Hz, 1H), 7.62- 7.55 (m, 3H)

^{13}C NMR (DMSO-d_6, 125 MHz, ppm): δ_C 162.2 (C), 161.5-159.5 (d, C-F), 152.4 (C), 146.1 (C), 133.1 (CH), 131.9 (CH), 130.8 (C), 129.1 (2xCH), 128.2 (2xCH), 123.6-123.5 (d, C_oH-C-F), 122.7-122.6 (d, C_m), 111.1-110.9 (d, C_oH-C-F).

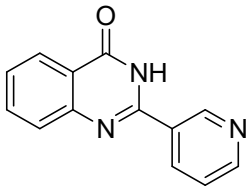
2-(Pyridin-2-yl)quinazolin-4(3*H*)-one (3qa)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 11.84 (s, 1H), 8.77 (d, J = 4.5 Hz, 1H), 8.47 (d, J= 8.0 Hz, 1H), 8.20 (d, J = 8.0 Hz, 1H), 8.08 (td, J = 8.0, 1.5 Hz, 1H), 7.88 (t, J= 8.0 Hz, 1H), 7.82 (d, J = 8.0 Hz, 1H), 7.67 (dd, J = 7.0, 5.5 Hz, 1H), 7.58 (t, J = 7.5 Hz, 1H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 160.8 (C), 150.0 (C), 149.0 (CH), 148.7 (C), 148.4 (C), 138.0 (CH), 134.7 (CH), 127.7 (CH), 127.3 (CH), 126.6 (CH), 126.1 (CH), 122.2 (CH), 122.0 (C).

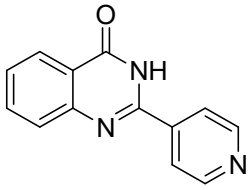
2-(Pyridin-3-yl)quinazolin-4(3*H*)-one (3ra)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 12.74 (s, 1H), 9.30 (d, J = 1.5 Hz, 1H), 8.76 (d, J = 3.5 Hz, 1H), 8.51- 8.49 (m, 1H), 8.17 (d, J= 7.5 Hz, 1H), 7.88- 7.85 (m, 1H), 7.77 (d, J = 8.0 Hz, 1H), 7.59 (dd, J=8.0, 5.0 Hz, 1H), 7.56 (t, J= 8.0 Hz, 1H).

^{13}C NMR (CDCl3, 125 MHz, ppm): δ_C 162.1 (C), 151.8 (CH), 150.8 (C), 148.7 (CH), 148.5 (C), 135.4 (CH), 134.7 (CH), 128.7 (CH), 127.6 (C), 126.9 (CH), 125.9 (C), 123.5 (CH), 121.1 (C).

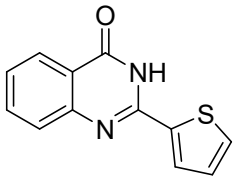
2-(Pyridin-4-yl)quinazolin-4(3*H*)-one (3sa)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 12.77 (s, 1H), 8.79 (s, 2H), 8.18 (d, J = 8.0 Hz, 1H), 8.12 (d, J = 5.0 Hz, 2H), 7.88 (t, J= 8.0 Hz, 1H), 7.80 (d, J = 8.0 Hz, 1H), 7.59 (t, J= 7.5 Hz, 1H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 162.0 (C), 150.5 (C), 150.3 (CH), 148.3 (C), 139.9 (C), 134.8 (CH), 127.8 (C), 127.4 (CH), 125.9 (C), 121.6 (CH), 121.5 (C).

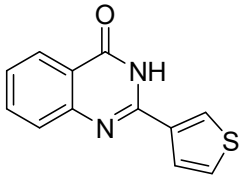
2-(2-Thiophen)quinazolin-4(3*H*)-one (3ta)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 12.65 (s, 1H), 8.23 (d, J = 3.5 Hz, 1H), 8.12 (d, J = 7.5 Hz, 1H), 7.87 (d, J= 9.5 Hz, 1H), 7.81 (d, J = 8.0 Hz, 1H), 7.65 (d, J = 8.5 Hz, 1H), 7.49 (t, J = 7.5, 1H), 7.24 (t, J = 4.5, 1H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 161.8 (C), 148.6 (C), 147.8 (C), 137.4 (C), 134.7 (CH), 132.2 (CH), 129.4 (CH), 128.5 (CH), 126.9 (CH), 126.3 (CH), 126.0 (CH), 121.0 (C).

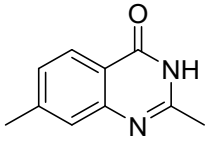
2-(3-Thiophen)quinazolin-4(3*H*)-one (3ua)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 12.47 (s, 1H), 8.61- 8.60 (m, 1H), 8.13 (d, J = 8.0 Hz, 1H), 7.88 (d, J= 5.0 Hz, 1H), 7.82 (t, J= 8.0 Hz, 1H), 7.72- 7.69 (m, 2H), 7.50 (t, J= 7.5 Hz, 1H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 162.1 (C), 148.9 (C), 148.3 (C), 135.4 (C), 134.6 (CH), 128.6 (CH), 127.4 (CH), 127.3 (CH), 127.0 (CH), 126.4 (CH), 125.9 (CH), 120.9 (C).

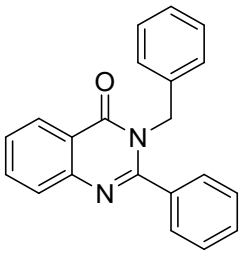
2,7-Dimethylquinazolin-4(3*H*)-one (3va)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 11.22 (br, 1H), 8.16 (d, J = 8.0 Hz, 1H), 7.47 (s, 1H), 7.29 (d, J = 8.0, 1H), 2.57 (s, 3H), 2.51 (s, 3H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 163.6 (C), 153.1 (C), 149.6 (C), 146.0 (C), 128.1 (CH), 126.8 (CH), 126.1 (CH), 117.9 (C), 22.2 (CH_3), 22.0 (CH_3).

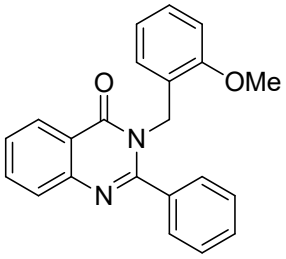
3-Benzyl-2-phenylquinazolin-4(3*H*)-one (3ab)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 8.38 (d, J = 8.0 Hz, 1H), 7.80-7.75 (m, 2H), 7.53 (ddd, J = 8.0, 6.0, 2.0 Hz, 1H), 7.47 (t, J = 7.5 Hz, 1H), 7.40 (t, J = 7.5 Hz, 2H), 7.34 (d, J = 7.5 Hz, 2H), 7.21-7.19 (m, 3H), 6.93-6.92 (m, 2H), 5.29 (s, 2H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 162.6 (C), 156.5 (C), 147.4 (C), 136.7 (C), 135.4 (C), 134.6 (CH), 130.0 (CH), 128.7 (2 x CH), 128.6 (2 x CH), 128.2 (2 x CH), 127.8 (CH), 127.6 (CH), 127.3 (CH), 127.2 (CH), 127.1 (2 x CH), 121.0 (C), 48.9 (CH_2).

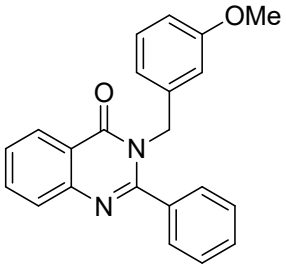
3-(2-Methoxybenzyl)-2-phenylquinazolin-4(3*H*)-one (3ac)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 8.37 (d, J = 8.0 Hz, 1H), 7.81- 7.75 (m, 2H), 7.53 (ddd, J = 8.0, 6.5, 1.5 Hz, 1H), 7.49- 7.45 (m, 1H), 7.41 (t, J = 8.0 Hz, 2H), 7.37- 7.36 (m, 2H), 7.13 (t, J = 8.0 Hz, 1H), 6.74 (d, J = 8.0 Hz, 2.0 Hz, 1H), 6.53 (d, J = 7.5 Hz, 1H), 6.46 (s, 1H), 5.24 (s, 2H), 3.70 (s, 3H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 162.6 (C), 156.9 (C), 156.5 (C), 147.5 (C), 135.5 (C), 134.5 (CH), 129.7 (CH), 128.5 (2 x CH), 128.4 (CH), 127.9 (2 x CH), 127.7 (CH) 127.2 (2 x CH), 127.1 (CH), 124.9 (C), 120.9 (C), 120.6 (CH), 110.2 (CH), 55.2 (CH_2), 44.7 (CH_3).

3-(3-Methoxybenzyl)-2-phenylquinazolin-4(3*H*)-one (3ad)

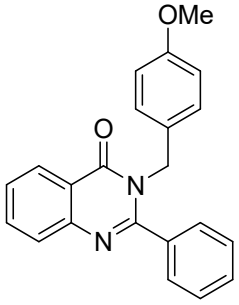


^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 8.37 (d, J = 8.0 Hz, 1H), 7.81- 7.75 (m, 2H), 7.53 (ddd, J = 8.0, 6.5, 1.5 Hz, 1H), 7.49- 7.45 (m, 1H), 7.41 (t, J = 8.0 Hz, 2H), 7.37- 7.36 (m, 2H), 7.13 (t, J =

8.0 Hz, 1H), 6.74 (d, *J* = 8.0 Hz, 2.0 Hz, 1H), 6.53 (d, *J* = 7.5 Hz, 1H), 6.46 (s, 1H), 5.24 (s, 2H), 3.70 (s, 3H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 162.6 (C), 159.8 (C), 156.5 (C), 147.4 (C), 138.3 (C), 135.4 (C), 134.7 (CH), 130.0 (CH), 129.7 (CH), 128.7 (2 x CH), 128.2 (2 x CH), 127.7 (CH), 127.3 (CH), 127.2 (CH), 121.0 (C), 119.4 (C), 112.9 (2 x CH), 55.3 (CH_2), 48.9 (CH_3).

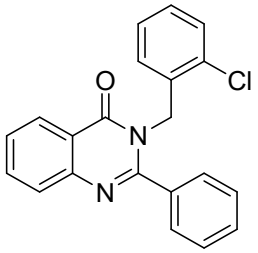
3-(4-Methoxybenzyl)-2-phenylquinazolin-4(3*H*)-one (3ae)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 8.38- 8.36 (m, 1H), 7.79-7.34 (m, 2H), 7.53-7.49 (m, 1H), 7.49- 7.47 (m, 1H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.37- 7.35 (m, 2H), 6.86-6.84 (m, 2H), 6.74- 6.71 (m, 2H) 5.22 (s, 2H), 3.74 (s, 3H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 162.5 (C), 156.4 (C), 160.0 (C), 156.4 (C), 147.3 (C), 135.4 (CH), 134.5 (CH), 129.9 (CH), 128.7 (C), 128.6 (2 x CH), 128.6 (2 x CH), 128.1 (2 x CH), 127.6 (CH), 127.1 (2 x CH), 121.0 (C), 113.9 (CH), 55.2 (CH_2), 48.2 (CH_3).

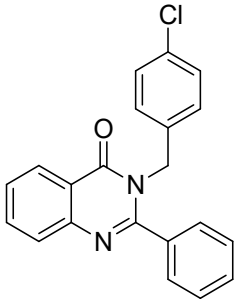
3-(2-Chlorobenzyl)-2-phenylquinazolin-4(3*H*)-one (3af)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 8.37 (d, *J* = 8.0 Hz, 1H), 7.83-7.79 (m, 2H), 7.55 (ddd, *J* = 8.0, 6.0, 2.5 Hz, 1H), 7.44 (m, 1H), 7.35 (t, *J* = 7.5 Hz, 2H), 7.31-7.27 (m, 3H), 7.20-7.17 (m, 2H), 6.97-6.95 (m, 1H), 5.30 (s, 2H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 162.4 (C), 156.5 (C), 147.4 (C), 134.9 (C), 134.7 (CH), 134.0 (C), 132.4 (C), 130.0 (CH), 129.5 (CH), 128.7 (2 x CH), 128.5 (CH), 127.8 (CH), 127.6 (2 x CH), 127.3 (CH), 127.2 (CH), 127.0 (2 x CH), 120.7 (C), 47.1 (CH_2).

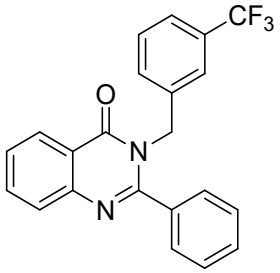
3-(4-Chlorobenzyl)-2-phenylquinazolin-4(3*H*)-one (3ag)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 8.36 (dd, J = 7.5, 1.0 Hz, 1H), 7.81-7.75 (m, 2H), 7.54 (ddd, J = 8.5, 7.0, 1.5 Hz, 1H), 7.50- 7.47 (m, 1H), 7.42 (t, J = 7.5 Hz, 2H), 7.35-7.33 (m, 2H), 7.18-7.16 (m, 2H), 7.85- 7.87 (m, 2H), 5.23 (s, 2H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 162.4 (C), 156.1 (C), 147.3 (C), 135.2 (C), 135.1 (C), 134.7 (CH), 133.4 (C), 130.0 (CH), 128.7 (2 x CH), 128.7 (2 x CH), 128.6 (2 x CH), 128.0 (2 x CH), 127.7 (CH), 127.3 (CH), 127.1 (CH), 120.8 (C), 48.2 (CH_2).

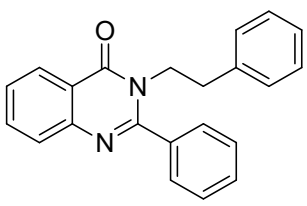
3-(3-Trifluoromethylbenzyl)-2-phenylquinazolin-4(3*H*)-one (3ah)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 8.33 (d, J = 8.0 Hz, 1H), 7.76-7.70 (m, 2H), 7.51- 7.48 (m, 1H), 7.45- 7.41 (m, 2H), 7.36 (t, J = 7.5 Hz, 2H), 7.29 (t, J = 8.0 Hz, 1H), 7.24 (d, J = 8.0 Hz, 2H), 7.17 (d, J = 8.0 Hz, 1H), 6.97 (s, 1H), 5.26 (s, 2H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 162.6 (C), 156.1 (C), 147.3 (C), 137.7 (C), 135.2 (C), 134.9 (CH), 130.2-131.0 (q, CF_3), 130.8 (CH), 130.3 (CH), 129.3 (CH), 128.9 (2 x CH), 128.1 (2 x CH), 127.9 (CH), 127.5 (CH), 127.3 (CH), 124.6-124.5 (d, C_oH-C-CF_3), 124.5-124.4 (d, C_oH-C-CF_3), 120.9 (C), 48.3 (CH_2).

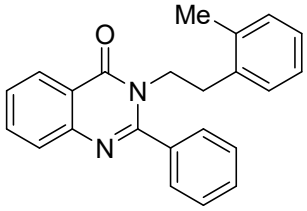
3-Phenylethyl-2-phenylquinazolin-4(3*H*)-one (3ai)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 8.37 (d, J = 8.0 Hz, 1H), 7.78-7.73 (m, 2H), 7.55- 7.48 (m, 4H), 7.40- 7.38 (m, 2H), 7.18 (m, 3H), 6.88 (m, 2H), 4.19 (d, J = 7.5 Hz, 2H), 2.91 (d, J = 2.5 Hz, 2H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 162.2 (C), 156.2 (C), 147.2 (C), 137.8 (C), 135.4 (C), 134.2 (CH), 129.8 (CH), 128.8 (4 x CH), 128.6 (2 x CH), 127.8 (2 x CH), 127.6 (CH), 127.1 (CH), 126.8 (CH), 126.7 (CH), 121.0 (C), 47.6 (CH_2), 34.7 (CH_2) .

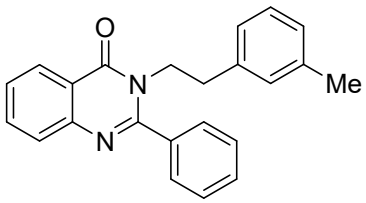
3-(2-Methylphenylethyl)-2-phenylquinazolin-4(3*H*)-one (3aj)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 8.38 (d, J = 8 Hz, 1H), 7.81-7.77 (m, 2H), 7.56- 7.47 (m, 4H), 7.40- 7.38 (m, 2H), 7.09 (dd, J = 7.5, 1.0 Hz, 1H), 7.05 (d, J = 7.0 Hz, 1H), 7.01 (td, J = 7.5, 0.5 Hz, 1H), 6.79 (d, J = 7 Hz, 1H), 4.18 (t, J = 7.5 Hz, 2H), 2.91 (t, J = 7.5 Hz, 2H), 2.01 (s, 3H).

^{13}C NMR (CDCl3, 125 MHz, ppm): δ_C 162.3 (C), 156.4 (C), 136.7 (CH), 135.9 (C), 134.7 (CH), 130.5 (CH), 130.1 (C), 129.8 (CH), 129.0 (3 x CH), 128.1 (3 x CH), 127.6 (C), 127.3 (C), 127.1 (CH), 126.9 (CH), 126.3 (CH), 121.0 (C), 46.3 (CH_2), 32.3 (CH_2), 18.8 (CH_3).

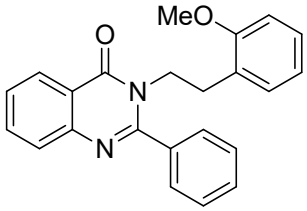
3-(3-Methylphenylethyl)-2-phenylquinazolin-4(3*H*)-one (3ak)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 8.37 (dd, J = 8.0, 1.0 Hz, 1H), 7.80-7.74 (m, 2H), 7.55- 7.48 (m, 4H), 7.40- 7.38 (m, 2H), 7.07 (t, J = 7.5 Hz, 1H), 6.99 (d, J = 7.5 Hz, 1H), 6.68- 6.65 (m, 2H), 4.19 (t, J = 8.0 Hz, 2H), 2.87 (t, J = 7.5 Hz, 2H), 2.22 (s, 3H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 162.3 (C), 156.3 (C), 147.3 (C), 138.4 (C), 137.8 (C), 135.5 (C), 134.6 (CH), 129.9 (CH), 129.8 (CH), 128.9 (2 x CH), 128.6 (CH), 128.0 (2 x CH), 127.7 (CH), 127.5 (CH), 127.2 (CH), 126.9 (CH), 125.9 (CH), 121.1 (C), 47.7 (CH_2), 34.7 (CH_2), 21.4 (CH_3).

3-(2-Methoxyphenylethyl)-2-phenylquinazolin-4(3*H*)-one (3al)

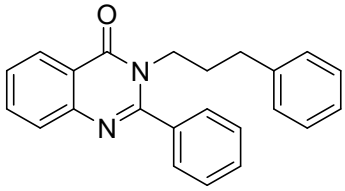


^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 8.38 (dd, J = 8.0, 1.0 Hz, 1H), 7.78-7.72 (m, 2H), 7.52 (ddd, J = 8.5, 8.0, 1.5 Hz, 1H), 7.47- 7.44 (m, 1H), 7.42- 7.38 (m, 2H), 7.19- 7.15 (m, 3H), 6.85- 6.83

(dd, J = 7.5, 2.0 Hz, 1H), 6.76 (td, J = 7.5, 1.0 Hz, 1H), 6.66 (d, J= 8.5 Hz, 1H), 4.28 (t, J = 8.0 Hz, 2H), 3.37 (s, 3H), 2.95 (t, J = 8.0 Hz, 2H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 162.5 (C), 157.8 (CH), 156.7 (C), 134.4 (C), 131.0 (CH), 129.5 (C), 128.6 (3 x CH), 128.2 (CH), 128.1 (3 x CH), 127.5 (C), 127.1 (CH), 126.9 (CH), 126.2 (C), 121.1 (C), 120.7 (CH), 110.2 (CH), 54.7 (CH_3), 46.3 (CH_2), 29.3 (CH_2) .

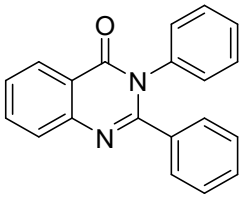
3-(3-Phenyl-1-propyl)-2-phenylquinazolin-4(3*H*)-one (3am)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 8.34- 8.32 (m, 1H), 7.77-7.71 (m, 2H), 7.52- 7.46 (m, 6H), 7.19- 7.16 (m, 2H), 7.13- 7.11 (m, 1H), 6.98 (d, J = 6.5 Hz, 2H), 3.99- 4.02 (m, 2H), 2.51 (t, J = 7.5 Hz, 2H), 1.92- 1.98 (m, 2H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 162.2 (C), 156.1 (C), 147.2 (C), 140.5 (C), 135.4 (C), 134.3 (CH), 129.8 (CH), 128.8 (2 x CH), 128.4 (2 x CH), 128.0 (2 x CH), 127.7 (2 x CH), 127.5 (CH), 127.0 (CH), 126.8 (CH), 126.0 (CH), 120.9 (C), 45.5 (CH_2), 32.9 (CH_2), 29.8 (CH_2).

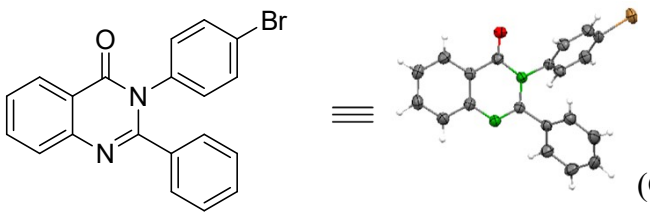
2,3-Diphenylquinazolin-4(3*H*)-one (3an)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 8.20 (d, J = 8.0 Hz, 1H), 7.91 (t, J = 7.5 Hz, 1H), 7.77 (d, J= 8.0 Hz, 1H), 7.61 (t, J = 8.0 Hz, 1H), 7.37 (d, J= 7.0 Hz, 2H), 7.34- 7.29 (m, 4H), 7.27- 7.20 (m, 4H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 161.4 (C), 155.2 (C), 147.3 (C), 137.8 (C), 135.6 (C), 134.8 (CH), 129.5 (2 x CH), 128.9 (2 x CH), 128.8 (CH), 128.6 (2 x CH), 128.2 (CH), 127.5 (2 x CH), 127.4 (CH), 127.2 (CH), 126.5 (CH), 120.7 (C).

3-(4-Bromophenyl)-2-phenylquinazolin-4(3*H*)-one (3ao)

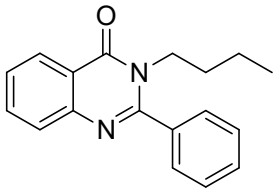


(CCDC number: 2057342)

^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 8.20 (d, J = 8.0 Hz, 1H), 7.91 (t, J = 8.0 Hz, 1H), 7.77 (d, J= 8.0 Hz, 1H), 7.61 (t, J = 8.0 Hz, 1H), 7.52 (d, J= 9.0 Hz, 2H), 7.39- 7.38 (m, 2H), 7.33 (d, J = 8.5 Hz, 2H), 7.29- 7.25 (m, 3H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 161.4 (C), 154.8 (C), 147.2 (C), 137.3 (C), 135.4 (C), 134.9 (CH), 131.7 (2 x CH), 131.6 (2 x CH), 129.1 (CH), 128.9 (2 x CH), 127.6 (2 x CH), 127.4 (CH), 127.2 (CH), 126.5 (CH), 121.3 (C), 120.7 (C).

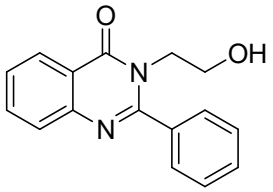
3-Butyl-2-phenylquinazolin-4(3*H*)-one (3ap)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 8.34- 8.32 (m, 1H), 7.77-7.72 (m, 2H), 7.54- 7.48 (m, 6H), 4.00- 3.97 (m, 2H), 1.62- 1.56 (m, 2H), 1.21- 1.14 (m, 2H), 0.76 (t, J = 2.5 Hz, 3H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 162.2 (C), 156.2 (C), 147.2 (C), 135.6 (C), 134.2 (CH), 129.8 (CH), 128.7 (2 x CH), 127.8 (2 x CH), 127.5 (CH), 126.9 (CH), 126.8 (CH), 121.0 (C), 45.7 (CH_2), 30.7 (CH_2), 19.9 (CH_2), 13.4 (CH_3).

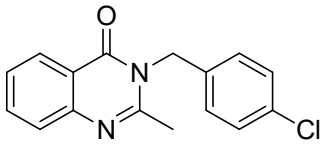
3-(2-Hydroxyethyl)-2-phenylquinazolin-4(3*H*)-one (3aq)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 8.31- 8.30 (m, 1H), 7.79-7.73 (m, 2H), 7.54- 7.50 (m, 6H), 4.22- 4.19 (m, 2H), 3.83- 3.81 (m, 2H), 2.94- 2.88 (m, 1H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 163.9 (C), 156.3 (C), 147.4 (C), 135.4 (C), 134.9 (CH), 130.1 (CH), 129.1 (2 x CH), 128.3 (2 x CH), 127.7 (CH), 127.4 (CH), 126.5 (CH), 120.7 (C), 61.7 (CH_2), 49.0 (CH_2).

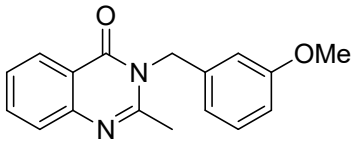
3-(4-Chlorobenzyl)- 2-methylquinazolin-4(3*H*)-one (3wg)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 8.13 (d, J = 7.0 Hz, 1H), 7.86- 7.83 (m, 1H), 7.66 (d, J= 8.0 Hz, 1H), 7.56- 7.52 (m, 2H), 7.34 (t, J= 7.0 Hz, 1H), 7.27 (t, J = 7.5 Hz, 1H), 6.81 (d, J = 7.5 Hz, 1H), 5.38 (s, 1H), 2.46 (s, 3H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 161.3 (C), 154.9 (C), 147.1 (C), 134.7 (CH), 133.4 (CH), 131.5 (C), 129.6 (CH), 129.0 (CH), 127.8 (CH), 126.7 (CH), 126.6 (CH), 126.4 (CH), 126.1 (CH), 119.7 (C), 44.7 (CH_2), 22.6 (CH_3).

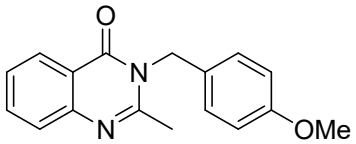
2-Methyl-3-(3-methoxybenzyl)quinazolin-4(3*H*)-one (3wd)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 8.15 (dd, J = 8.0, 1.5 Hz, 1H), 7.84- 7.80 (m, 1H), 7.62 (d, J= 8.0 Hz, 1H), 7.51 (t, J = 7.5Hz, 1H), 7.25 (t, J = 8.0 Hz, 1H), 6.85 (dd, J = 8.0, 2.0 Hz, 1H), 6.78 (m, 1H), 6.69 (d, J = 7.5 Hz, 1H), 5.35 (s, 2H), 3.72 (s, 3H), 2.48 (s, 3H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 161.5 (C), 159.5 (C), 155.1 (C), 147.1 (C), 138.1 (C), 134.5 (CH), 130.0 (C), 126.6 (CH), 126.5 (CH), 126.4 (CH), 119.8 (CH), 118.1 (CH), 112.5 (CH), 112.4 (CH), 55.0 (CH_2), 46.2 (CH_3), 22.9 (CH_3).

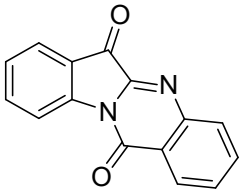
2-Methyl-3-(4-methoxybenzyl)quinazolin-4(3*H*)-one (3we)



^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ_H 8.15 (dd, J = 8.0, 1.5 Hz, 1H), 7.82 (ddd, J = 8.5, 7.5, 1.5 Hz, 1H), 7.62 (d, J= 8.0 Hz, 1H), 7.53- 7.50 (m, 1H), 7.25 (t, J = 8.0 Hz, 1H), 6.85 (dd, J = 8.0, 2.0 Hz, 1H), 6.78 (m, 1H), 6.69 (d, J = 7.5 Hz, 1H), 5.35 (s, 2H), 3.72 (s, 3H), 2.48 (s, 3H).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ_C 161.0 (C), 154.9 (C), 147.0 (C), 138.3 (C), 134.3 (C), 128.8 (2 x CH), 128.6 (2 x CH), 126.6 (CH), 126.5 (CH), 126.2 (CH), 126.1 (CH), 119.9 (C), 45.6 (CH_2), 33.6 (CH_3), 22.7 (CH_3).

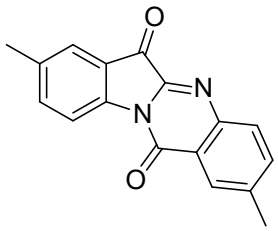
Indolo[2,1-*b*]quinazoline-6,12-dione (4aa)



^{1}H NMR (500 MHz, DMSO-d_6, ppm): δ_H 8.49 (d, J = 8.0 Hz, 1H), 8.33 (d, J = 8.0 Hz, 1H), 7.95 (d, J = 3.5 Hz, 2H), 7.89- 7.86 (m, 2H), 7.76- 7.73 (m, 1H), 7.48 (t, J = 7.5 Hz, 1H).

^{13}C NMR (125 MHz, DMSO-d_6, ppm): δ_C 182.5 (C), 157.7 (C), 146.5 (C), 145.9 (C), 145.0 (C), 137.7 (CH), 135.2 (CH), 129.9 (CH), 129.8 (CH), 126.9 (2 x CH), 124.7 (CH), 123.3 (C), 122.3 (C), 117.0 (CH).

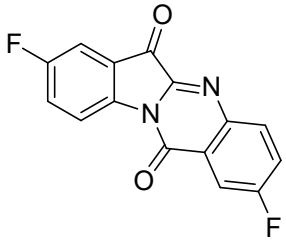
2,8-dimethylindolo[2,1-*b*]quinazoline-6,12-dione (4bb)



^{1}H NMR (500 MHz, DMSO-d_6, ppm): δ_H 8.34 (d, J = 8.0 Hz, 1H), 8.11 (s, 1H), 7.83 (d, J = 8.0 Hz, 1H), 7.75 (dd, J = 8.5, 1.5 Hz, 1H), 7.68- 7.66 (m, 2H), 2.52 (s, 3H), 2.41 (s, 3H).

^{13}C NMR (125 MHz, DMSO-d_6, ppm): δ_C 182.5 (C), 157.4 (C), 144.6 (C), 144.4 (C), 143.9 (C), 140.2 (C), 138.1 (CH), 136.6 (C), 136.1 (CH), 129.8 (CH), 126.5 (CH), 124.7 (CH), 123.1 (C), 122.4 (C), 116.8 (CH), 21.0 (CH3), 20.4 (CH3).

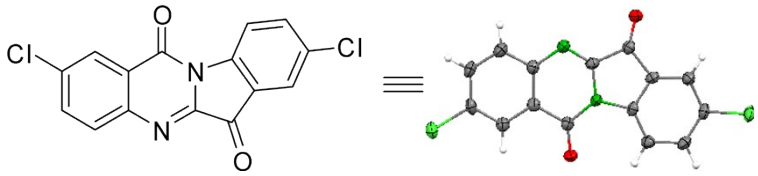
2,8-Difluoroindolo[2,1-*b*]quinazoline-6,12-dione (4cc)



^{1}H NMR (500 MHz, DMSO-d_6, ppm): δ_H 8.49 (dd, J = 8.5, 4.0 Hz, 1H), 8.07- 8.03 (m, 2H), 7.85 (td, J = 8.5, 3.5 Hz, 1H), 7.81 (dd, J = 7.0, 2.5 Hz, 1H), 7.74 (td, J = 9.0, 2.5 Hz, 1H).

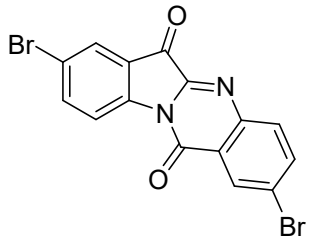
^{13}C NMR (125 MHz, DMSO-d_6, ppm): δ_C 181.4 (C), 163.1 (C), 161.4 (C), 160.3 (C-F), 156.8 (C), 144.9 (C), 142.7 (C-F), 132.8 (C_mH-CF), 125.1 (C), 125.0 (C), 123.9 (C_oH- CF), 123.4 (C_oH- CF), 118.9 (C_mH-CF), 112.4 (C_oH- CF), 111.7 (C_oH- CF).

NMR data of **2,8-dichloroindolo[2,1-*b*]quinazoline-6,12-dione (4dd)** was not collected because of its very poor solubility in various deuterated solvents.



X-ray crystal structure of compound **4dd (**CCDC number: 2057341)

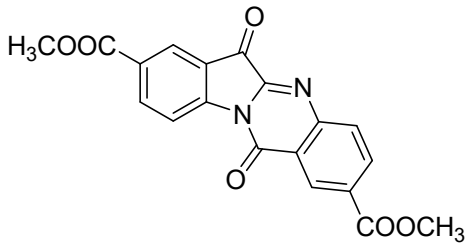
2,8-Dibromoindolo[2,1-*b*]quinazoline-6,12-dione (4ee)



^{1}H NMR (500 MHz, DMSO-d_6, ppm): δ_H 8.41- 8.39 (m, 2H), 8.14 (dd, J = 8.5, 2.5 Hz 1H), 8.09-8.06 (m, 2H), 7.92 (d, J = 8.5 Hz, 1H).

^{13}C NMR (125 MHz, DMSO-d_6, ppm): δ_C 182.5 (C), 157.4 (C), 144.6 (C), 144.4 (C), 143.9 (C), 140.2 (C), 138.1 (CH), 136.96(C), 136.1 (CH), 129.8 (CH), 126.5 (CH), 124.7 (CH), 123.1 (C), 122.4 (C), 116.8 (CH).

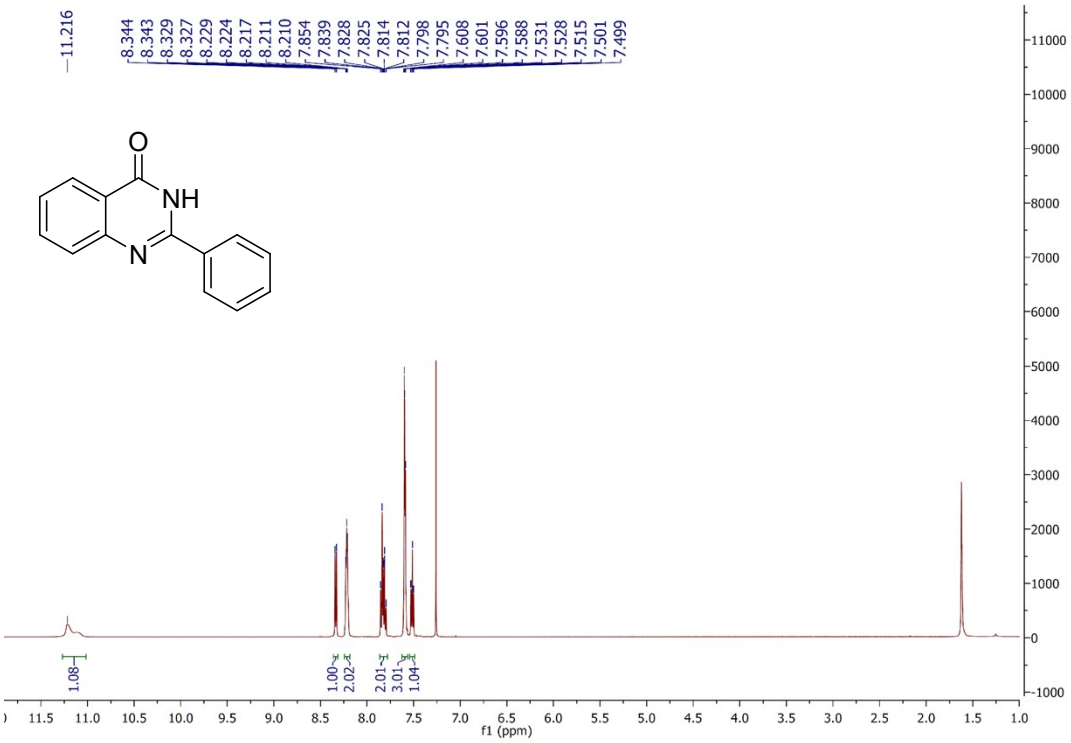
Dimethyl 6,12-dioxo-6,12-dihydroindolo[2,1-*b*]quinazoline-2,8-dicarboxylate (4ff)

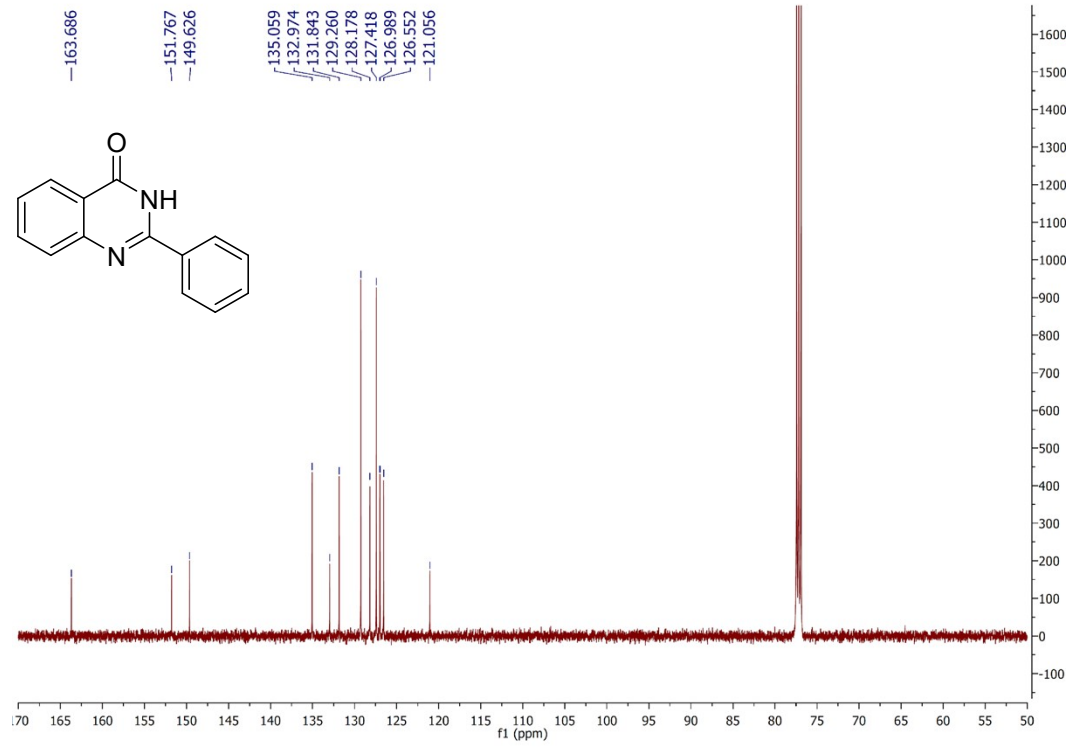


^{1}H NMR (500 MHz, DMSO-d_6, ppm): δ_H 8.83 (s, 1H), 8.62 (d, J = 8.5 Hz, 1H), 8.45 (dd, J = 14.0, 8.5 Hz, 2H), 8.30 (s, 1H), 8.10 (d, J = 8.5 Hz, 1H), 3.96 (s, 3H), 3.93 (s, 3H).

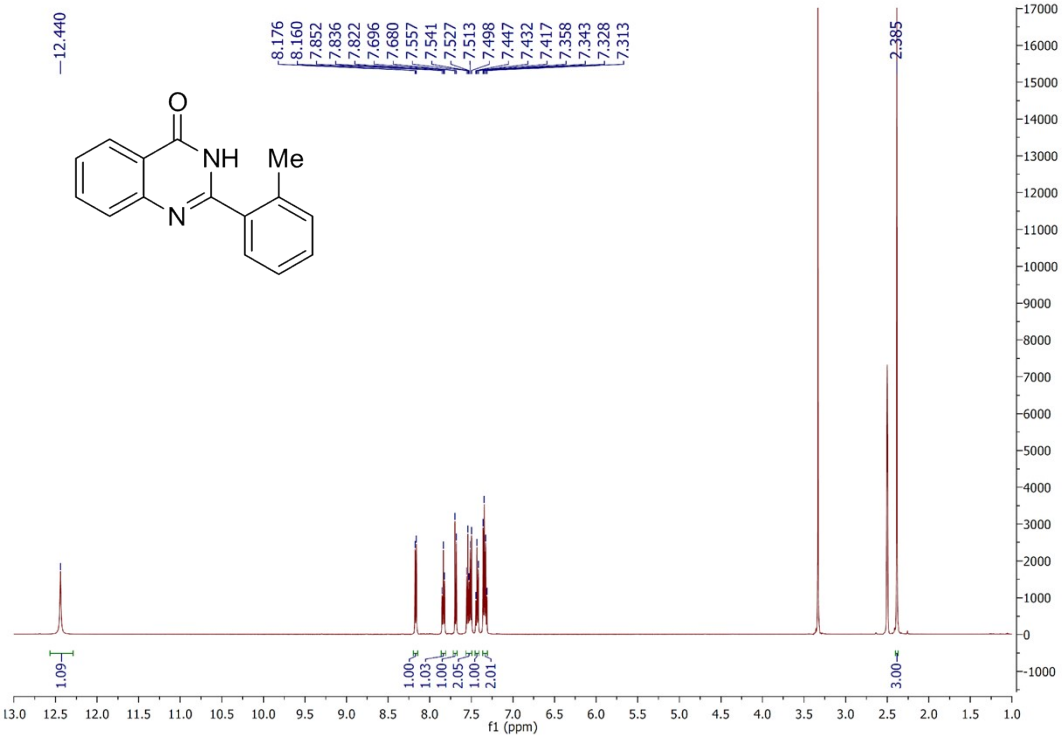
The ^{13}C-NMR data was not collected because of its very poor solubility in various deuterated solvents.

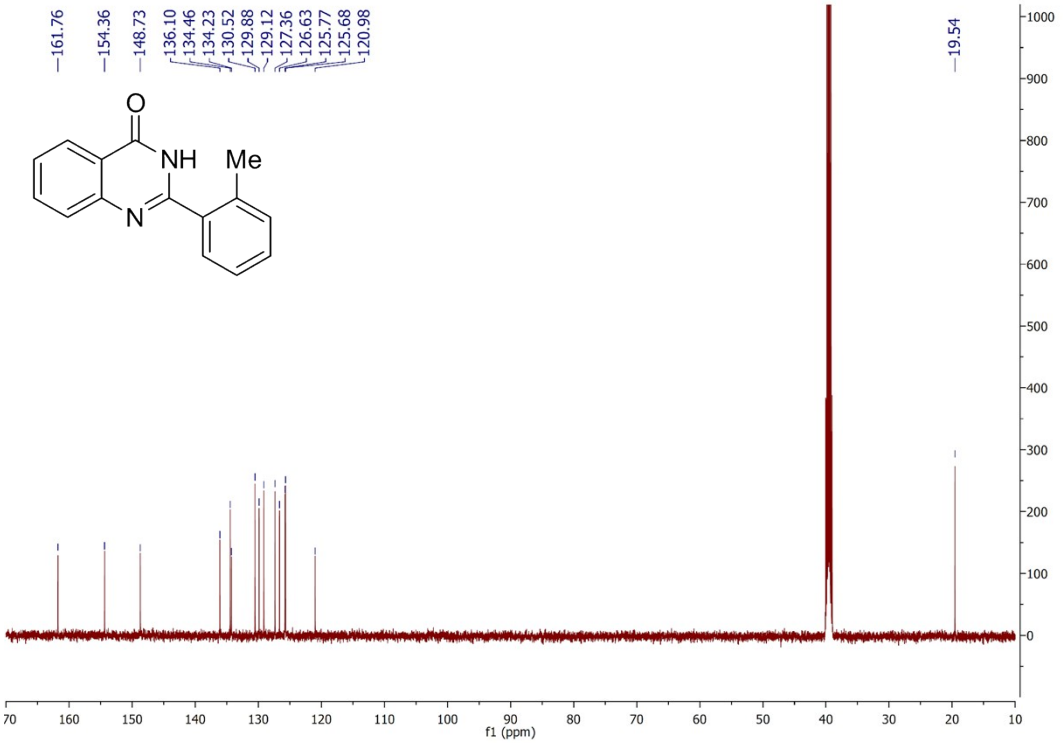
2-Phenylquinazolin-4(3*H*)-one (3aa)



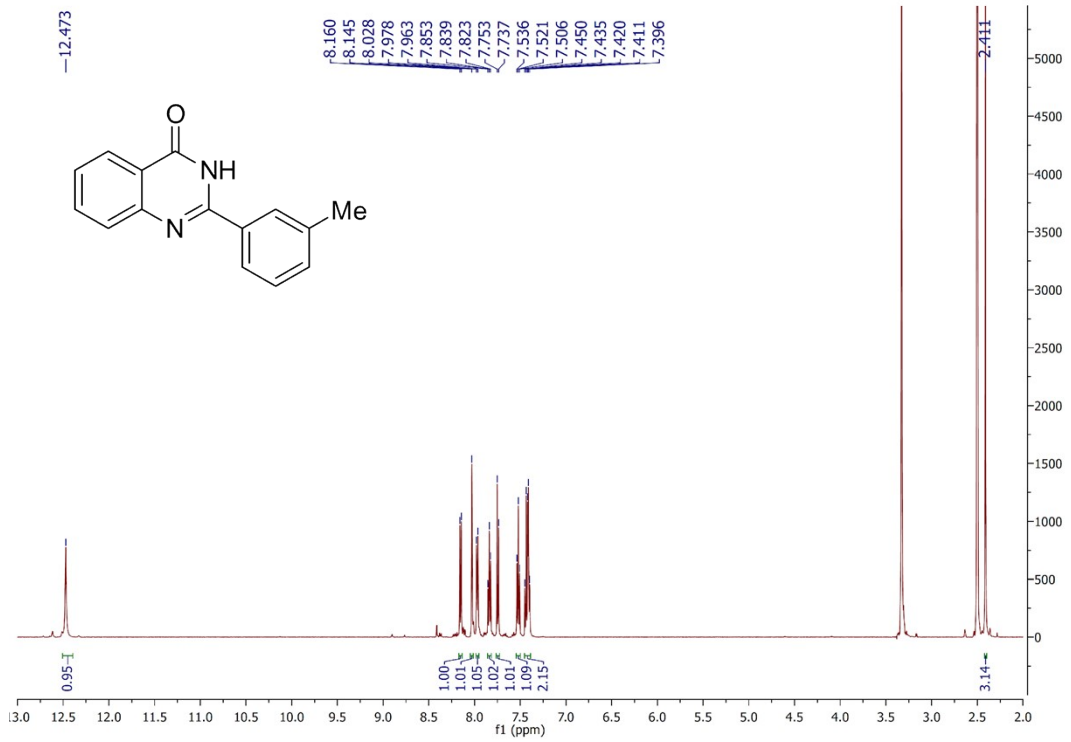


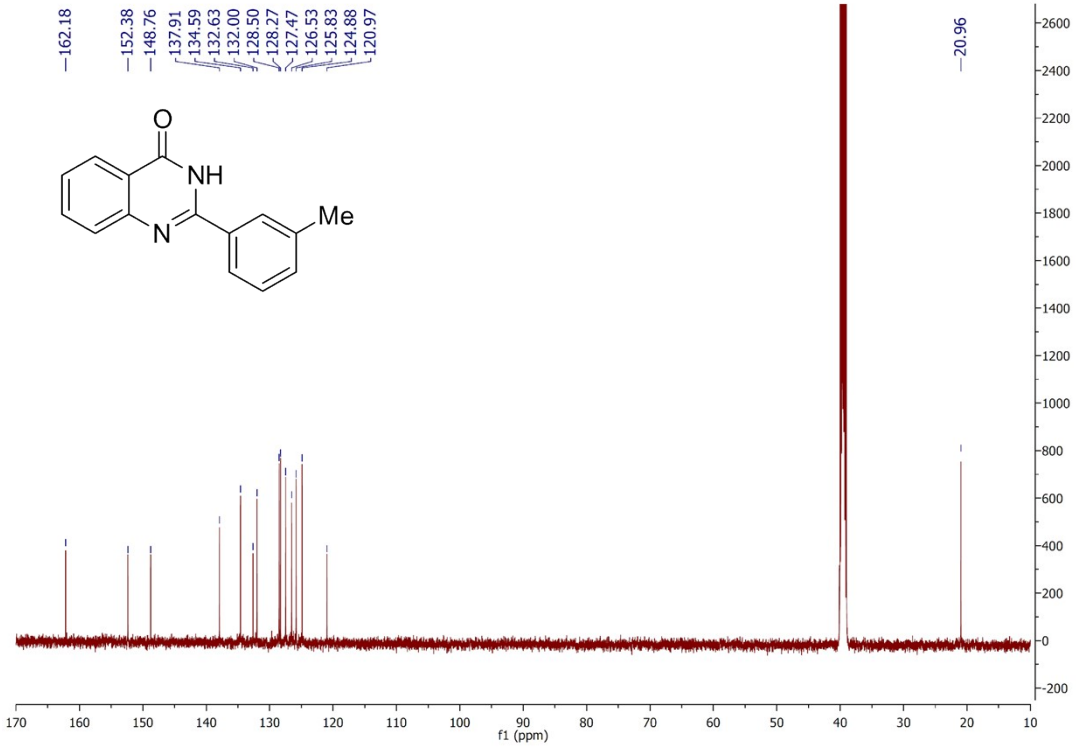
2-(2-Methylphenyl)quinazolin-4(3*H*)-one (3ba)



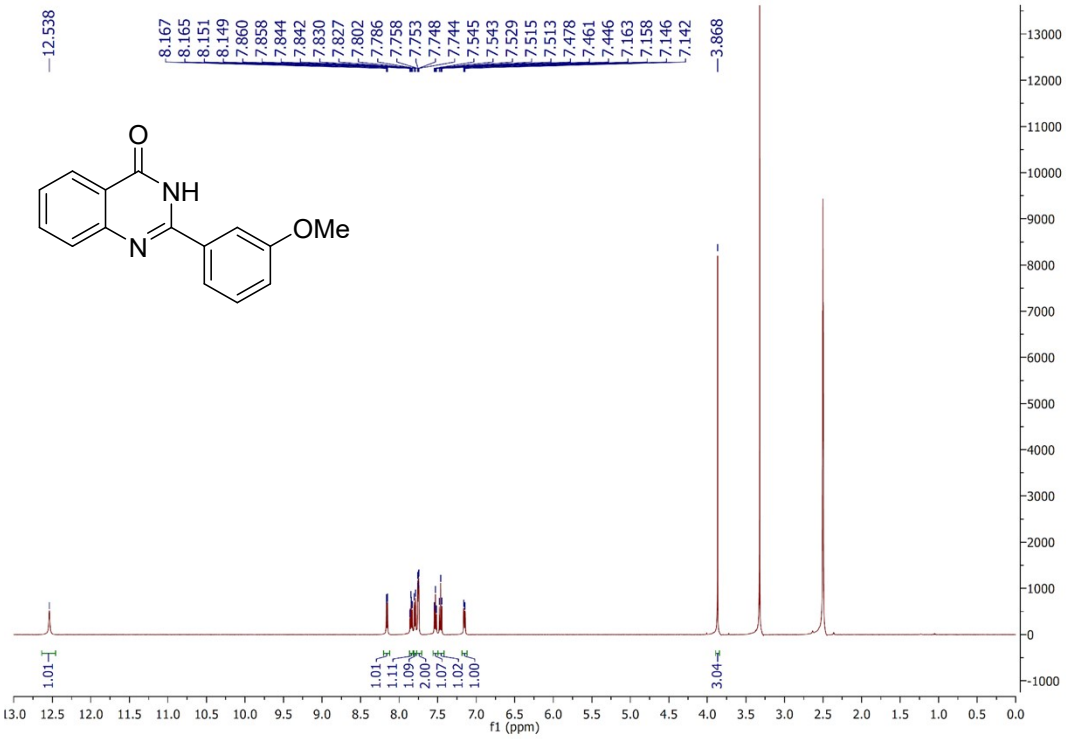


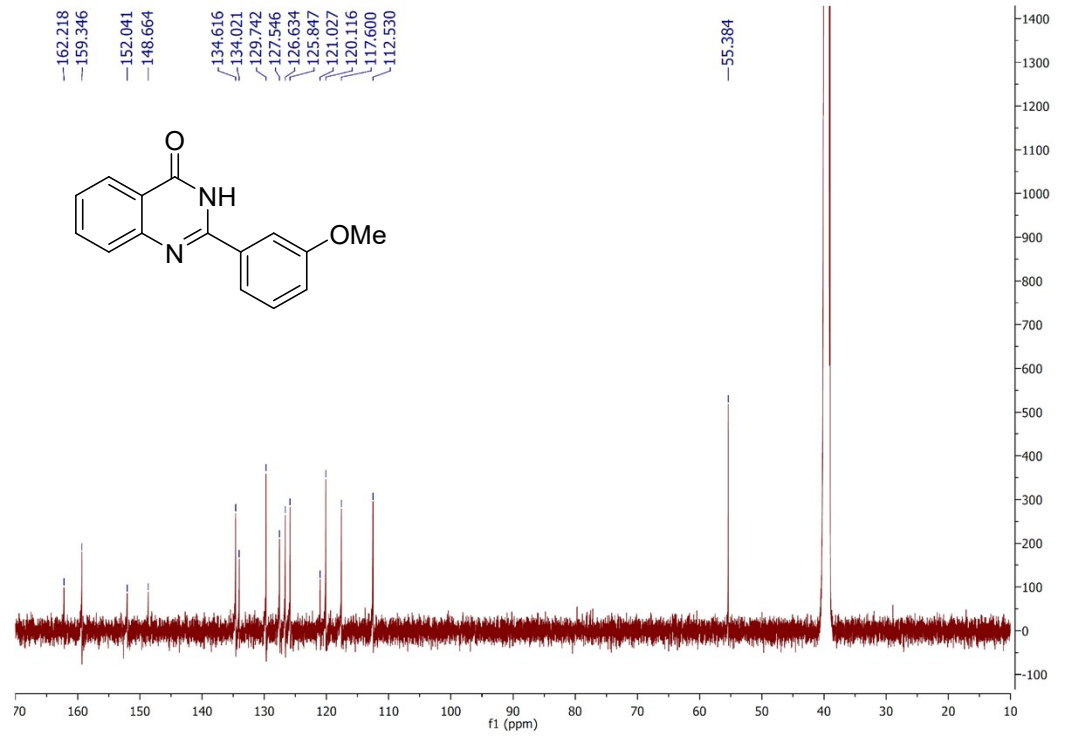
2-(3-Methylphenyl)quinazolin-4(3*H*)-one (3ca)



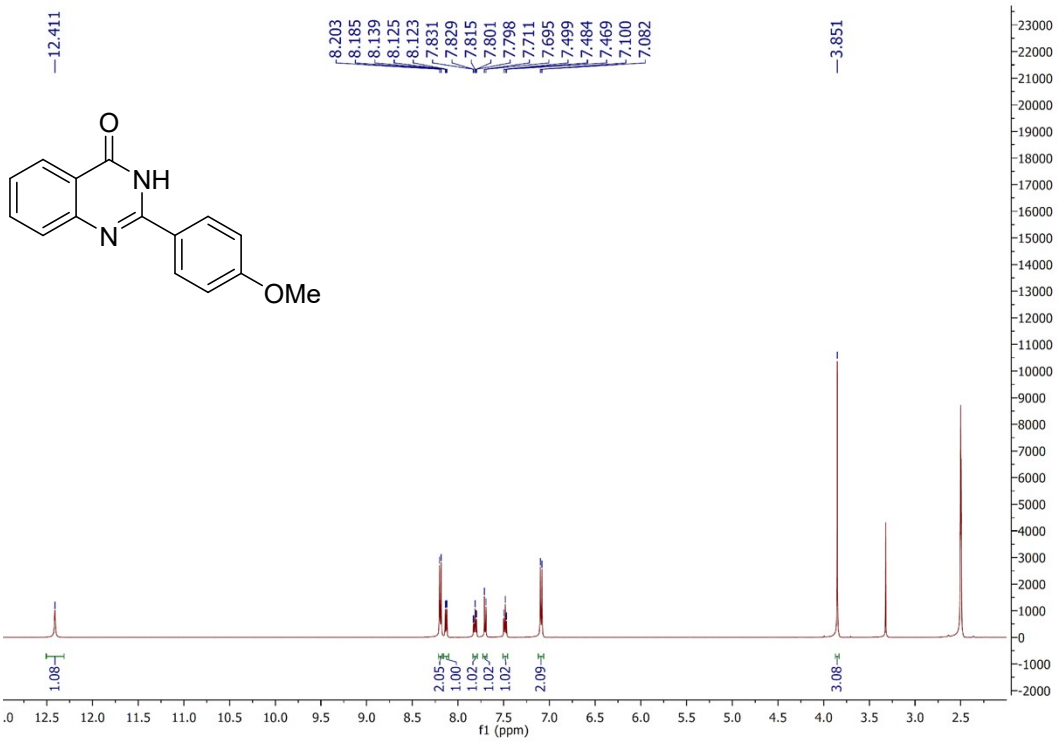


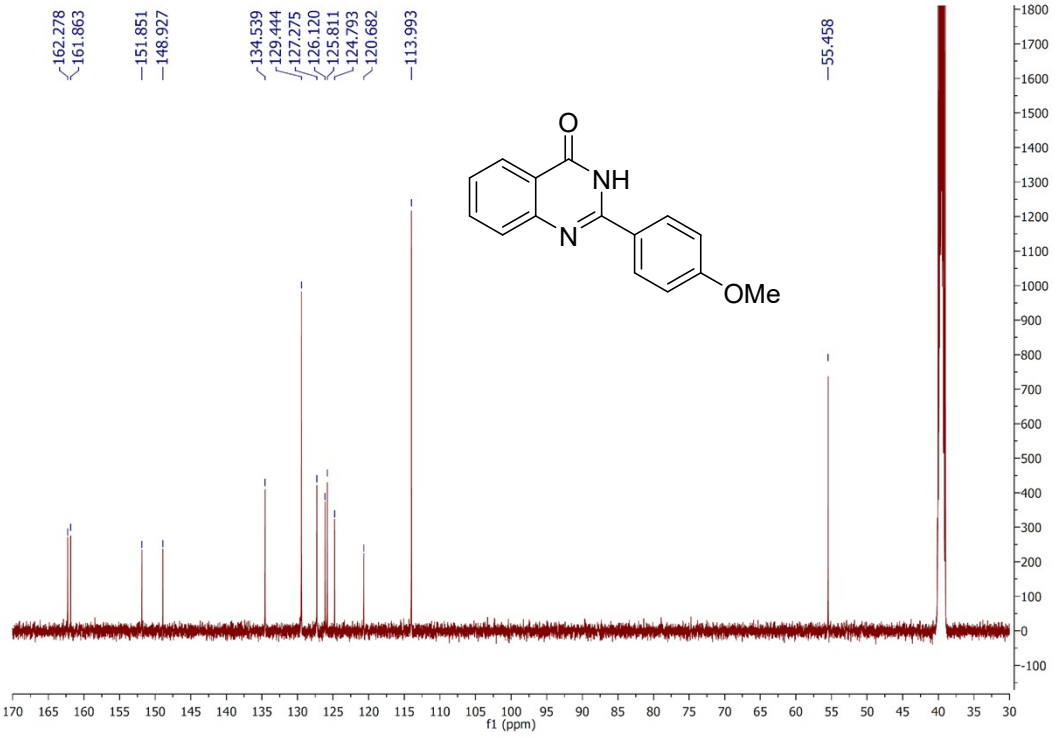
2-(3-Methoxyphenyl)quinazolin-4(3*H*)-one (3da)



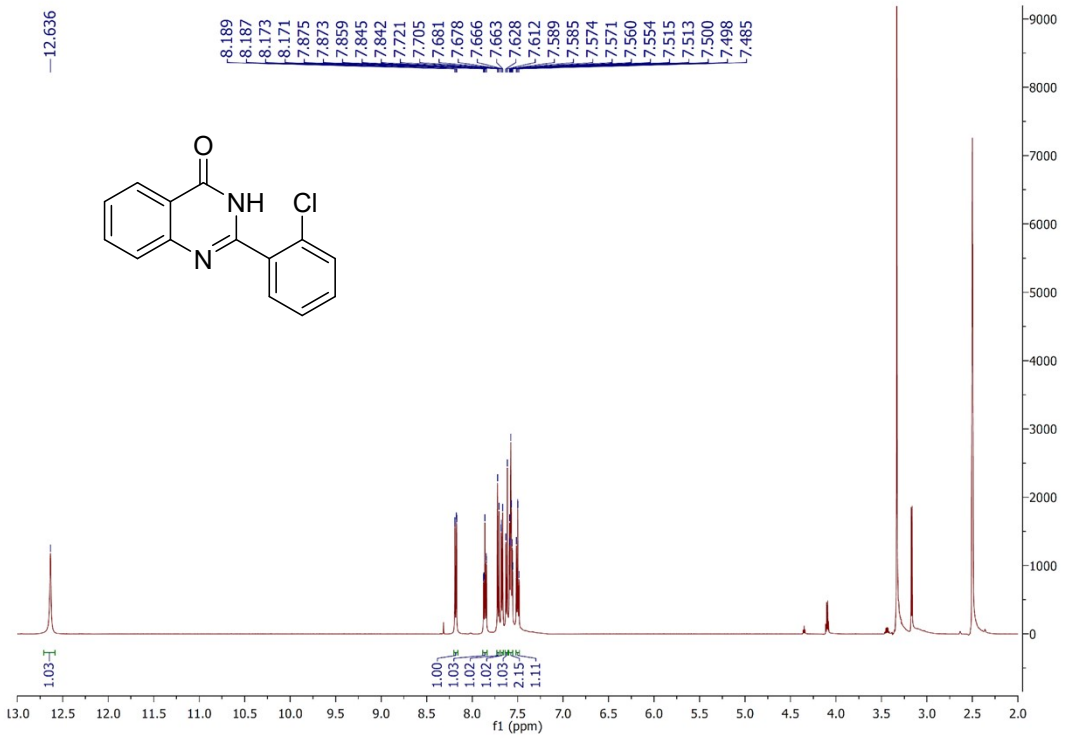


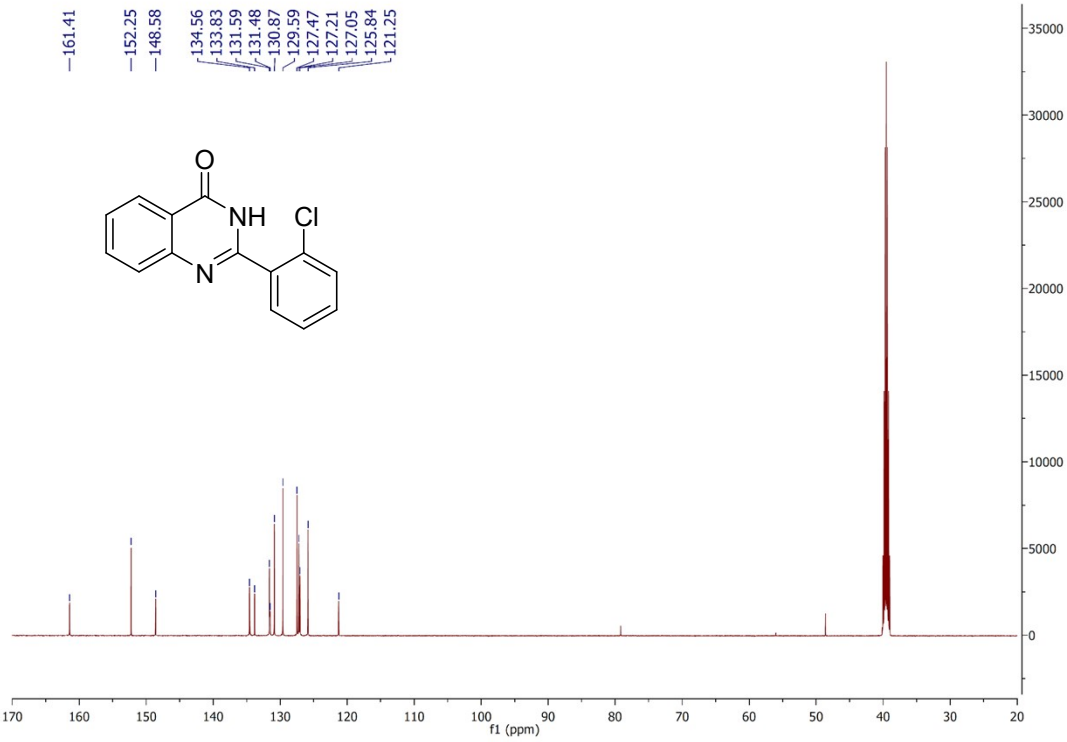
2-(4-Methoxyphenyl)quinazolin-4(*3H*)-one (3ea)



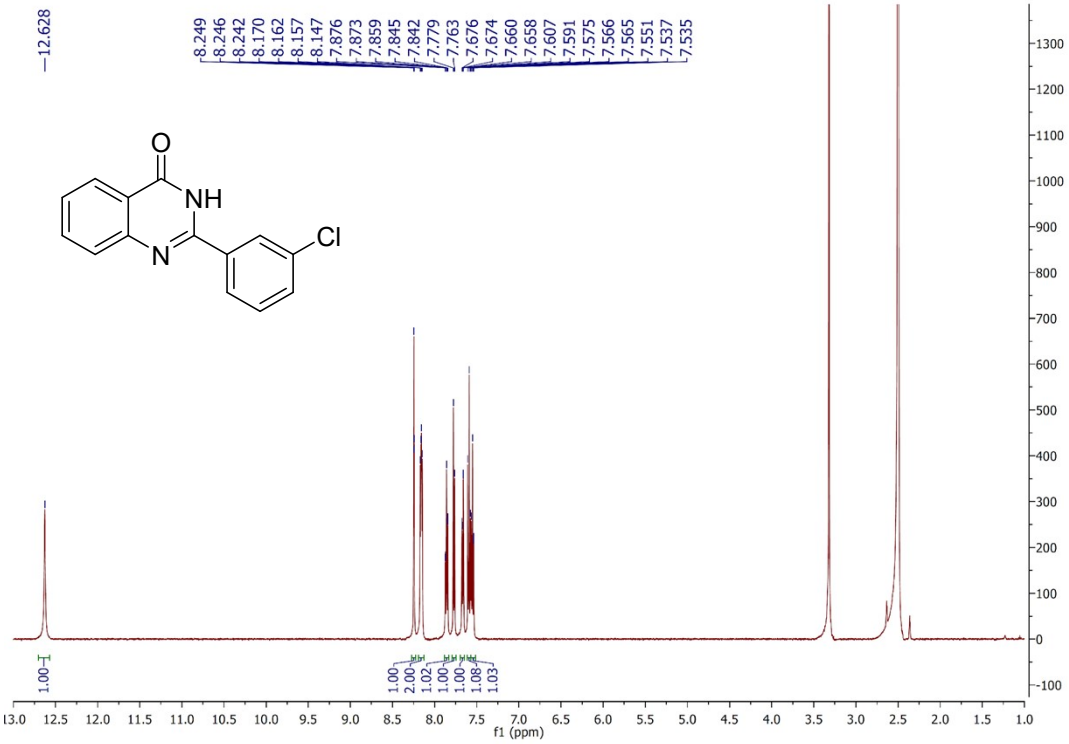


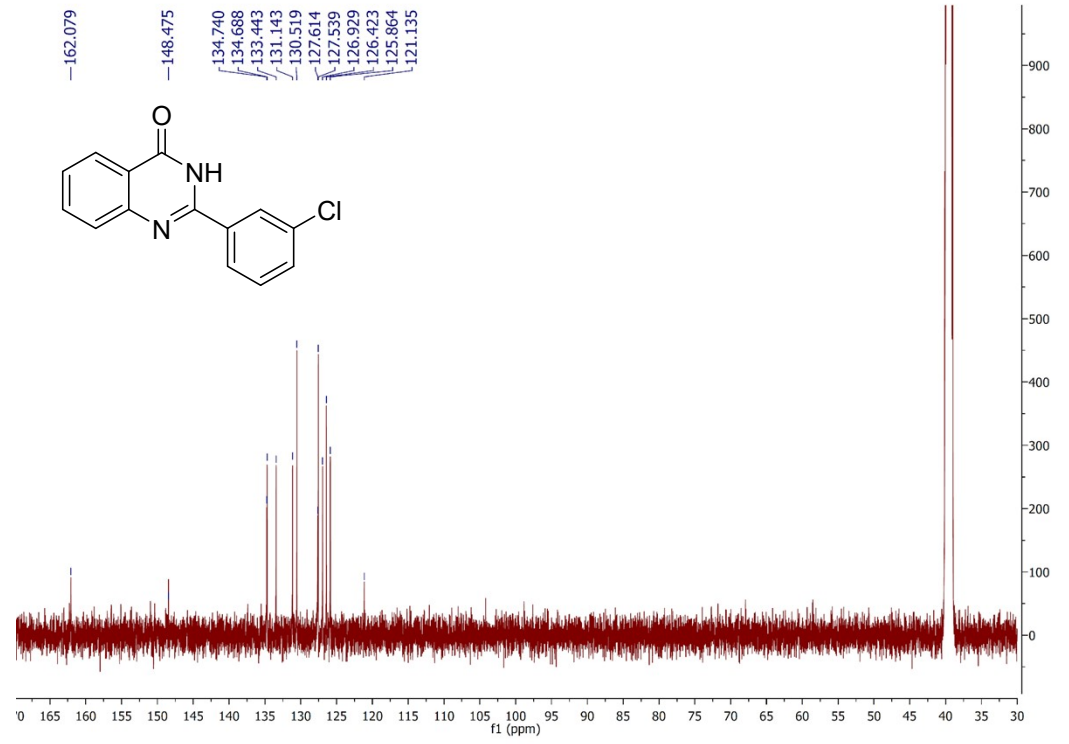
2-(2-Chlorophenyl)quinazolin-4(*3H*)-one (3fa)



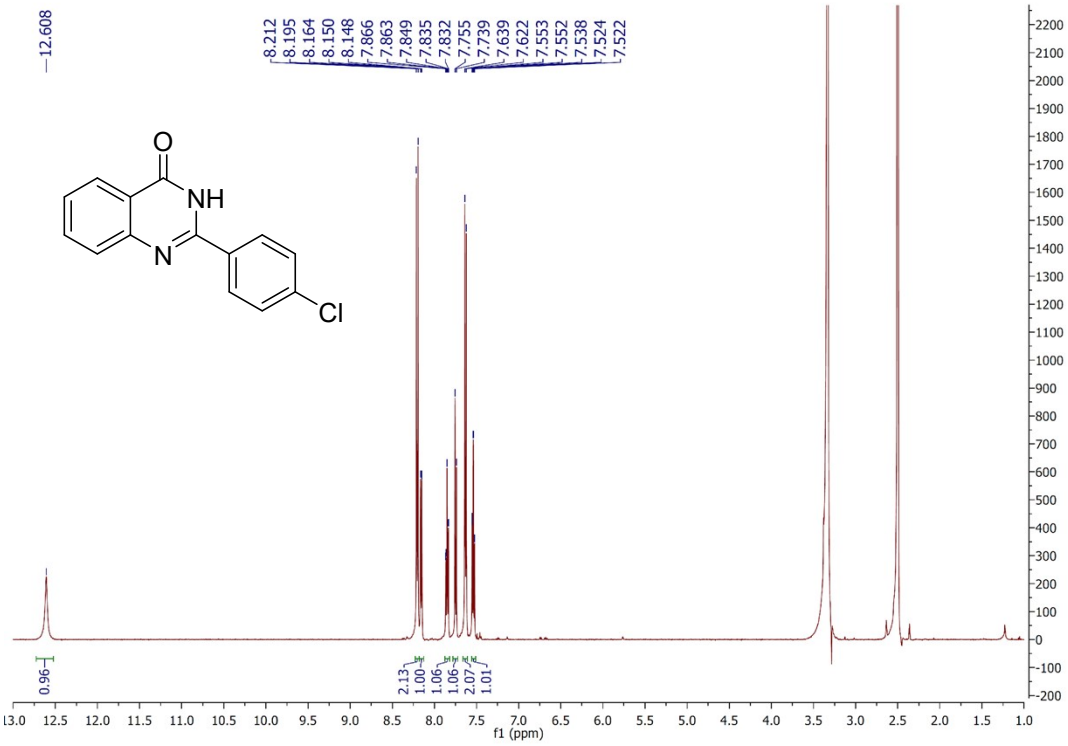


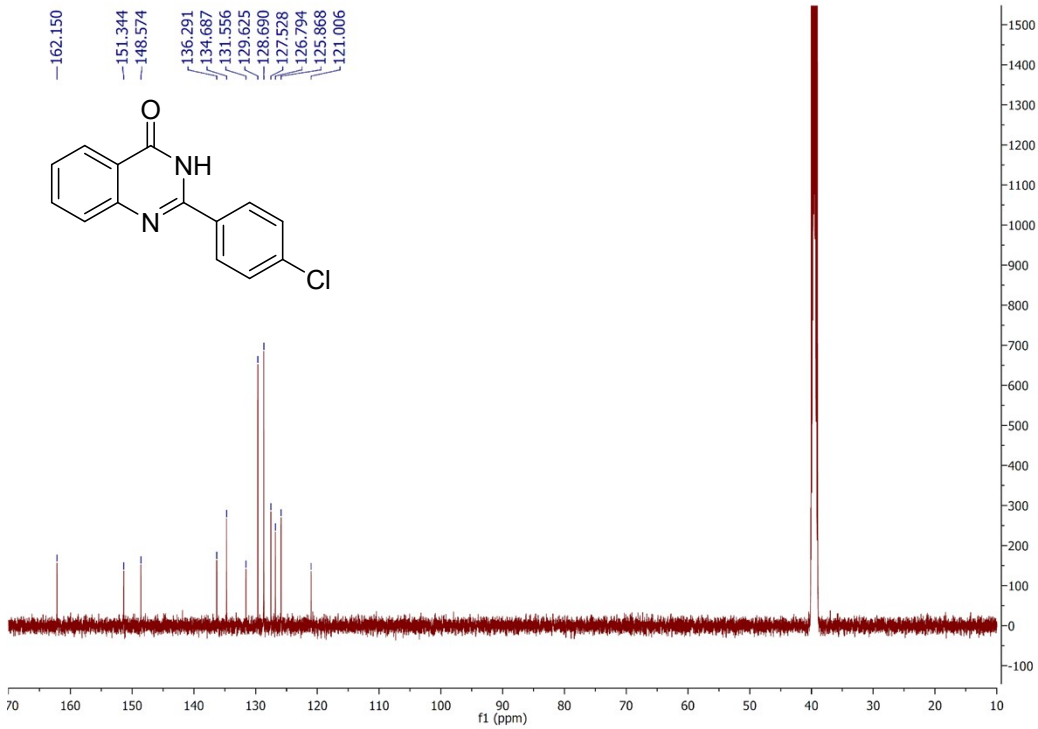
2-(3-Chlorophenyl)quinazolin-4(*3H*)-one (3ga)



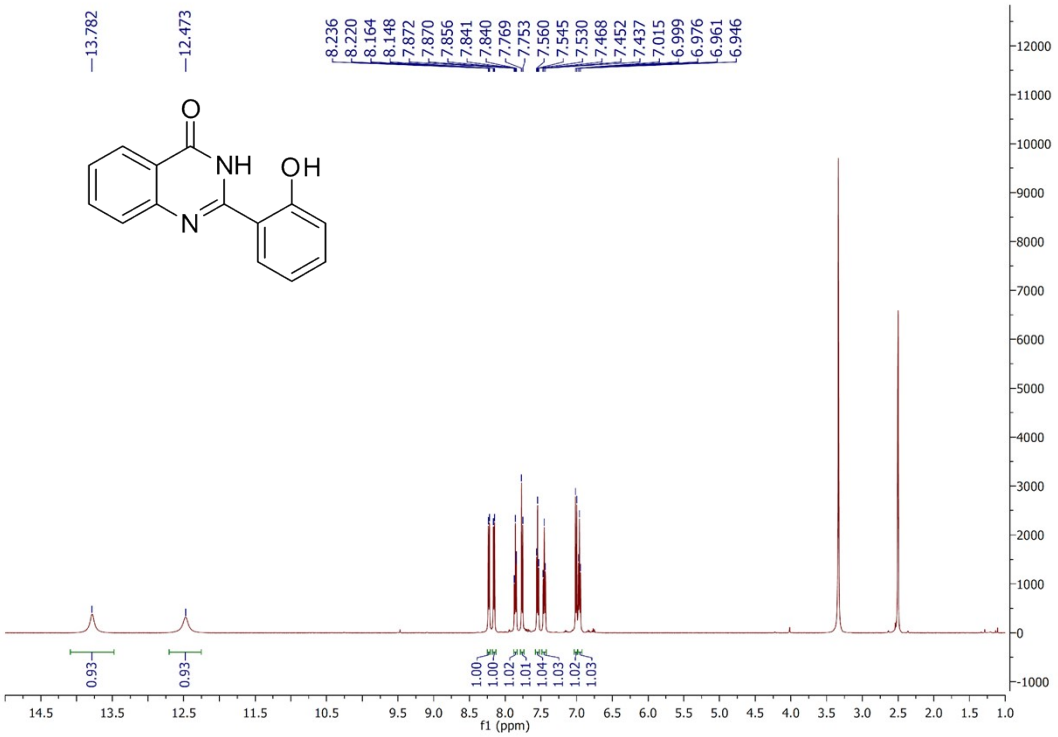


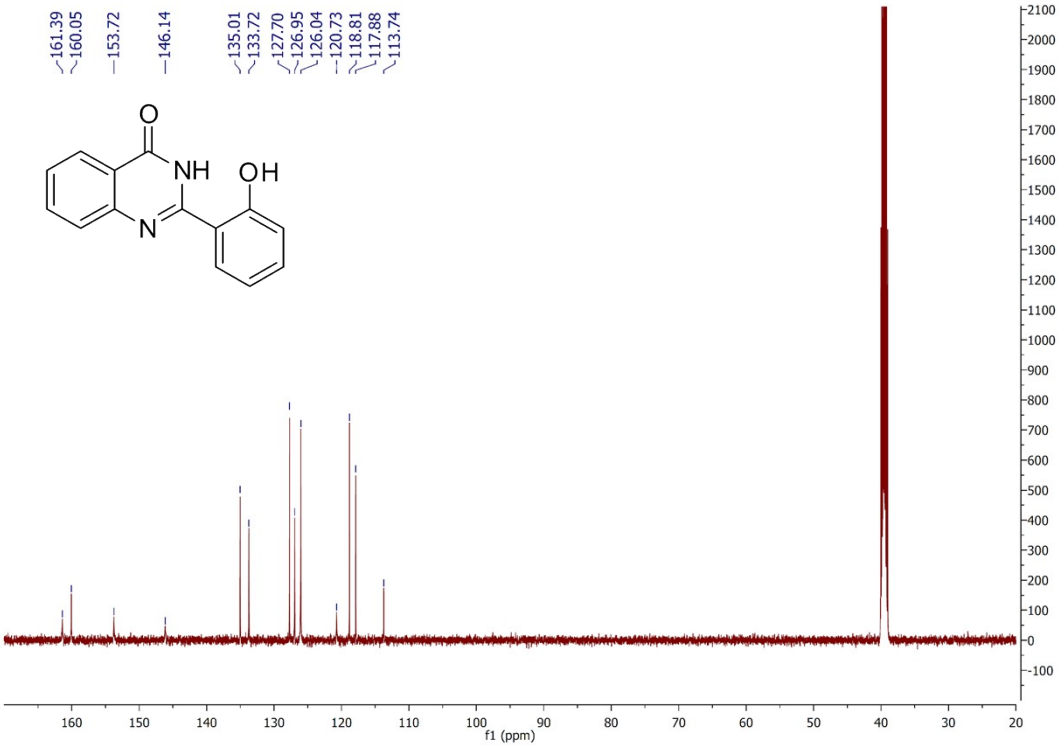
2-(4-Chlorophenyl)quinazolin-4(*3H*)-one (3ha)



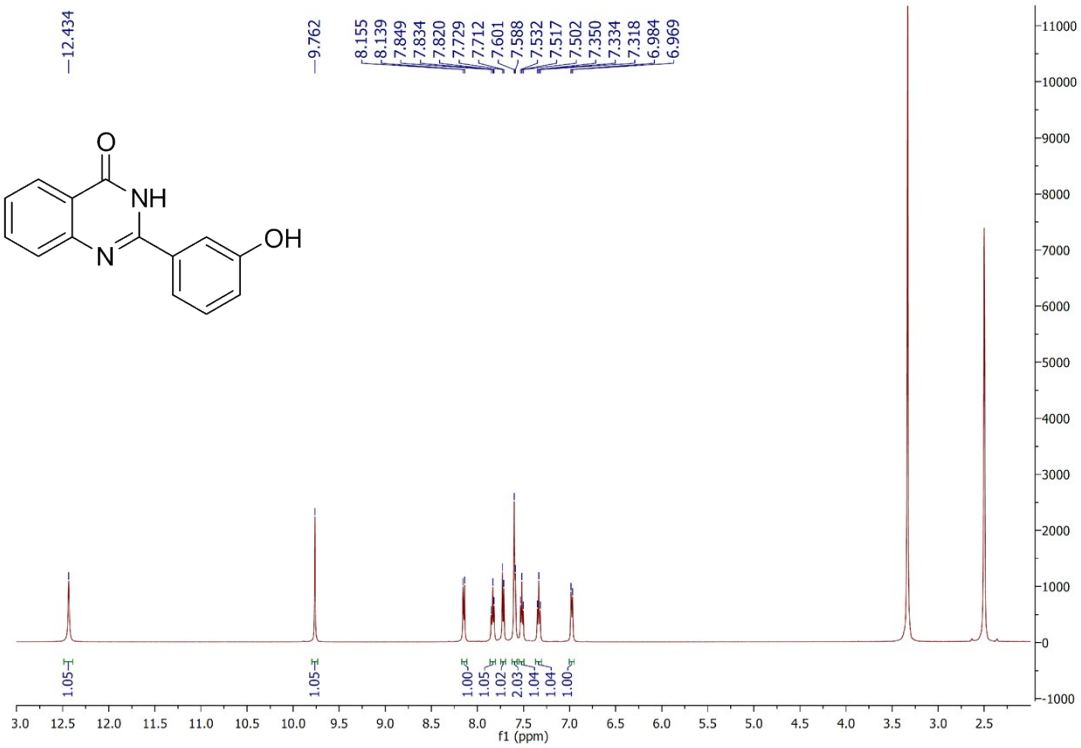


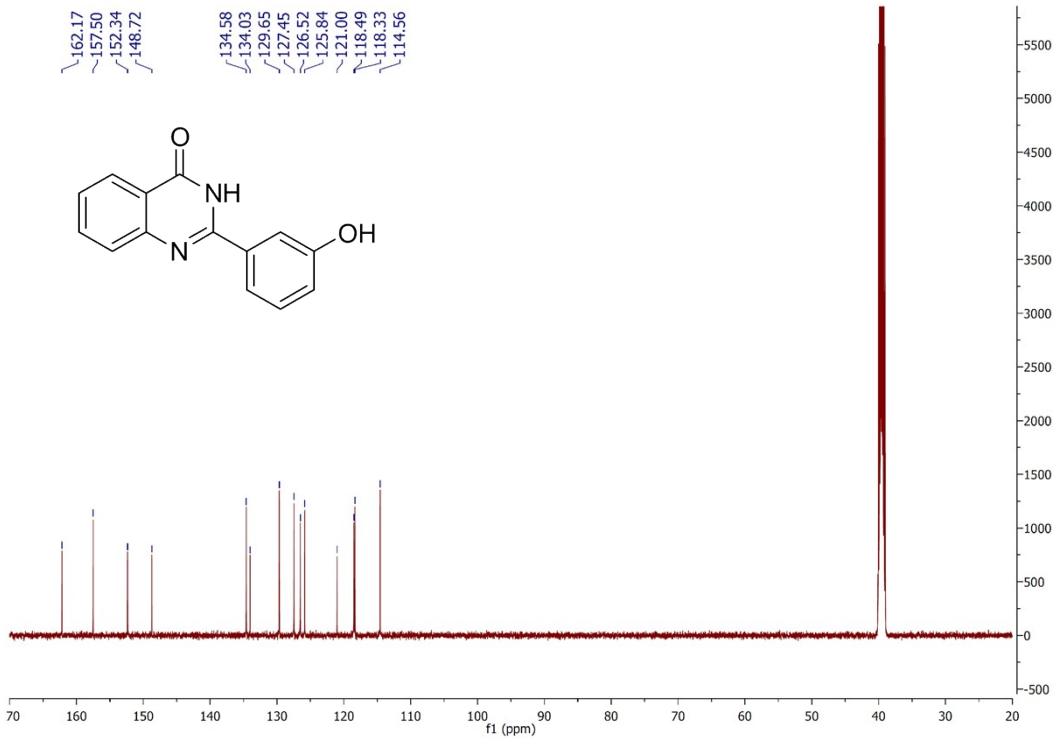
2-(2-Hydroxyphenyl)quinazolin-4(3*H*)-one (3ia)



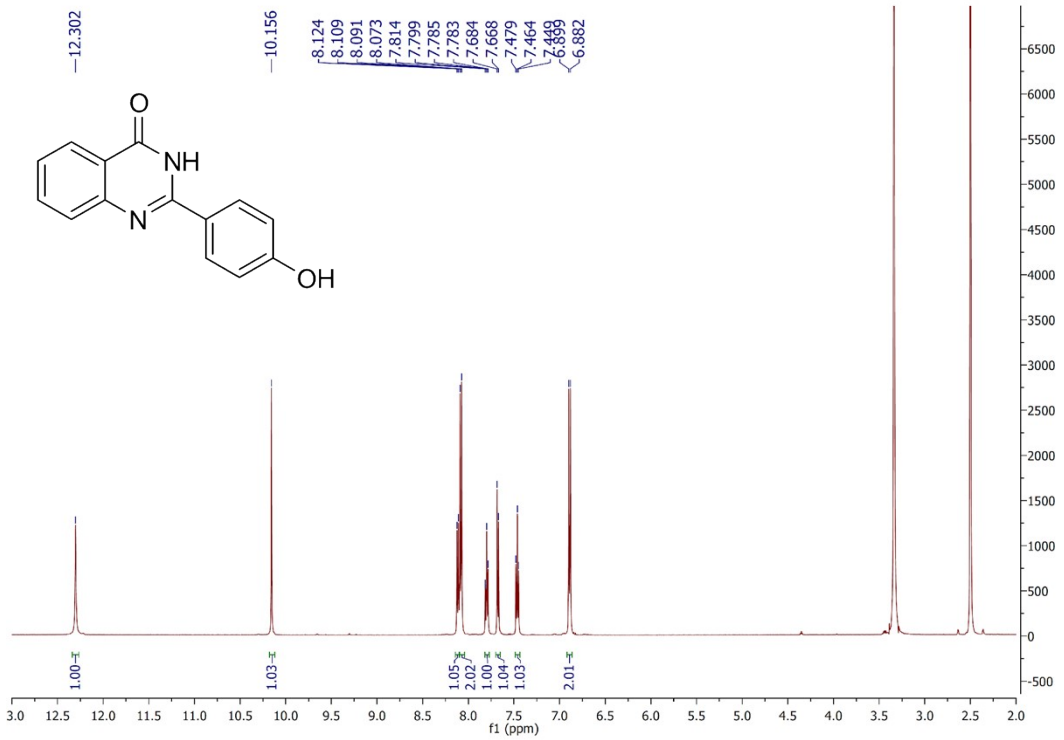


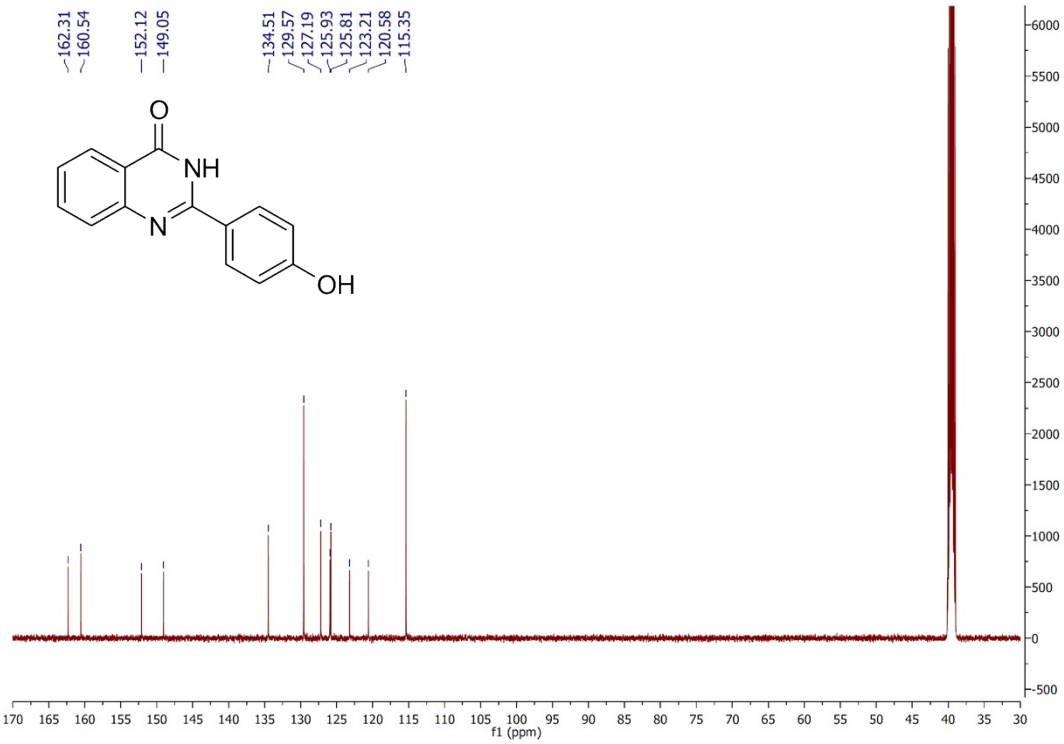
2-(3-Hydroxyphenyl)quinazolin-4(3*H*)-one (3ja)



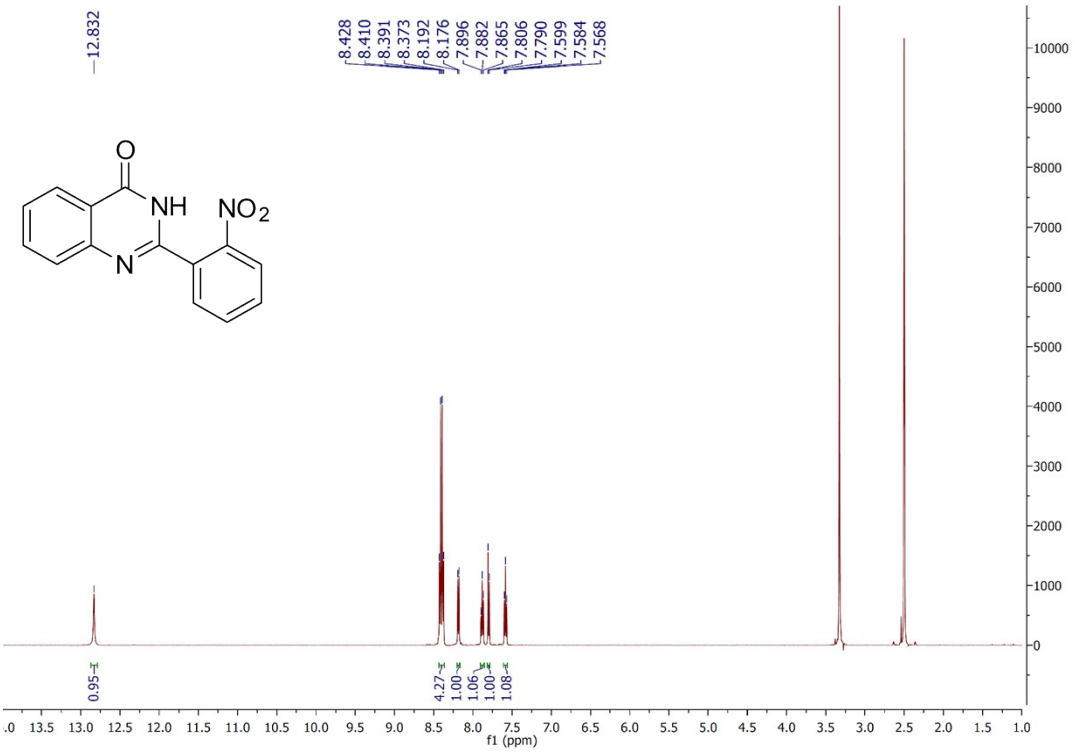


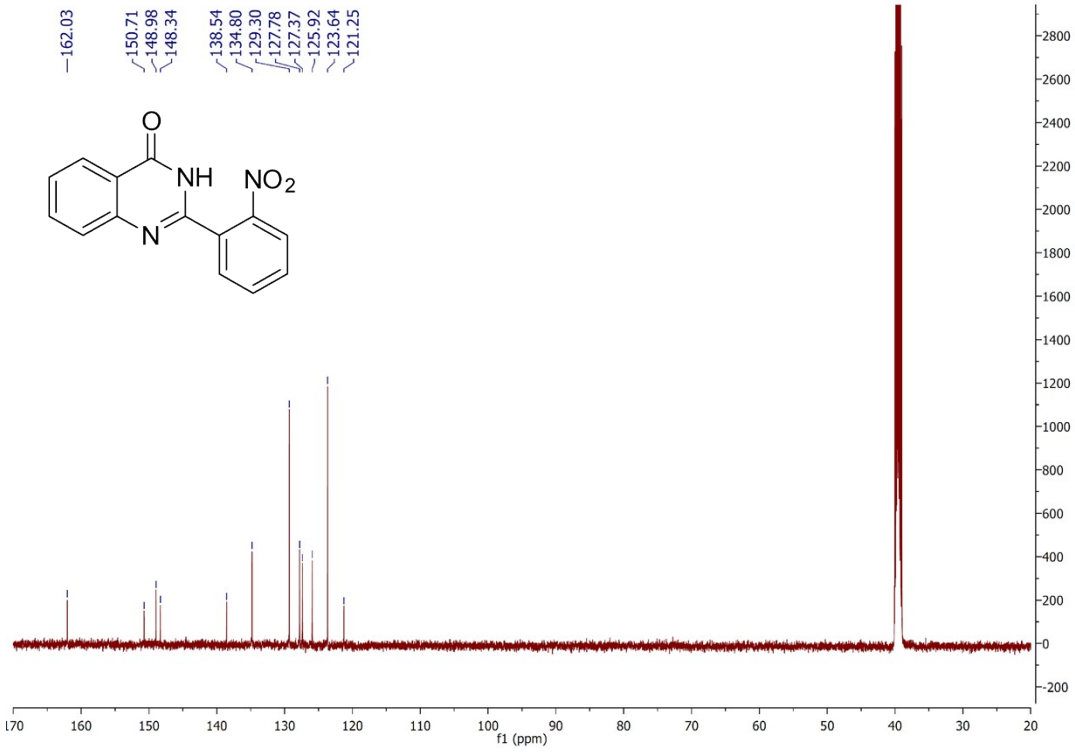
2-(4-Hydroxyphenyl)quinazolin-4(3*H*)-one (3ka)



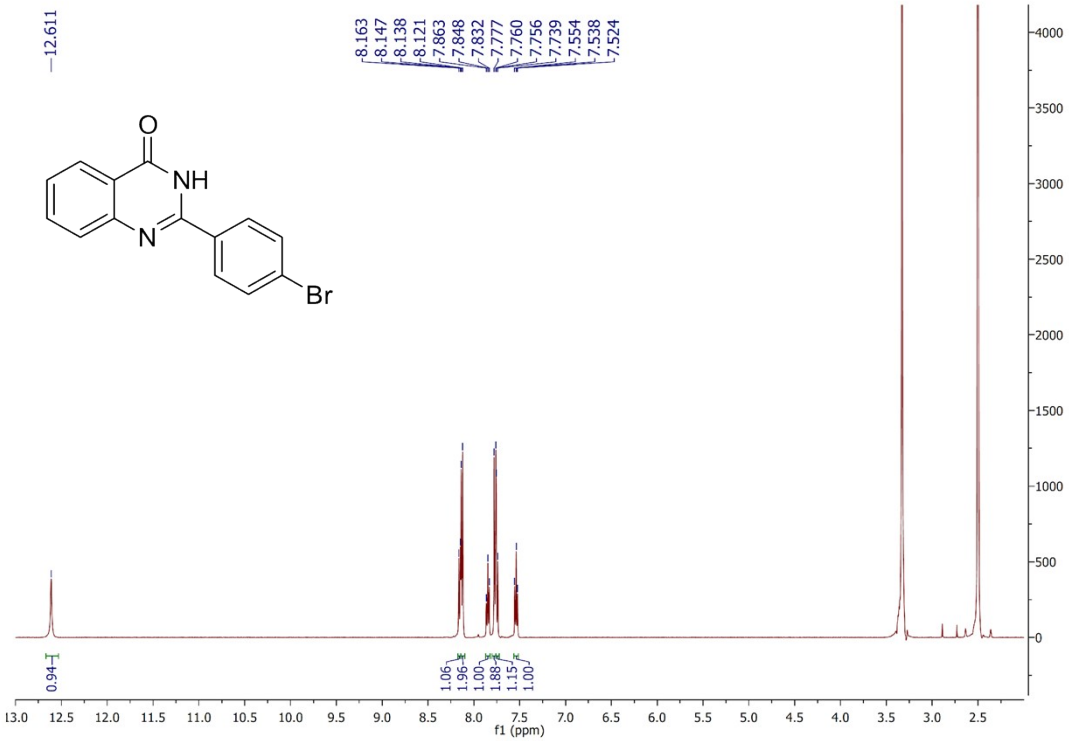


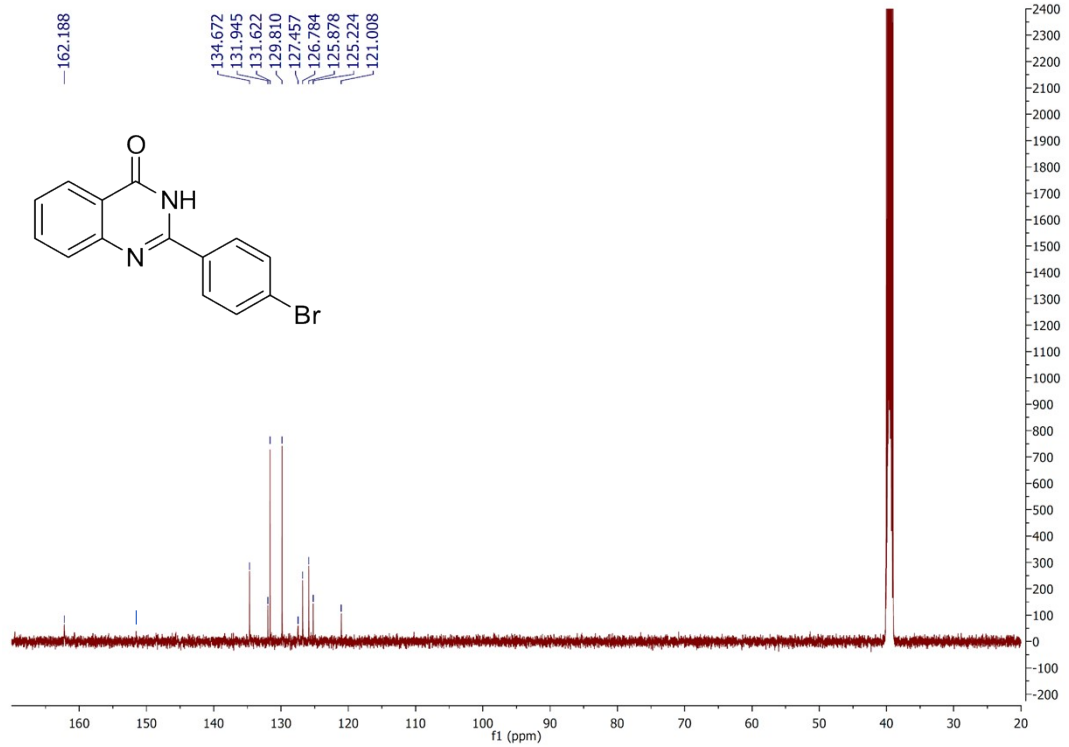
2-(2-Nitrophenyl)quinazolin-4(3*H*)-one (3la)



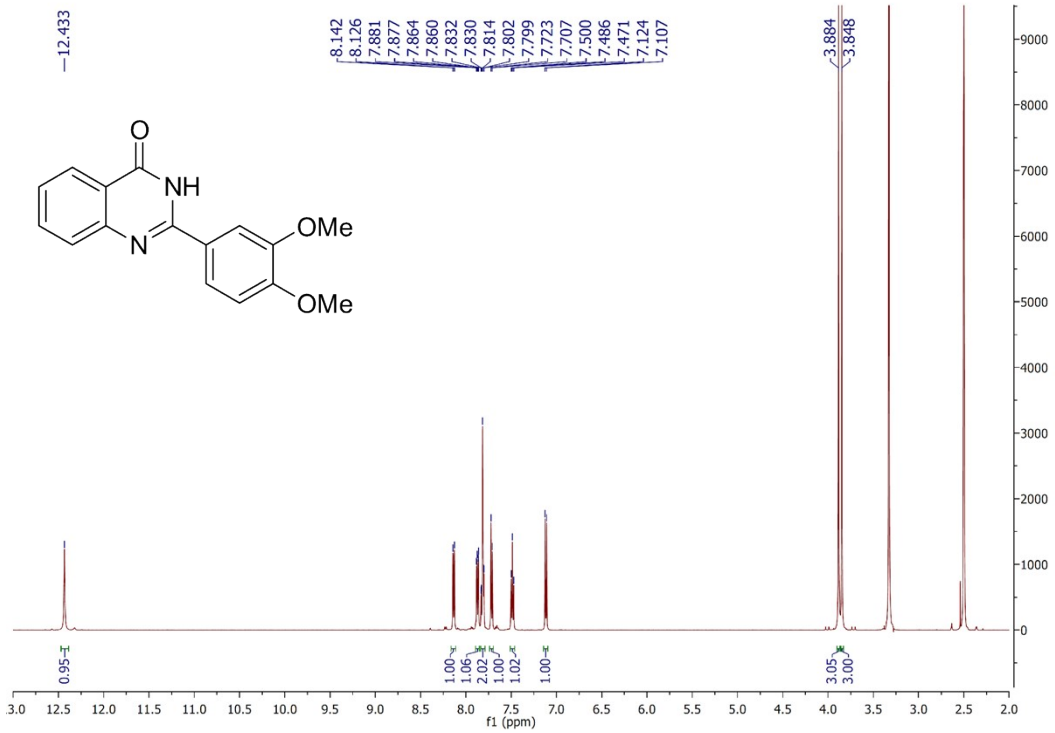


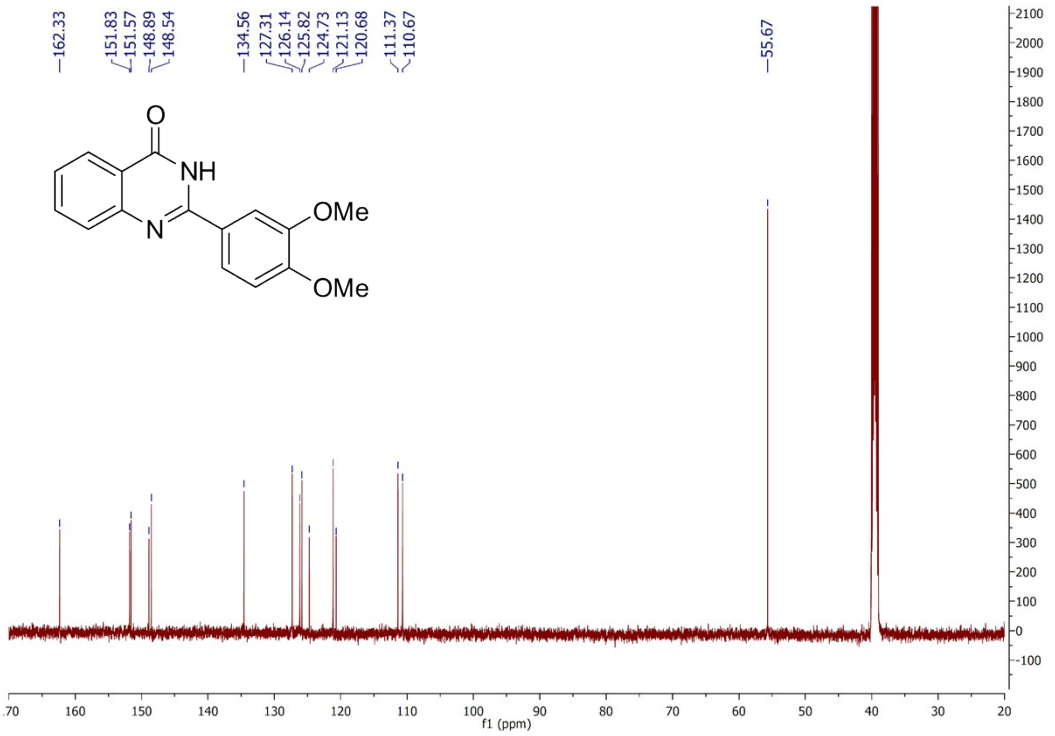
2-(4-Bromophenyl)quinazolin-4(3*H*)-one (3ma)



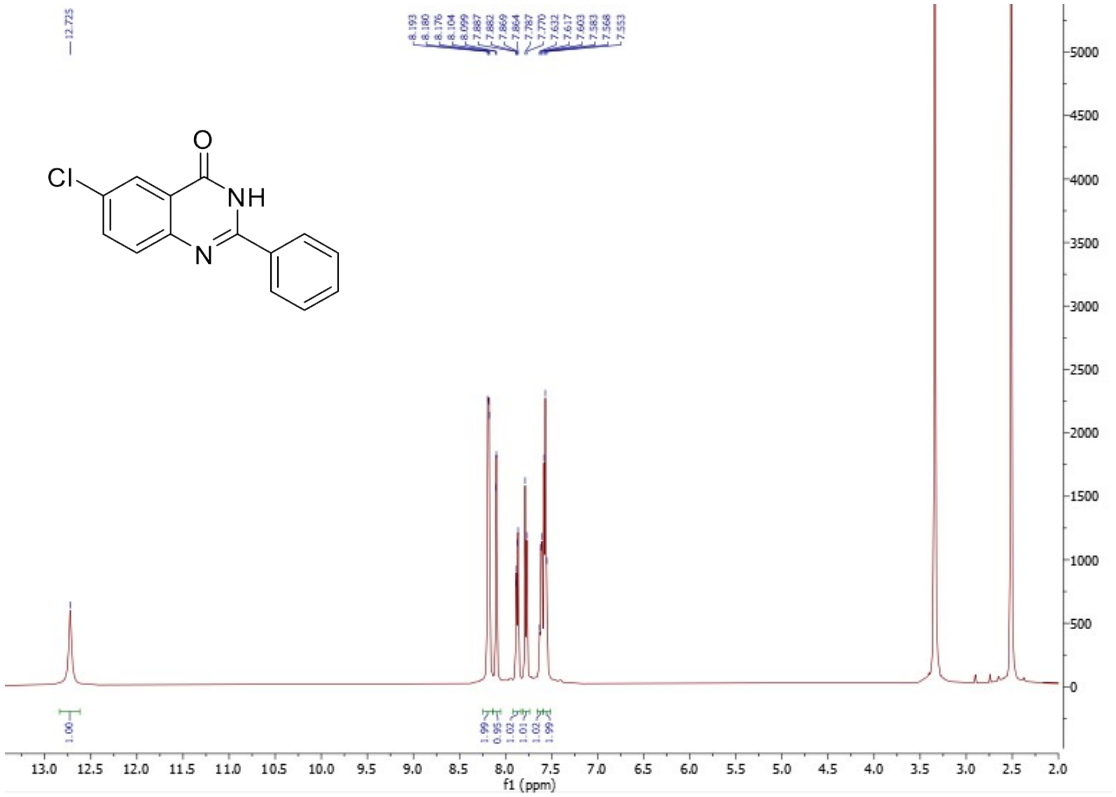


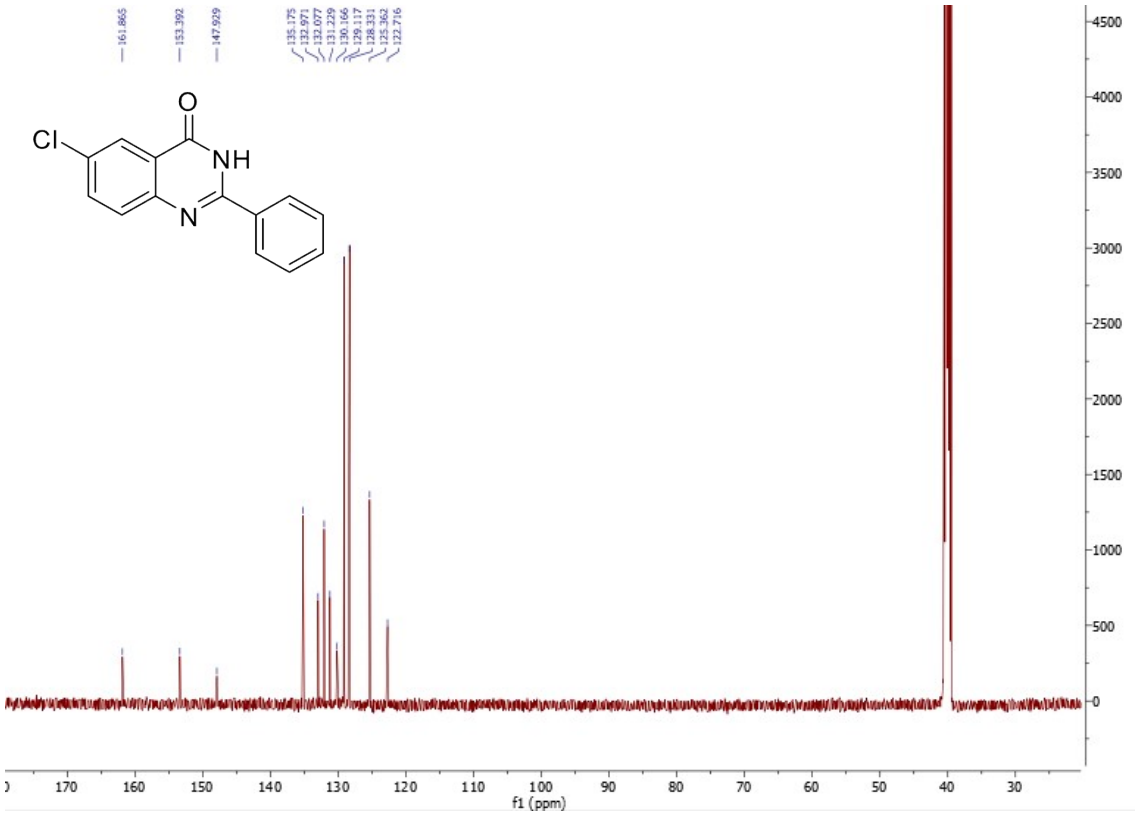
2-(3,4-Dimethoxyphenyl)quinazolin-4(3*H*)-one (3na)



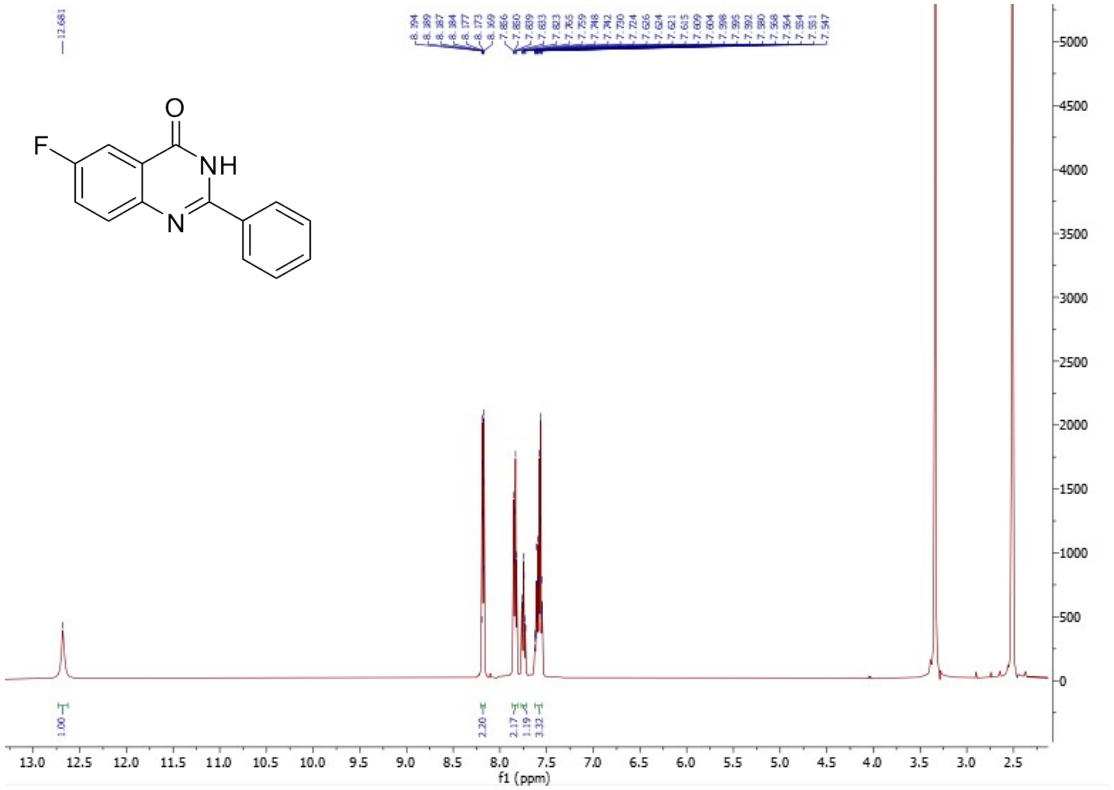


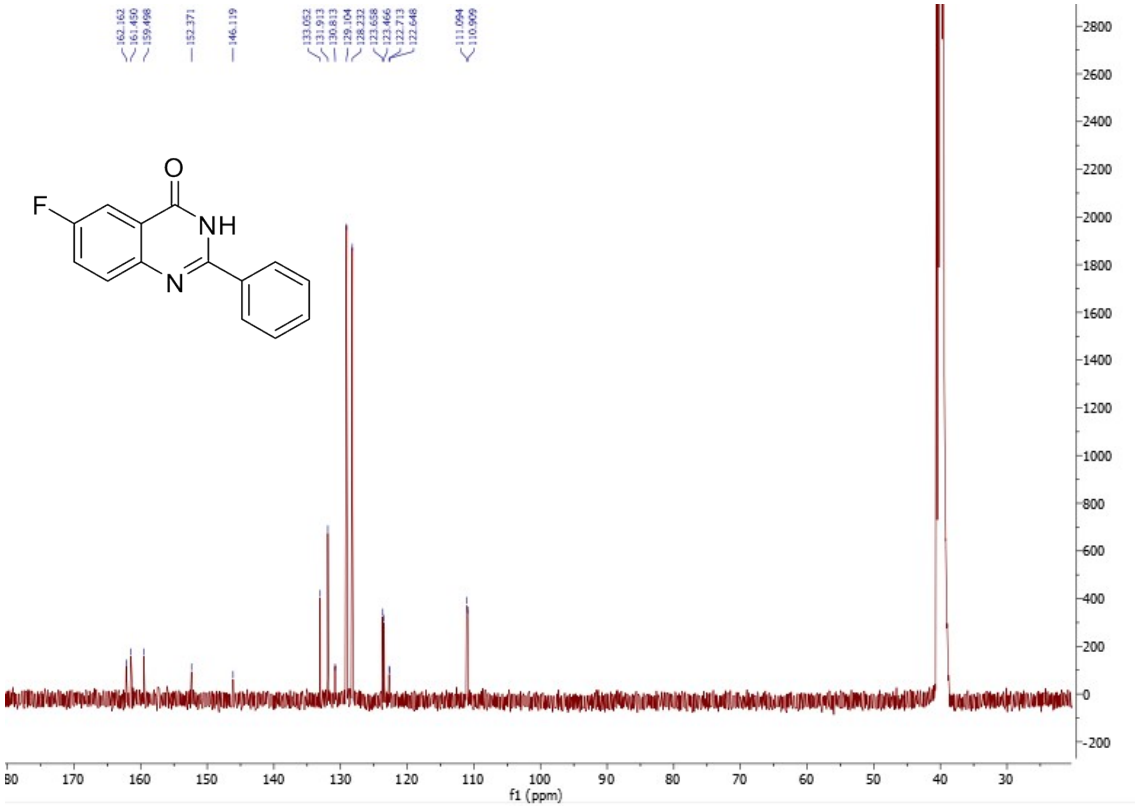
6-Chloro-2-phenylquinazolin-4(3*H*)-one (3oa)



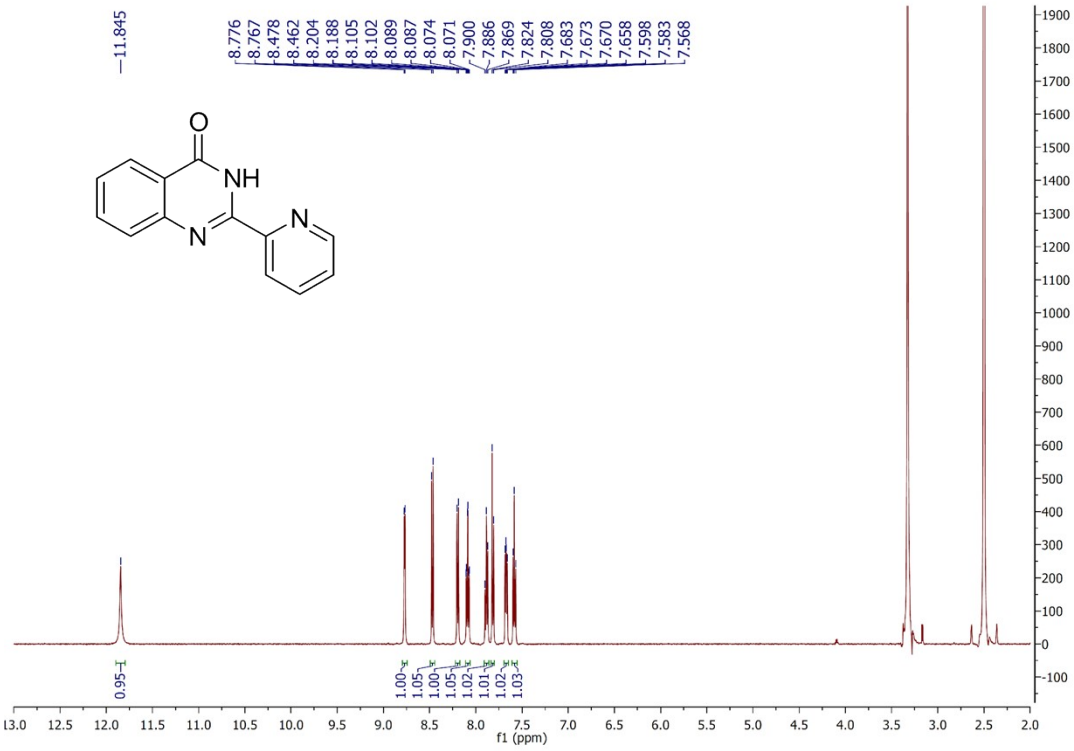


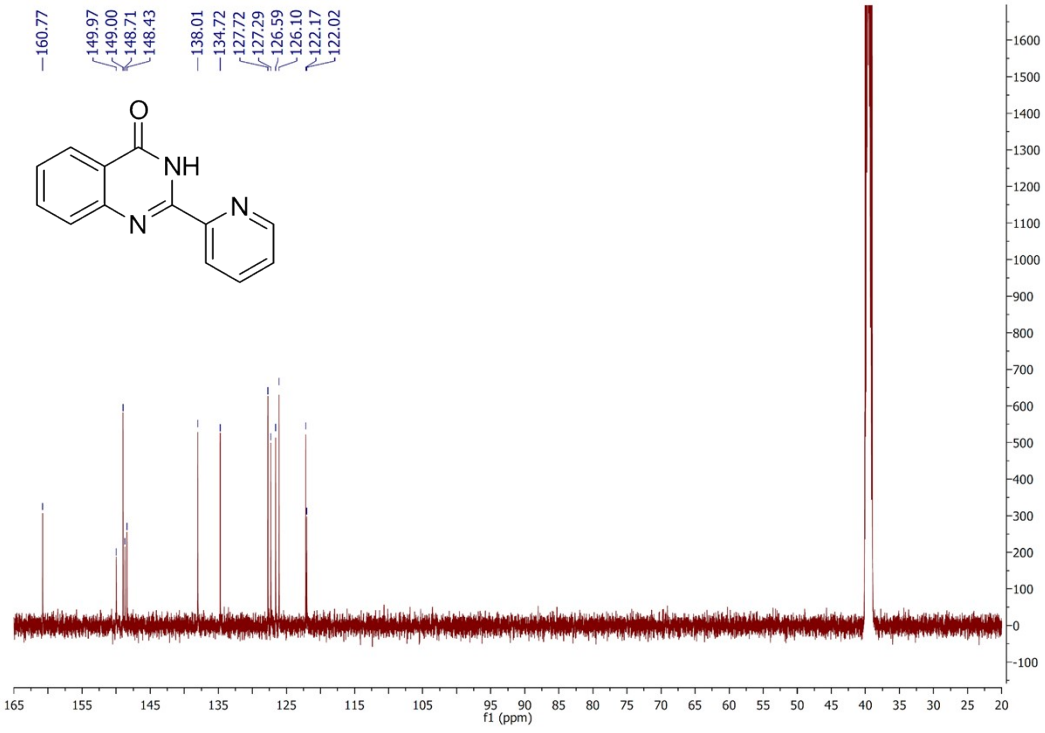
6-Fluoro-2-phenylquinazolin-4(3*H*)-one (3pa)



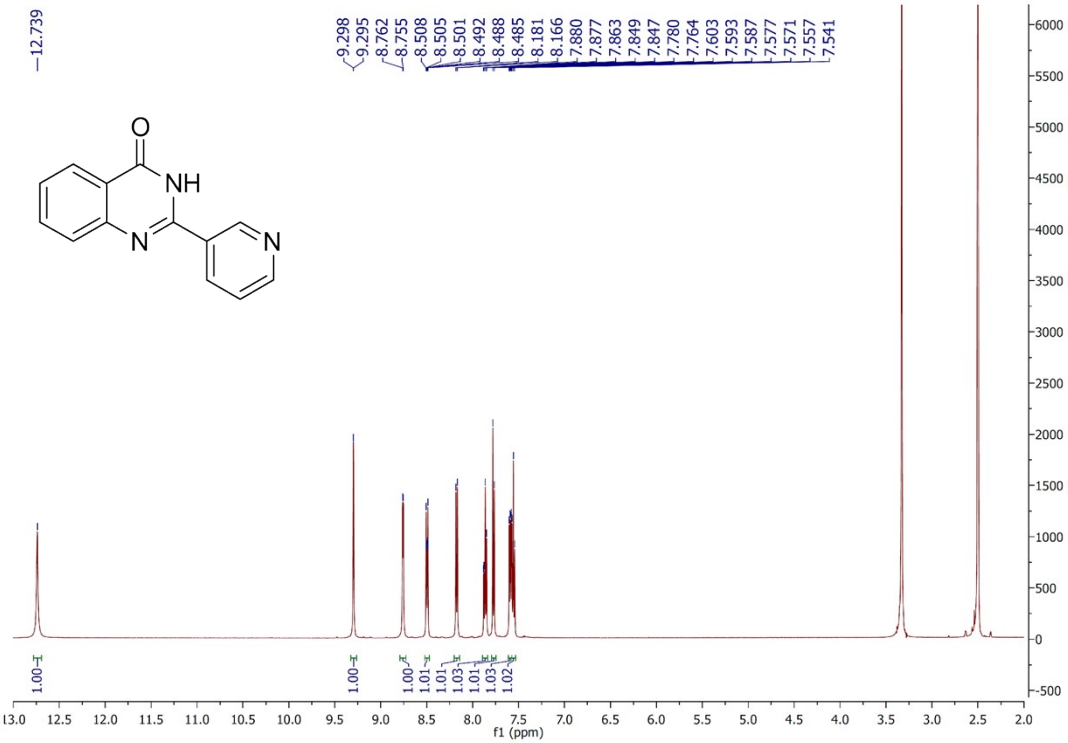


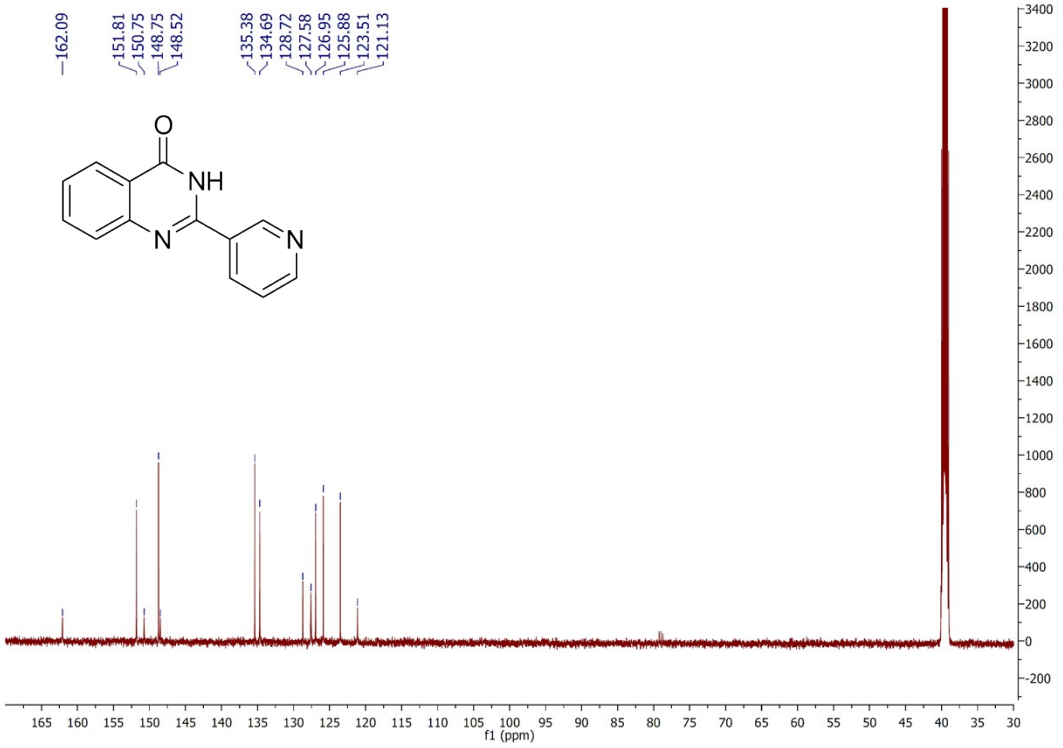
2-(Pyridin-2-yl)quinazolin-4(3*H*)-one (3qa)



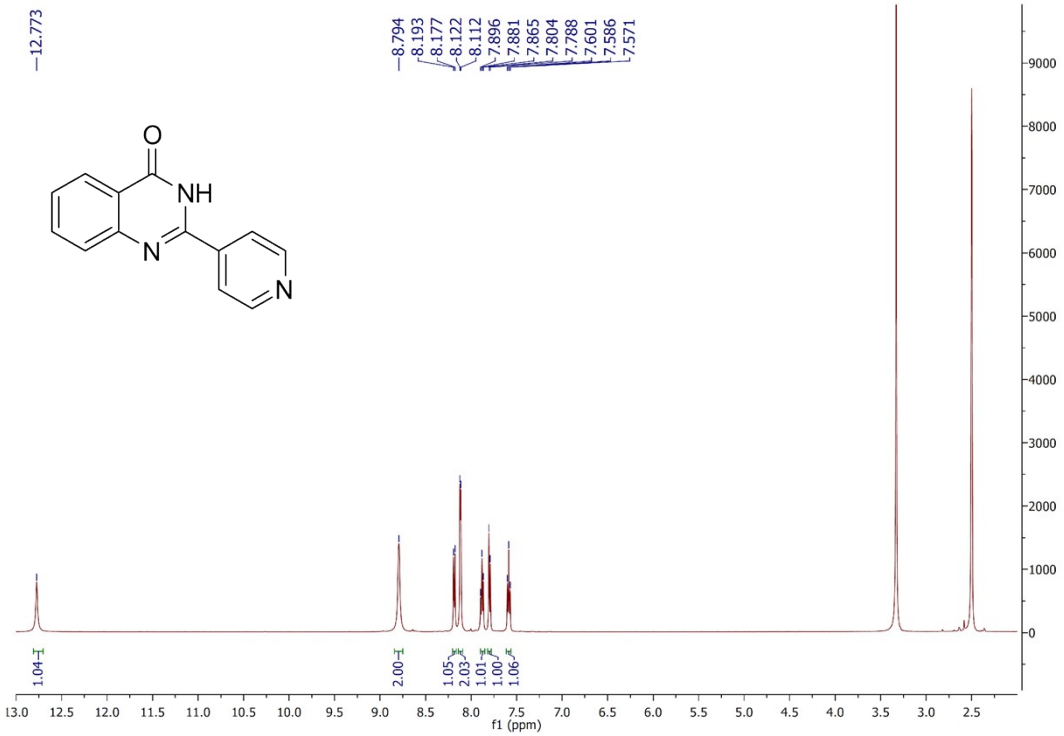


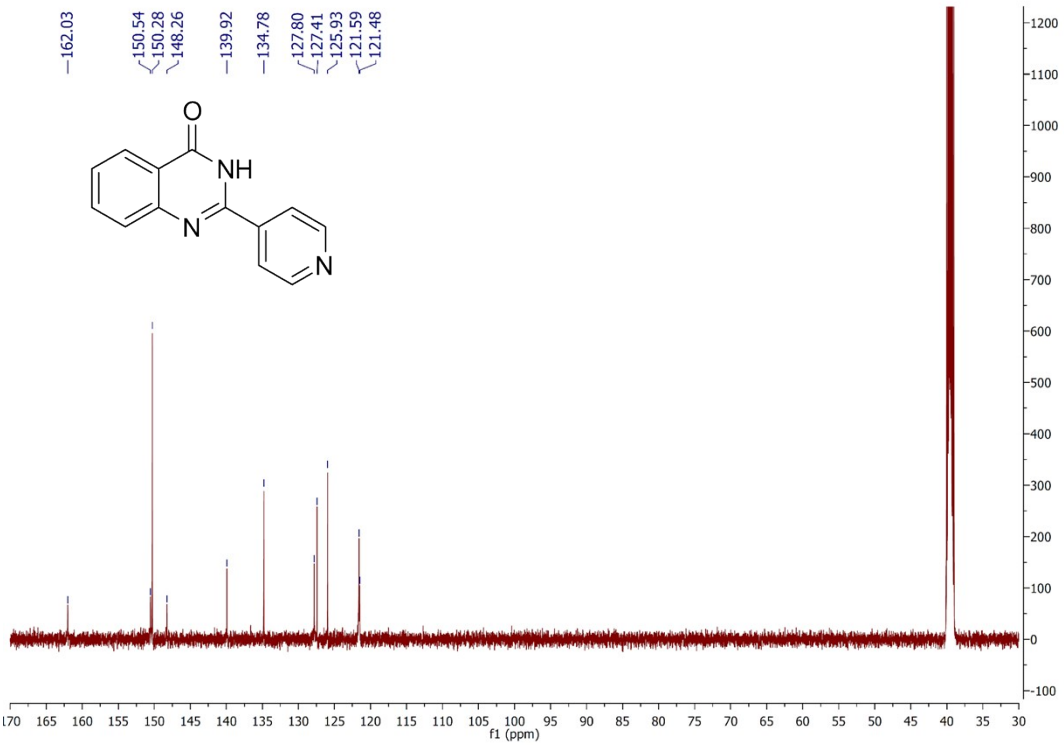
2-(Pyridin-3-yl)quinazolin-4(3*H*)-one (3ra)



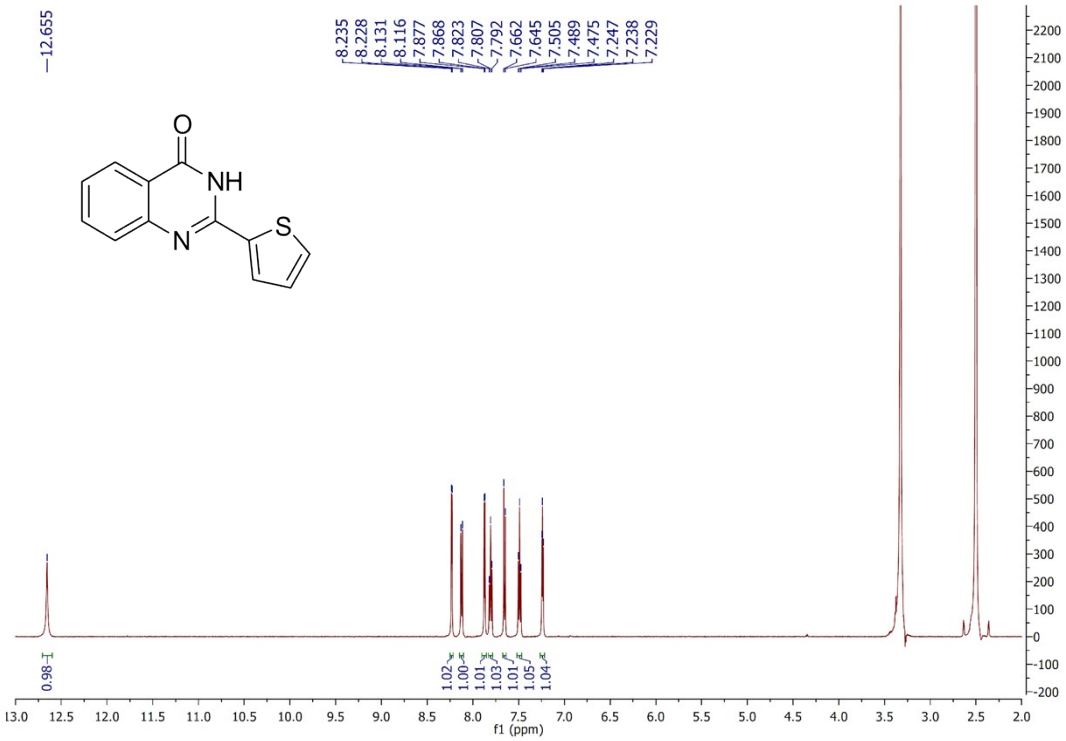


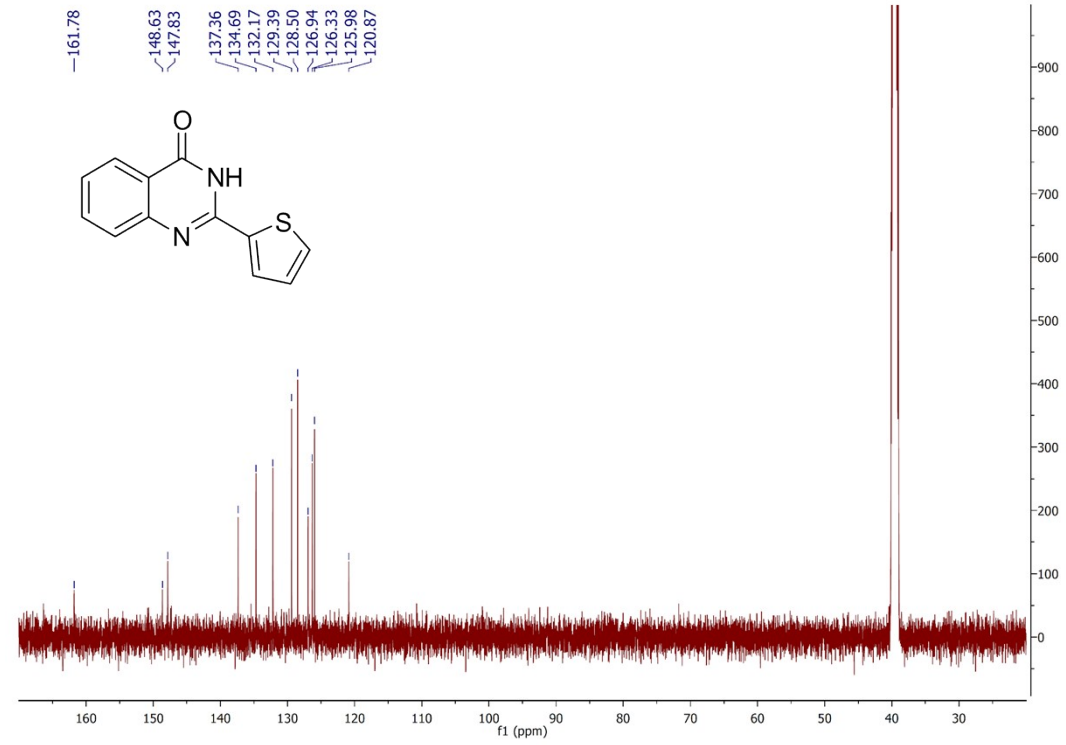
2-(Pyridin-4-yl)quinazolin-4(3*H*)-one (3sa)



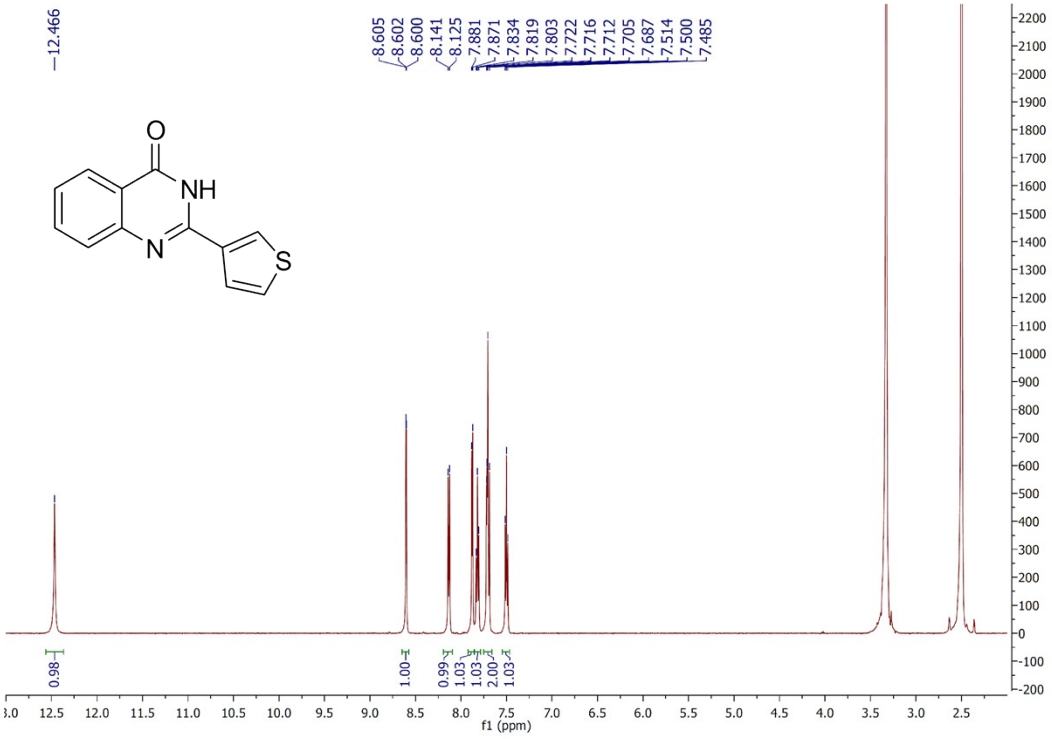


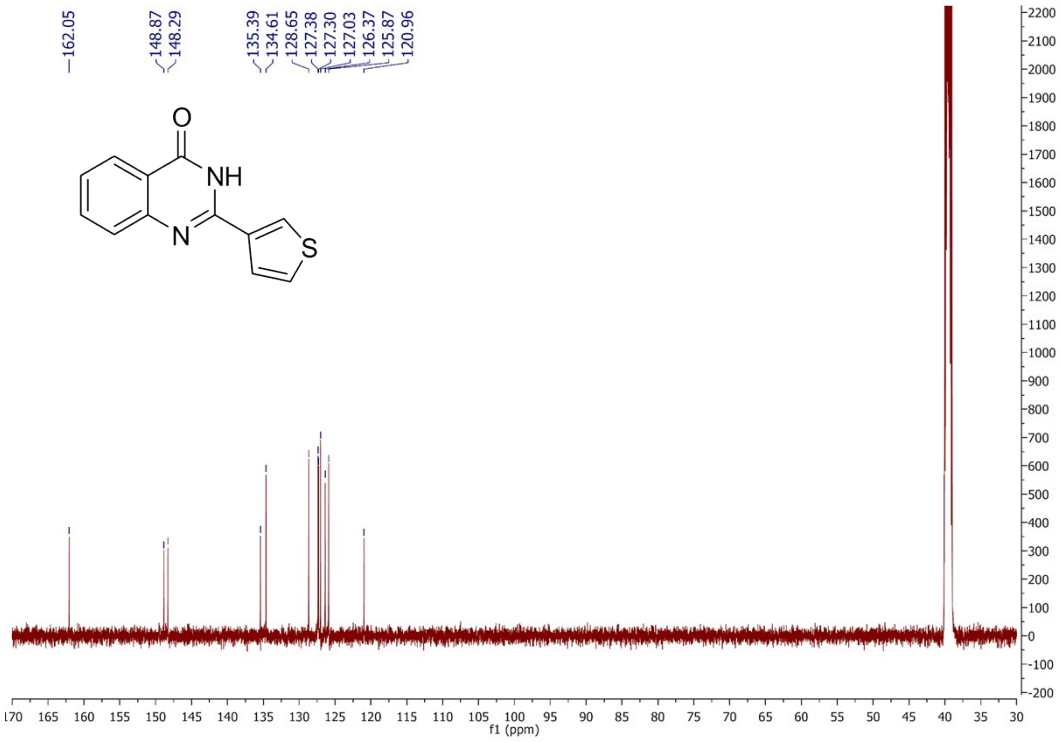
2-(2-Thiophen)quinazolin-4(3*H*)-one (3ta)



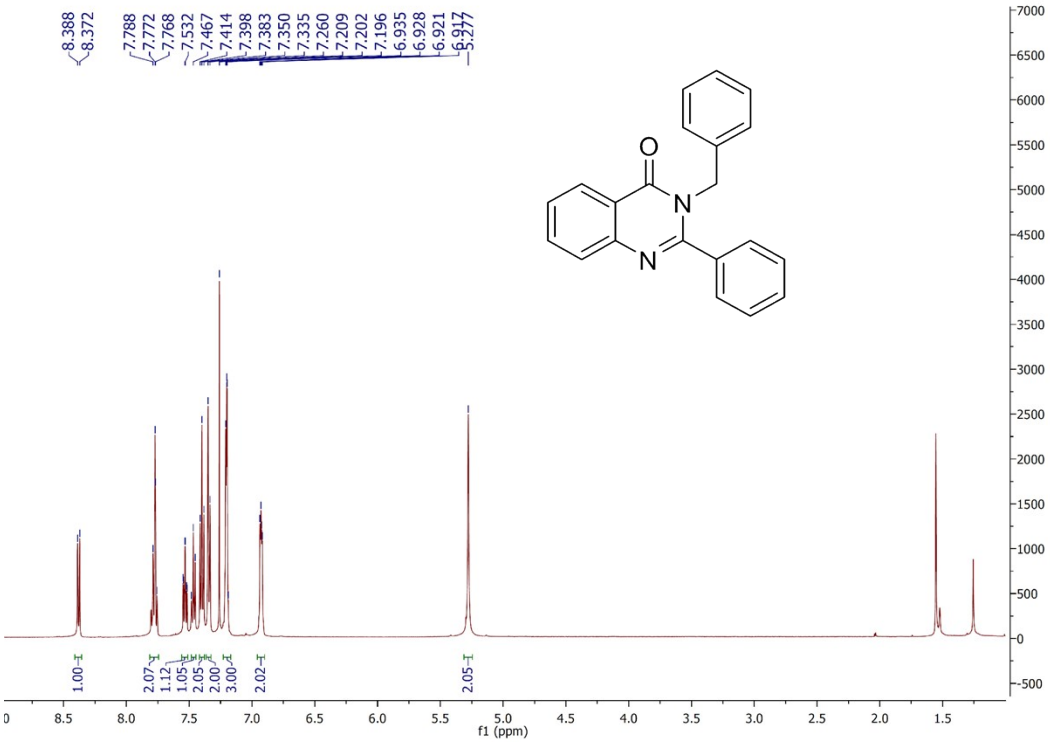


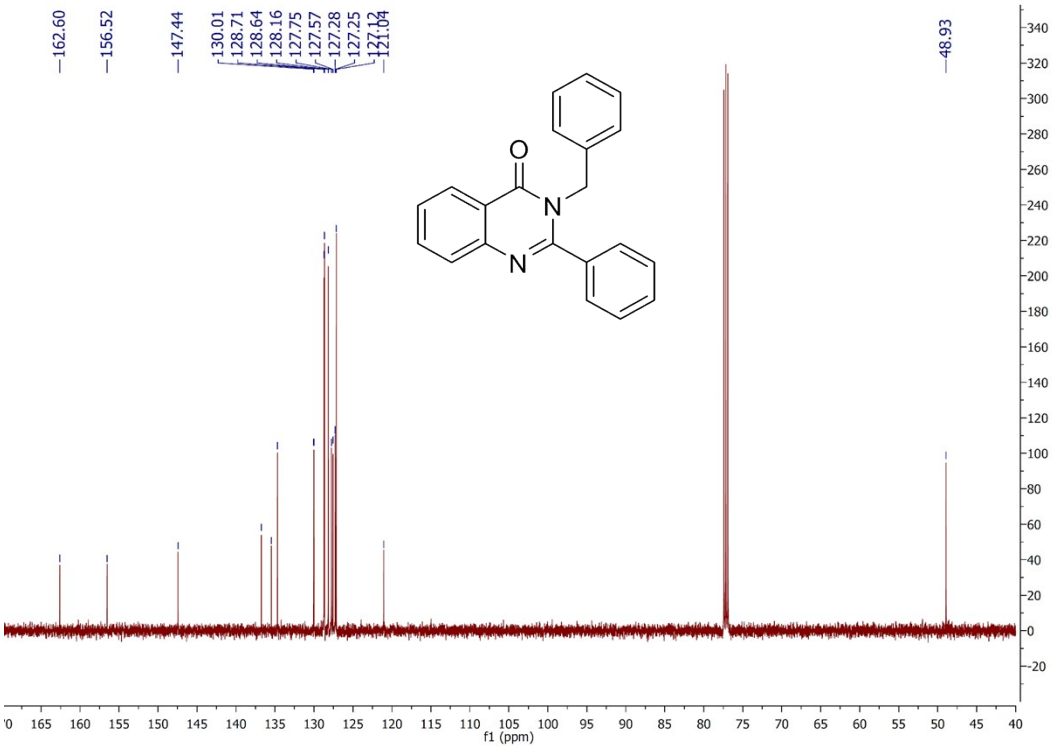
2-(3-Thiophen)quinazolin-4(3*H*)-one (3ua)



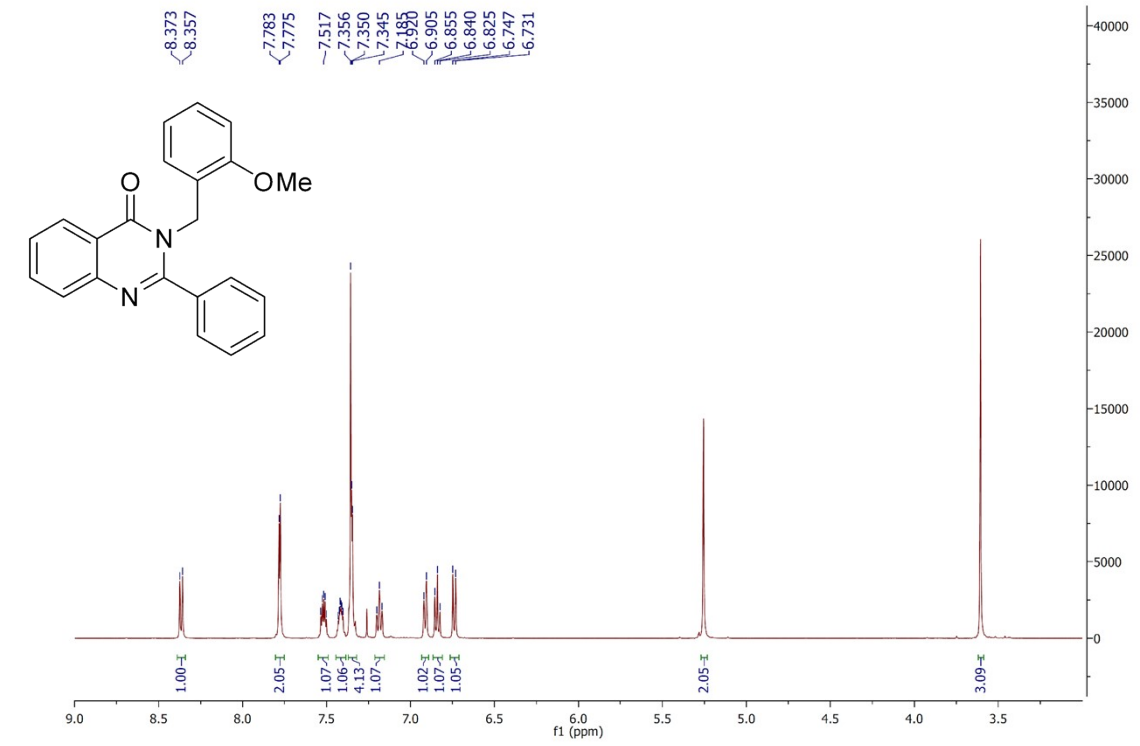


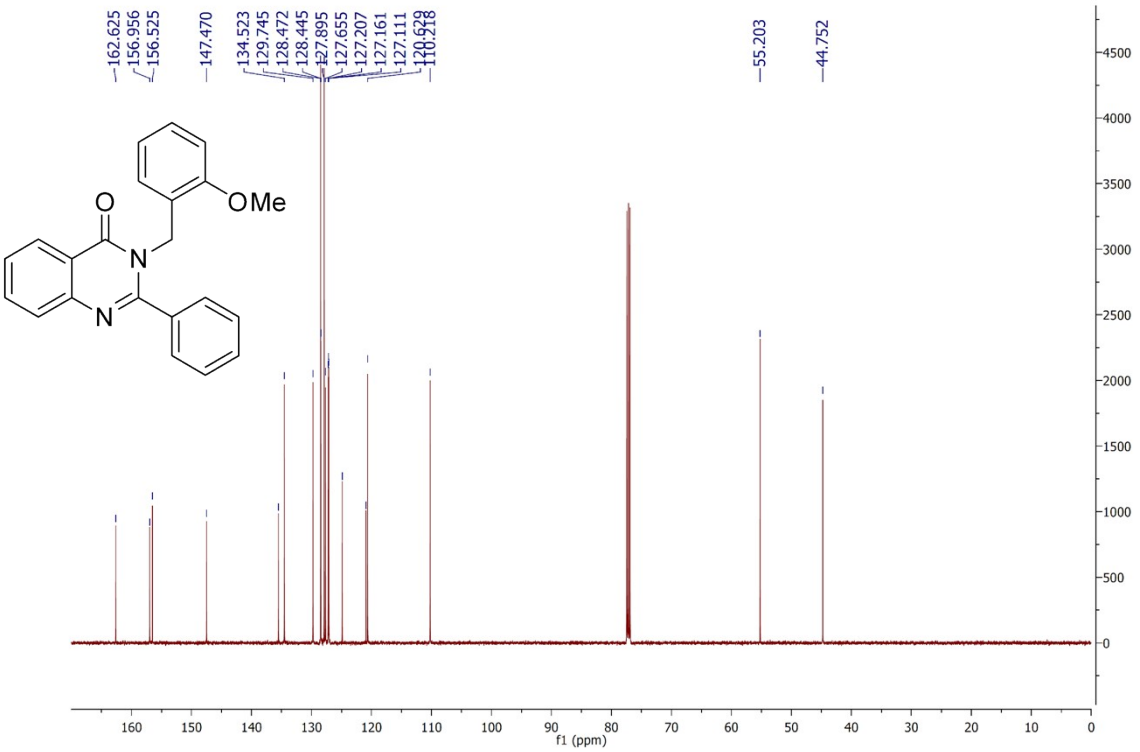
3-Benzyl-2-phenylquinazolin-4(3*H*)-one (3ab)



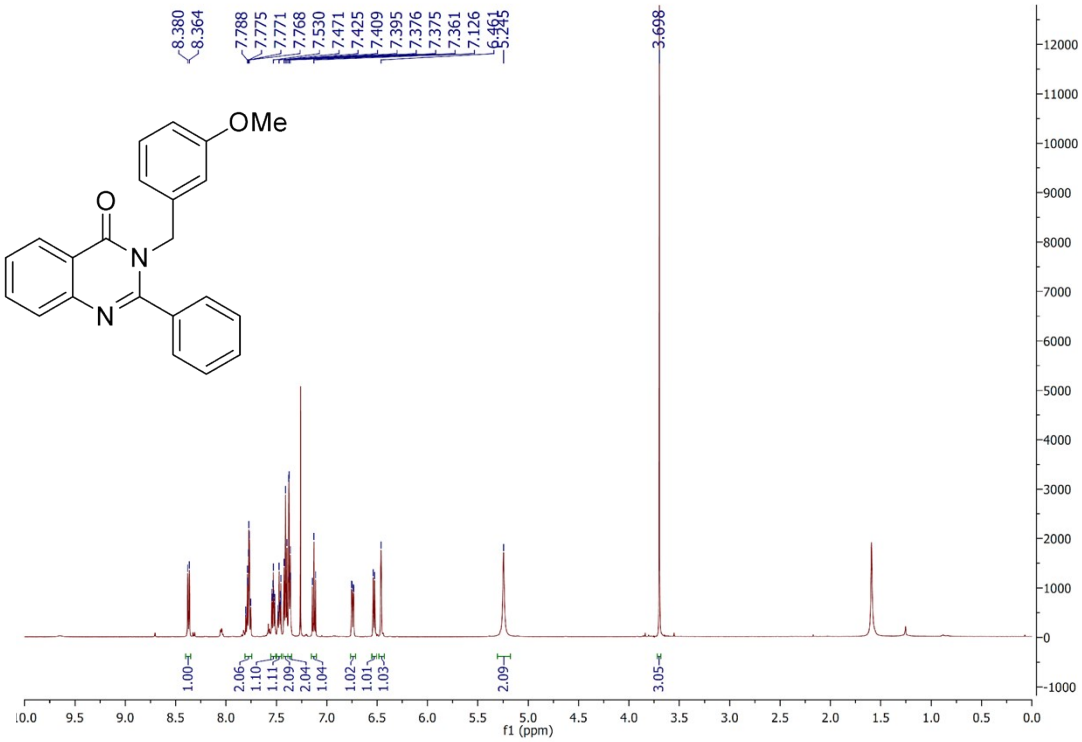


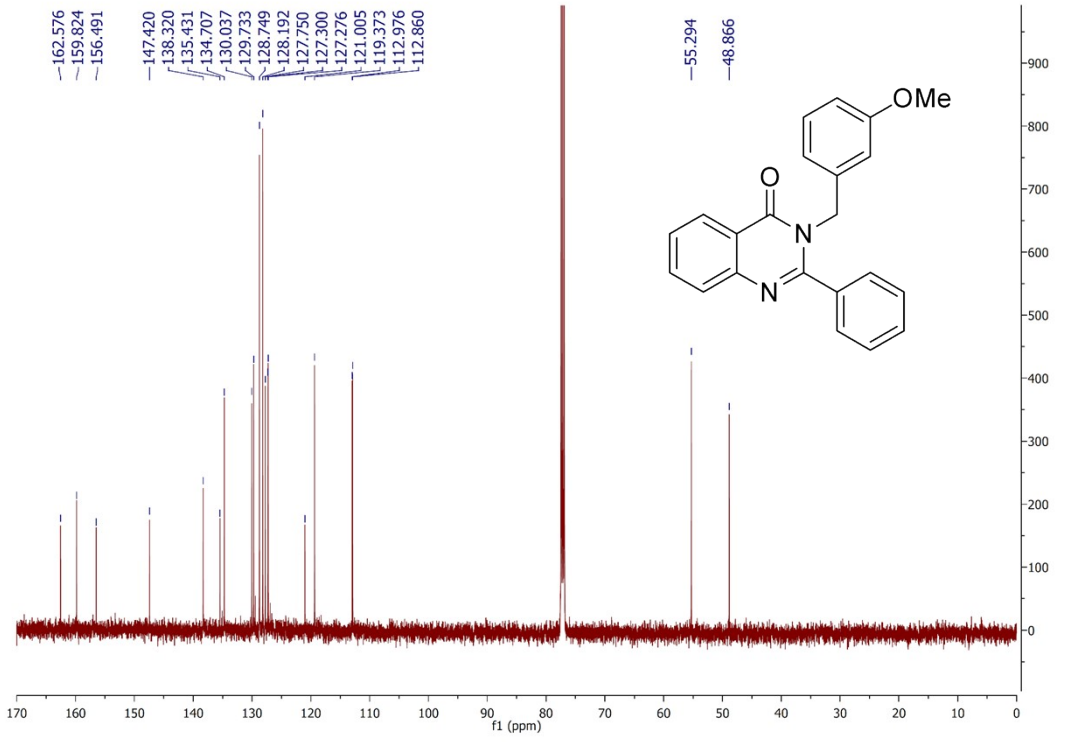
3-(2-Methoxybenzyl)-2-phenylquinazolin-4(3*H*)-one (3ac)



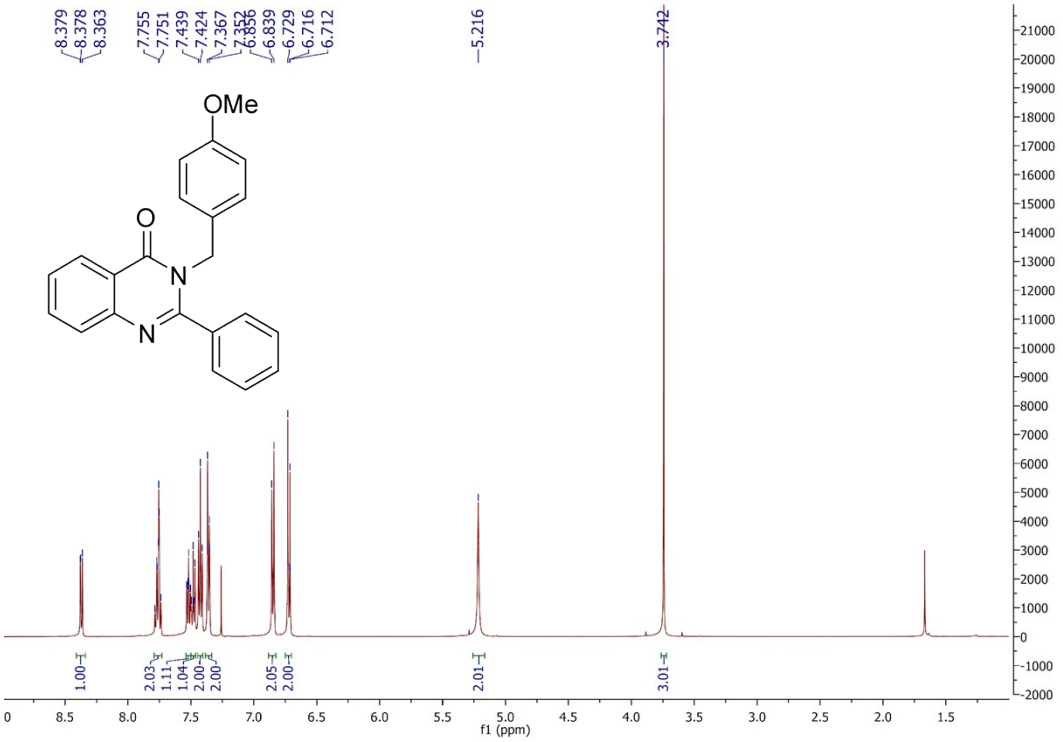


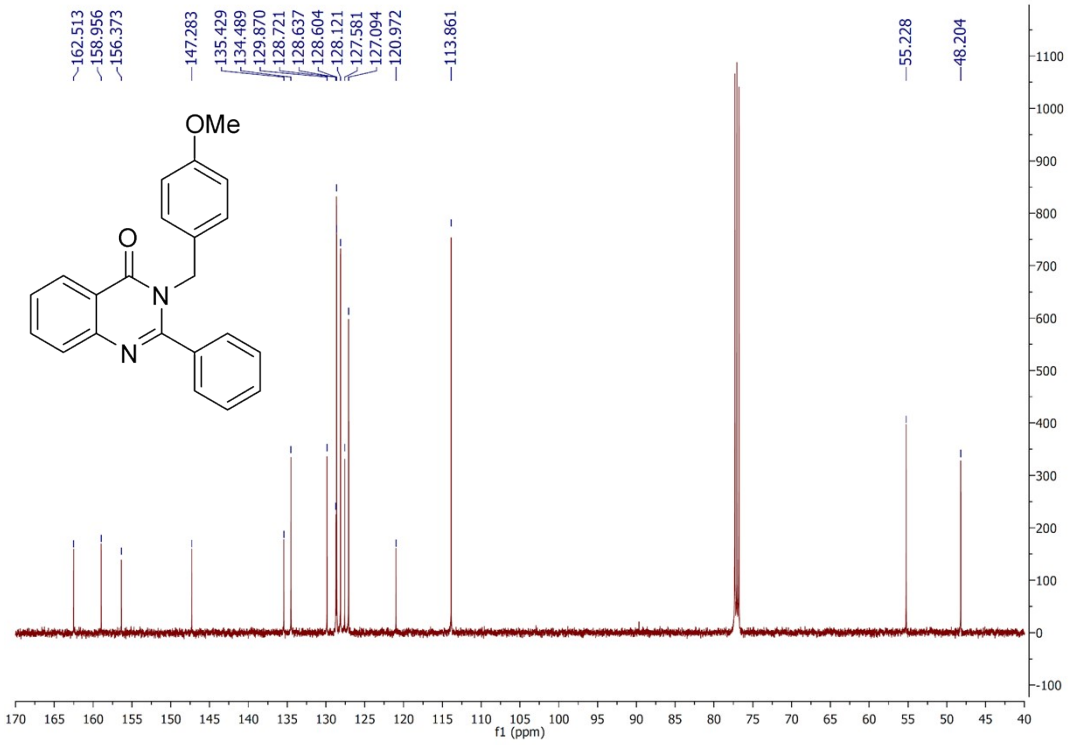
3-(3-Methoxybenzyl)-2-phenylquinazolin-4(3*H*)-one (3ad)



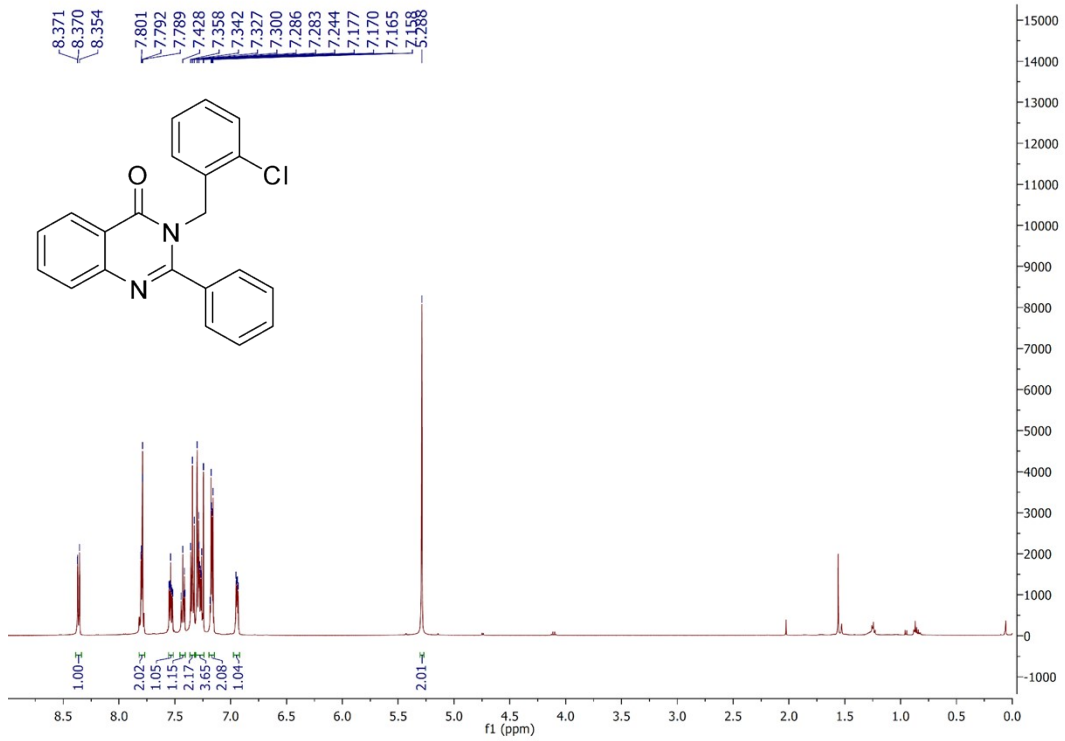


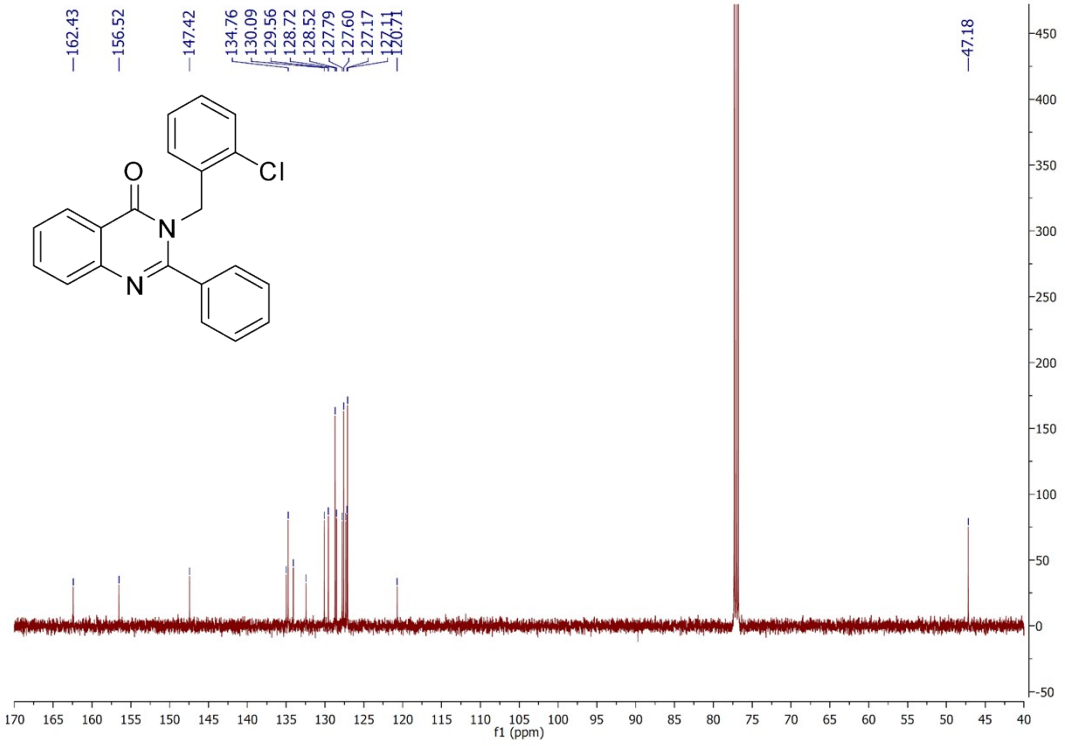
3-(4-Methoxybenzyl)-2-phenylquinazolin-4(3*H*)-one (3ae)



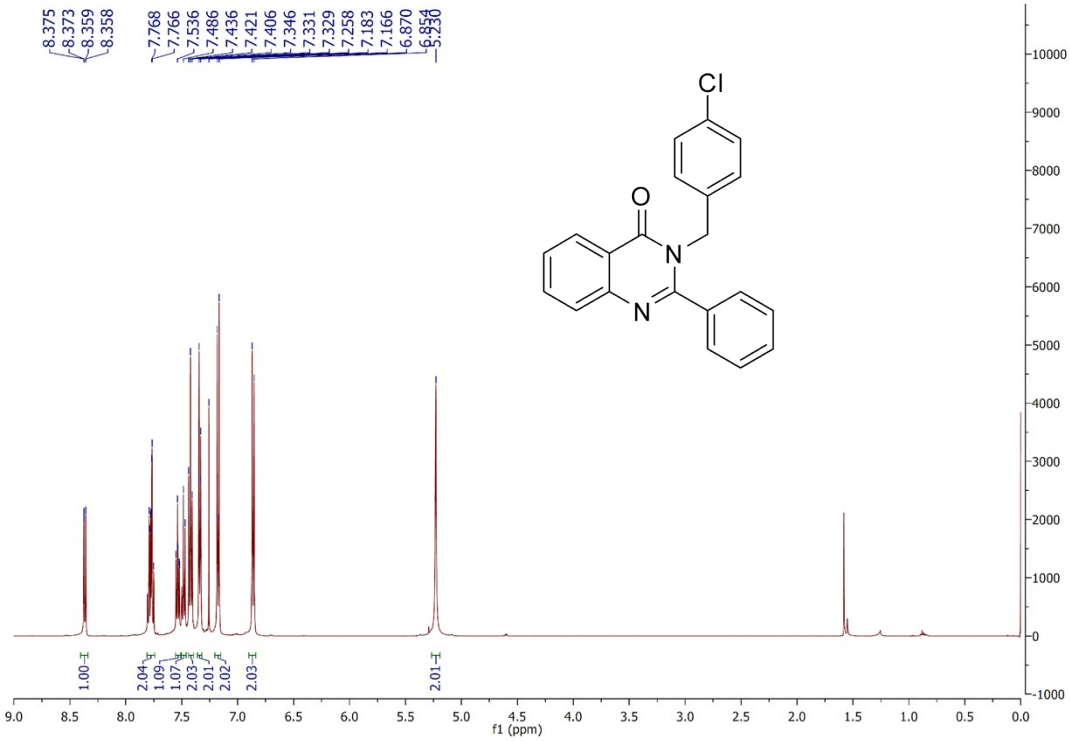


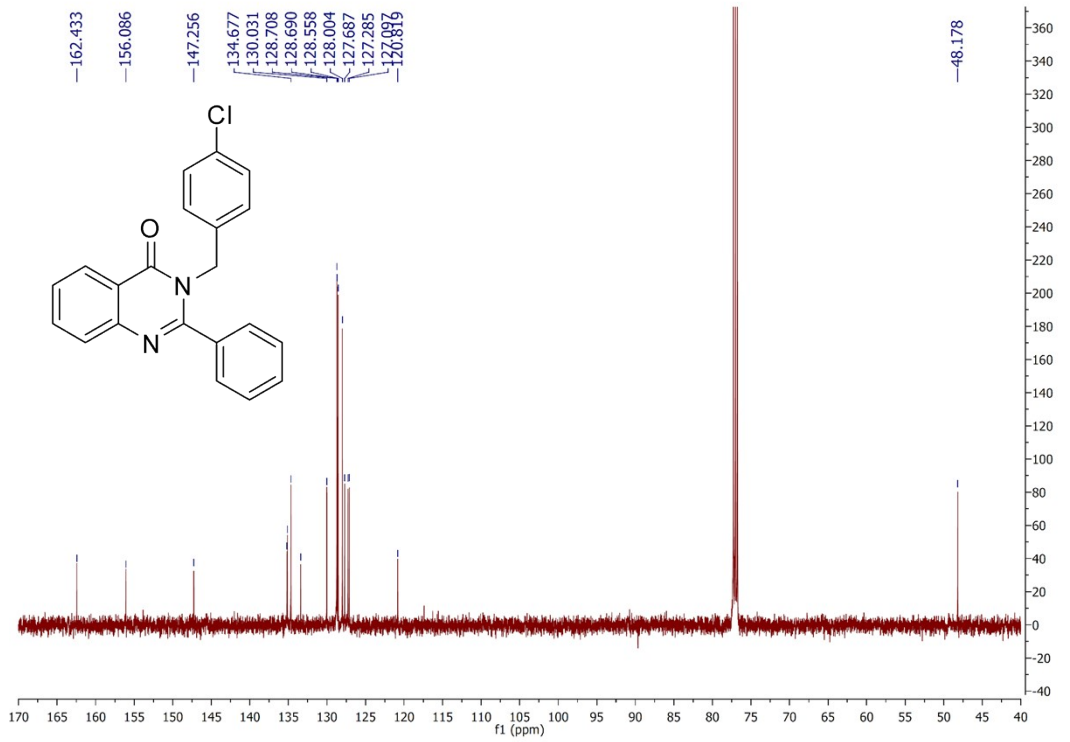
3-(2-Chlorobenzyl)-2-phenylquinazolin-4(3*H*)-one (3af)



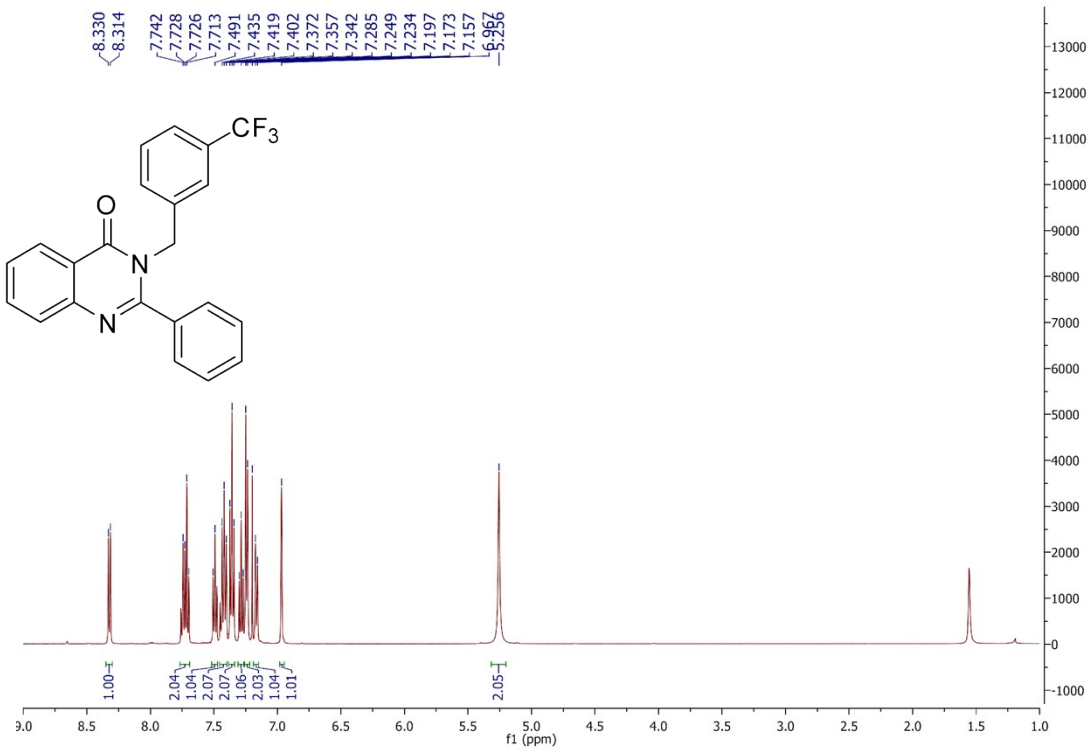


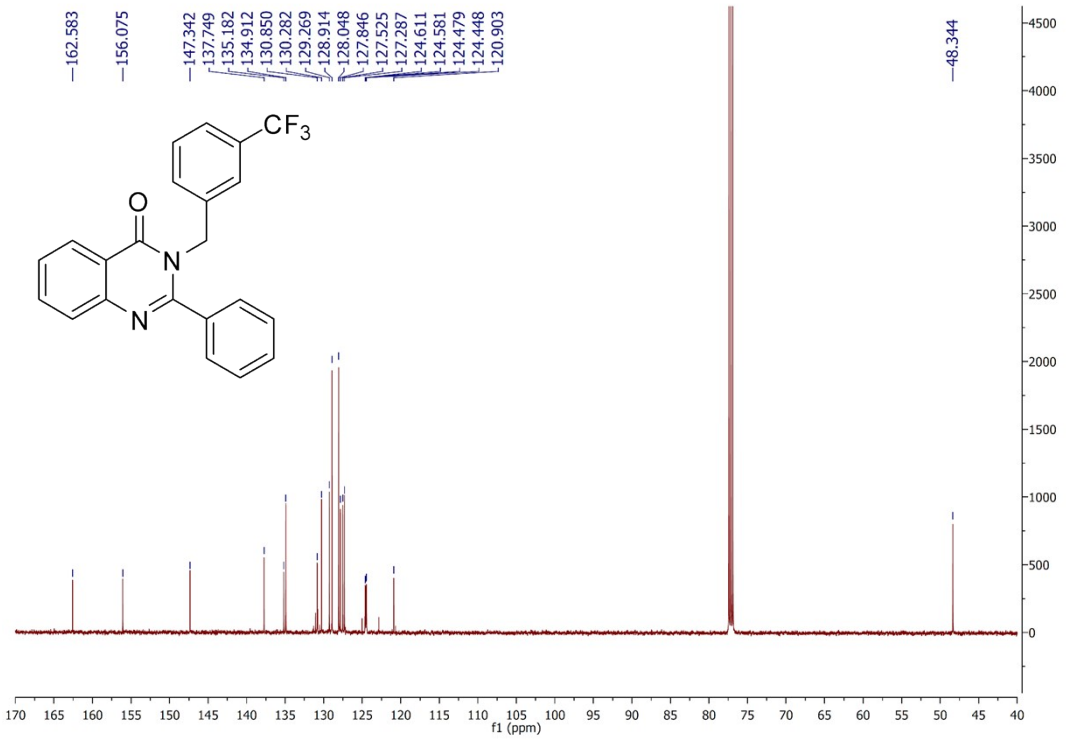
3-(4-Chlorobenzyl)-2-phenylquinazolin-4(3*H*)-one (3ag)



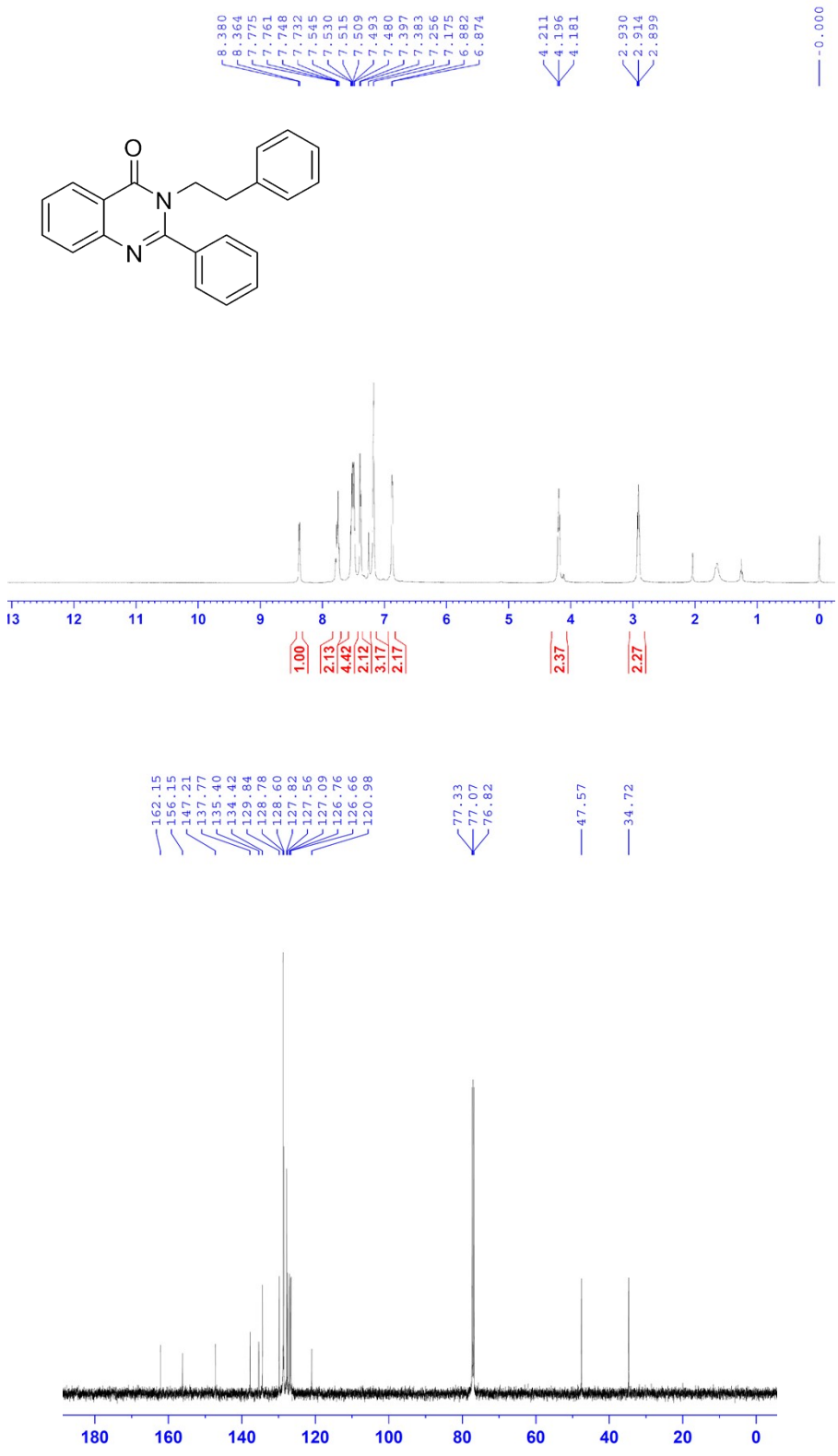


3-(3-Trifluoromethylbenzyl)-2-phenylquinazolin-4(3*H*)-one (3ah)

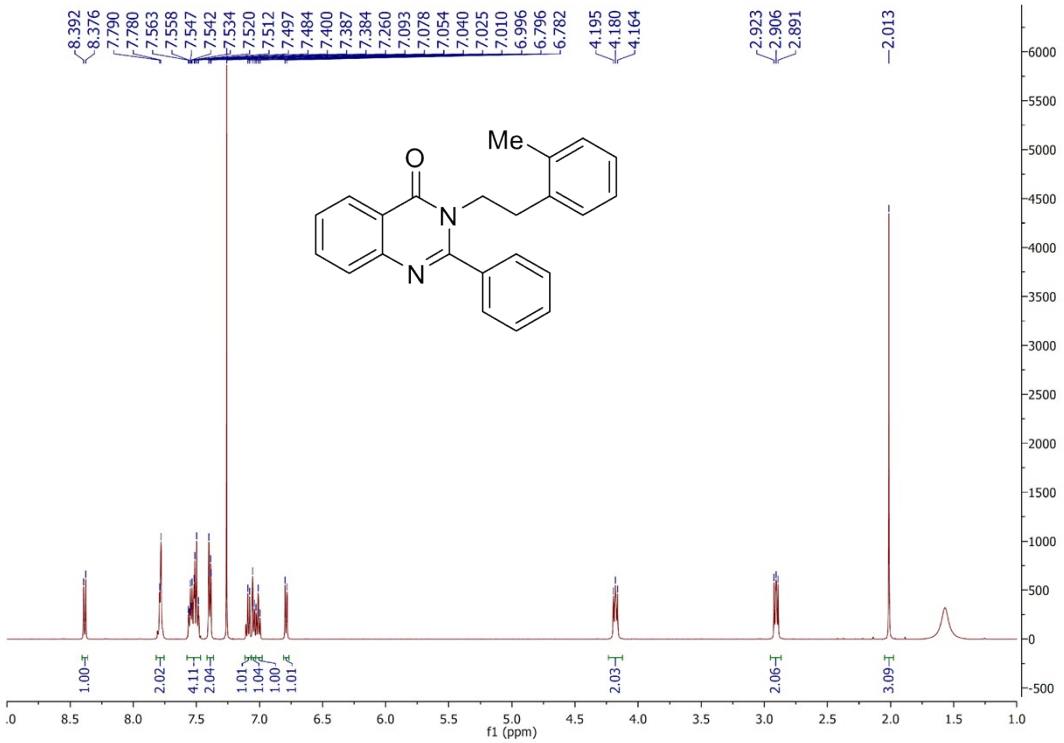


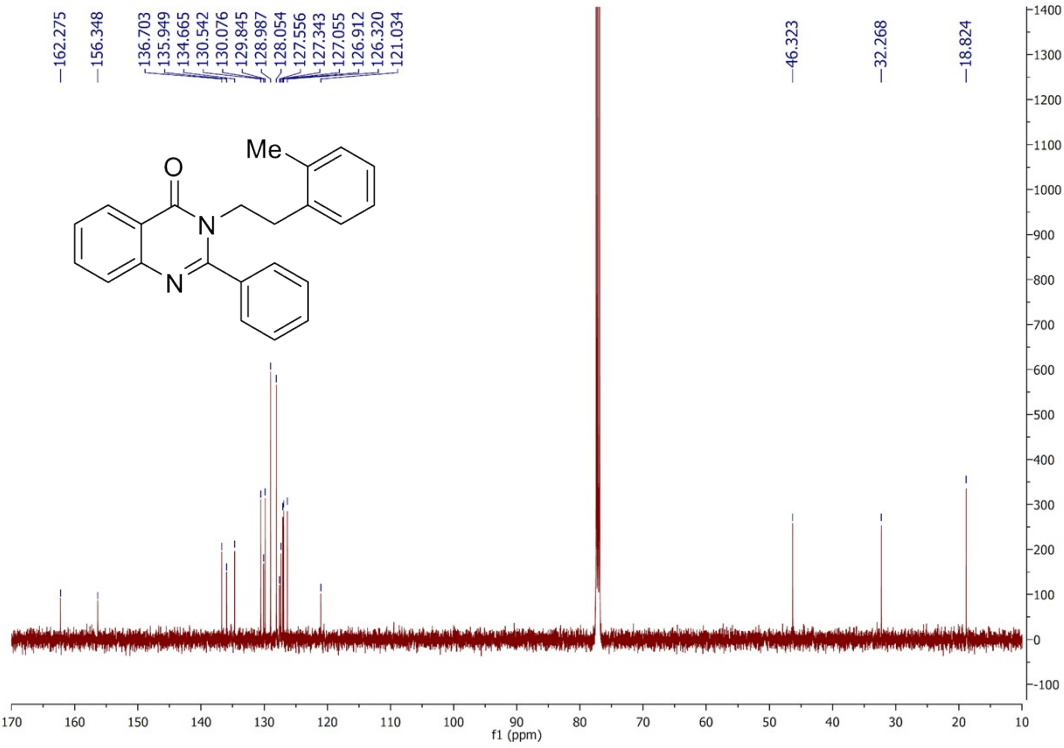


3-Phenylethyl-2-phenylquinazolin-4(3*H*)-one (3ai)

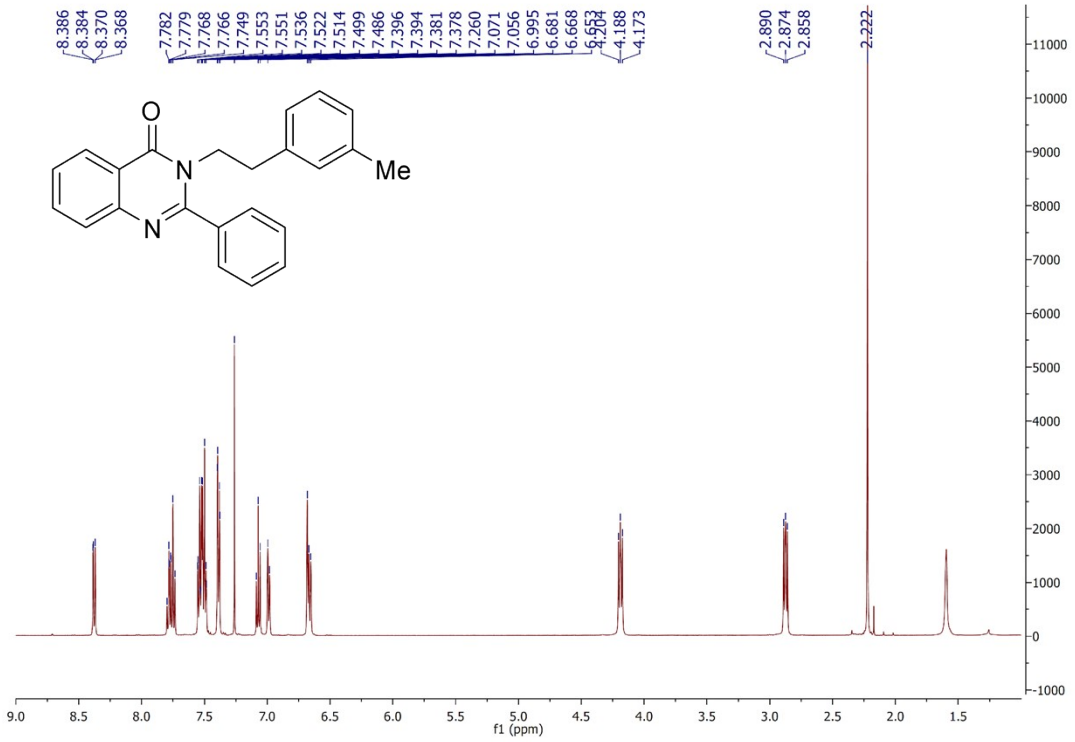


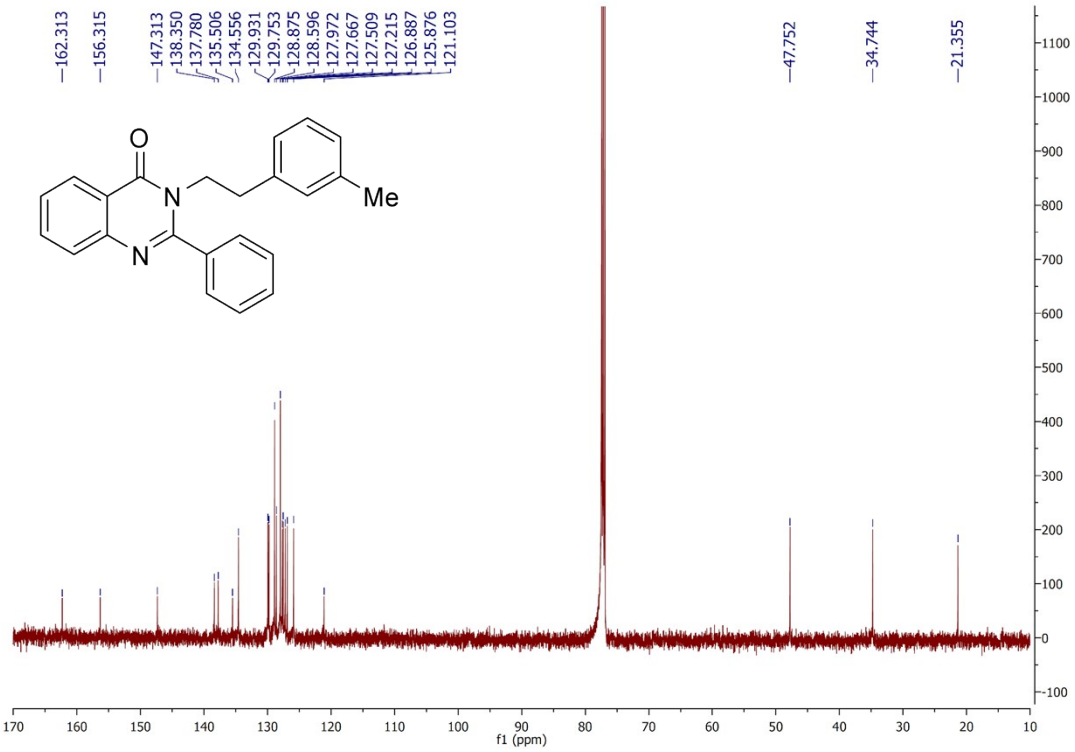
3-(2-Methylphenylethyl)-2-phenylquinazolin-4(3*H*)-one (3aj)



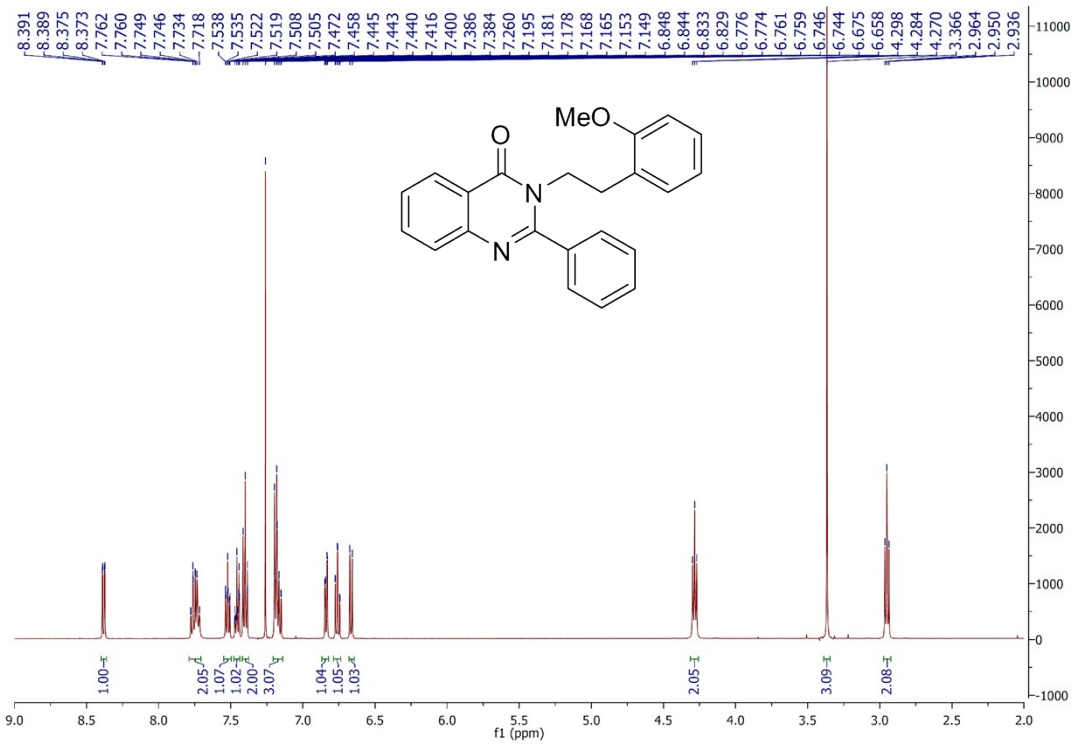


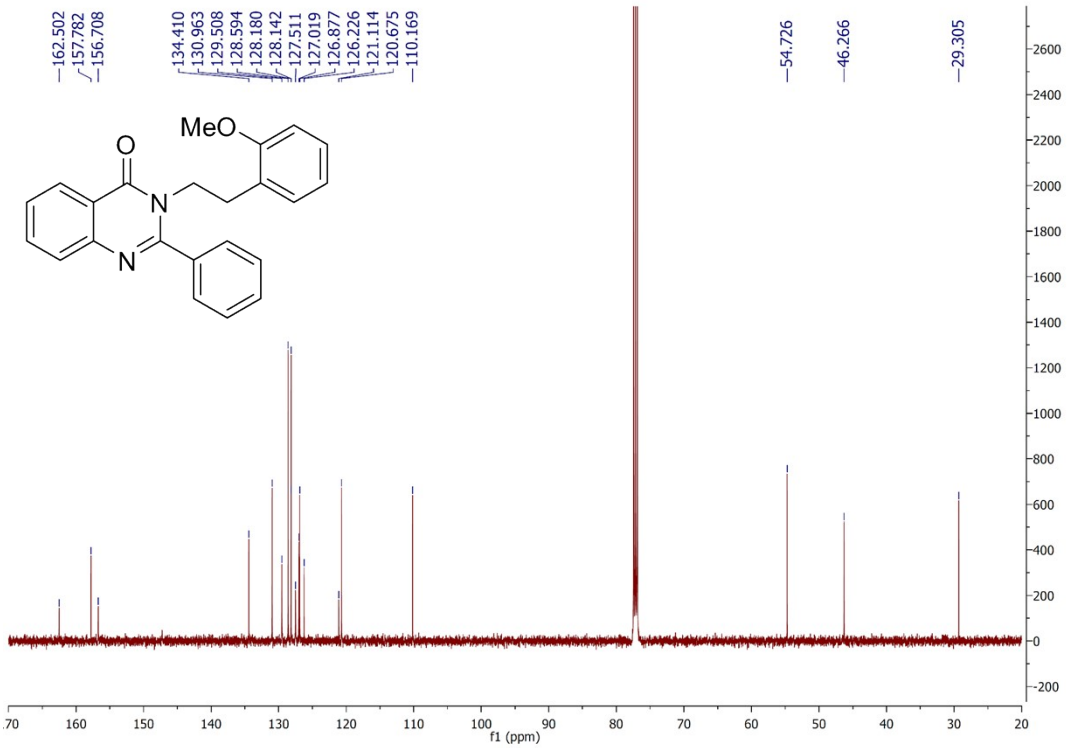
3-(3-Methylphenylethyl)-2-phenylquinazolin-4(3*H*)-one (3ak)



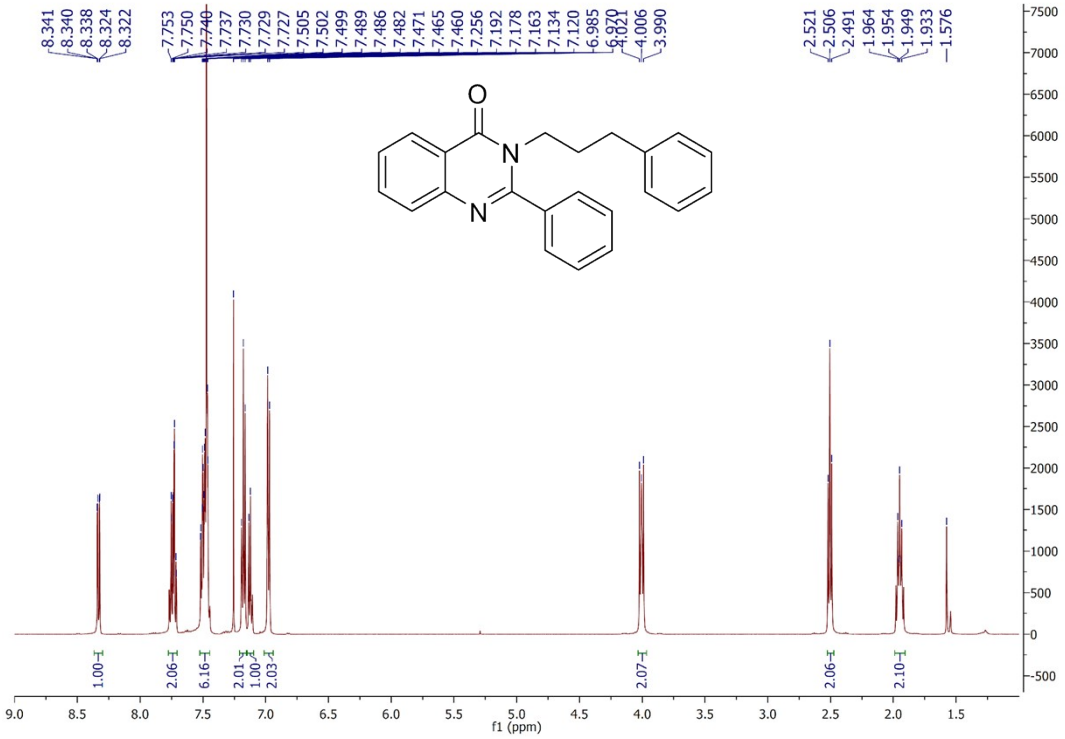


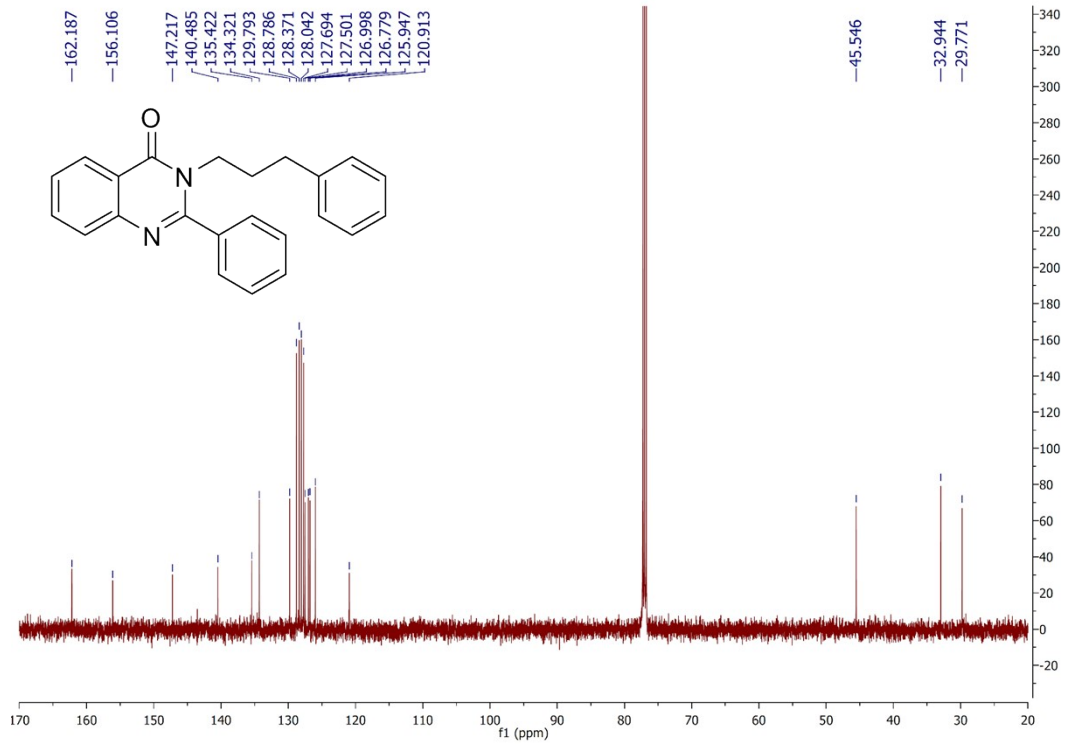
3-(2-Methoxyphenylethyl)-2-phenylquinazolin-4(3*H*)-one (3al)



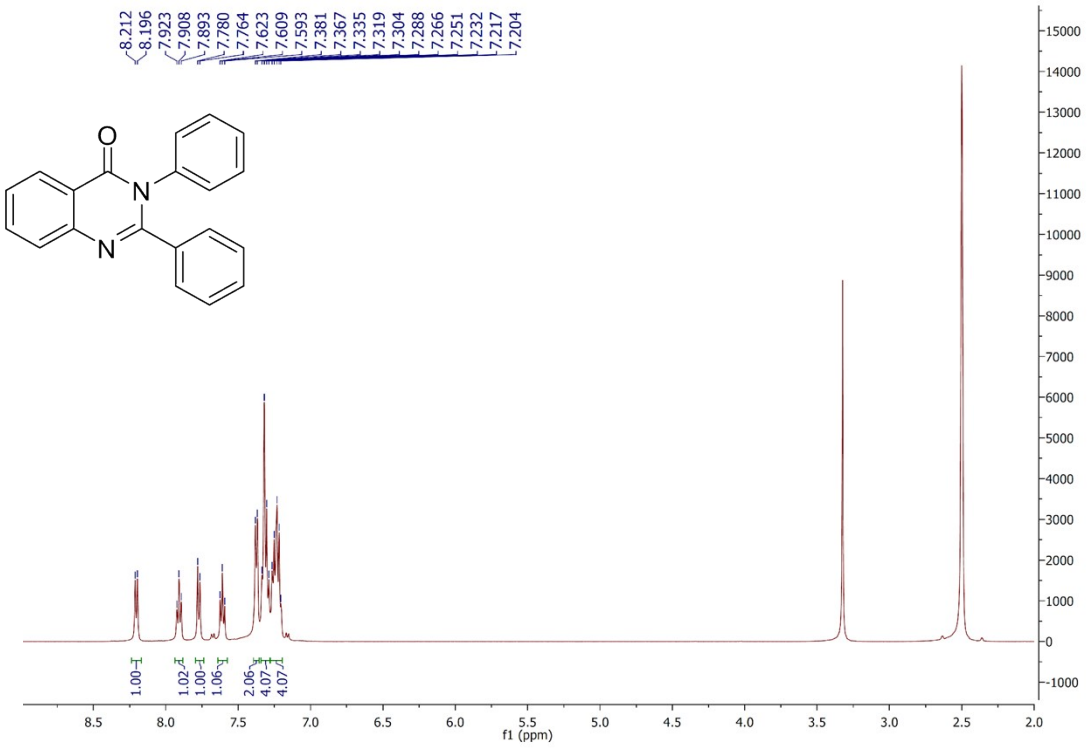


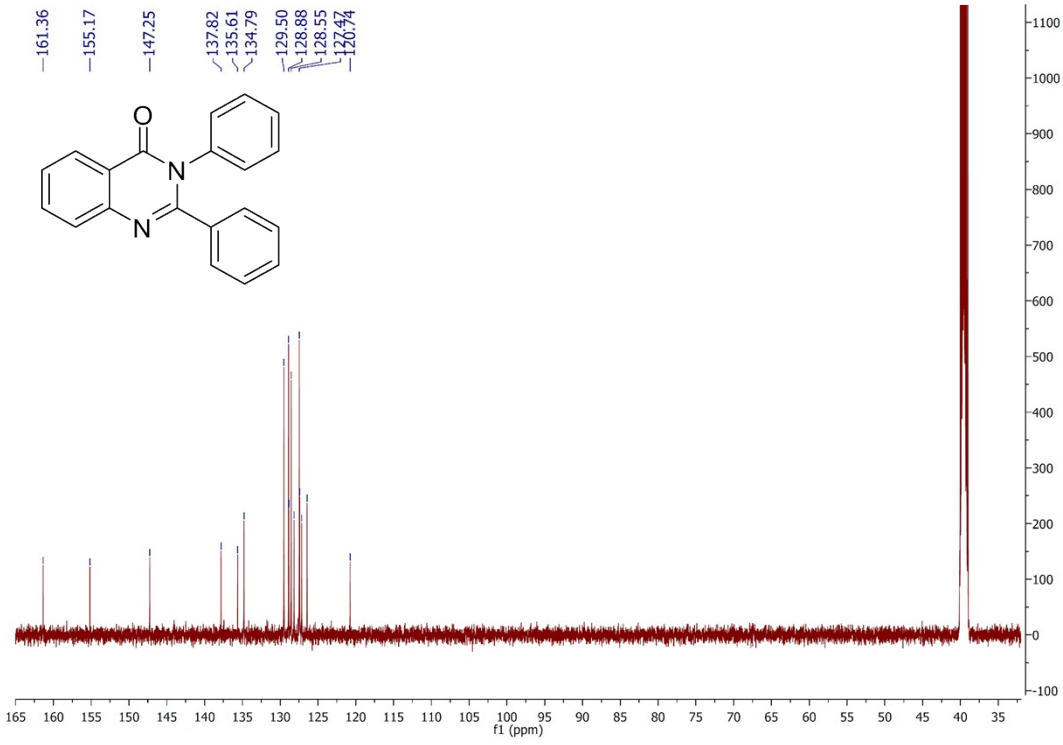
3-(3-Phenyl-1-propyl)-2-phenylquinazolin-4(3*H*)-one (3am)



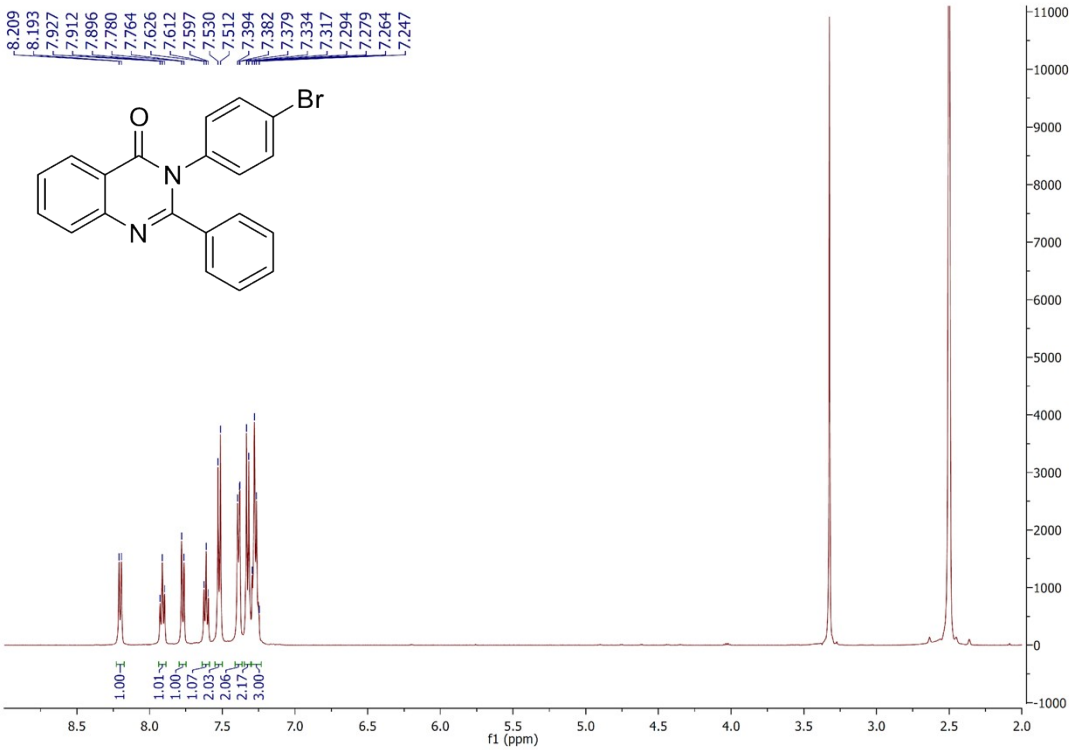


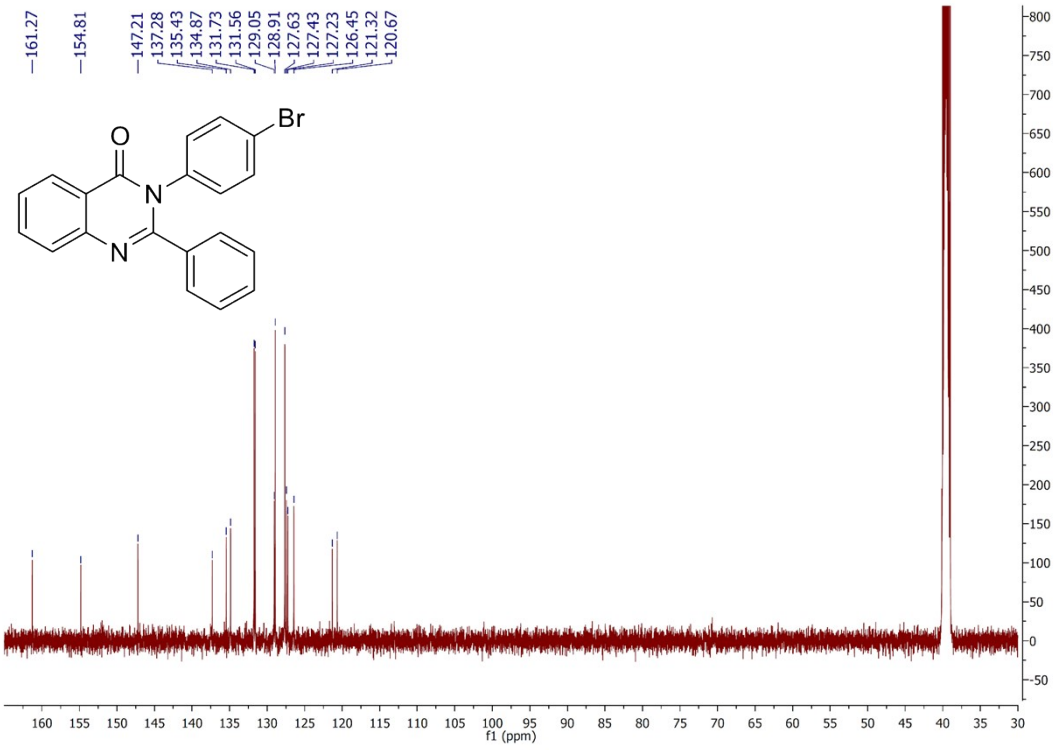
2,3-Diphenylquinazolin-4(3*H*)-one (3an)



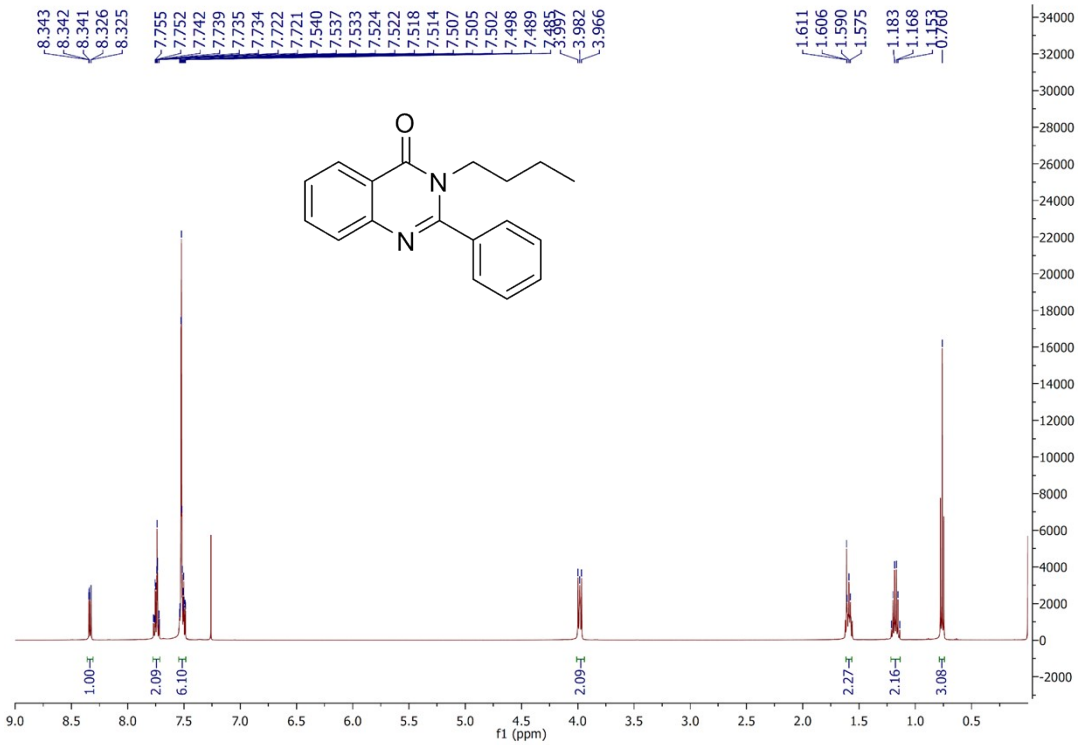


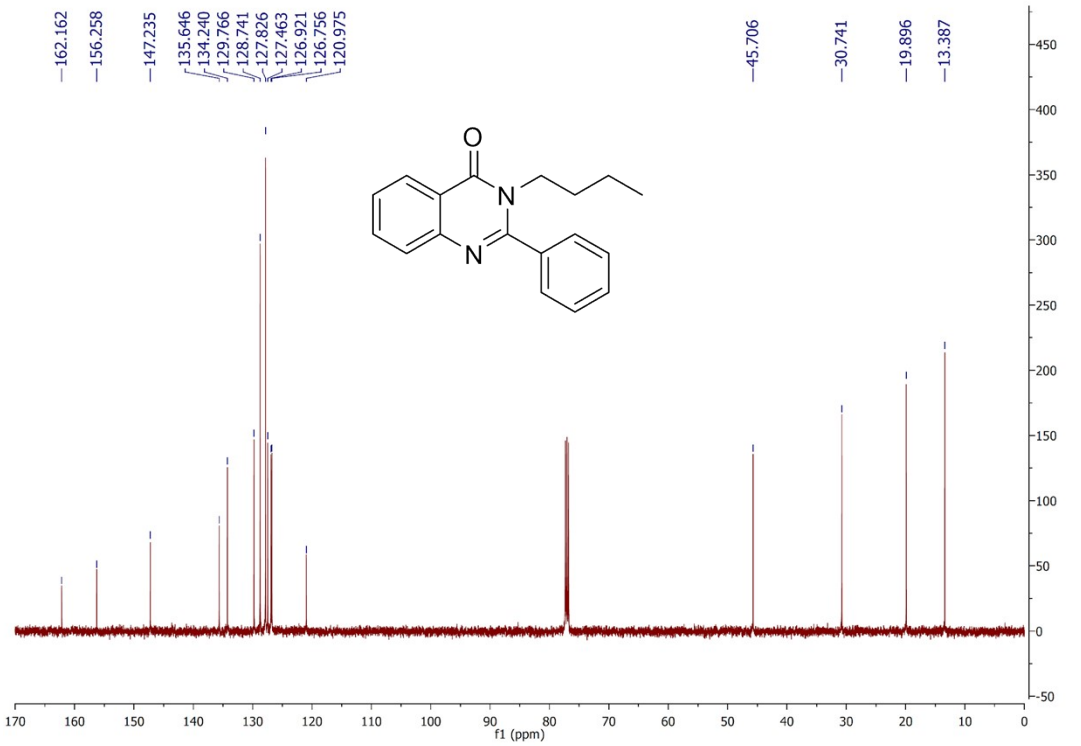
3-(4-Bromophenyl)-2-phenylquinazolin-4(3*H*)-one (3ao)



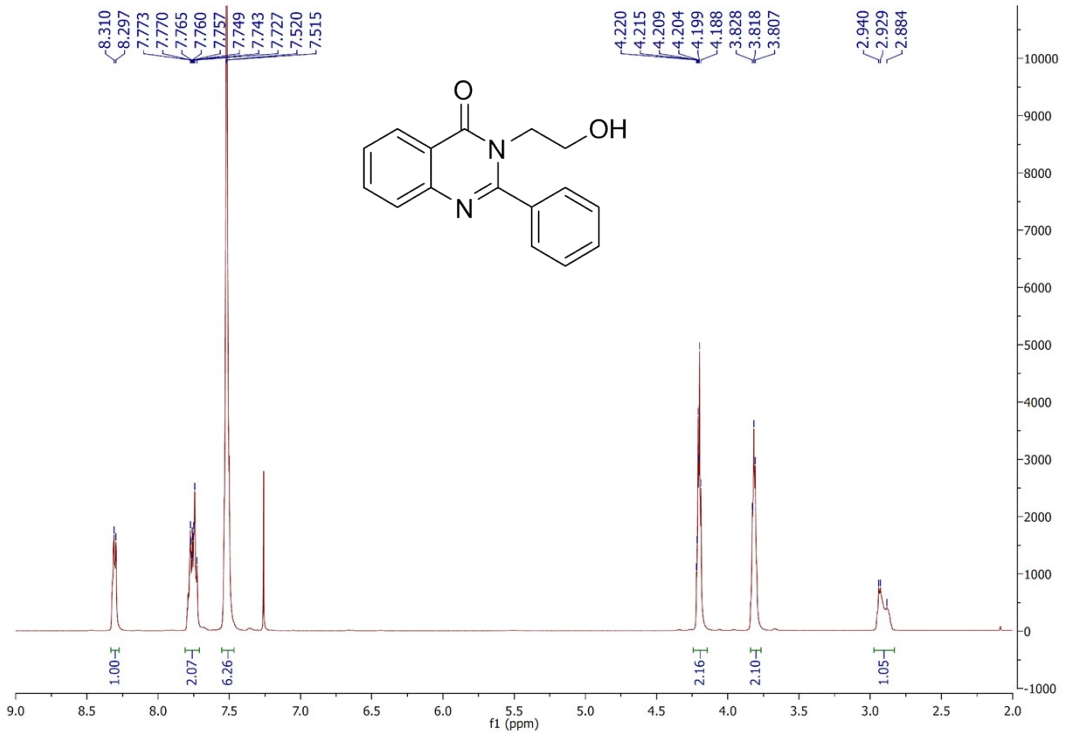


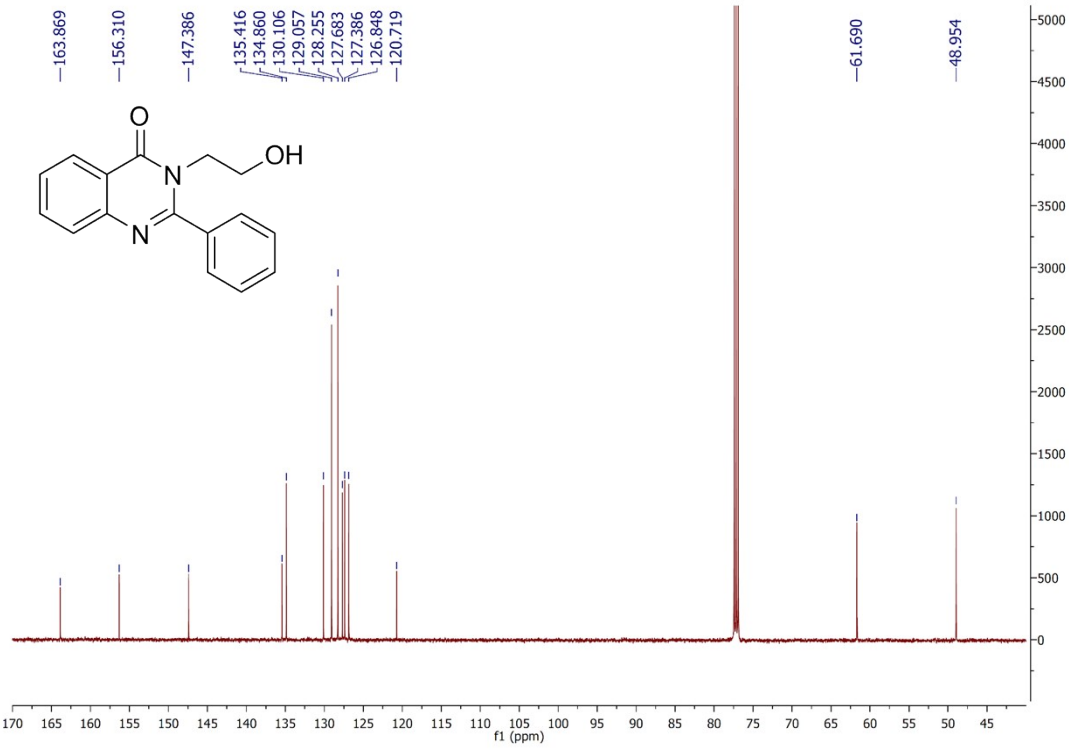
3-Butyl-2-phenylquinazolin-4(3*H*)-one (3ap)



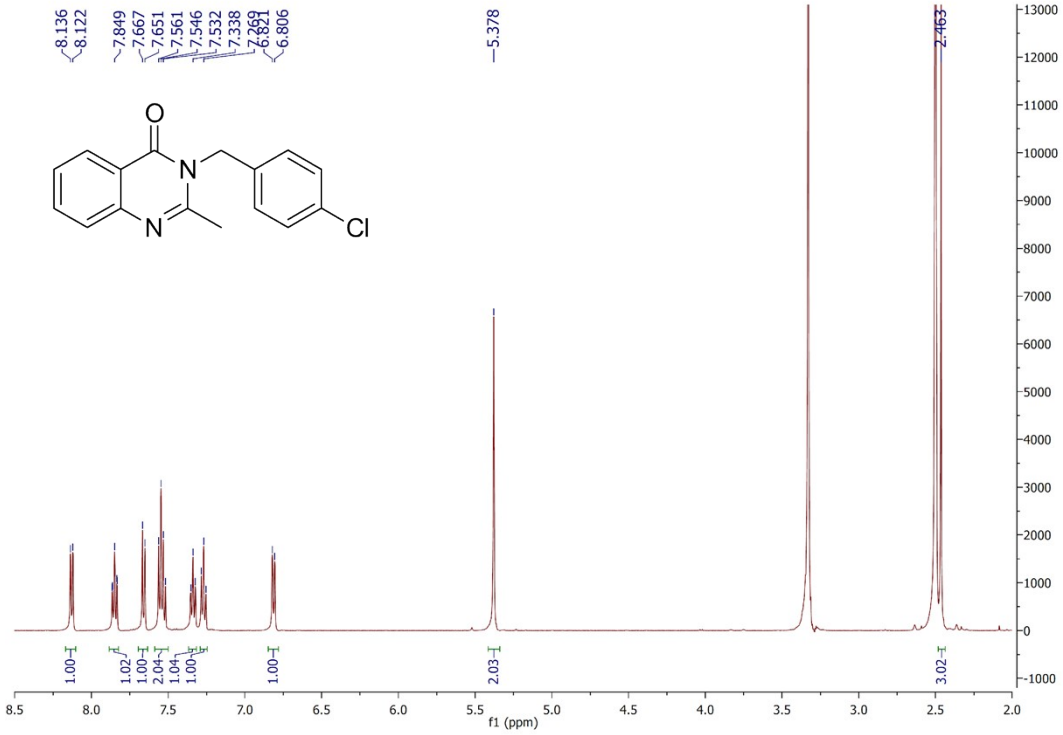


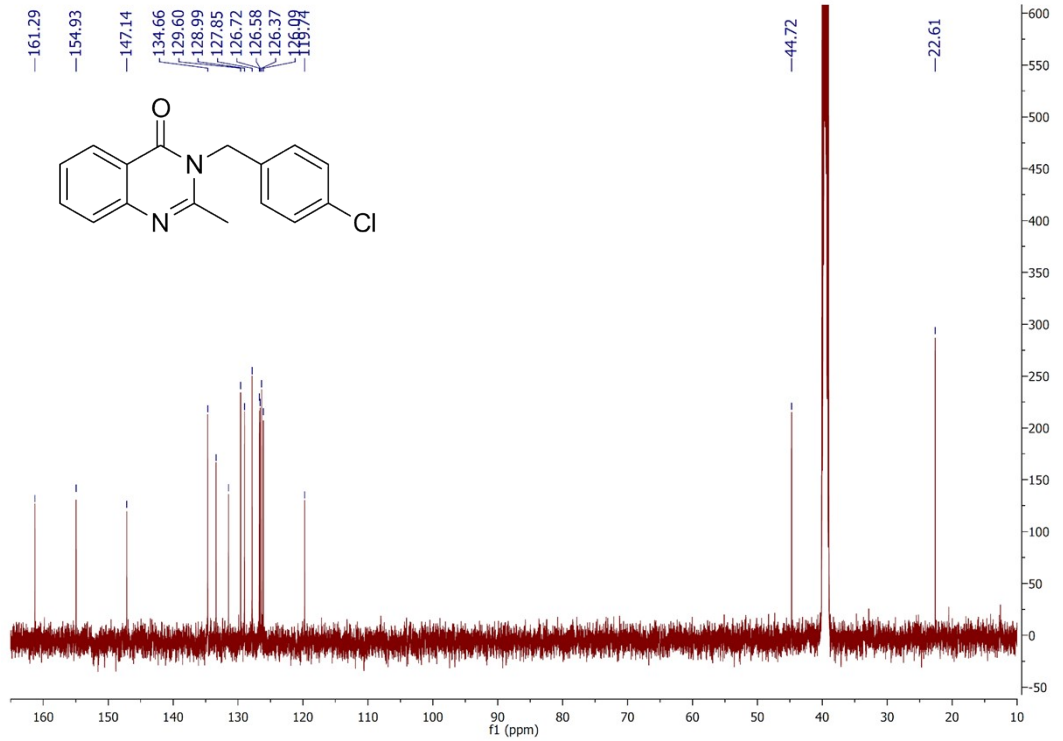
3-(2-Hydroxyethyl)-2-phenylquinazolin-4(3*H*)-one (3aq)



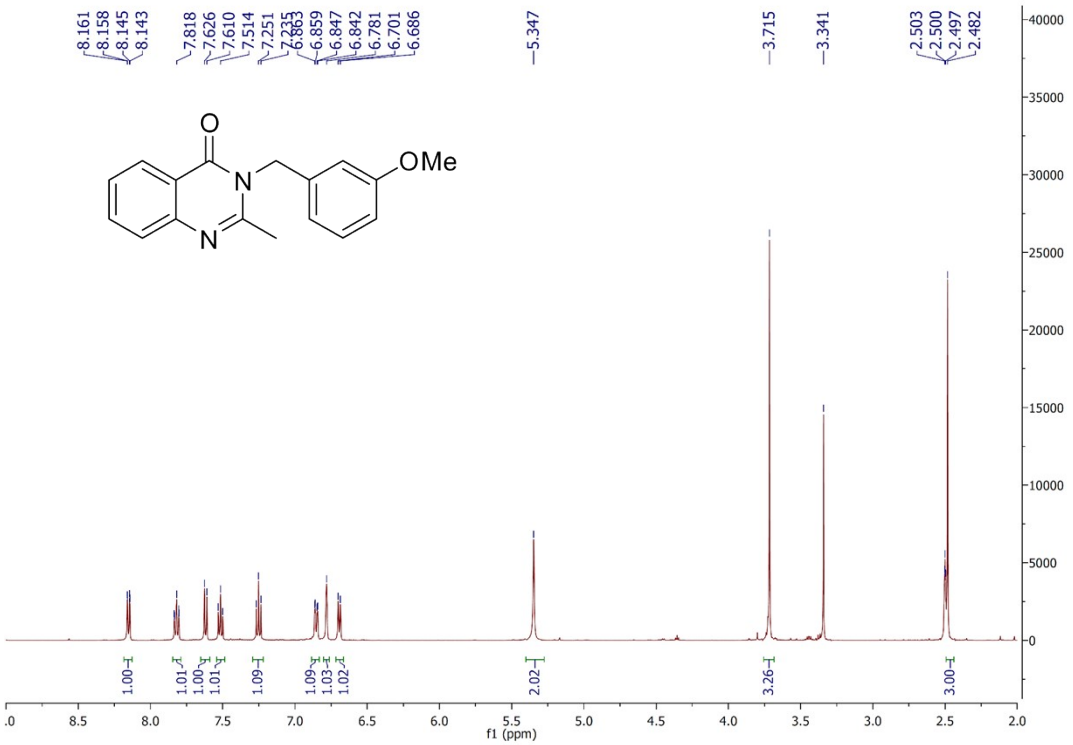


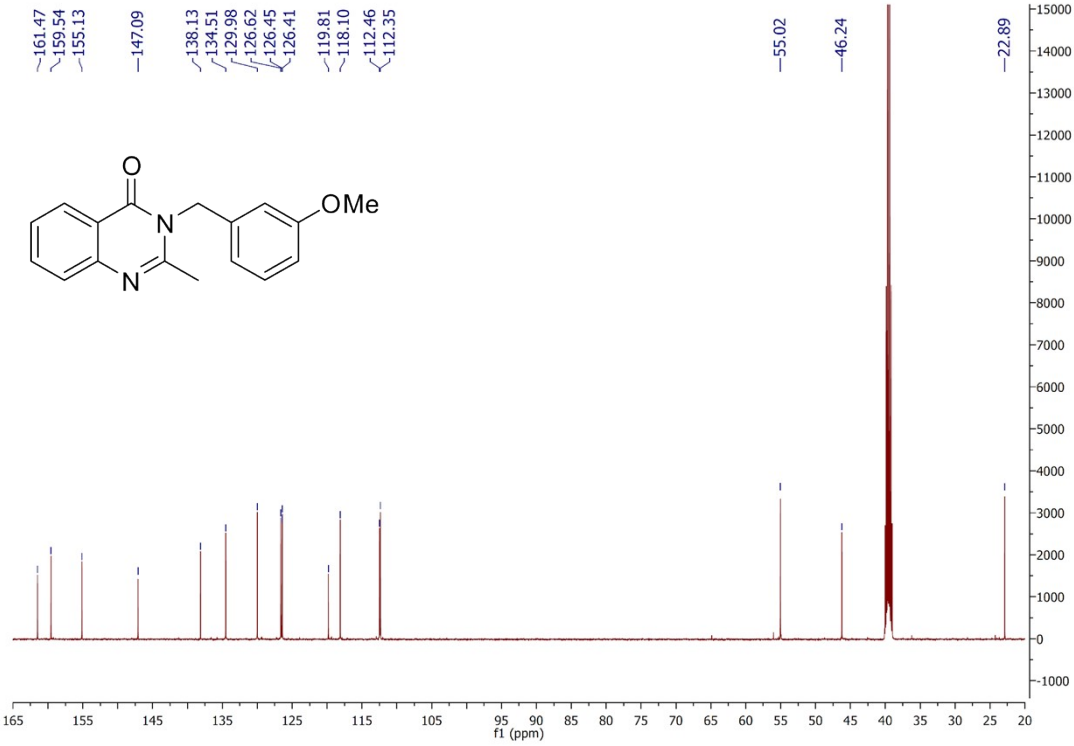
3-(4-Chlorobenzyl)- 2-methylquinazolin-4(3*H*)-one (3wg)



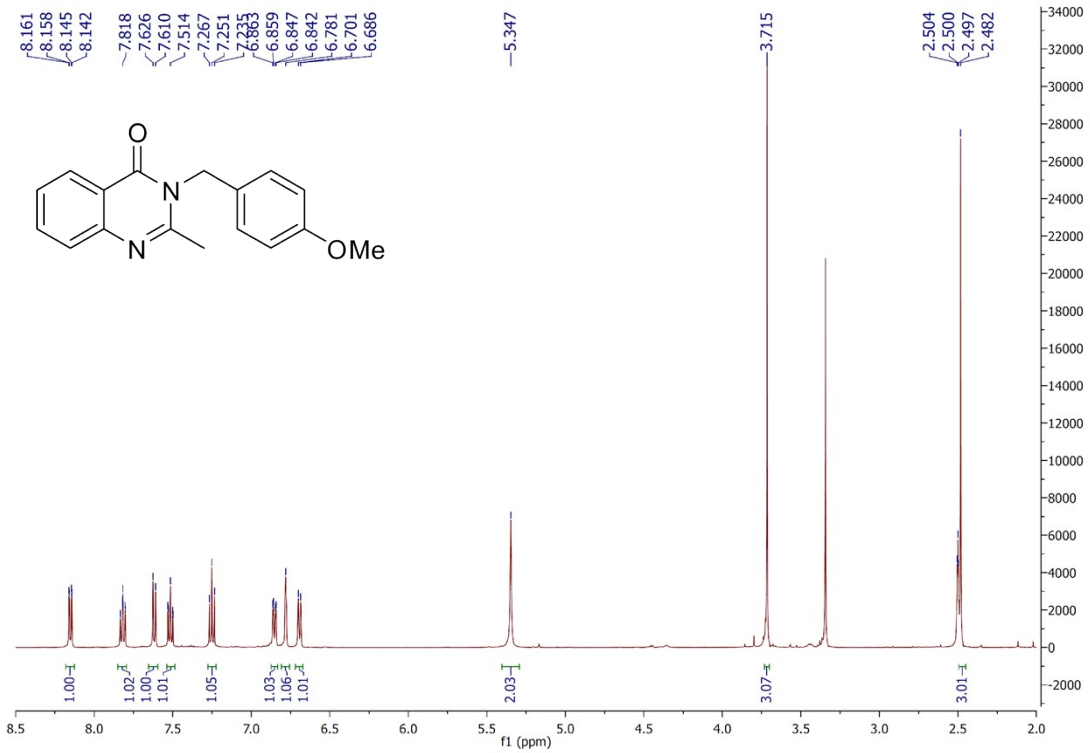


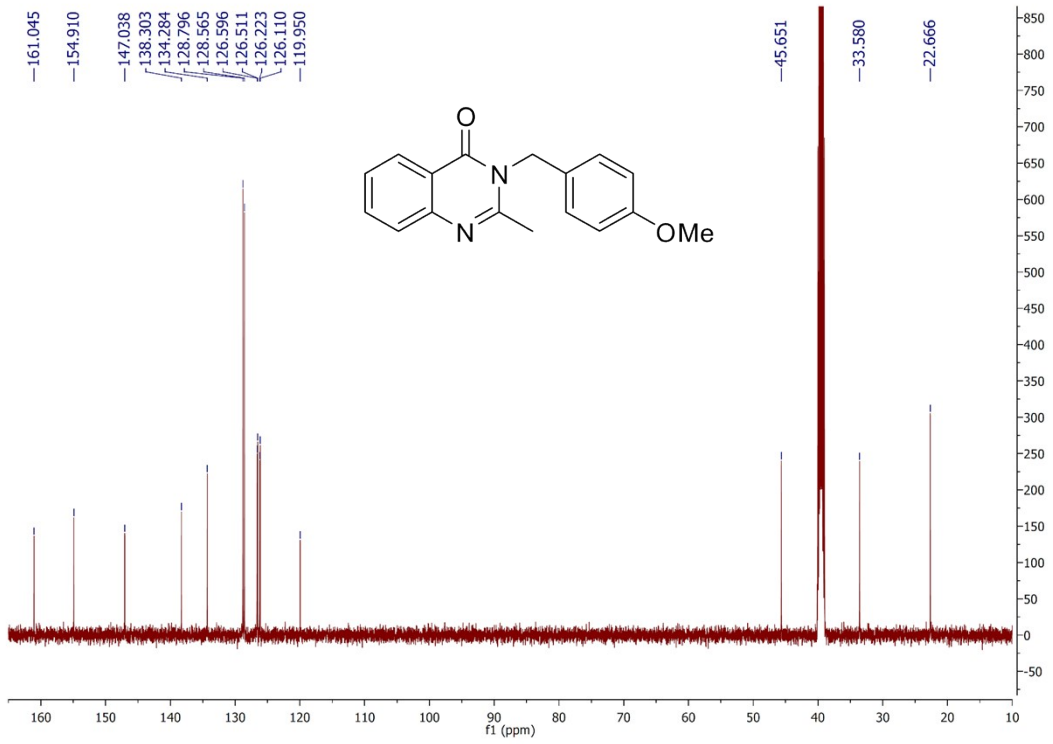
2-Methyl-3-(3-methoxybenzyl)quinazolin-4(3*H*)-one (3wd)



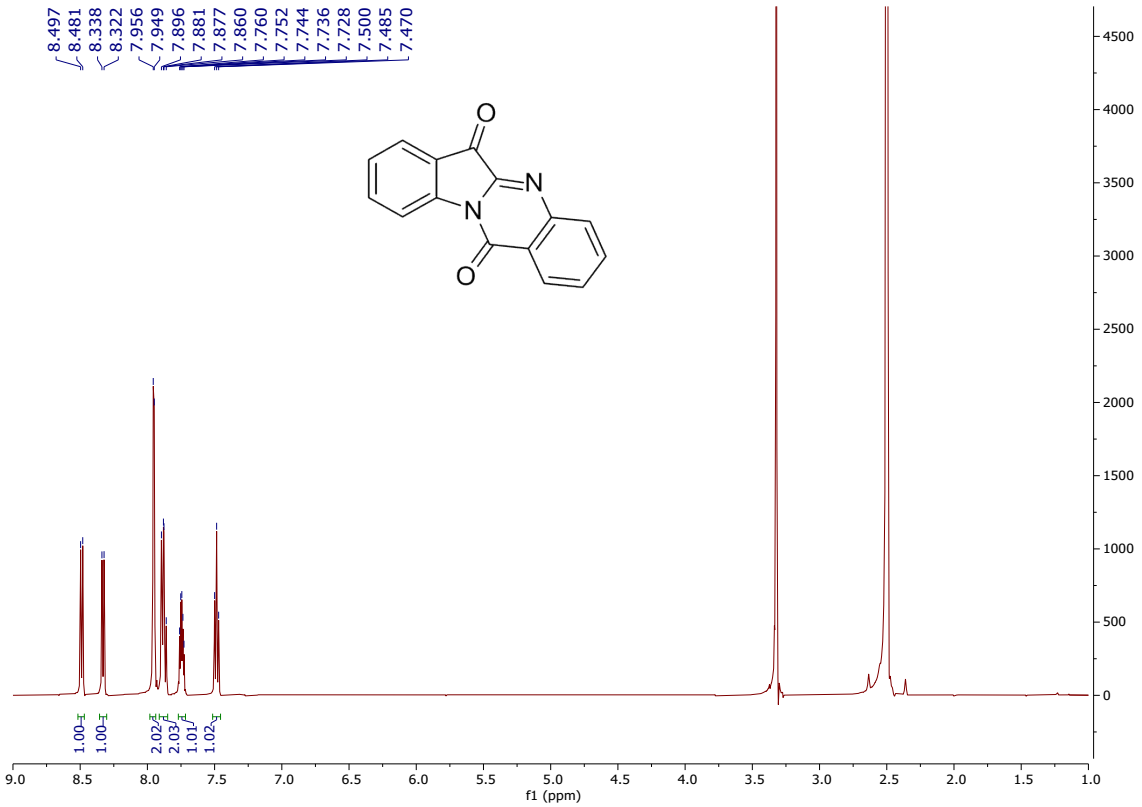


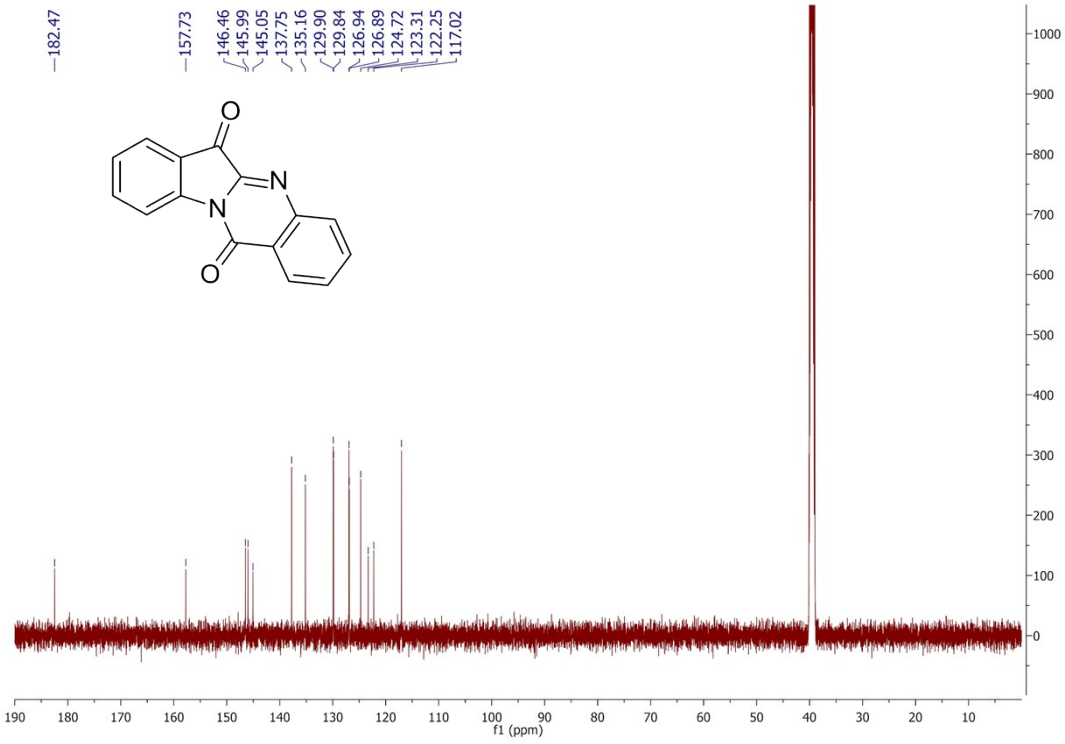
2-Methyl-3-(4-methoxybenzyl)quinazolin-4(3*H*)-one (3we)



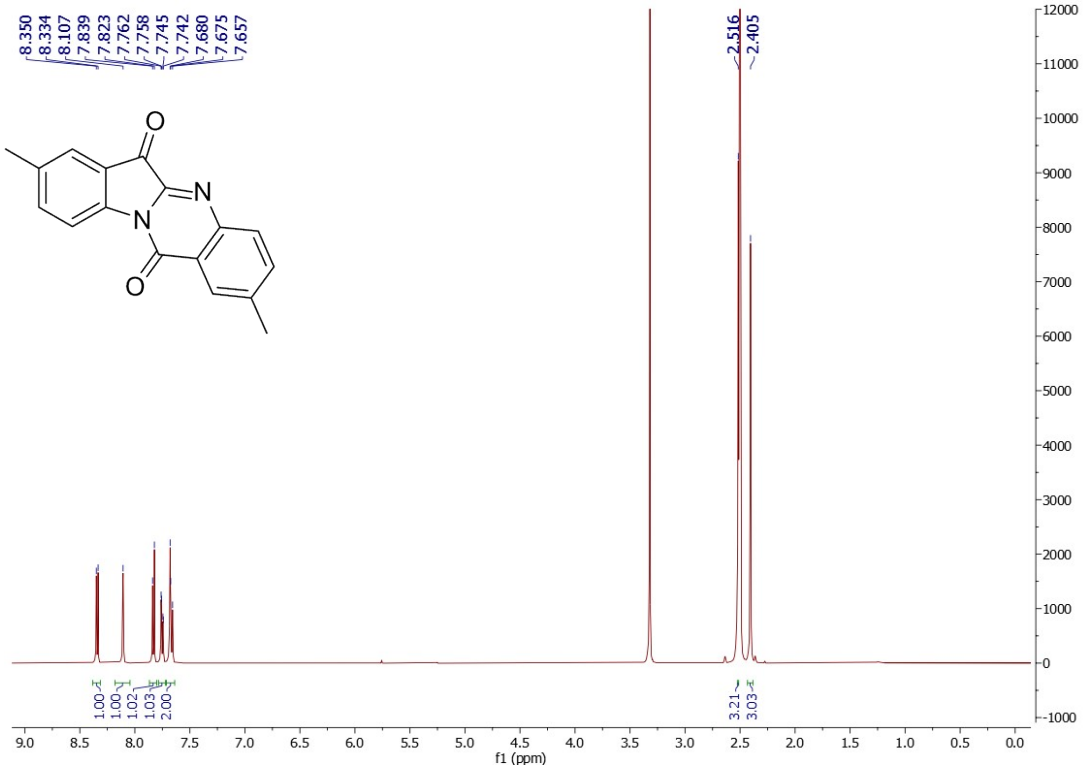


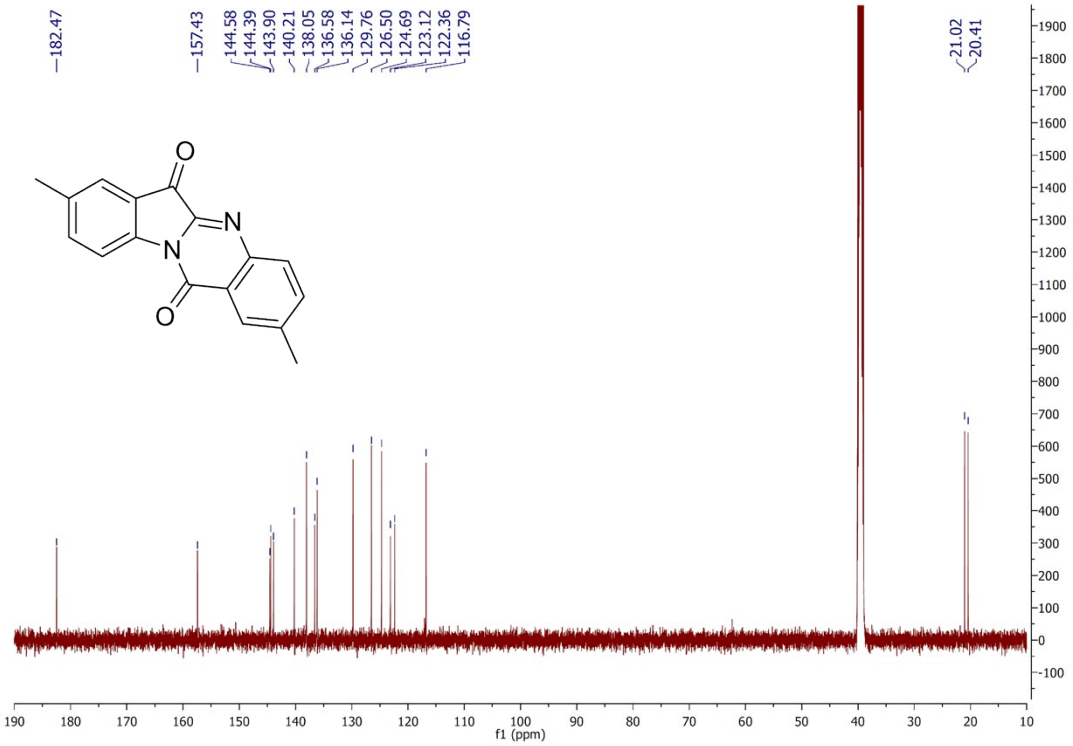
Indolo[2,1-*b*]quinazoline-6,12-dione (4aa)



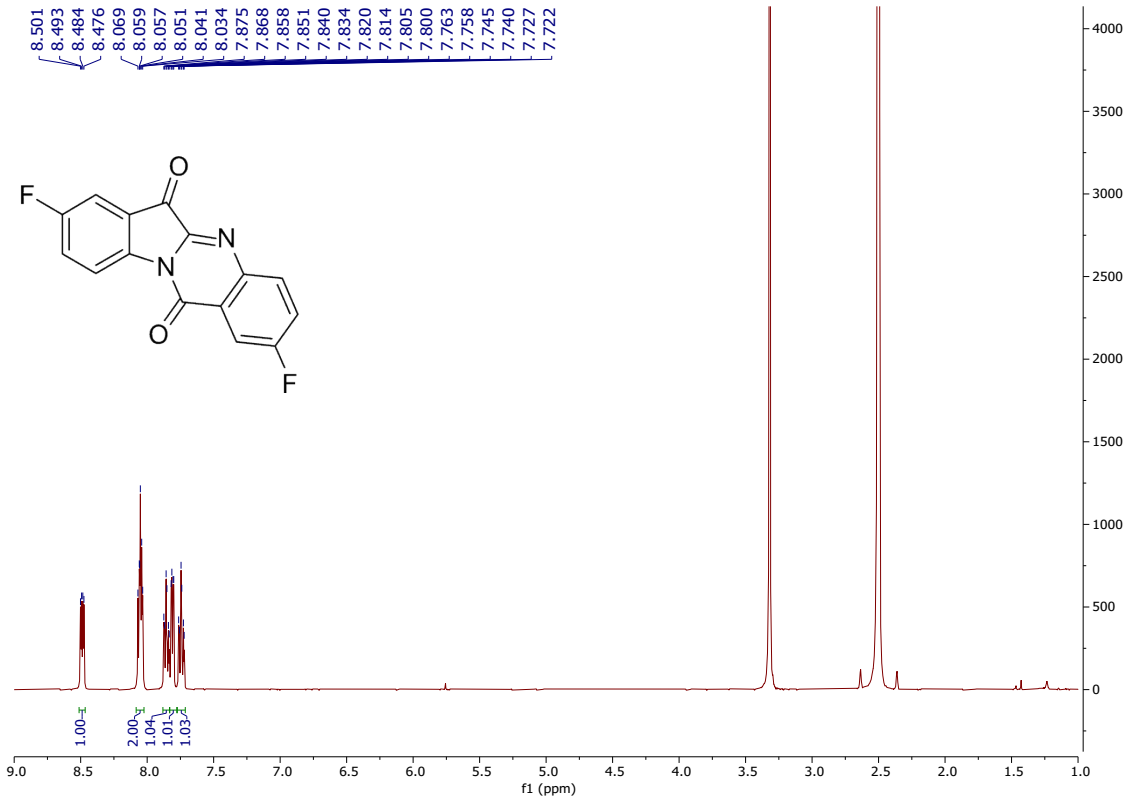


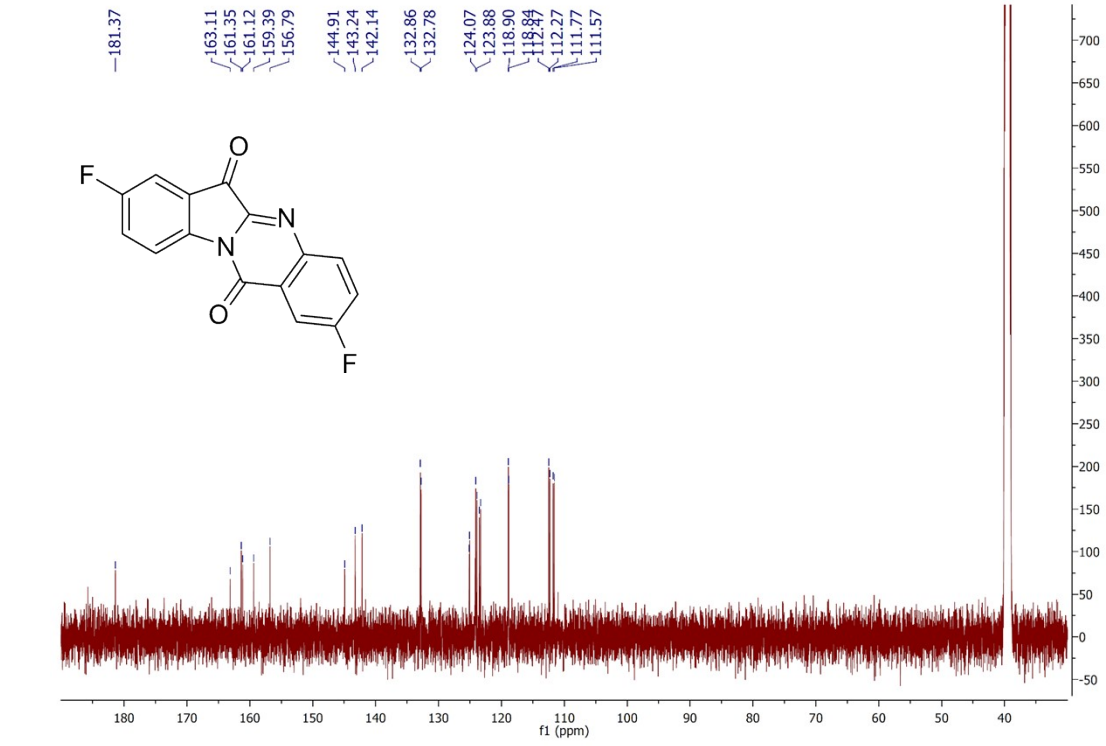
2,8-Dimethylindolo[2,1-*b*]quinazoline-6,12-dione (4bb)



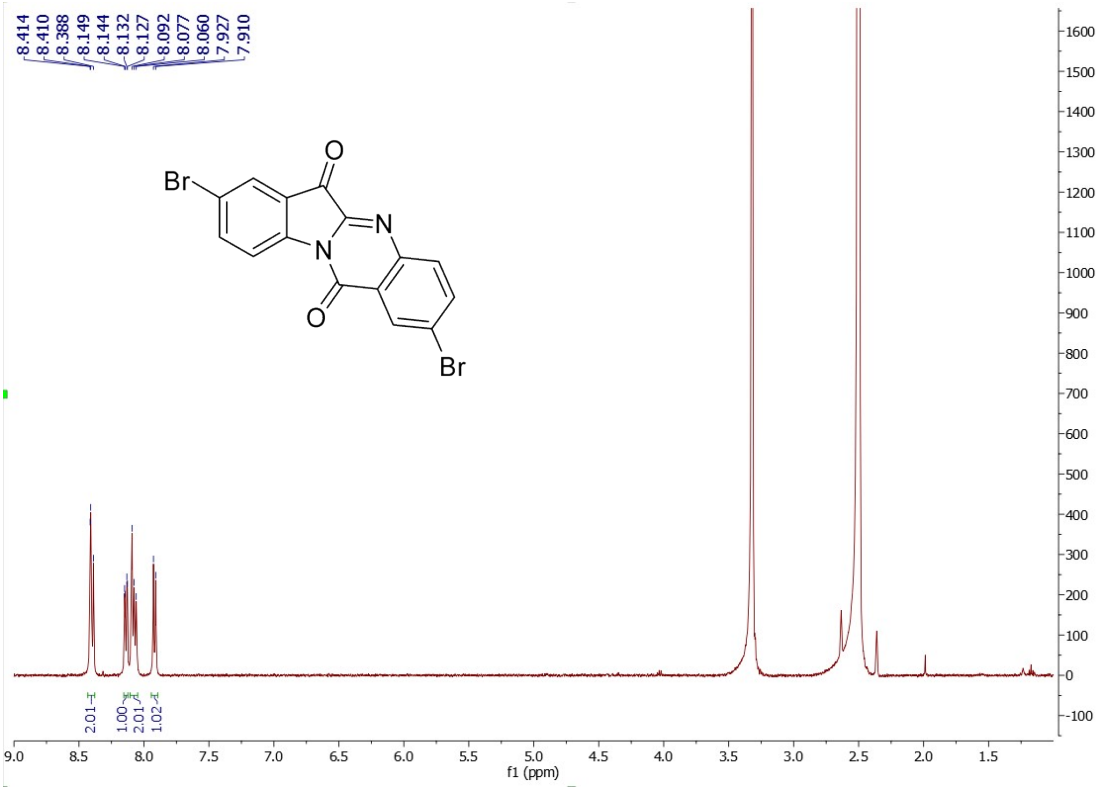


2,8-Difluoroindolo[2,1-*b*]quinazoline-6,12-dione (4cc)





2,8-Dibromoindolo[2,1-*b*]quinazoline-6,12-dione (4ee)



Dimethyl 6,12-dioxo-6,12-dihydroindolo[2,1-*b*]quinazoline-2,8-dicarboxylate (4ff)