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SUPPORTING INFORMATION

Unveiling the Untapped Potential of Bertagnini's Salts in Microwave-Assisted Synthesis of Quinazolinones

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GENERAL INFORMATION AND EXPERIMENTAL PROCEDURE

Commercially available reagents were purchased from Acros, Aldrich, Strem Chemicals, Alfa-Aesar, TCI Europe and used as received. All reactions were monitored by thin-layer chromatography (TLC) performed on glass-backed silica gel 60 F254, 0.2 mm plates (Merck), and compounds were visualized under UV light (254 nm). All reactions were performed using microwave instrument (Model: DISCOVER SP; SERIAL NO: DC8609; MODEL NO: 909155). The eluents were technical grade. ^{1}H and ^{13}C NMR spectra were recorded on a Varian 600 MHz and Bruker Avance III HD 600 MHz NMR spectrometer and were calibrated using trimethylsilane (TMS). Proton chemical shifts are expressed in parts per million (ppm, δ scale) and are referred to the residual hydrogen in the solvent ($CHCl_3$, 7.260 ppm or DMSO 2.50 ppm). Data are represented as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet and/or multiple resonances, bs = broad singlet, and combination of thereof), coupling constant (*J*) in Hertz (Hz) and integration. Carbon chemical shifts are expressed in parts per million (ppm, δ scale) and are referenced to the carbon resonances of the NMR solvent ($CDCl_3$, δ 77.16 ppm or δ DMSO-d_6 δ 39.52 ppm). Deuterated NMR solvents were obtained from Aldrich. Infrared (IR) spectral was recorded in the Jasco FTIR-4X (MODEL: PKS-D1) instrument and data are reported in wavenumber (cm^{-1}). Positive ESI-MS spectra were recorded on a high-resolution LTQ Orbitrap Elite™ mass spectrometer (Thermo Fisher Scientific, Waltham, MA, USA). The solutions were infused into the ESI source at a flow rate of 5.00 μL/min. Spectra were recorded with a resolution of 120,000 (FWHM). Instrument conditions were as follows: spray voltage 3500 V, capillary temperature 275 °C, sheath gas 12 (arbitrary units),

auxiliary gas 3 (arbitrary units), sweep gas 0 (arbitrary units), probe heater temperature 50 °C. Yields refer to pure isolated materials after filtration only (No column chromatography).

Instrumental details of Microwave

Model: DISCOVER SP
SERIAL NO: DC8609
MODEL NO: 909155
VOLTS: 180/240 VAC
MAX. MICROWAVE POWER: 300 W
MAX. CUR: 6.3 A
MAX PWR: 1100
FREQ: 50/60 Hz.

Pictorial diagram of Microwave instrument

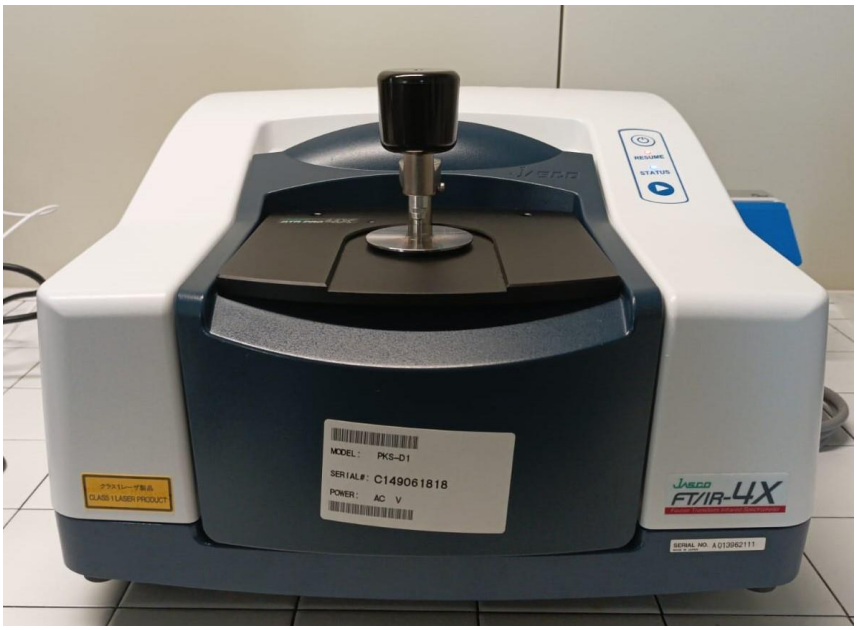
FTIR Instrumental details

Jasco FTIR-4X

MODEL: PKS-D1

SERIAL#: C149061818

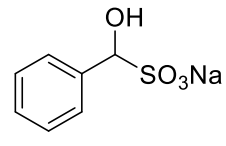
POWER: AC V



Procedure A. GENERAL PROCEDURE FOR THE SYNTHESIS OF 2-PHENYLQUINAZOLIN-4(3*H*)-ONE

Anthranilamide (0.5 mmol) and sodium hydroxy(phenyl)methanesulfonate (**2a**) (0.5 mmol) were placed in a 10 mL microwave vial equipped with a stir bar. After addition of 2 mL of water the vial was capped properly, then the reaction mixture underwent microwave irradiation at 100 °C with stirring for 10 hours. The resulting solid crude product was then filtered and washed with water to yield 2-phenylquinazolin-4(3*H*)-one (**3aa**). In certain instances, the crude reaction mixture was quenched by pouring it into ice water to enhance product yield.

LIST OF BERTAGNINI'S SALTS:



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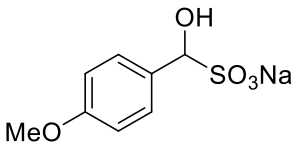

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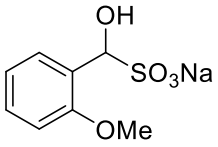

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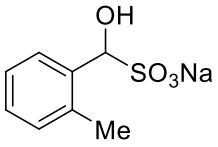

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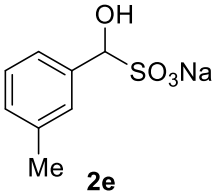

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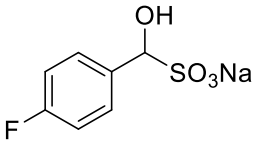

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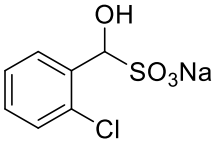

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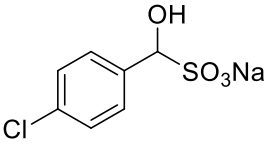

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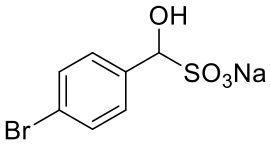

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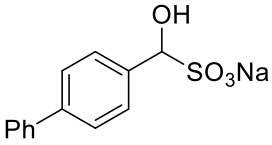

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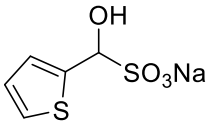
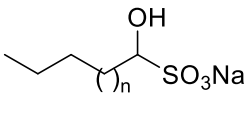
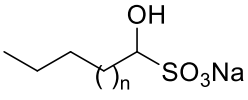


2k



n = X

2l



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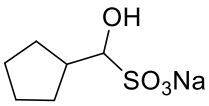
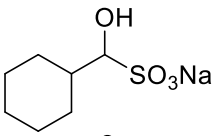
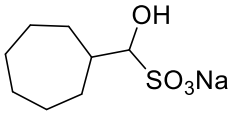
2m



2n

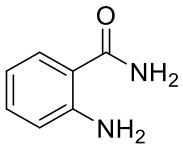


2o

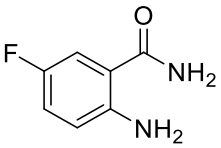


2p

LIST OF ANTHRANILAMIDES:



1a



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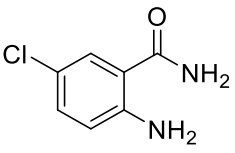
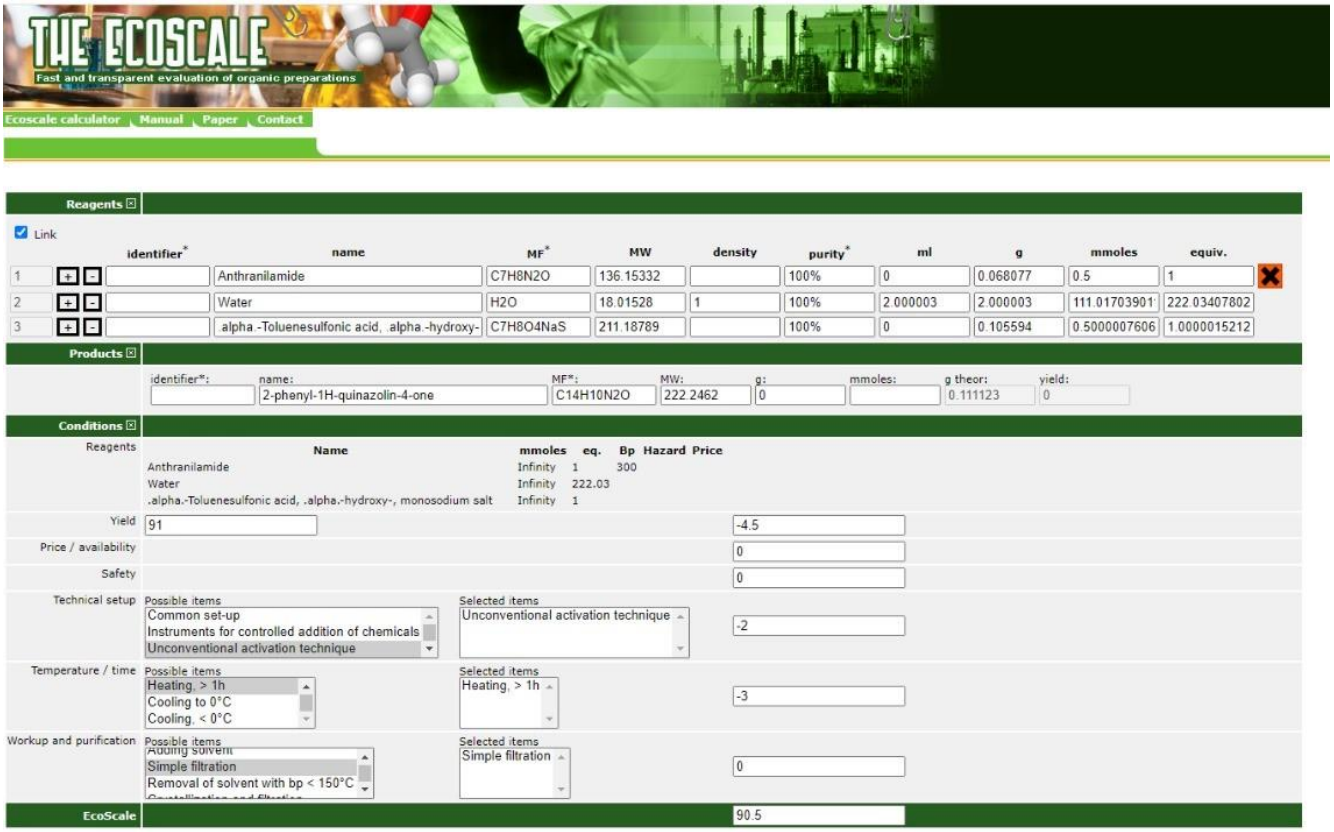


1c

Table S1. Calculation of Ecoscale score[a]

The Eco-scale Score for the microwave asssited synthesis of 2-Phenylquinazolin-4(3*H*)-one (**3aa)**

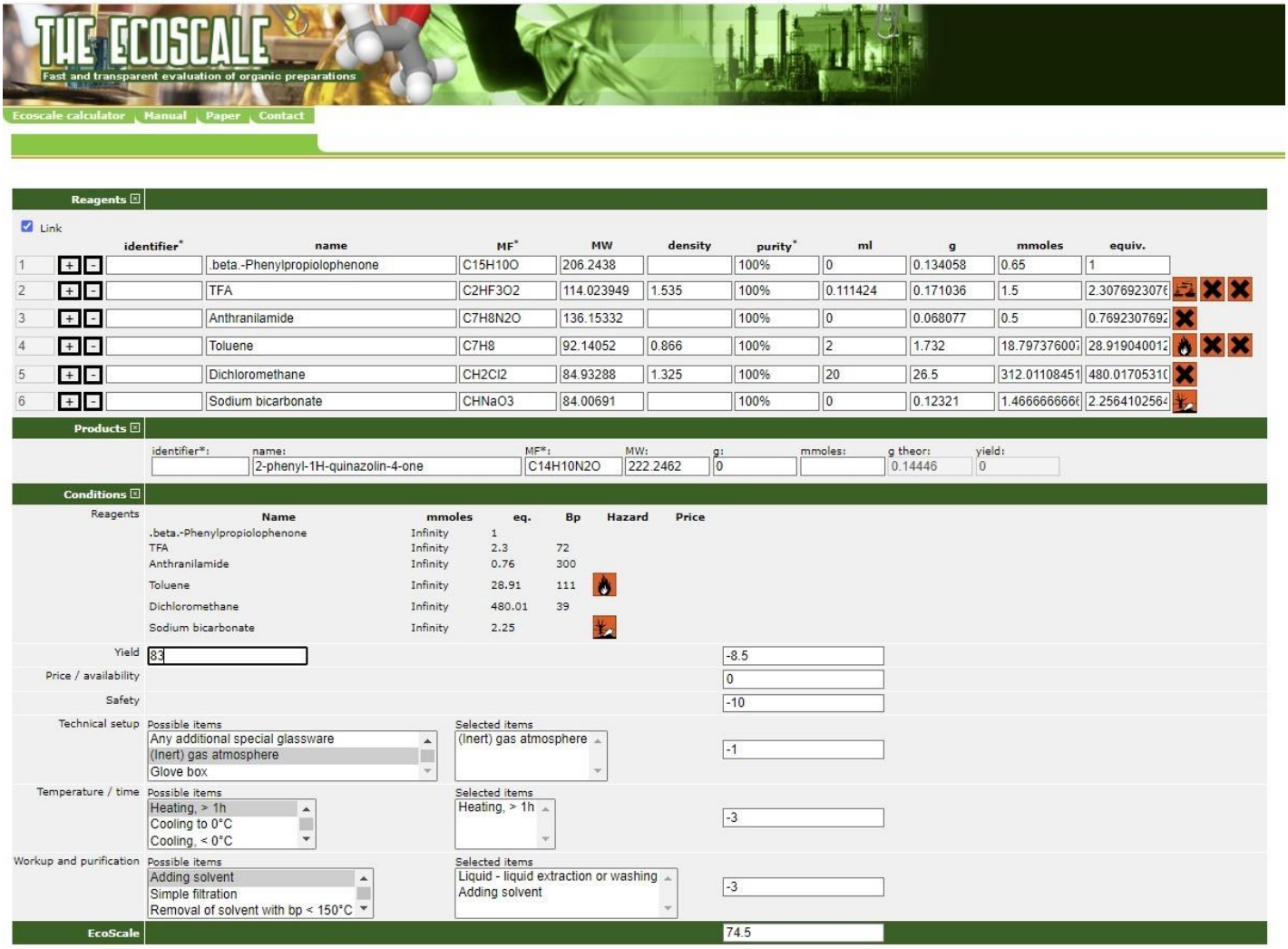


Entry	Parameters	Penalty Points
1	Yield (91%)	-4.5
2	Price/availability	0
3	Safety	0
4	Technical set-up (Common set-up)	-2
5	Temperature/time (r.t.; < 24 h)	-3
6	Work-up and purification (Adding solvent, Simple filtration, removal of solvent with bp <150 °C)	0
	EcoScale Score	90.5

[a] Values calculated using the eco scale calculator software available at the link: http://ecoscale.cheminfo.org/calculator

The Eco-scale Score for the reported synthesis of 2-Phenylquinazolin-4(3*H*)-one (**3aa)**

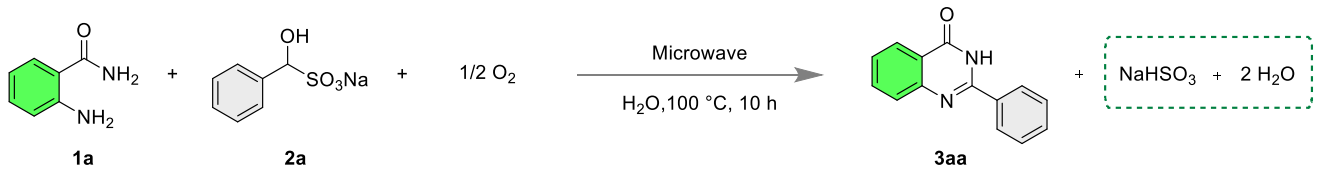
Yang, X.; Cheng, G.; Shen, J.; Kuai, C.; Cui, X,. *Org. Chem. Front.* **2015,** *2*, 366-368.



Entry	Parameters	Penalty Points
1	Yield (83%)	-8.5
2	Price/availability	0
3	Safety	-10
4	Technical set-up (Common set-up)	-1
5	Temperature/time (r.t.; < 24 h)	-3
6	Work-up and purification (Adding solvent, Simple filtration, removal of solvent with bp <150 °C)	-3
	EcoScale Score	74.5

[a]Values calculated using the eco scale calculator software available at the link: http://ecoscale.cheminfo.org/calculator

Calculation of the Green Chemistry Metrics for the the microwave asssited synthesis of 2-Phenylquinazolin-4(3*H*)-one (3aa)



1a	**2a**		**3aa**	
Molecular Weight: 136,15	Molecular Weight: 210,18	Molecular Weight: 16,00	Molecular Weight: 222,25	Molecular Weight: 140,08
0.5 mmol	0.5 mmol	0.5 mmol	0.455 mmol	
			91% yield	
68.07 mg	**105.1 mg**	**8,00 mg**	**(101,1 mg)**	**70,04 mg**

Solvent: 2000 mg

$$\text{Atom Economy } (\textit{AE}) = \frac{\textit{mass of desired product}}{\textit{total mass of reagents}} = \frac{222{,}25}{136{,}15 + 210{,}18 + 16{,}00} \times 100 = \frac{222{,}25}{362{,}33} \times 100 = \mathbf{61{,}3}$$

$$\text{Enviromental factor } (\textit{E}) = \frac{\textit{mass of total waste}}{\textit{mass of desired product}} = \frac{(70{,}04 + 2000)\ \text{mg}}{101{,}1\ \text{mg}} = \frac{2070.04\ \text{mg}}{101{,}1\ \text{mg}} = \mathbf{20{,}4}$$

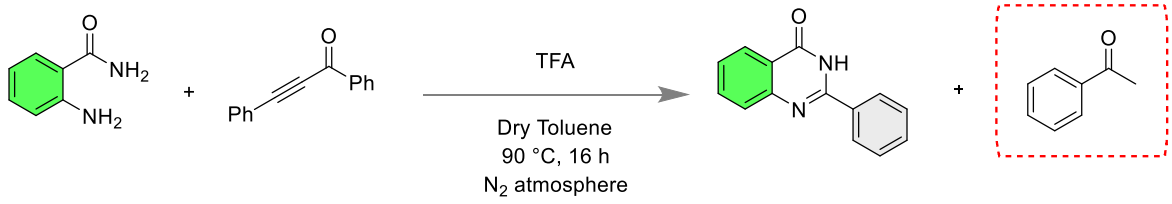
Work-up: H_2O (6000 mg)

$$\textit{E} \text{ (after purification: filtration and washing)} = \frac{(70{,}04 + 2000 + 6000)\ \text{mg}}{101.1\ \text{mg}} = \frac{8070{,}04\ \text{mg}}{101.1\ \text{mg}} = \mathbf{79{,}8}$$

$$\text{Reaction Mass Effinciecy } (\textit{RMS}) = \frac{\textit{actual mass of desired product}}{\textit{total mass of reagents}} = \frac{101{,}1\ \text{mg}}{(68{,}07 + 105{,}1 + 8{,}00)\ \text{mg}} \times 100 = \frac{101{,}10\ \text{mg}}{181{,}17\ \text{mg}} \times 100 = \mathbf{55{,}8}$$

Calculation of the Green Chemistry Metrics for the reported synthesis of 2-Phenylquinazolin-4(3*H*)-one (3aa)

Yang, X.; Cheng, G.; Shen, J.; Kuai, C.; Cui, X,. *Org. Chem. Front.* **2015,** *2*, 366-368.



Molecular Weight: 136,15	Molecular Weight: 206,24	Molecular Weight: 114.02	Molecular Weight: 222,25	Molecular Weight: 120,15
0.5 mmol	0.65 mmol	1.5 mmol	0.415	
			83% yield	
68.07 mg	**134.1 mg**	**171.03 mg**	**(92.23 mg)**	**60.08 mg**

Excess Reagent : **30,94 mg + 171,03 mg**

Solvent: **1734,00 mg**

Atom Economy (***AE***) = $\frac{\textit{mass of desired product}}{\textit{total mass of reagents}} = \frac{222,25}{136,15 + 206,24} \times 100 = \frac{222,25}{342,39} \times 100 =$ **64,9**

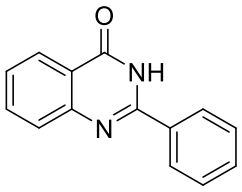
Enviromental factor (***E***) = $\frac{\textit{mass of total waste}}{\textit{mass of desired product}} = \frac{(30,94 + 171,03 + 60,08 + 1734,00)\ mg}{92,23\ mg} = \frac{1996,05\ mg}{92,23\ mg} =$ **21,6**

Work-up: DCM (300 mL, 399000,00 mg, H_2O (30 mL, 30000,00 mg), $NaHCO_3$ 126,01 mg + EtOH (1000,00 mg)

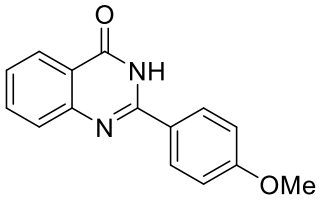
E (after purification: filtration and washing = $\frac{(30,94 + 171,03 + 60,08 + 1734,00 + 399000,00 + 30000,00 + 126,01 + 1000,00)\ mg}{92.23\ mg} = \frac{432131,06\ mg}{92.23\ mg} =$ **4684,61**

Reaction **M**ass **E**ffinciecy (***RMS***)= $\frac{\textit{actual mass of desired product}}{\textit{total mass of reagents}} = \frac{92,23\ mg}{(68,07 + 134,10)\ mg} \times 100 = \frac{92,23\ mg}{202,17\ mg} \times 100 =$ **45,6**

CHARACTERIZATION DATA OF THE SYNTHESIZED COMPOUNDS

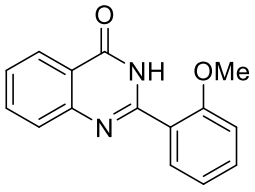


2-Phenylquinazolin-4(3*H*)-one (**3aa**):[1] The title compound was synthesized according to the general procedure **A**; White solid; Yield: 91% (101 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.53 (s, 1H), 8.20 – 8.13 (m, 3H), 7.82 (t, *J* = 7.2 Hz, 1H), 7.74 (d, *J* = 8.4 Hz, 1H), 7.60 – 7.48 (m, 4H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 162.3, 152.3, 148.8, 134.6, 132.7, 131.4, 128.6, 127.8, 127.5, 126.6, 125.9, 121.0.



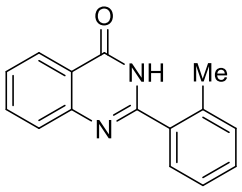
2-(4-Methoxyphenyl)quinazolin-4(3*H*)-one (3ab):[2] The title compound was synthesized according to the general procedure **A**; White solid; Yield: 78% (98.5 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.39 (s, 1H), 8.19 (d, *J* = 5.4 Hz, 2H), 8.13 (s, 1H), 7.80 (s, 1H), 7.70 (s, 1H), 7.47 (s, 1H), 7.08 (s, 2H), 3.84 (s, 3H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 162.3, 161.9, 151.8, 148.9, 134.5, 129.4, 127.3, 126.1, 125.8, 124.8, 120.7, 113.9, 55.4.

2-(2-Methoxyphenyl)quinazolin-4(3*H*)-one (3ac):[3] The title compound was synthesized according

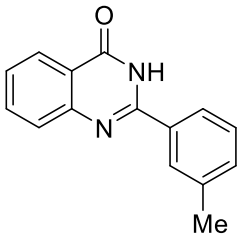


to the general procedure **A**; White solid; Yield: 69% (87 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.08 (s, 1H), 8.15 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.85 – 7.79 (m, 1H), 7.71 (dd, *J* = 12.0, 4.8 Hz, 2H), 7.56 – 7.51 (m, 2H), 7.19 (d, *J* = 8.4 Hz, 1H), 7.10 (t, *J* = 7.2 Hz, 1H), 3.86 (s, 3H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 161.3, 157.2, 152.4, 148.9, 134.4, 132.2, 130.5, 127.3, 126.6, 125.8, 122.6, 120.9, 120.5, 111.9, 55.8.

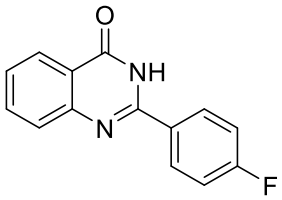
2-(o-Tolyl)quinazolin-4(3*H*)-one (**3ad**)[4]: The title compound was synthesized according to the general procedure **A**; White solid; Yield: 65% (77 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.43 (s, 1H), 8.17 (d, J = 7.8 Hz, 1H), 7.83 (t, J = 7.2 Hz, 1H), 7.69 (d, J = 7.8 Hz, 1H), 7.54 (d, J = 7.2 Hz, 1H), 7.53 – 7.49 (m, 1H), 7.43 (t, J = 7.2 Hz, 1H), 7.36 – 7.30 (m, 2H), 2.39 (s, 3H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 161.8, 154.4, 148.7, 136.1, 134.4, 134.2, 130.5, 129.9, 129.1, 127.4, 126.6, 125.8, 125.7, 120.9, 19.5.



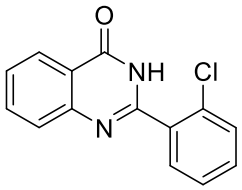
2-(m-Tolyl)quinazolin-4(3*H*)-one (3ae):[5] The title compound was synthesized according to the general procedure **A**; White solid; Yield: 74% (88 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.45 (s, 1H), 8.15 (d, J = 7.2 Hz, 1H), 8.02 (s, 1H), 7.97 (d, J = 7.8 Hz, 1H), 7.85 – 7.81 (m, 1H), 7.74 (d, J = 7.8 Hz, 1H), 7.54 – 7.49 (m, 1H), 7.45 – 7.37 (m, 2H), 2.40 (s, 3H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 162.2, 152.4, 148.8, 137.9, 134.6, 132.7, 132.0, 128.5, 128.3, 127.5, 126.5, 125.9, 124.9, 120.9, 20.9.



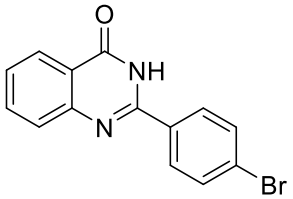
2-(4-Fluorophenyl)quinazolin-4(3*H*)-one (3af):[6] The title compound was synthesized according to the general procedure **A**; White solid; Yield: 83% (99.5 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.55 (s, 1H), 8.27 – 8.22 (m, 2H), 8.15 (d, J = 7.8 Hz, 1H), 7.82 (t, J = 7.2 Hz, 1H), 7.72 (d, J = 8.4 Hz, 1H), 7.51 (t, J = 7.2 Hz, 1H), 7.38 (t, J = 8.4 Hz, 2H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 164.1 (d, $^{1}J_{C\text{-}F}$ = 249.4 Hz), 162.2, 151.4, 148.7, 134.6, 130.4 (d, $^{3}J_{C\text{-}F}$ = 9.0 Hz), 129.2 (d, $^{4}J_{C\text{-}F}$ = 2.5 Hz), 127.5, 126.6, 125.9, 120.9, 115.6 (d, $^{2}J_{C\text{-}F}$ = 21.9 Hz).



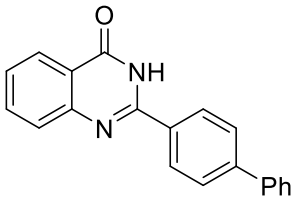
2-(2-Chlorophenyl)quinazolin-4(3*H*)-one (**3ag**):[7] The title compound was synthesized according to the general procedure **A**; White solid; Yield: 63% (81 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.65 (s, 1H), 8.18 (dd, J = 7.8, 1.2 Hz, 1H), 7.88 – 7.82 (m, 1H), 7.71 (d, J = 7.8 Hz, 1H), 7.67 (dd, J = 7.8, 1.2 Hz, 1H), 7.63 – 7.60 (m, 1H), 7.58 – 7.55 (m, 2H), 7.50 (td, J = 7.8, 1.2 Hz, 1H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 161.5, 152.3, 148.5, 134.6, 133.8, 131.6, 131.5, 130.9, 129.6, 127.4, 127.2, 127.1, 125.9, 121.2.



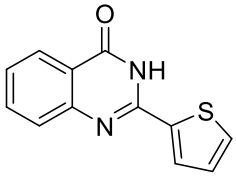
2-(4-Bromophenyl)quinazolin-4(3*H*)-one (3ai):[1] The reaction was performed in DMSO solvent and reaction mixture was poured into water to get the solid precipitate. Further crude product was washed with excess water to obtain the pure product. White solid; Yield: 86% (129 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.60 (s, 1H), 8.15 (dd, J = 7.8, 1.2 Hz, 1H), 8.13 (s, 1H), 8.11 (s, 1H), 7.86 – 7.81 (m, 1H), 7.76 (d, J = 1.8 Hz, 1H), 7.75 (d, J = 2.4 Hz, 1H), 7.73 (s, 1H), 7.55 – 7.51 (m, 1H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 162.2, 151.5, 148.5, 134.7, 131.9, 131.6, 129.8, 127.4, 126.8, 125.9, 125.2, 120.9.



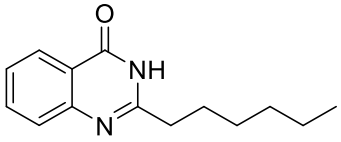
2-([1,1'-Biphenyl]-4-yl)quinazolin-4(3*H*)-one (**3aj**):[5] The title compound was synthesized according to the general procedure **A**; White solid; Yield: 81% (120.5 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.58 (s, 1H), 8.30 (d, J = 7.8 Hz, 2H), 8.17 (d, J = 7.8 Hz, 1H), 7.84 (t, J = 9.0 Hz, 3H), 7.76 (d, J = 3.6 Hz, 3H), 7.56 – 7.47 (m, 3H), 7.42 (t, J = 7.2 Hz, 1H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 162.3, 151.9, 148.7, 142.9, 138.9, 134.6, 131.5, 129.1, 128.4, 128.2, 127.4, 126.8, 126.7, 126.6, 125.9, 120.9.



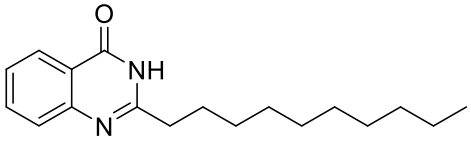
2-(Thiophen-2-yl)quinazolin-4(3*H*)-one (3ak):[8] The title compound was synthesized according to the general procedure **A**; White solid; Yield: 67% (76 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.48 (s, 1H), 8.12 (d, J = 7.8 Hz, 1H), 7.99 (s, 1H), 7.80 (t, J = 7.6 Hz, 1H), 7.68 (d, J = 8.1 Hz, 1H), 7.63 (d, J = 2.7 Hz, 1H), 7.48 (t, J = 7.5 Hz, 1H), 6.74 (s, 1H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 161.6, 148.7, 146.6, 146.1, 144.0, 134.6, 127.2, 126.4, 125.9, 121.2, 114.5, 112.5.



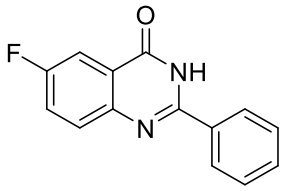
2-Hexylquinazolin-4(3*H*)-one (3al):[9] The title compound was synthesized according to the general procedure **A**; White solid; Yield: 73% (84 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.14 (s, 1H), 8.07 (dd, J = 7.8, 1.2 Hz, 1H), 7.77 – 7.72 (m, 1H), 7.58 (d, J = 7.8 Hz, 1H), 7.46 – 7.41 (m, 1H), 2.60 – 2.55 (m, 2H), 1.73 – 1.66 (m, 2H), 1.31 – 1.26 (m, 2H), 1.27 – 1.19 (m, 4H), 0.86 – 0.79 (m, 3H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 161.9, 157.6, 149.0, 134.3, 126.8, 125.9, 125.7, 120.8, 34.6, 30.9, 28.2, 26.8, 21.9, 13.9.



2-Decylquinazolin-4(3*H*)-one (3am):[10] The title compound was synthesized according to the general procedure **A**; White solid; Yield: 68% (97 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.13 (s, 1H), 8.07 (dd, J = 7.8, 1.2 Hz, 1H), 7.78 – 7.73 (m, 1H), 7.57 (d, J = 7.8 Hz, 1H), 7.46 – 7.41 (m, 1H), 2.61 – 2.54 (m, 2H), 1.73 – 1.66 (m, 2H), 1.33 – 1.25 (m, 5H), 1.25 – 1.14 (m, 9H), 0.84 – 0.81 (m, 3H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 161.9, 157.6, 148.9, 134.3, 126.8, 125.9, 125.7, 120.8, 34.5, 31.3, 28.9, 28.9, 28.7, 28.5, 26.8, 22.1, 13.9.

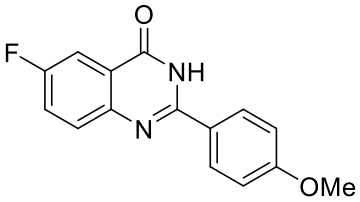


6-Fluoro-2-phenylquinazolin-4(3*H*)-one (3ba):[11] The title compound was synthesized according to



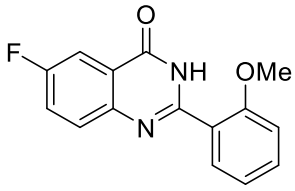
the general procedure **A**; White solid; Yield: 89% (107 mg); 89%; ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.65 (s, 1H), 8.17 (s, 1H), 8.16 – 8.15 (m, 1H), 7.84 – 7.82 (m, 1H), 7.81 (d, J = 5.6 Hz, 1H), 7.72 (td, J = 8.4, 3.0 Hz, 1H), 7.59 (d, J = 7.2 Hz, 1H), 7.56 – 7.53 (m, 2H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 161.6, 159.9 (d, $^{1}J_{C\text{-}F}$ = 245.5 Hz), 151.8, 145.6, 132.6, 131.4, 130.3 (d, $^{3}J_{C\text{-}F}$ = 8.3 Hz), 128.6, 127.7, 123.1 (d, $^{2}J_{C\text{-}F}$ = 24.1 Hz), 122.2 (d, $^{3}J_{C\text{-}F}$ = 8.6 Hz), 110.5 (d, $^{2}J_{C\text{-}F}$ = 23.3 Hz).

6-Fluoro-2-(4-methoxyphenyl)quinazolin-4(3*H*)-one (3bb):[12] The title compound was synthesized



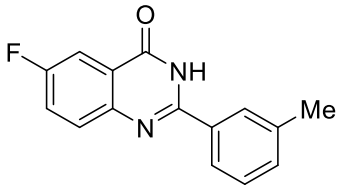
according to the general procedure **A**; White solid; Yield: 82% (111 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.51 (s, 1H), 8.17 (s, 2H), 7.83 - 7.66 (m, 3H), 7.09 (s, 2H), 3.85 (s, 3H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 161.9, 159.7 (d, $^{1}J_{C\text{-}F}$ = 245.7 Hz), 151.5, 145.8, 130.0, 129.4, 124.6, 123.1, 122.9, 121.8 (d, $^{3}J_{C\text{-}F}$ = 10.6 Hz), 114.0, 110.4 (d, $^{2}J_{C\text{-}F}$ = 23.4 Hz), 55.5.

6-Fluoro-2-(2-methoxyphenyl)quinazolin-4(3*H*)-one (**3bc**):[12] The title compound was synthesized according to the general procedure **A**; White solid; Yield: 78% (106 mg); ^{1}H NMR (600 MHz, DMSO-

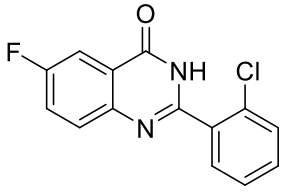


d_6) δ 12.22 (s, 1H), 7.82 (dd, J = 8.4, 3.0 Hz, 1H), 7.79 – 7.76 (m, 1H), 7.73 – 7.70 (m, 1H), 7.69 – 7.67 (m, 1H), 7.56 – 7.52 (m, 1H), 7.19 (d, J = 8.4 Hz, 1H), 7.09 (t, J = 7.2 Hz, 1H), 3.86 (s, 3H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 160.7, 159.9 (d, $^{1}J_{C\text{-}F}$ = 245.3 Hz), 157.1, 151.9, 145.9, 132.3, 130.4, 130.2 (d, $^{3}J_{C\text{-}F}$ = 8.3 Hz), 122.9 (d, $^{2}J_{C\text{-}F}$ = 24.0 Hz), 122.5, 122.2 (d, $^{3}J_{C\text{-}F}$ = 8.4 Hz), 120.4, 111.9, 110.4 (d, $^{2}J_{C\text{-}F}$ = 23.3 Hz), 55.8.

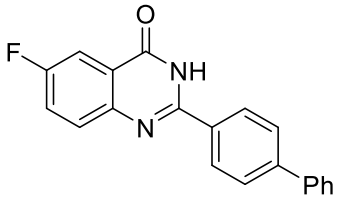
6-Fluoro-2-(m-tolyl)quinazolin-4(3*H*)-one (**3be**)**:** The title compound was synthesized according to the general procedure **A**; White solid; Yield: 87% (110 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.58 (s, 1H), 8.00 (s, 1H), 7.95 (d, J = 6.6 Hz, 1H), 7.81 (d, J = 6.0 Hz, 2H), 7.72 (d, J = 6.0 Hz, 1H), 7.46 – 7.37 (m, 2H), 2.40 (s, 3H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 161.7, 159.9 (d, $^{1}J_{C\text{-}F}$ = 244.8 Hz), 151.9, 145.6, 137.9, 132.5, 132.0, 130.3, 130.2 (d, $^{4}J_{C\text{-}F}$ = 4.9 Hz), 128.4 (d, $^{3}J_{C\text{-}F}$ = 7.9 Hz), 124.9, 123.1 (d, $^{2}J_{C\text{-}F}$ = 24.2 Hz), 122.2 (d, $^{3}J_{C\text{-}F}$ = 8.7 Hz), 110.5 (d, $^{2}J_{C\text{-}F}$ = 23.2 Hz); FTIR $\tilde{\nu}$ max = 3116, 3075, 1675, 1571, 1484, 1294, 879 cm^{-1}; HRMS: calculated for $C_{15}H_{12}FN_2O$: 255.0928 $[M+H]^+$; found: 255.0939.



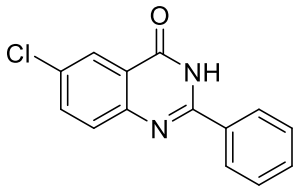
2-(2-Chlorophenyl)-6-fluoroquinazolin-4(3*H*)-one (3bg): The title compound was synthesized according to the general procedure **A**; White solid; Yield: 67% (92 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.76 (s, 1H), 7.85 (dd, J = 8.4, 3.0 Hz, 1H), 7.80 (dd, J = 8.4, 4.8 Hz, 1H), 7.74 (td, J = 8.4, 3.0 Hz, 1H), 7.67 (dd, J = 7.8, 1.8 Hz, 1H), 7.63 – 7.60 (m, 1H), 7.57 (td, J = 7.8, 1.8 Hz, 1H), 7.50 (td, J = 7.8, 1.2 Hz, 1H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 160.9, 160.3 (d, $^{1}J_{C\text{-}F}$ = 246.0 Hz), 151.8, 145.4, 133.6, 131.7, 131.5, 130.9, 130.4 (d, $^{3}J_{C\text{-}F}$ = 10.0 Hz), 129.6, 127.3, 123.1 (d, $^{2}J_{C\text{-}F}$ = 24.1 Hz), 122.5 (d, $^{3}J_{C\text{-}F}$ = 8.4 Hz), 110.6 (d, $^{2}J_{C\text{-}F}$ = 23.3 Hz); FTIR $\tilde{\nu}$ max = 3045, 2977, 1679, 1604, 1481, 927, 763 cm^{-1}; HRMS: calculated for $C_{14}H_9ClFN_2O$: 275.0387 $[M+H]^+$; found: 275.0396.



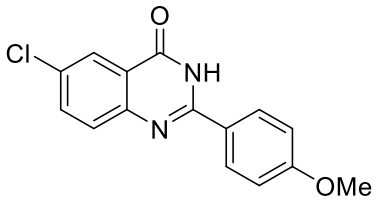
2-([1,1'-Biphenyl]-4-yl)-6-fluoroquinazolin-4(3*H*)-one (**3bj**): The title compound was synthesized according to the general procedure **A**; White solid; Yield: 58% (92 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.70 (s, 1H), 8.29 (s, 2H), 7.86 (s, 4H), 7.78 (s, 3H), 7.55 - 7.49 (m, 3H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 161.7, 159.9 (d, J = 246.1 Hz), 157.4, 154.1, 151.5, 145.7, 142.9, 138.9, 130.3, 129.1, 128.4, 128.2, 126.8 (d, $^{3}J_{C-F}$ = 13.3 Hz), 123.1 (d, $^{2}J_{C-F}$ = 23.5 Hz), 122.2, 110.5 (d, $^{2}J_{C-F}$ = 22.4 Hz); FTIR $\tilde{\nu}$ max = 3029, 2952, 1660, 1596, 1481, 1301, 836 cm^{-1}; HRMS: calculated for $C_{20}H_{14}FN_2O$: 317.1090 $[M+H]^+$; found: 317.1103.



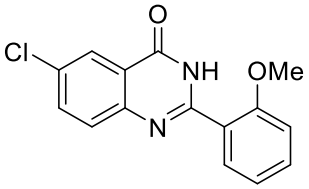
6-Chloro-2-phenylquinazolin-4(3*H*)-one (**3ca**):[1] The title compound was synthesized according to the general procedure **A**; White solid; Yield: 69% (89 mg); ^{1}H NMR (600 MHz, DMSO-d$_6$) δ 12.71 (s, 1H), 8.18 (s, 2H), 8.09 (s, 1H), 7.86 (s, 1H), 7.77 (s, 1H), 7.60 (s, 1H), 7.56 (s, 2H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 161.3, 152.9, 147.5, 134.7, 132.4, 131.6, 130.8, 129.7, 128.6, 127.8, 124.9, 122.2.



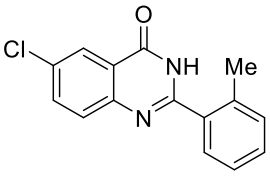
6-Chloro-2-(4-methoxyphenyl)quinazolin-4(3*H*)-one (3cb):[13] The title compound was synthesized according to the general procedure **A**; White solid; Yield: 58% (83 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.56 (s, 1H), 8.19 (s, 1H), 8.17 (s, 1H), 8.06 (d, J = 2.4 Hz, 1H), 7.83 (dd, J = 8.4, 2.4 Hz, 1H), 7.72 (d, J = 8.4 Hz, 1H), 7.09 (d, J = 8.8 Hz, 2H), 3.85 (s, 3H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 162.0, 161.3, 152.4, 147.7, 134.6, 130.2, 129.6, 129.5, 124.8, 124.5, 121.9, 114.0, 55.5.



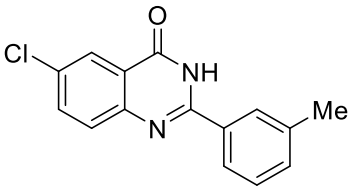
6-Chloro-2-(2-methoxyphenyl)quinazolin-4(3*H*)-one (**3cc**):[14] The title compound was synthesized according to the general procedure **A**; White solid; Yield: 59% (85 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.27 (s, 1H), 8.08 (d, *J* = 2.4 Hz, 1H), 7.85 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.70 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.56 – 7.51 (m, 1H), 7.20 (d, *J* = 8.4 Hz, 1H), 7.09 (t, *J* = 7.8 Hz, 1H), 3.86 (s, 3H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 160.3, 157.1, 152.8, 147.8, 134.5, 132.4, 130.8, 130.5, 129.6, 124.8, 122.4, 122.2, 120.4, 111.9, 55.8.



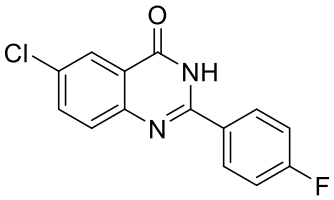
6-Chloro-2-(o-tolyl)quinazolin-4(3*H*)-one (**3cd**):[15] The title compound was synthesized according to the general procedure **A**; White solid; Yield: 53% (72 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.61 (s, 1H), 8.10 (d, *J* = 2.4 Hz, 1H), 7.86 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.71 (d, *J* = 8.4 Hz, 1H), 7.51 (d, *J* = 7.2 Hz, 1H), 7.44 (t, *J* = 7.2 Hz, 1H), 7.35 (d, *J* = 8.4 Hz, 1H), 7.32 (d, *J* = 7.2 Hz, 1H), 2.38 (s, 3H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 160.8, 154.9, 147.4, 136.2, 134.5, 133.9, 130.8, 130.6, 130.0, 129.6, 129.1, 125.7, 124.8, 122.2, 19.5.



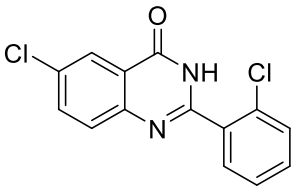
6-Chloro-2-(m-tolyl)quinazolin-4(3*H*)-one (**3ce**): The title compound was synthesized according to the general procedure **A**; White solid; Yield: 56% (76 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.63 (s, 1H), 8.08 (d, *J* = 2.4 Hz, 1H), 8.01 (s, 1H), 7.96 (d, *J* = 7.2 Hz, 1H), 7.85 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.76 (d, *J* = 8.4 Hz, 1H), 7.45 – 7.40 (m, 2H), 2.41 (s, 3H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 161.3, 152.9, 137.9, 134.8, 134.7, 132.9, 132.4, 132.2, 130.7, 129.7, 128.5, 128.4, 124.9, 124.9, 20.9; FTIR $\tilde{\nu}$ max = 3023, 2925, 1671, 1579, 1467, 1309, 842 cm^{-1}; HRMS: calculated for $C_{15}H_{12}ClN_2O$: 271.0638 $[M+H]^+$; found: 271.0649.



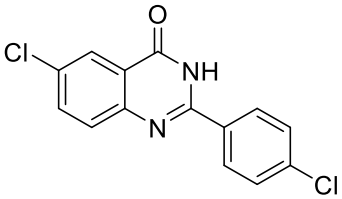
6-Chloro-2-(4-fluorophenyl)quinazolin-4(3*H*)-one (**3cf**):[16] The title compound was synthesized according to the general procedure **A**; White solid; Yield: 65% (89 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.73 (s, 1H), 8.26 – 8.21 (m, 2H), 8.08 (d, J = 2.4 Hz, 1H), 7.85 (dd, J = 8.4, 2.4 Hz, 1H), 7.75 (d, J = 8.4 Hz, 1H), 7.39 (t, J = 8.4 Hz, 2H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 164.1 (d, $^{1}J_{C\text{-}F}$ = 249.9 Hz), 161.3, 151.9, 147.4, 134.7, 130.8, 130.5 (d, $^{3}J_{C\text{-}F}$ = 9.0 Hz), 129.7, 128.9 (d, $^{4}J_{C\text{-}F}$ = 2.8 Hz), 124.9, 122.1, 115.7 (d, $^{2}J_{C\text{-}F}$ = 22.0 Hz).



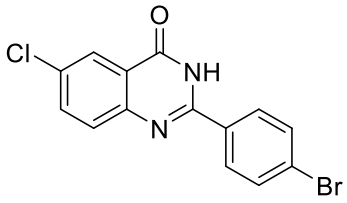
6-Chloro-2-(2-chlorophenyl)quinazolin-4(3*H*)-one (**3cg**):[16] The title compound was synthesized according to the general procedure **A**; White solid; Yield: 61% (89 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.82 (s, 1H), 8.12 (d, J = 2.4 Hz, 1H), 7.89 (dd, J = 8.4, 2.4 Hz, 1H), 7.75 (d, J = 8.4 Hz, 1H), 7.67 (dd, J = 7.2, 1.2 Hz, 1H), 7.62 (d, J = 8.4 Hz, 1H), 7.58 (td, J = 7.2, 1.2 Hz, 1H), 7.50 (t, J = 7.2 Hz, 1H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 160.5, 152.7, 147.3, 134.7, 133.5, 131.8, 131.4, 131.4, 130.9, 129.7, 129.6, 127.2, 124.9, 122.5.



6-Chloro-2-(4-chlorophenyl)quinazolin-4(3*H*)-one (**3ch**):[16] The title compound was synthesized according to the general procedure **A**; White solid; Yield: 64% (93 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.67 (s, 1H), 8.20 (d, J = 7.8 Hz, 2H), 8.09 (s, 1H), 7.85 (d, J = 8.4 Hz, 1H), 7.76 (d, J = 8.4 Hz, 1H), 7.62 (d, J = 7.8 Hz, 2H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 161.3, 152.3, 141.4, 139.2, 136.3, 134.4, 129.8, 129.5, 128.5, 127.6, 124.7, 122.2.

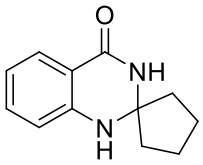


2-(4-Bromophenyl)-6-chloroquinazolin-4(3*H*)-one (3ci):[17] The title compound was synthesized



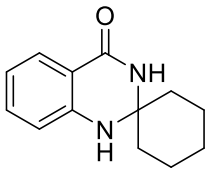
according to the general procedure **A**; White solid; Yield: 76% (127 mg); ^{1}H NMR (600 MHz, DMSO-*d*$_6$) δ 12.66 (s, 1H), 8.14 (s, 1H), 8.12 (s, 1H), 8.08 (d, *J* = 2.5 Hz, 1H), 7.84 (dd, *J* = 8.7, 2.5 Hz, 1H), 7.76 (d, *J* = 8.4 Hz, 3H); ^{13}C NMR (151 MHz, DMSO-*d*$_6$) δ 161.4, 152.2, 134.4, 131.4, 131.4, 130.6, 129.7, 129.4, 128.8, 125.1, 124.7, 122.2.

1'*H*-spiro[cyclopentane-1,2'-quinazolin]-4'(3'*H*)-one (**3an**)[18] The title compound was synthesized



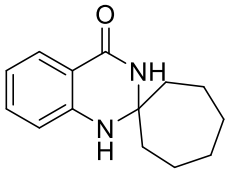
according to the general procedure **A**; White solid; Yield: 56% (56.6 mg); ^{1}H NMR (600 MHz, DMSO-*d*$_6$) δ 8.07 (s, 1H), 7.57 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.25 – 7.14 (m, 1H), 6.72 (s, 1H), 6.69 (d, *J* = 7.8 Hz, 1H), 6.63 (t, *J* = 7.8 Hz, 1H), 1.83 – 1.75 (m, 4H), 1.68 – 1.63 (m, 4H); ^{13}C NMR (151 MHz, DMSO-*d*$_6$) δ 163.5, 147.5, 133.0, 127.3, 116.6, 114.6, 114.3, 77.1, 39.3, 21.9.

1'*H*-spiro[cyclohexane-1,2'-quinazolin]-4'(3'*H*)-one (**3ao**):[18] The title compound was synthesized



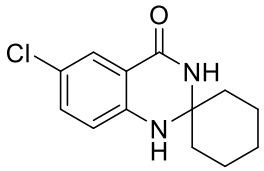
according to the general procedure **A**; White solid; Yield: 73% (79 mg); ^{1}H NMR (600 MHz, DMSO-*d*$_6$) δ 7.90 (s, 1H), 7.56 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.24 – 7.16 (m, 1H), 6.80 (d, *J* = 7.8 Hz, 1H), 6.62 (d, *J* = 7.8 Hz, 1H), 6.60 (d, *J* = 5.4 Hz, 1H), 1.78 – 1.67 (m, 2H), 1.65 – 1.58 (m, 2H), 1.58 – 1.51 (m, 4H), 1.46 – 1.36 (m, 1H), 1.29 – 1.20 (m, 1H); ^{13}C NMR (151 MHz, DMSO-*d*$_6$) δ 163.2, 146.8, 133.1, 127.1, 116.5, 114.6, 114.5, 67.8, 37.2, 24.6, 20.9.

1'*H*-spiro[cycloheptane-1,2'-quinazolin]-4'(3'*H*)-one (3ap):[18] The reaction was performed in



DMSO solvent and reaction mixture was poured into water to get the solid precipitate. Further crude product was washed with excess water to obtaine the pure product. White solid; Yield: 84% (97 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.00 (s, 1H), 7.55 (dd, J = 7.8, 1.2 Hz, 1H), 7.23 – 7.16 (m, 1H), 6.71 (s, 1H), 6.70 (s, 1H), 6.62 – 6.58 (m, 1H), 1.92 – 1.81 (m, 4H), 1.51 (s, 8H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 162.9, 146.7, 133.1, 127.1, 116.3, 114.4, 114.3, 71.9, 41.0, 29.2, 20.9.

6'-Chloro-1'*H*-spiro[cyclohexane-1,2'-quinazolin]-4'(3'*H*)-one (3co):[18] The title compound was



synthesized according to the general procedure **A**; White solid; Yield: 86 % (108 mg); ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.10 (s, 1H), 7.49 (d, J = 2.4 Hz, 1H), 7.24 (dd, J = 8.4, 2.4 Hz, 1H), 6.87 – 6.78 (m, 2H), 1.78 – 1.70 (m, 2H), 1.63 – 1.57 (m, 2H), 1.57 – 1.50 (m, 4H), 1.47 – 1.38 (m, 1H), 1.27- 1.19 (m, 1H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 162.0, 145.5, 132.9, 126.2, 120.1, 116.6, 115.6, 68.0, 37.1, 24.5, 20.8.

NMR SPECTRA

^{1}H NMR (600 MHz, DMSO-d_6)

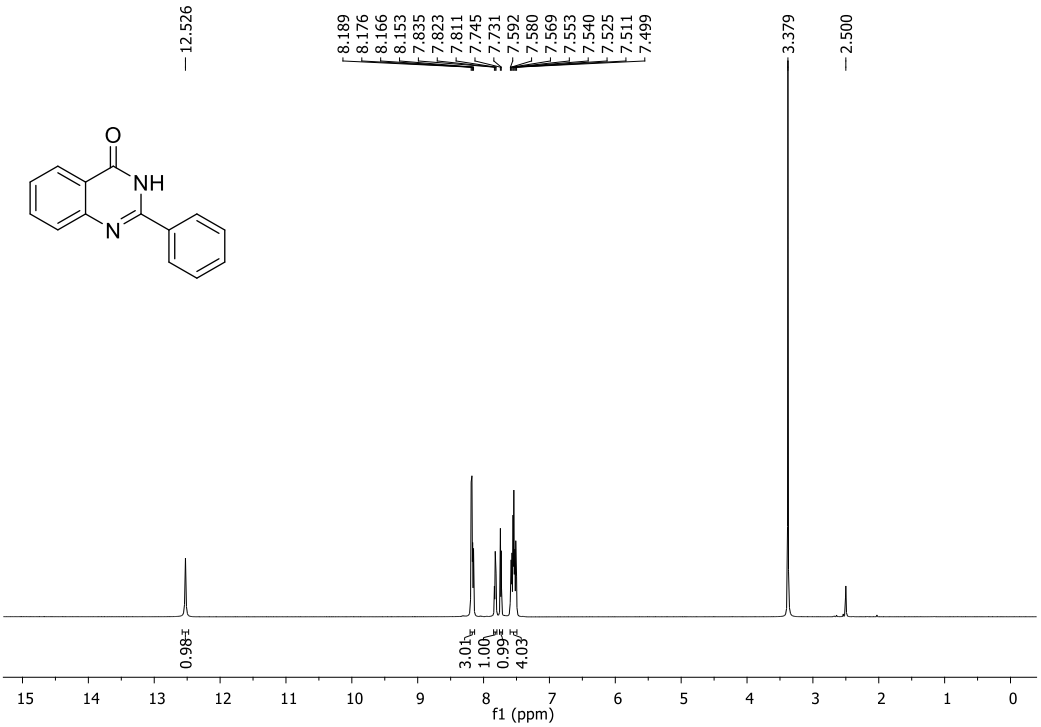


Figure S1. ^{1}H NMR spectrum of 2-Phenylquinazolin-4(3*H*)-one (**3aa**)

^{13}C NMR (151 MHz, DMSO-d_6)

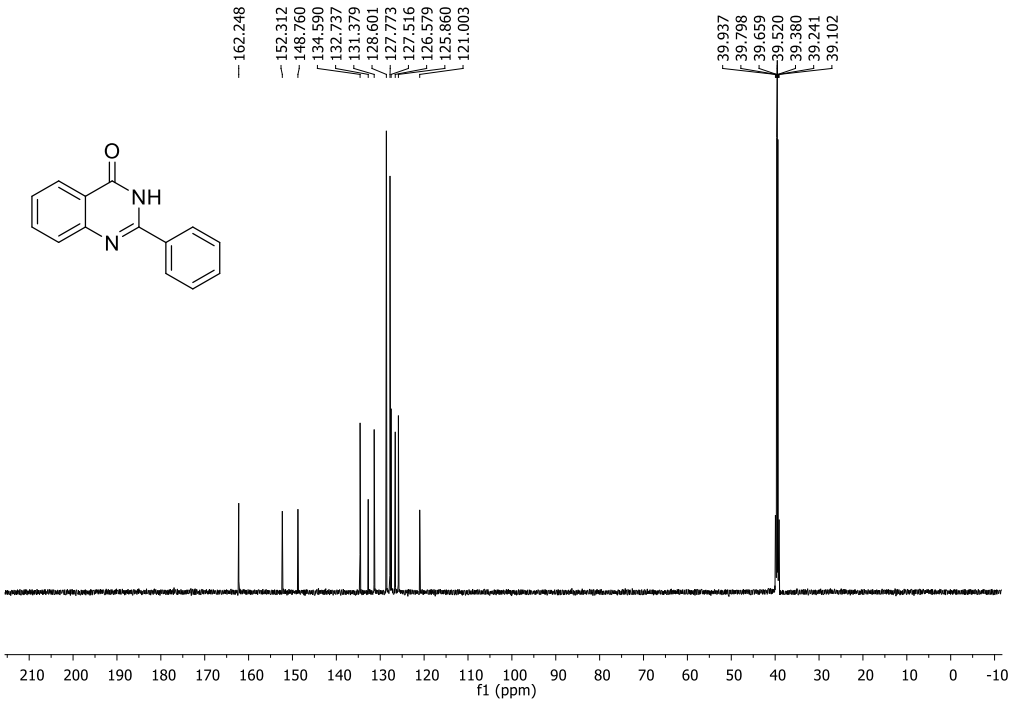


Figure S2. ^{13}C NMR spectrum of 2-Phenylquinazolin-4(3*H*)-one (**3aa**)

^{1}H NMR (600 MHz, DMSO-d_6)

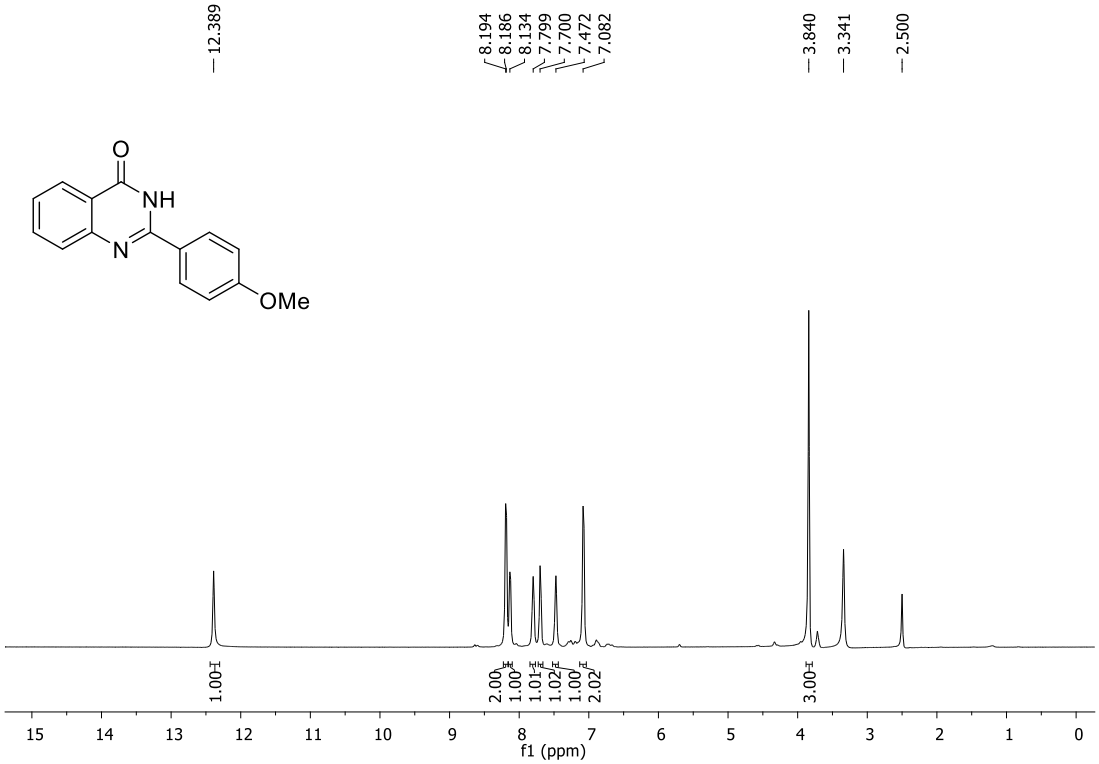


Figure S3. ^{1}H NMR spectrum of 2-(4-Methoxyphenyl)quinazolin-4(3*H*)-one (**3ab**)

^{13}C NMR (151 MHz, DMSO-d_6)

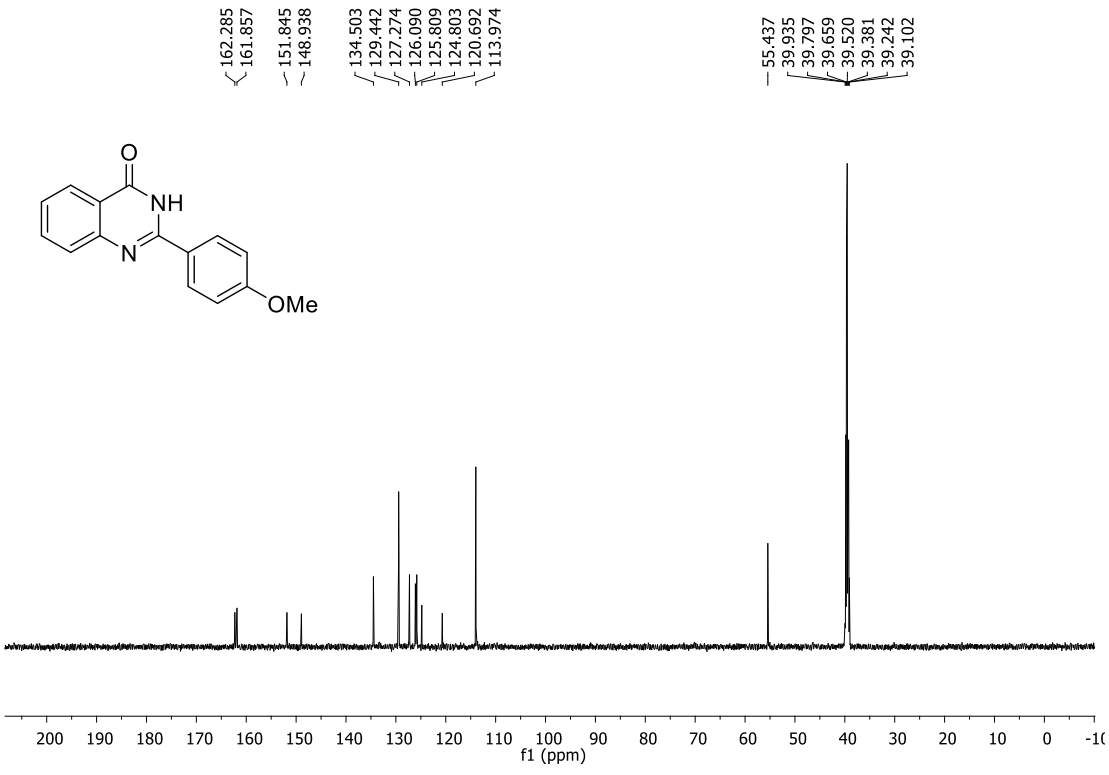


Figure S4. ^{13}C NMR spectrum of 2-(4-Methoxyphenyl)quinazolin-4(3*H*)-one (**3ab**)

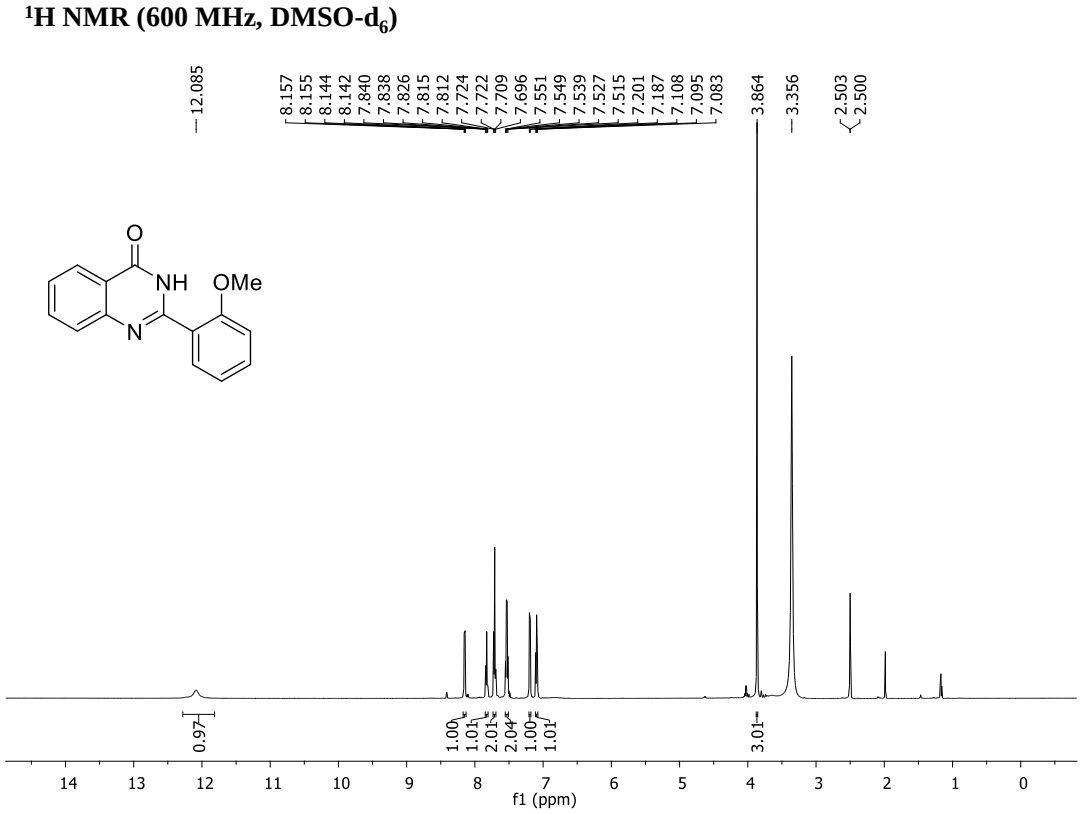


Figure S5. ^{1}H NMR spectrum of 2-(2-Methoxyphenyl)quinazolin-4(3*H*)-one (**3ac**)

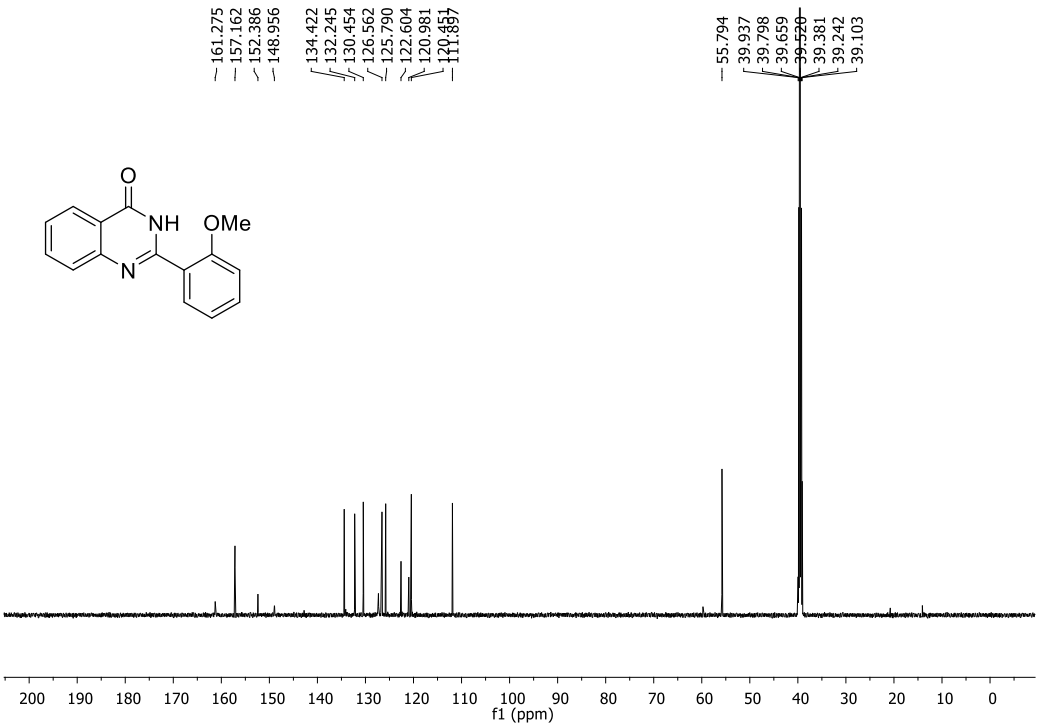


Figure S6. ^{13}C NMR spectrum of 2-(2-Methoxyphenyl)quinazolin-4(3*H*)-one (**3ac**)

^{1}H NMR (600 MHz, DMSO-d$_6$)

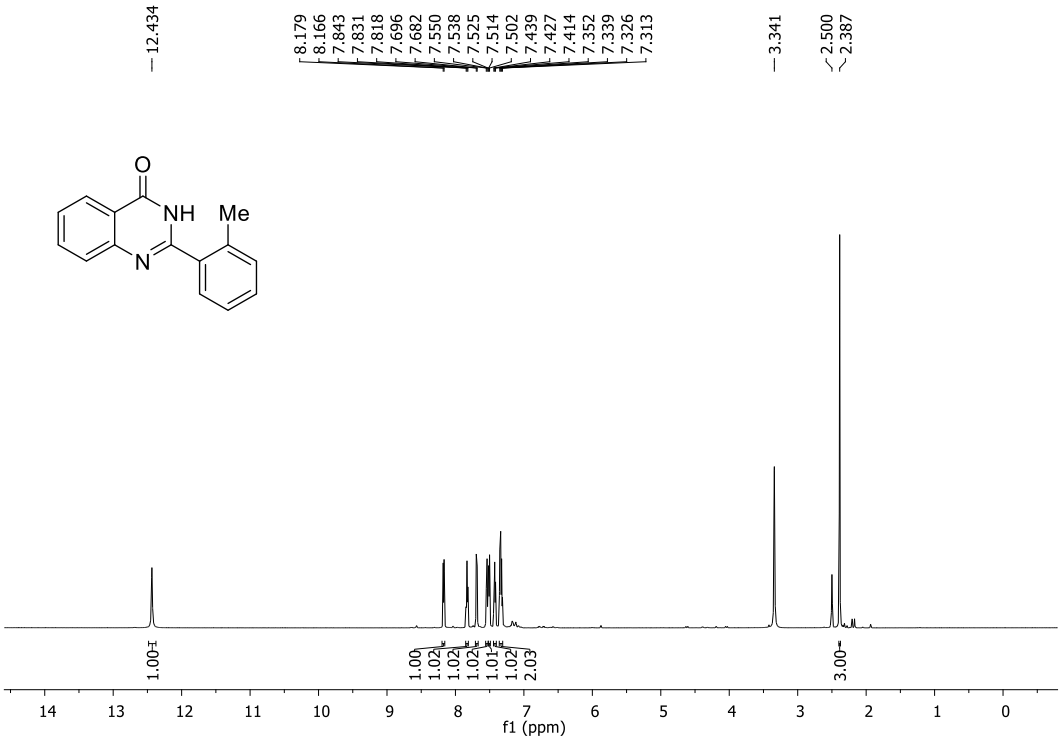


Figure S7. ^{1}H NMR spectrum of 2-(o-Tolyl)quinazolin-4(3*H*)-one (**3ad**)

^{13}C NMR (151 MHz, DMSO-d$_6$)

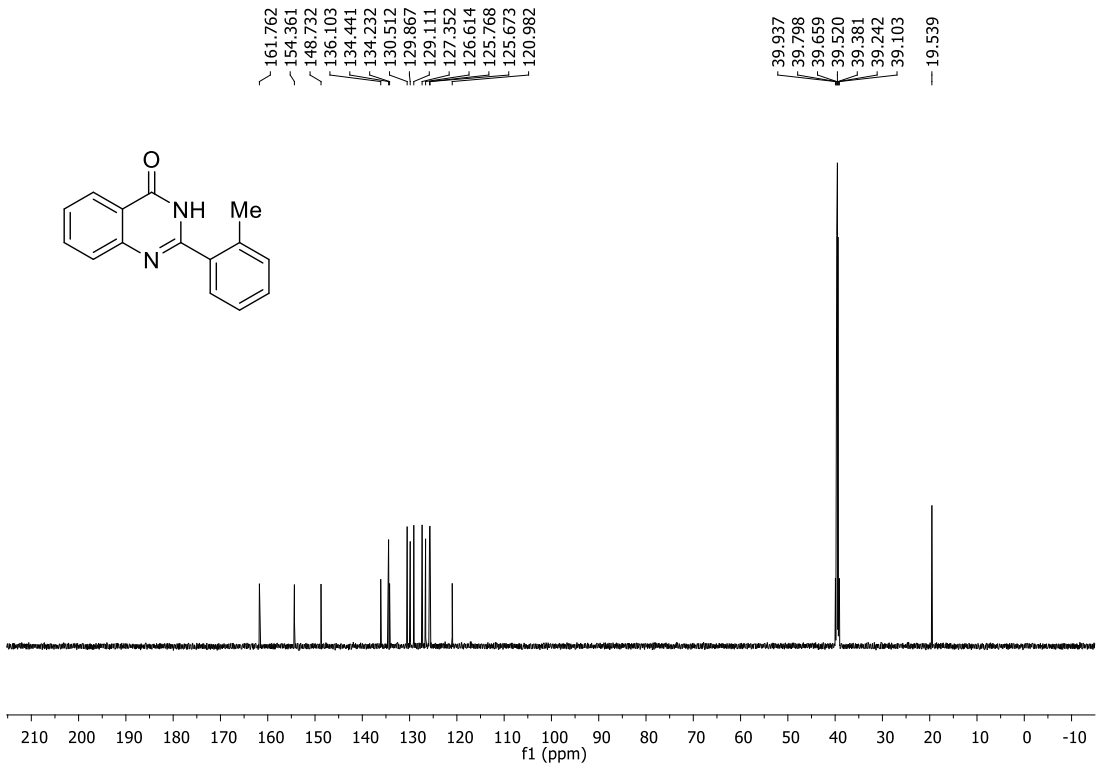


Figure S8. ^{13}C NMR spectrum of 2-(o-Tolyl)quinazolin-4(3*H*)-one (**3ad**)

^{1}H NMR (600 MHz, DMSO-d$_6$)

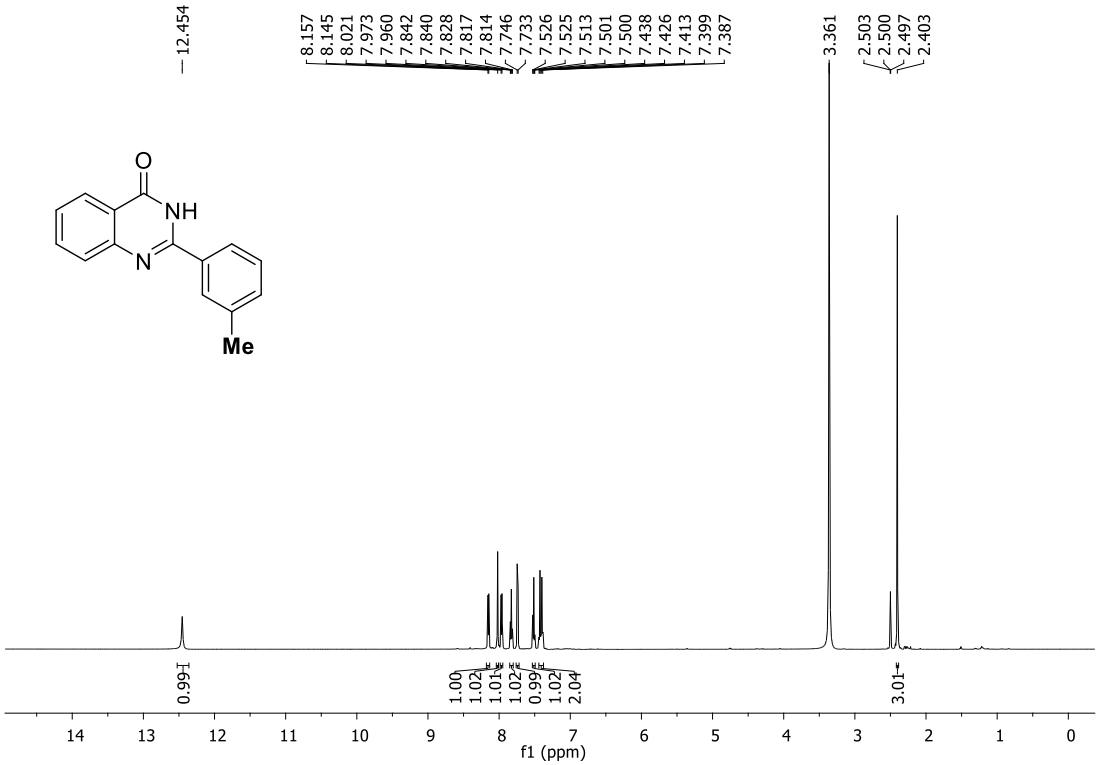


Figure S9. ^{1}H NMR spectrum of 2-(m-Tolyl)quinazolin-4(3*H*)-one (**3ae**)

^{13}C NMR (151 MHz, DMSO-d$_6$)

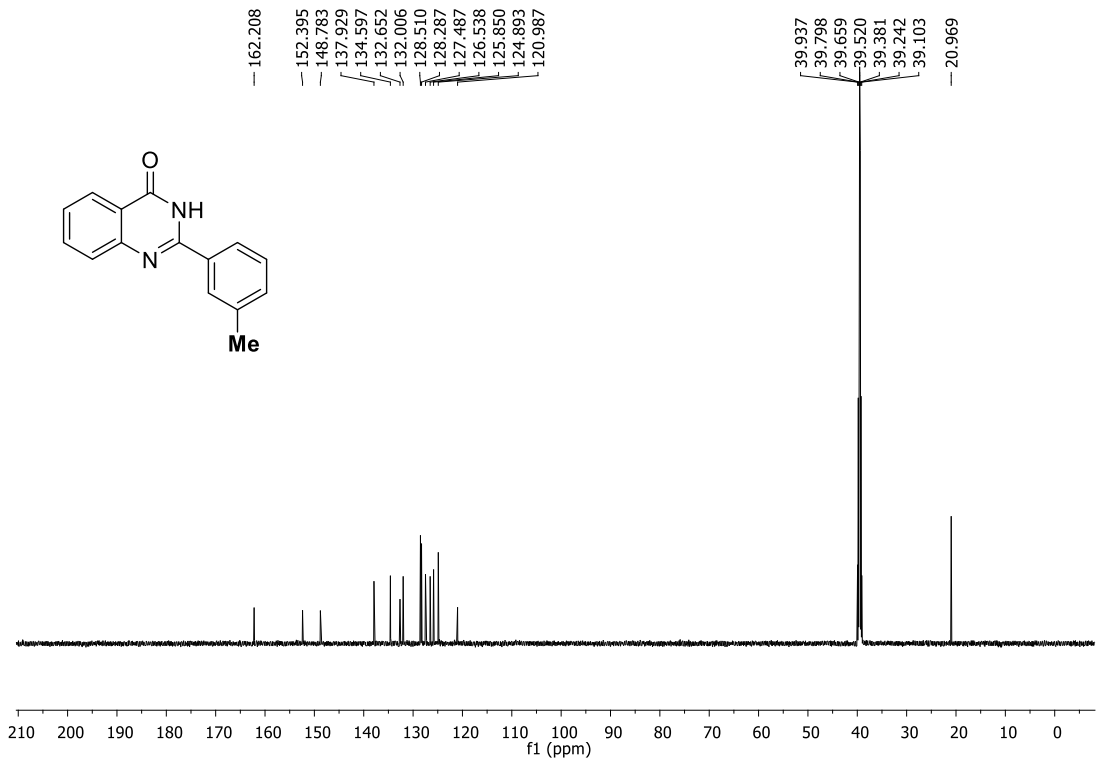


Figure S10. ^{13}C NMR spectrum of 2-(m-Tolyl)quinazolin-4(3*H*)-one (**3ae**)

^{1}H NMR (600 MHz, DMSO-d$_6$)

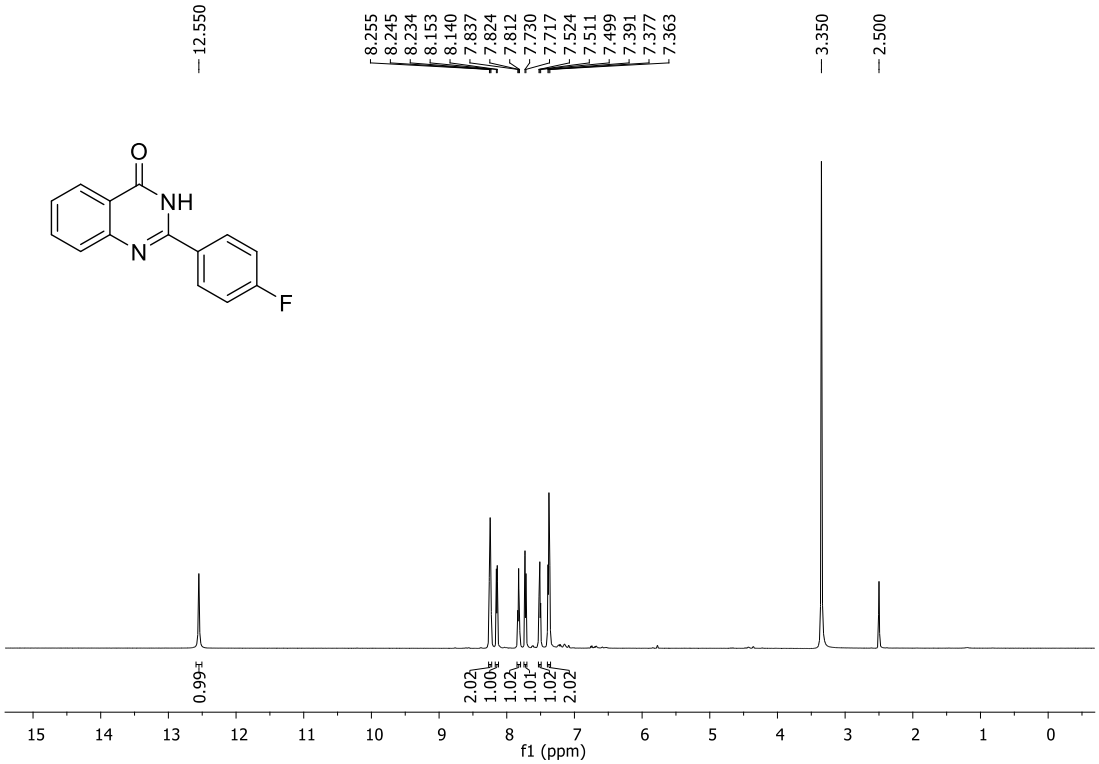


Figure S11. ^{1}H NMR spectrum of 2-(4-Fluorophenyl)quinazolin-4(3*H*)-one (**3af**)

^{13}C NMR (151 MHz, DMSO-d$_6$)

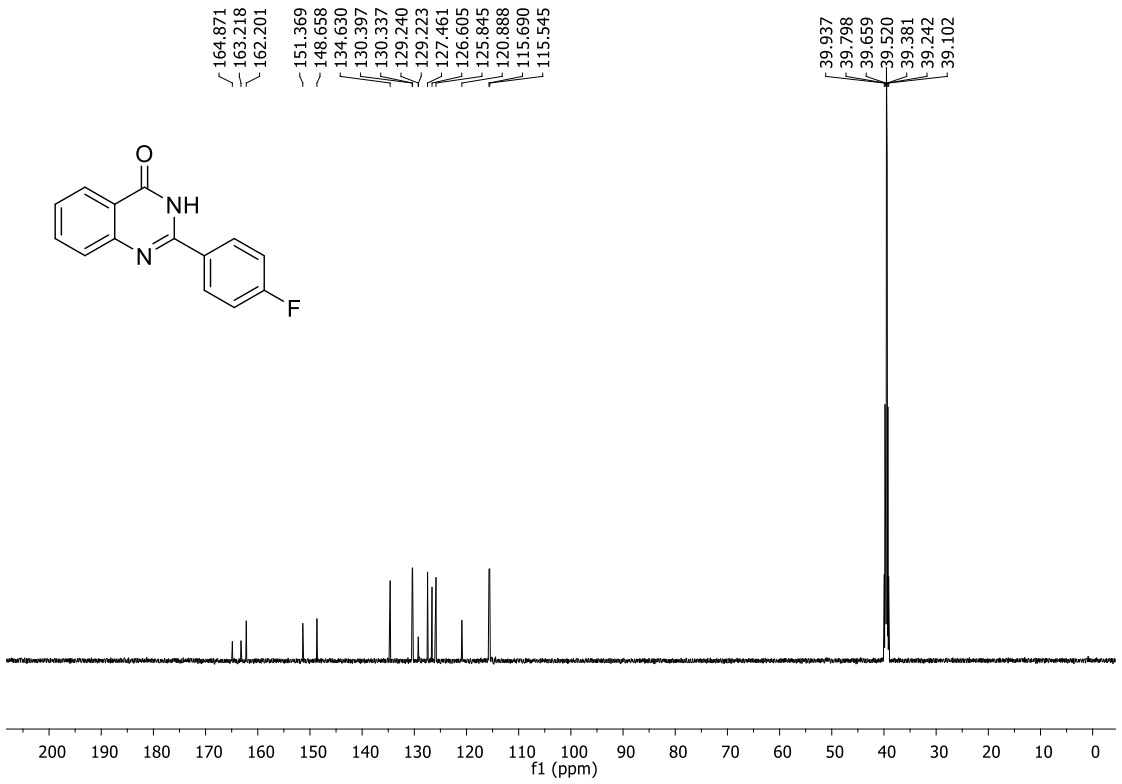


Figure S12. ^{13}C NMR spectrum of 2-(4-Fluorophenyl)quinazolin-4(3*H*)-one (**3af**)

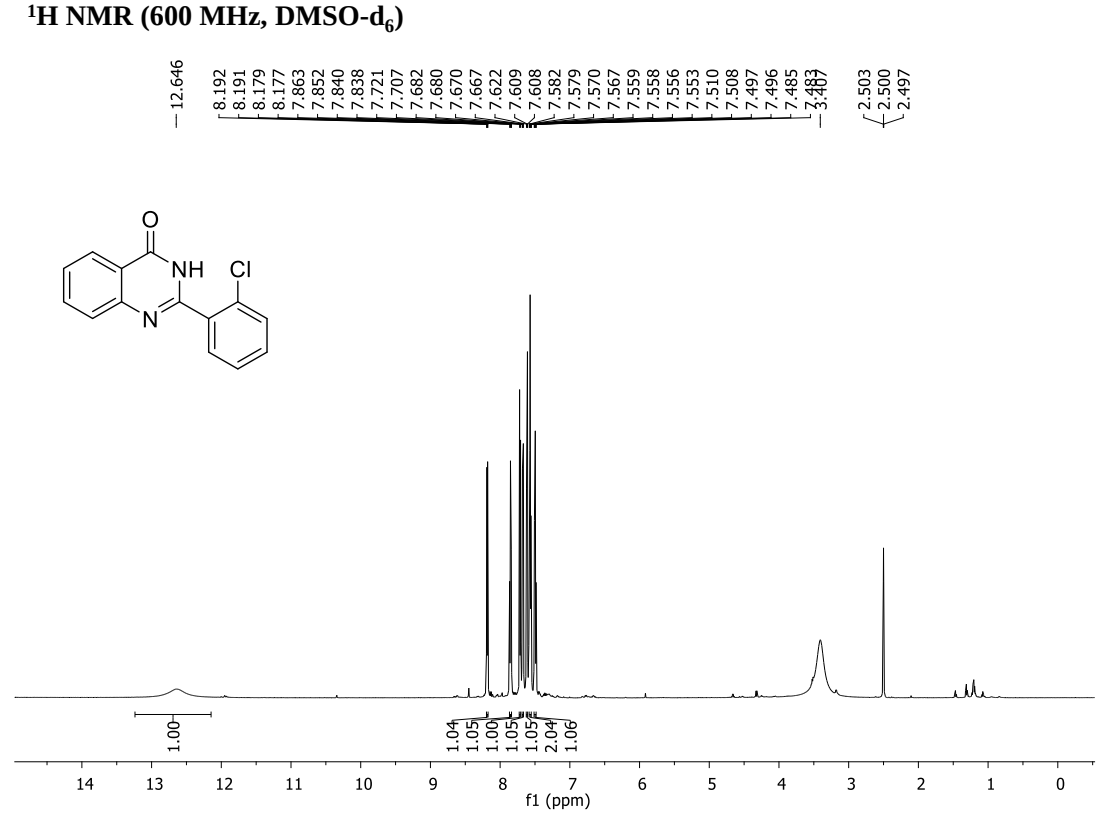


Figure S13. ^{1}H NMR spectrum of 2-(2-Chlorophenyl)quinazolin-4(3*H*)-one (**3ag**)

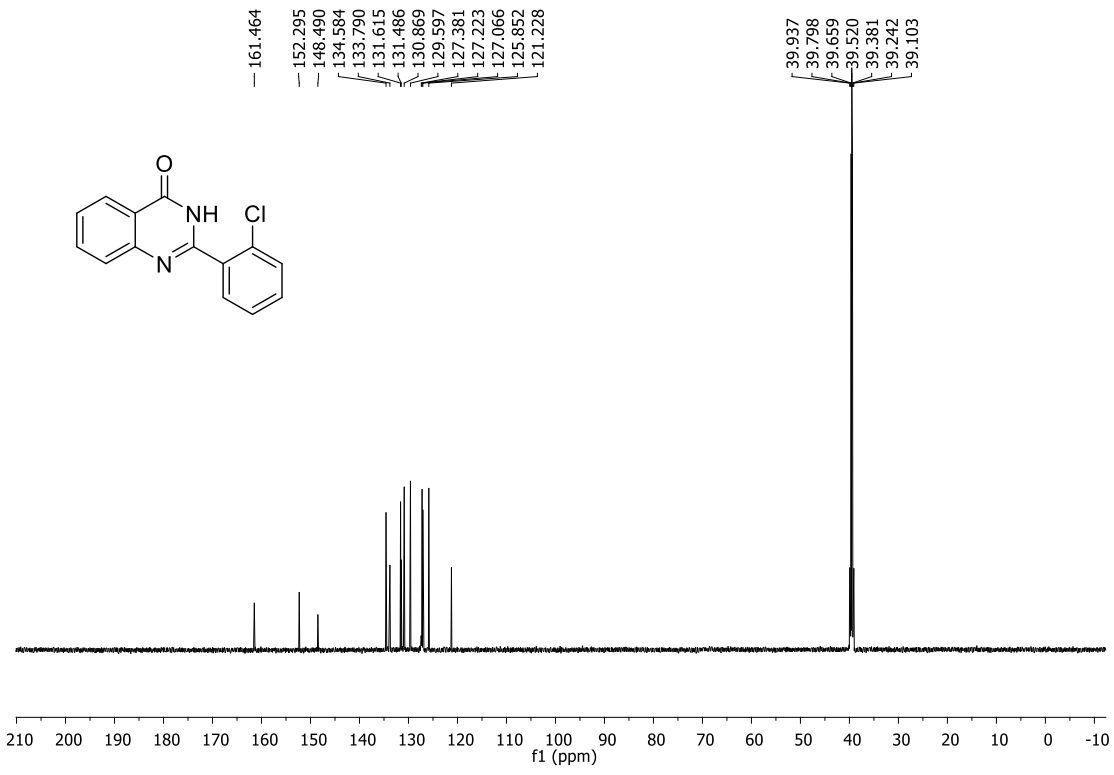


Figure S14. ^{13}C NMR spectrum of 2-(2-Chlorophenyl)quinazolin-4(3*H*)-one (**3ag**)

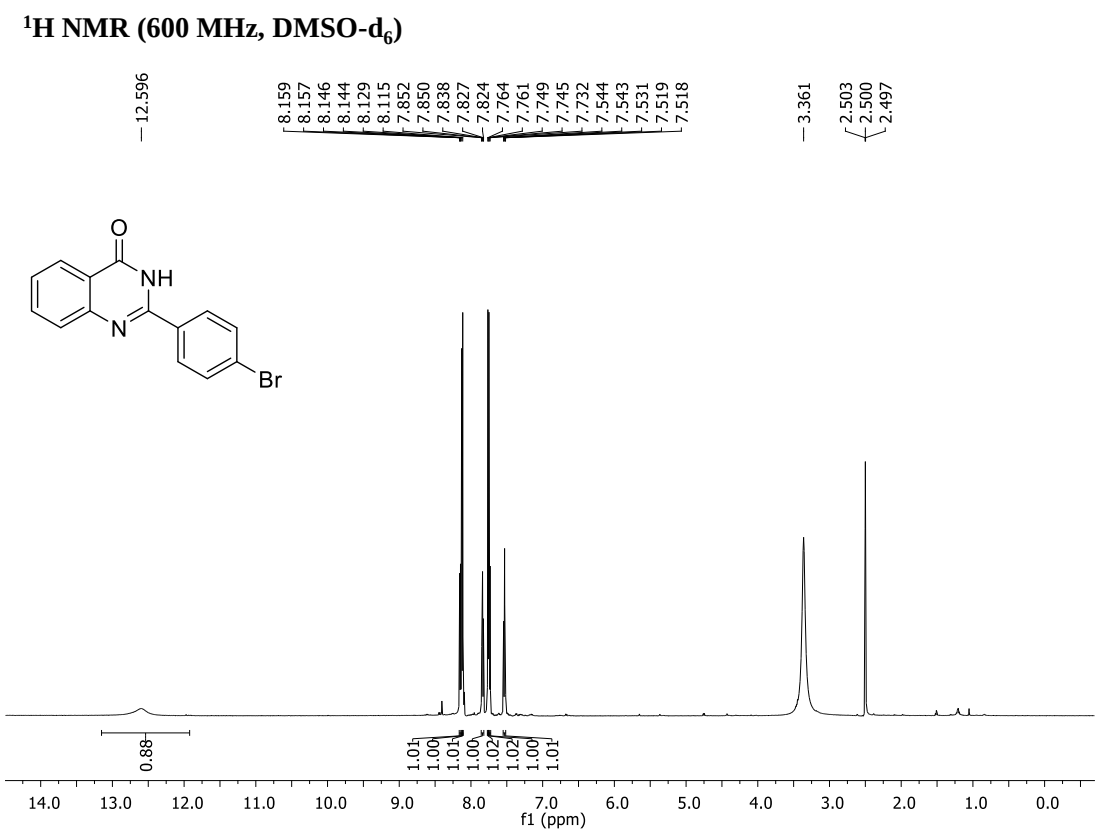


Figure S15. ^{1}H NMR spectrum of 2-(4-Bromophenyl)quinazolin-4(3*H*)-one (**3ai**)

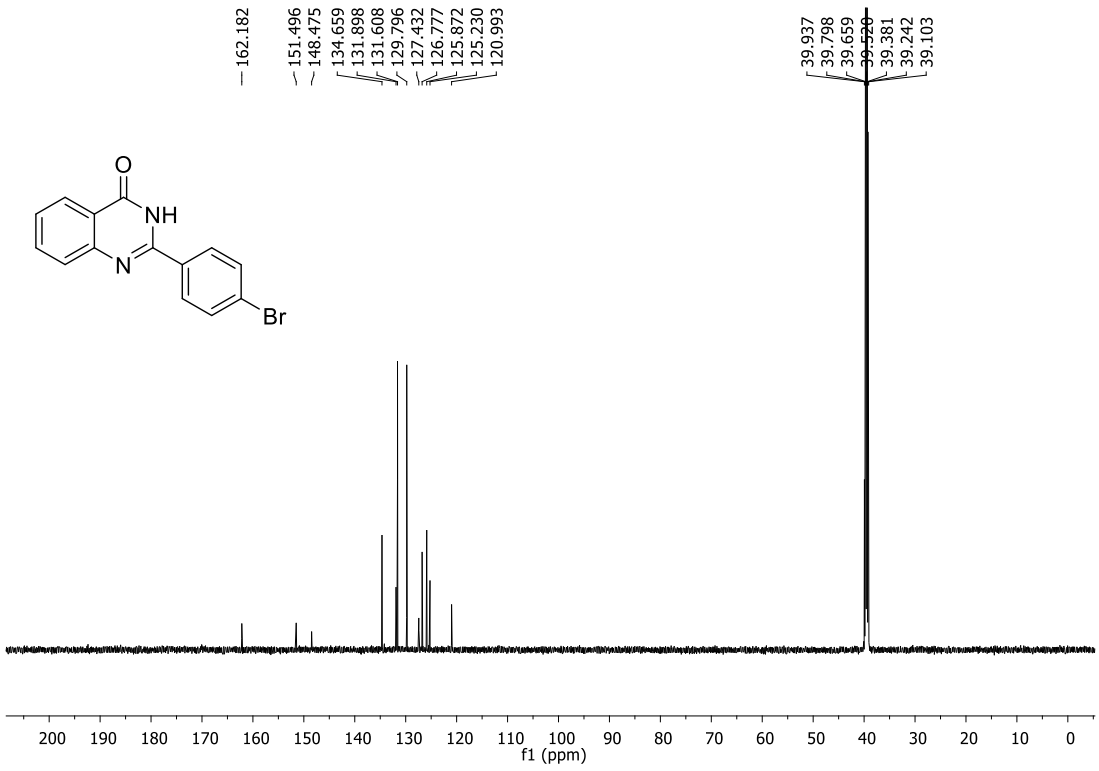


Figure S16. ^{13}C NMR spectrum of 2-(4-Bromophenyl)quinazolin-4(3*H*)-one (**3ai**)

^{1}H NMR (600 MHz, DMSO-d$_6$)

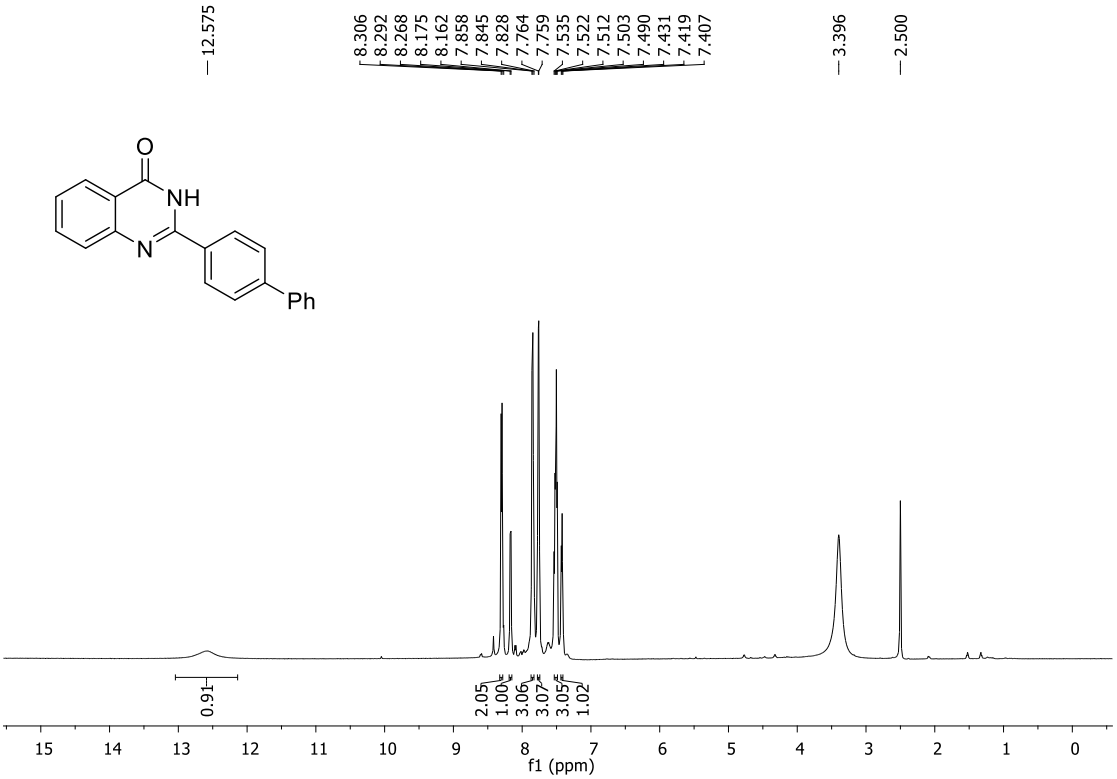


Figure S17. ^{1}H NMR spectrum of 2-([1,1'-Biphenyl]-4-yl)quinazolin-4(3*H*)-one (**3aj**)

^{13}C NMR (151 MHz, DMSO-d$_6$)

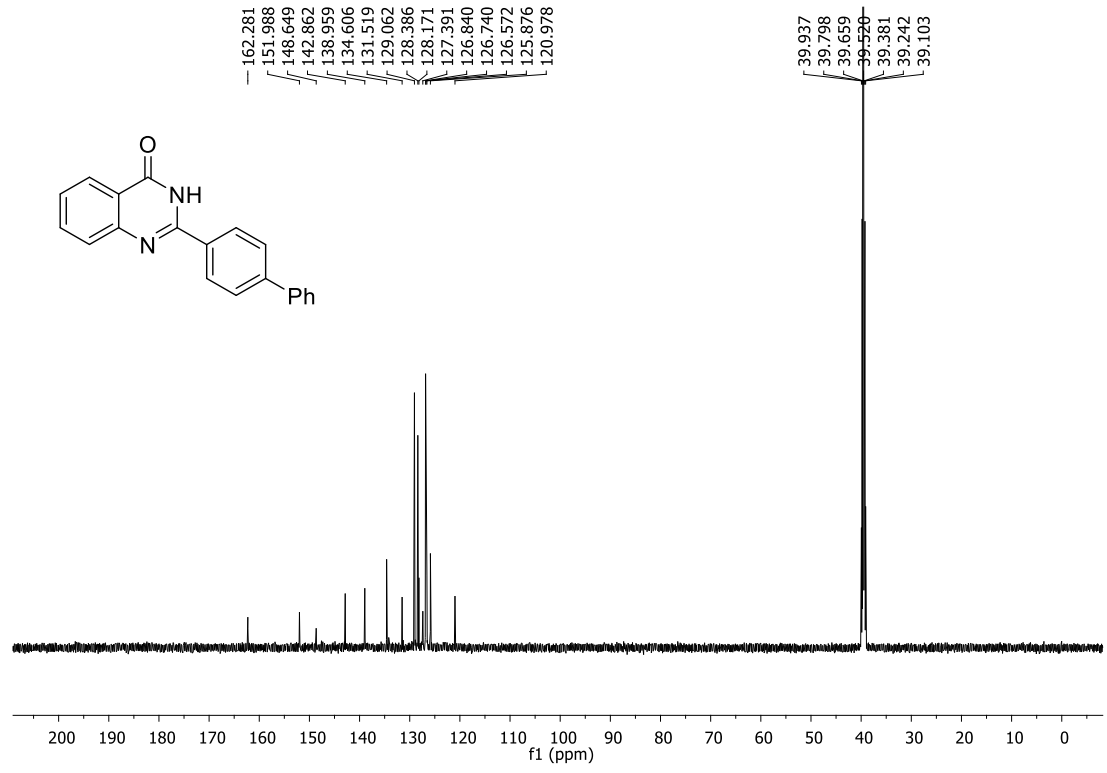


Figure S18. ^{13}C NMR spectrum of 2-([1,1'-Biphenyl]-4-yl)quinazolin-4(3*H*)-one (**3aj**)

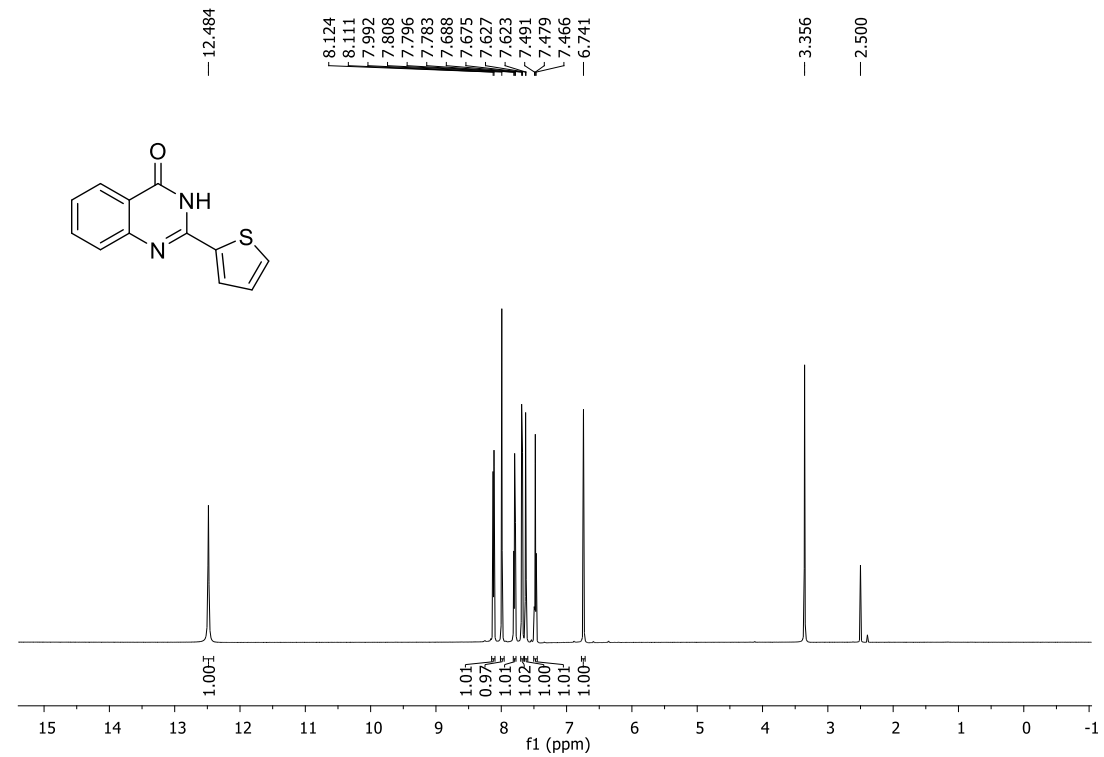


Figure S19. ^{1}H NMR spectrum of 2-(Thiophen-2-yl)quinazolin-4(3*H*)-one (**3ak**)

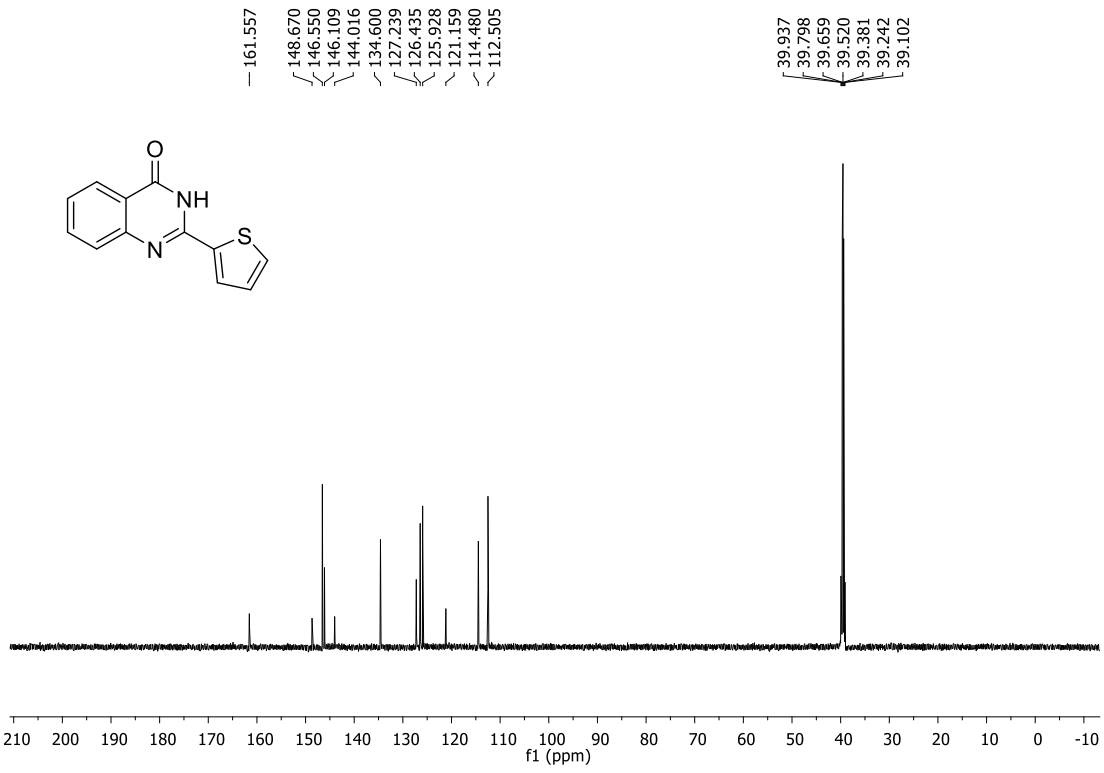


Figure S20. ^{13}C NMR spectrum of 2-(Thiophen-2-yl)quinazolin-4(3*H*)-one (**3ak**)

^{1}H NMR (600 MHz, DMSO-d_6)

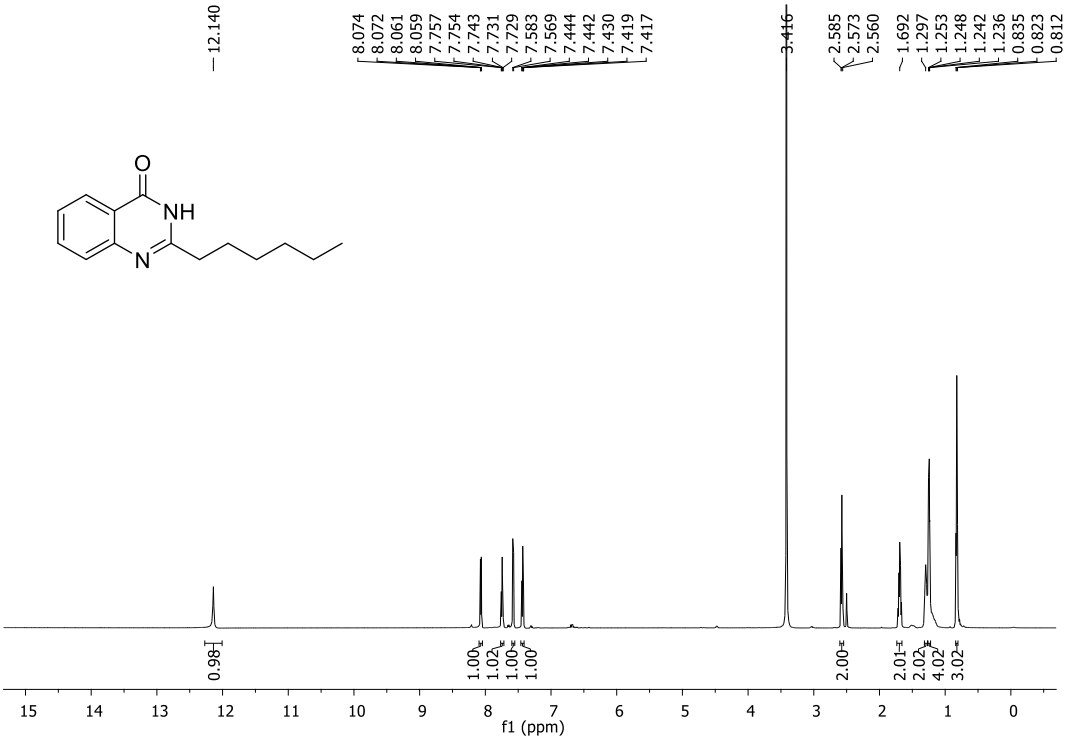


Figure S21. ^{1}H NMR spectrum of 2-Hexylquinazolin-4(3*H*)-one (**3al**)

^{13}C NMR (151 MHz, DMSO-d_6)

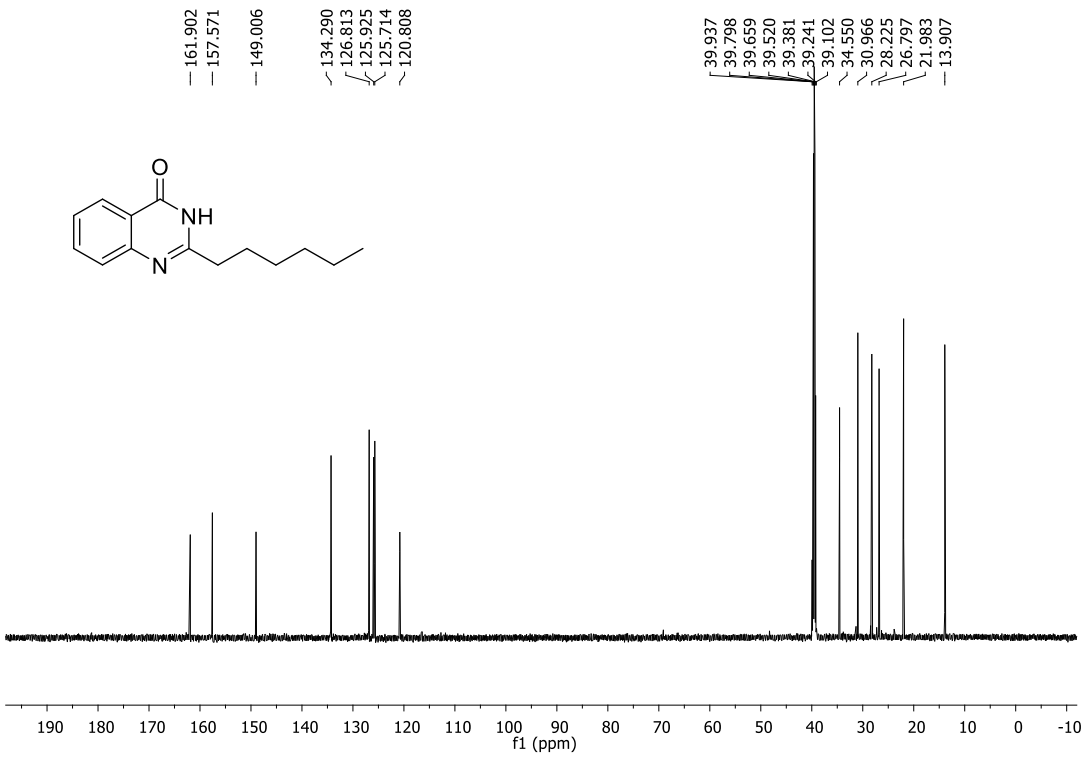


Figure S22. ^{13}C NMR spectrum of 2-Hexylquinazolin-4(3*H*)-one (**3al**)

^{1}H NMR (600 MHz, DMSO-d_6)

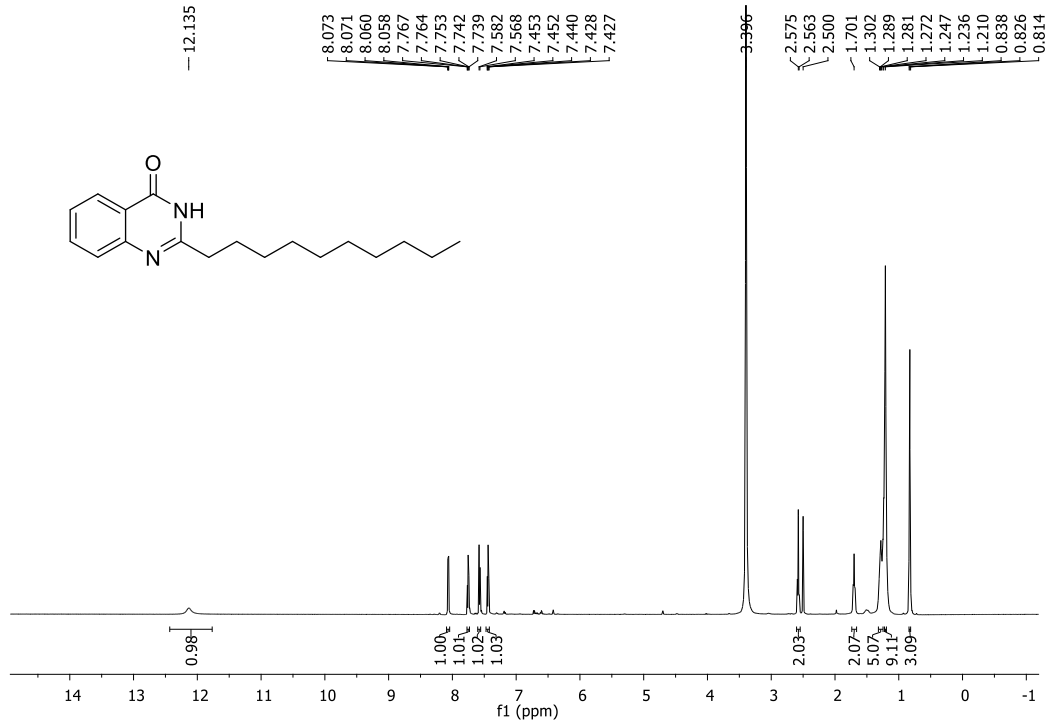


Figure S23. ^{1}H NMR spectrum of 2-Decylquinazolin-4(3*H*)-one (**3am**)

^{13}C NMR (151 MHz, DMSO-d_6)

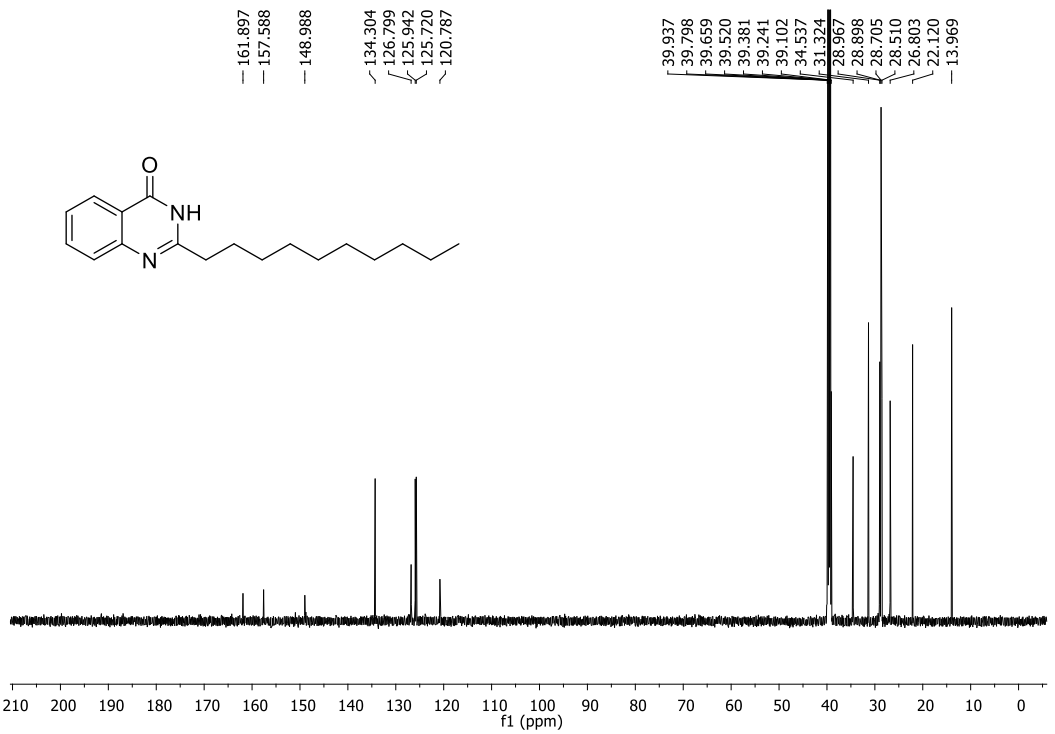


Figure S24. ^{13}C NMR spectrum of 2-Decylquinazolin-4(3*H*)-one (**3am**)

^{1}H NMR (600 MHz, DMSO-d_6)

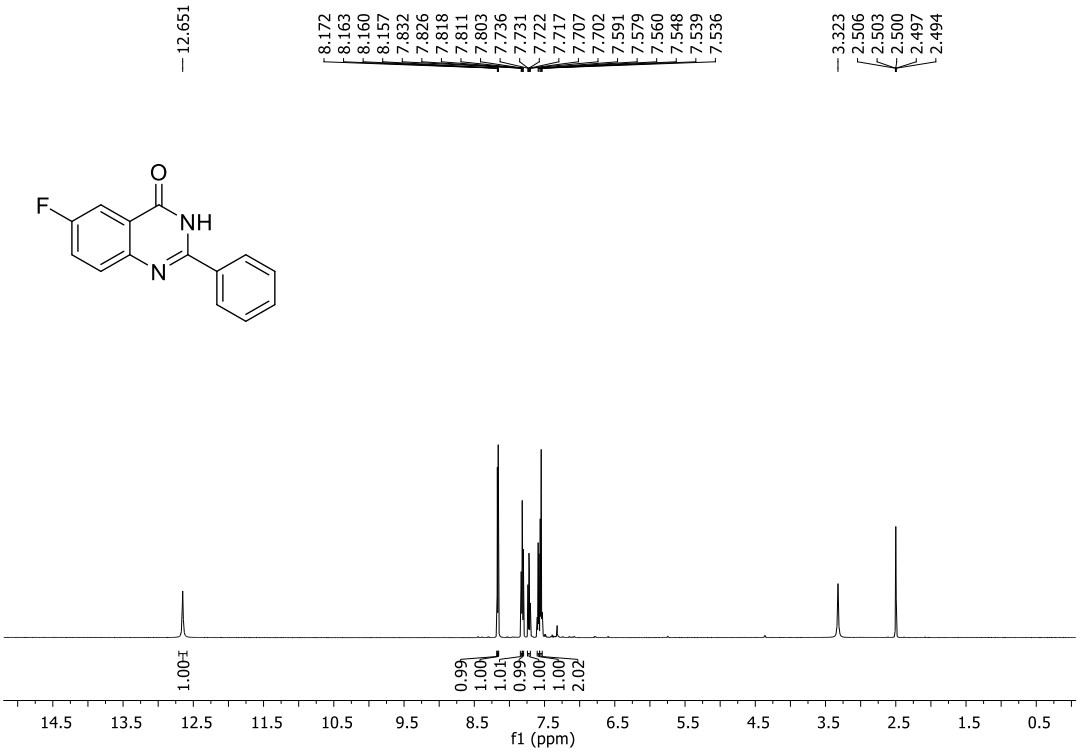


Figure S25. ^{1}H NMR spectrum of 6-Fluoro-2-phenylquinazolin-4(3*H*)-one (**3ba**)

^{13}C NMR (151 MHz, DMSO-d_6)

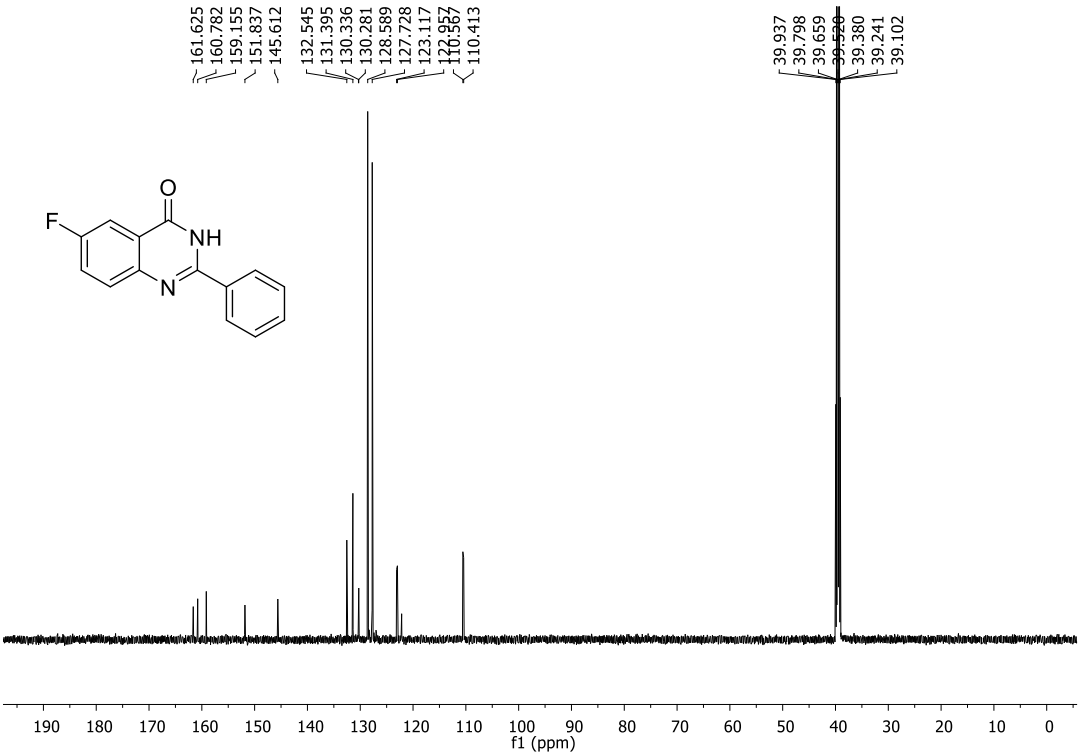


Figure S26. ^{13}C NMR spectrum of 6-Fluoro-2-phenylquinazolin-4(3*H*)-one (**3ba**)

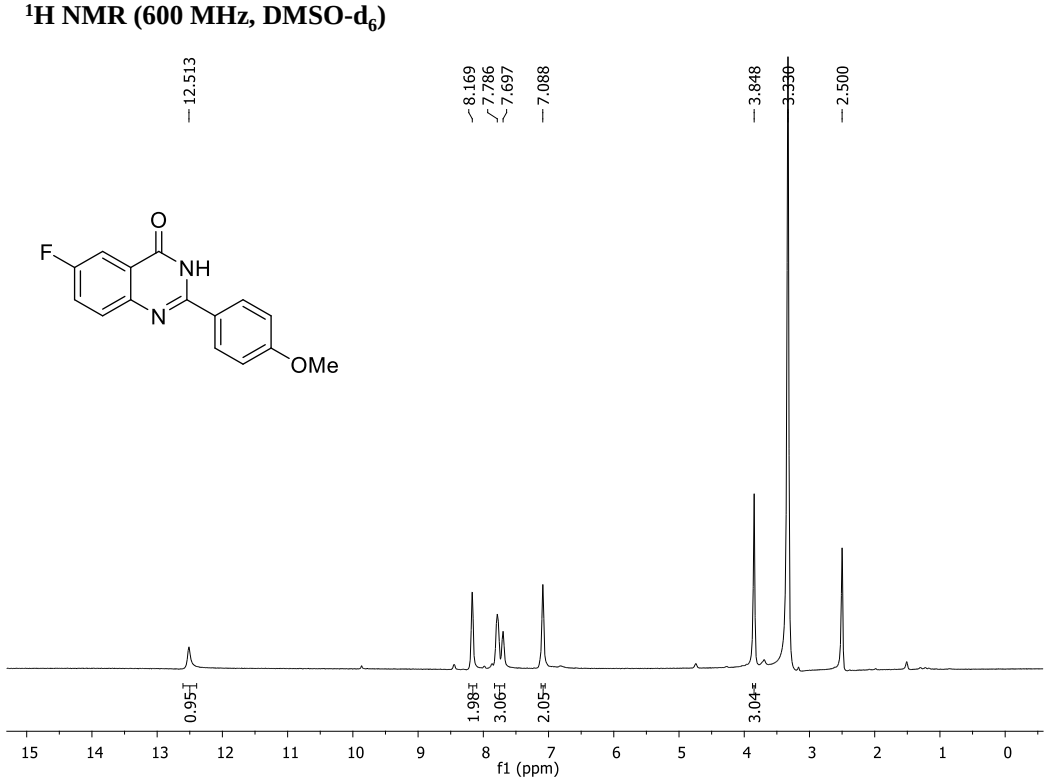


Figure S27. [1]H NMR spectrum of 6-Fluoro-2-(4-methoxyphenyl)quinazolin-4(3*H*)-one (**3bb)**

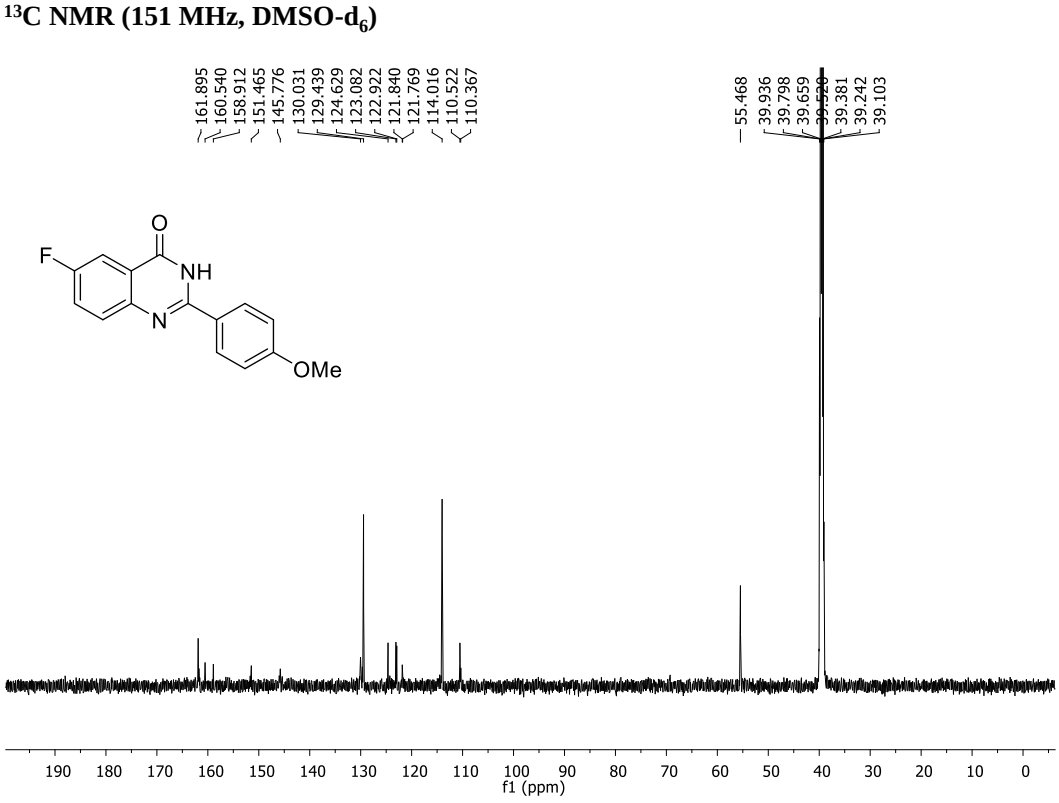


Figure S28. [13]C NMR spectrum of 6-Fluoro-2-(4-methoxyphenyl)quinazolin-4(3*H*)-one (**3bb)**

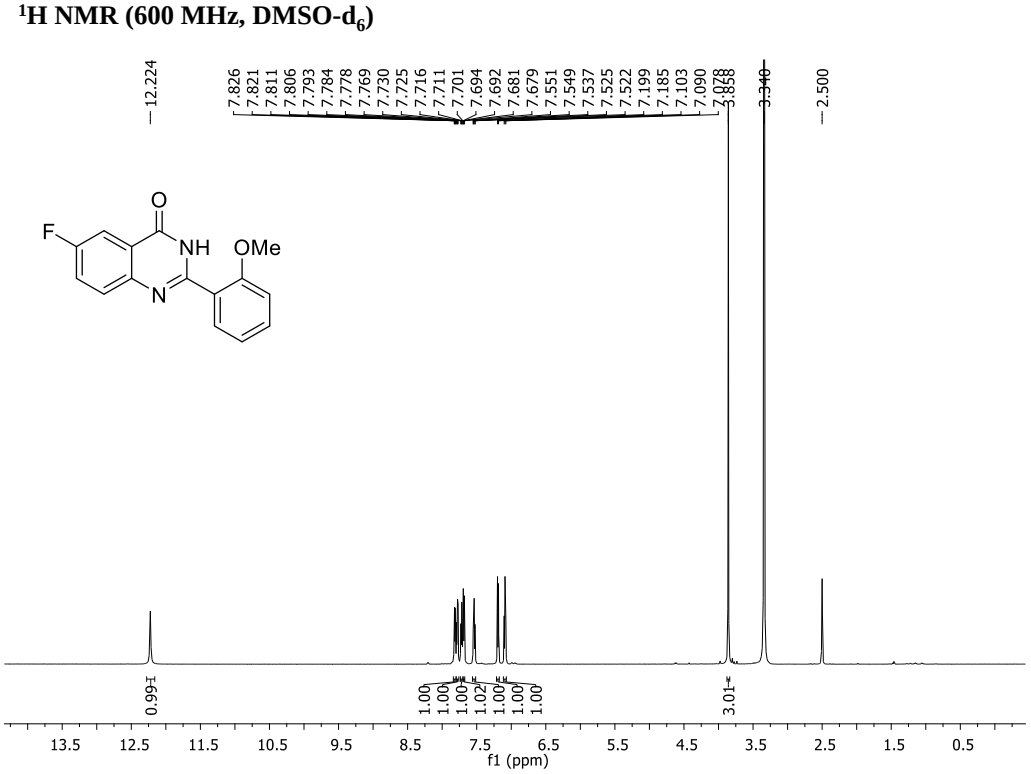


Figure S29. ^{1}H NMR spectrum of 6-Fluoro-2-(2-methoxyphenyl)quinazolin-4(3*H*)-one **(3bc)**

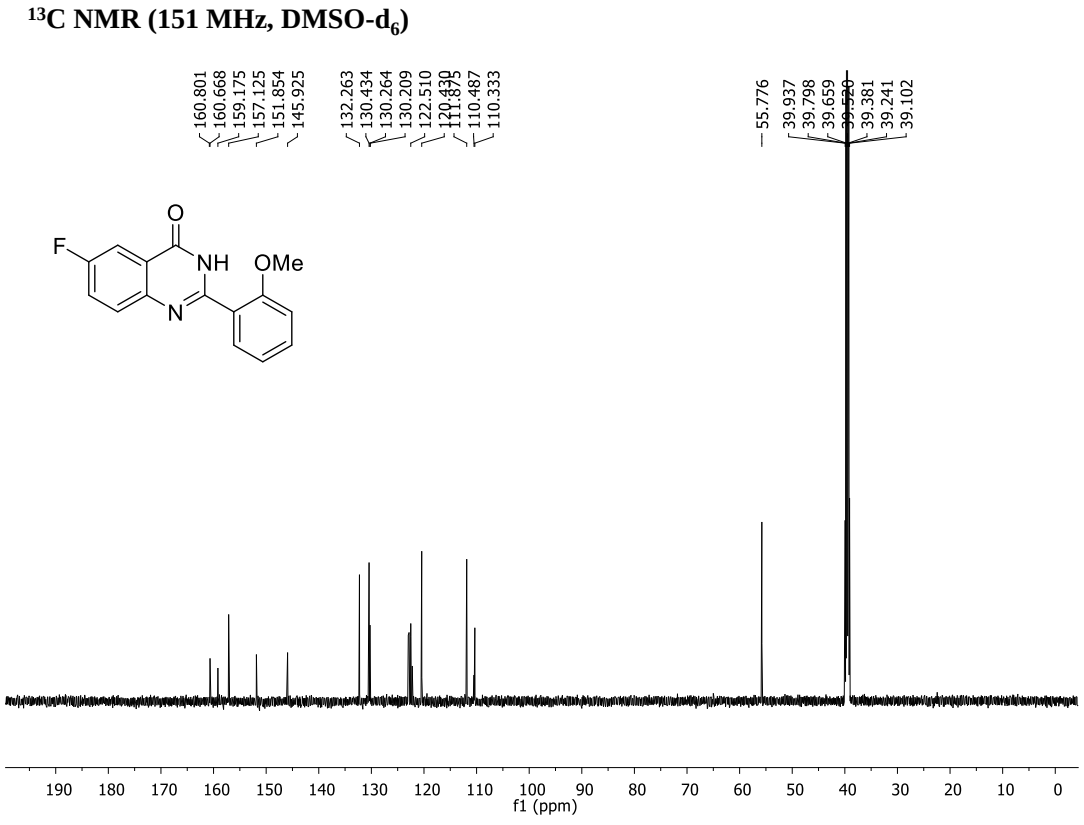


Figure S30. ^{13}C NMR spectrum of 6-Fluoro-2-(2-methoxyphenyl)quinazolin-4(3*H*)-one **(3bc)**

^{1}H NMR (600 MHz, DMSO-d_6)

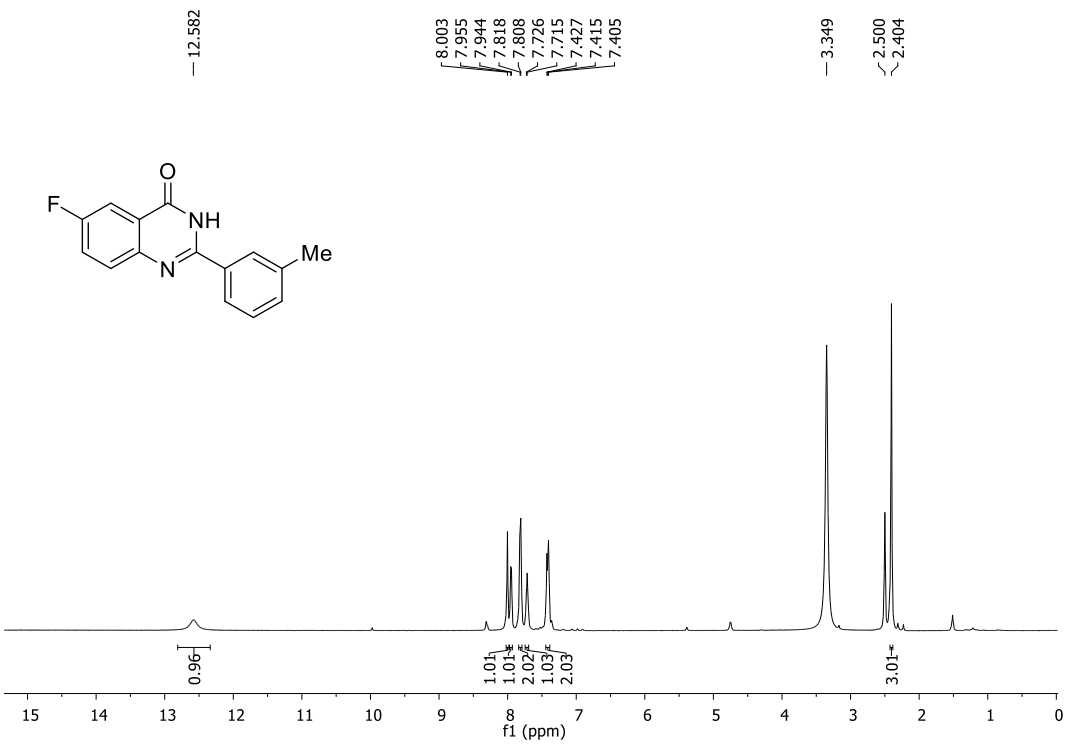


Figure S31. ^{1}H NMR spectrum of 6-Fluoro-2-(m-tolyl)quinazolin-4(3*H*)-one (**3be)**

^{13}C NMR (151 MHz, DMSO-d_6)

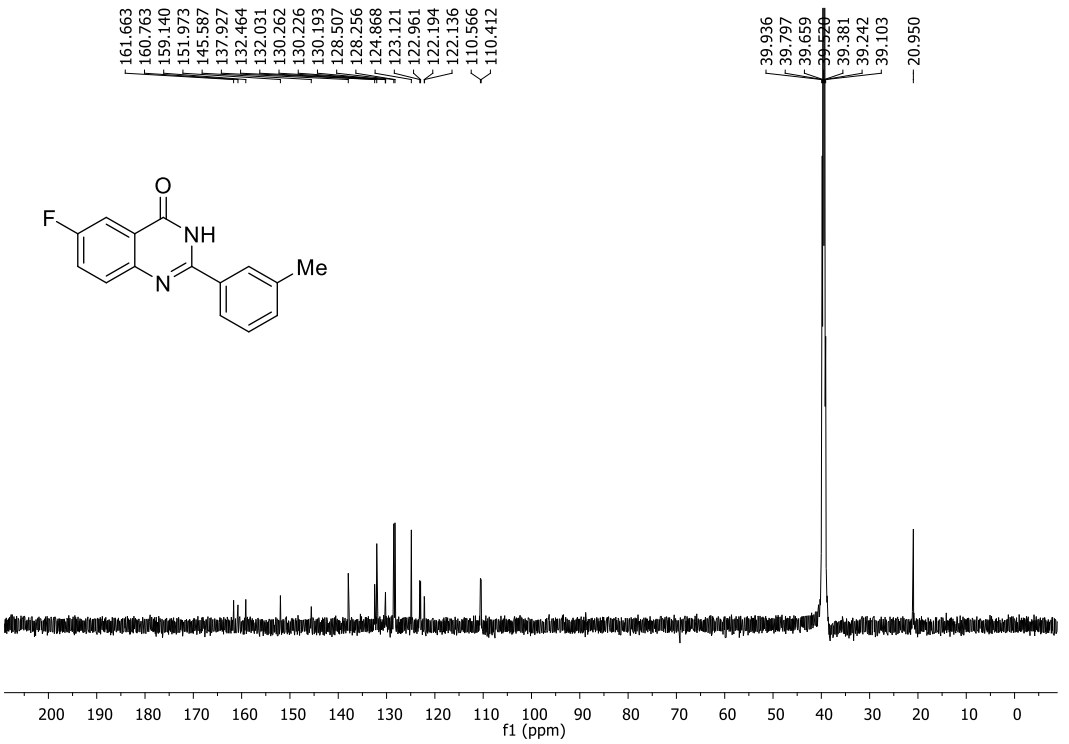


Figure S32. ^{13}C NMR spectrum of 6-Fluoro-2-(m-tolyl)quinazolin-4(3*H*)-one (**3be)**

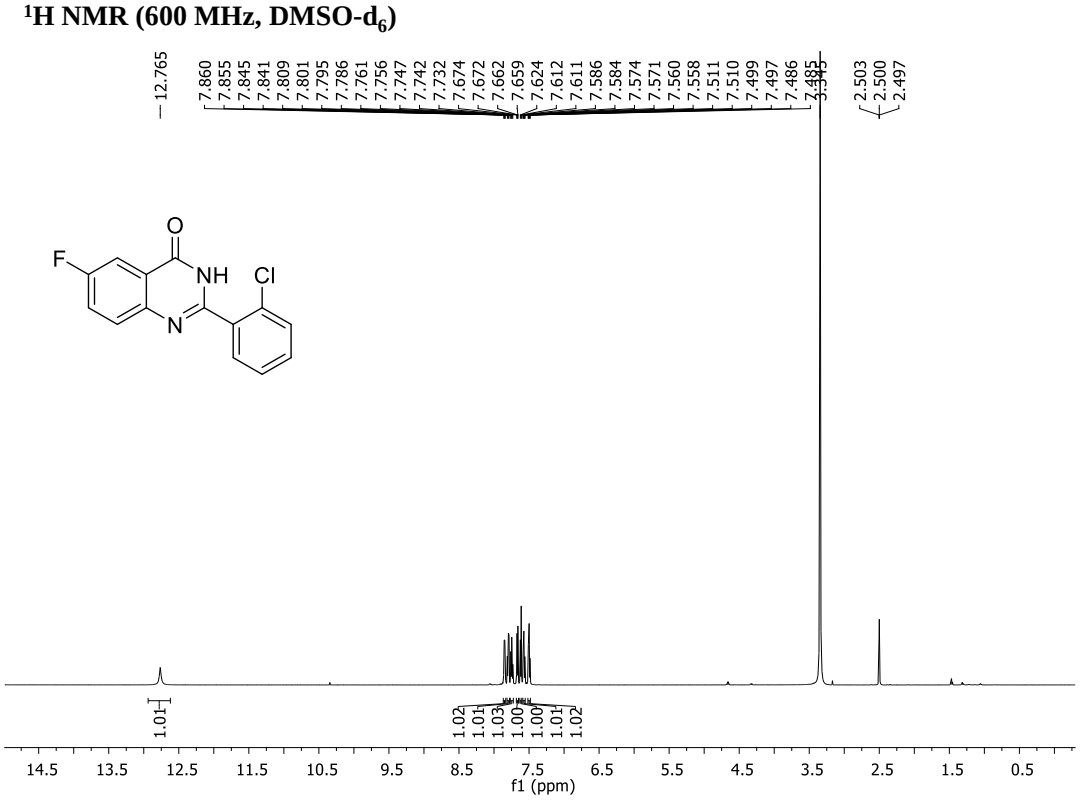


Figure S33. ^{1}H NMR spectrum of 2-(2-Chlorophenyl)-6-fluoroquinazolin-4(3*H*)-one (**3bg**)

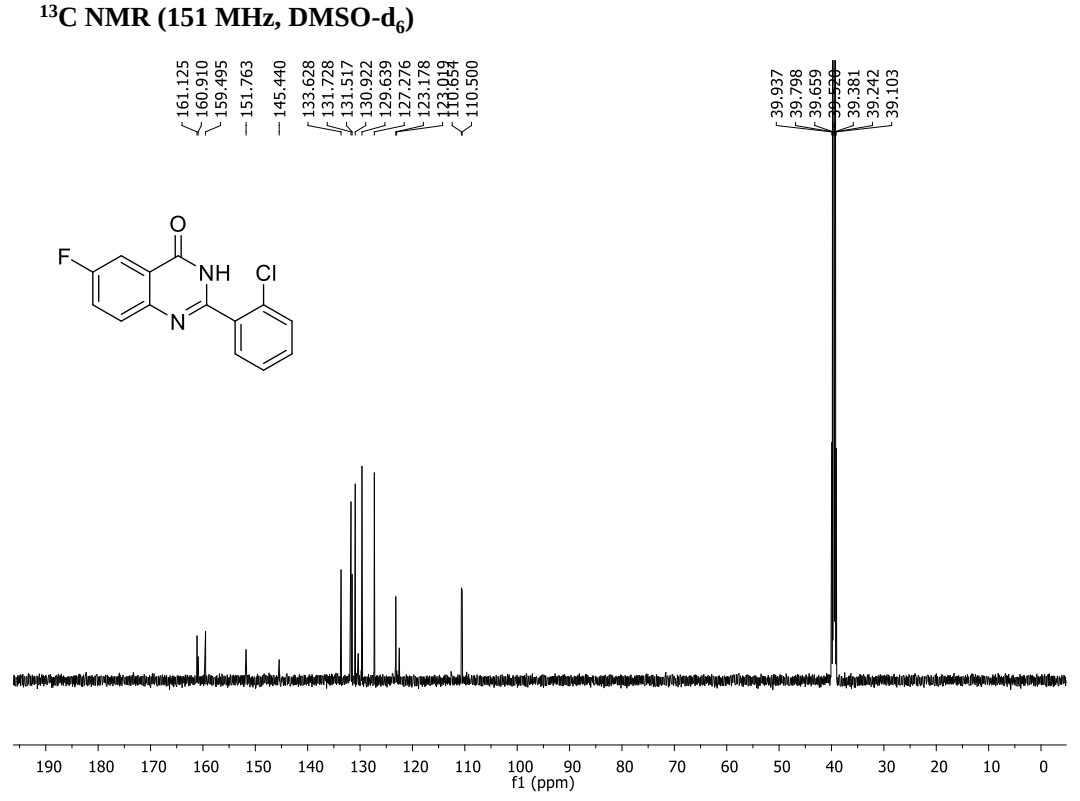


Figure S34. ^{13}C NMR spectrum of 2-(2-Chlorophenyl)-6-fluoroquinazolin-4(3*H*)-one (**3bg**)

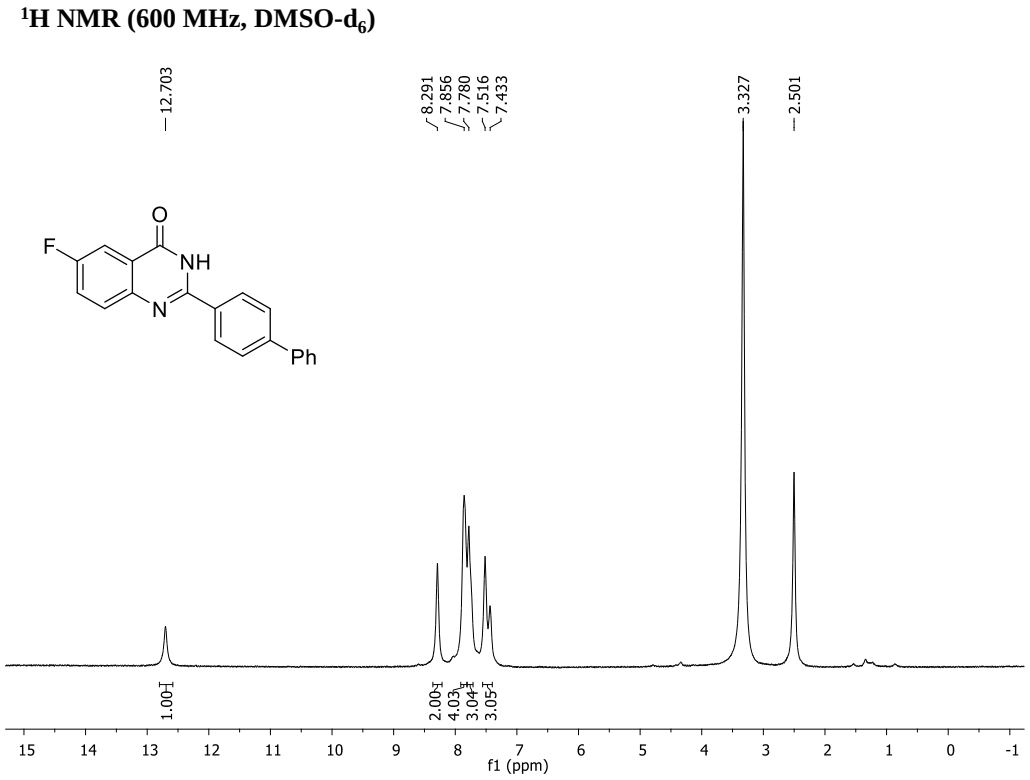


Figure S35. ^{1}H NMR spectrum of 2-([1,1'-Biphenyl]-4-yl)-6-fluoroquinazolin-4(3*H*)-one (**3bj**)

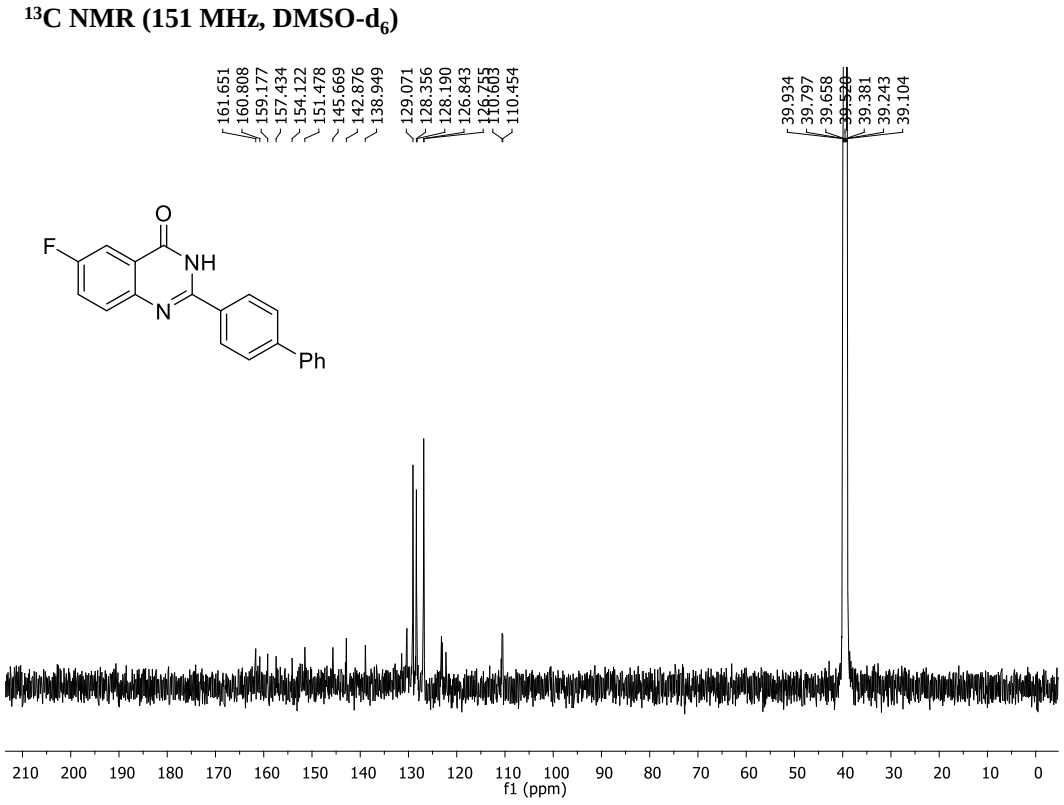


Figure S36. ^{13}C NMR spectrum of 2-([1,1'-Biphenyl]-4-yl)-6-fluoroquinazolin-4(3*H*)-one (**3bj**)

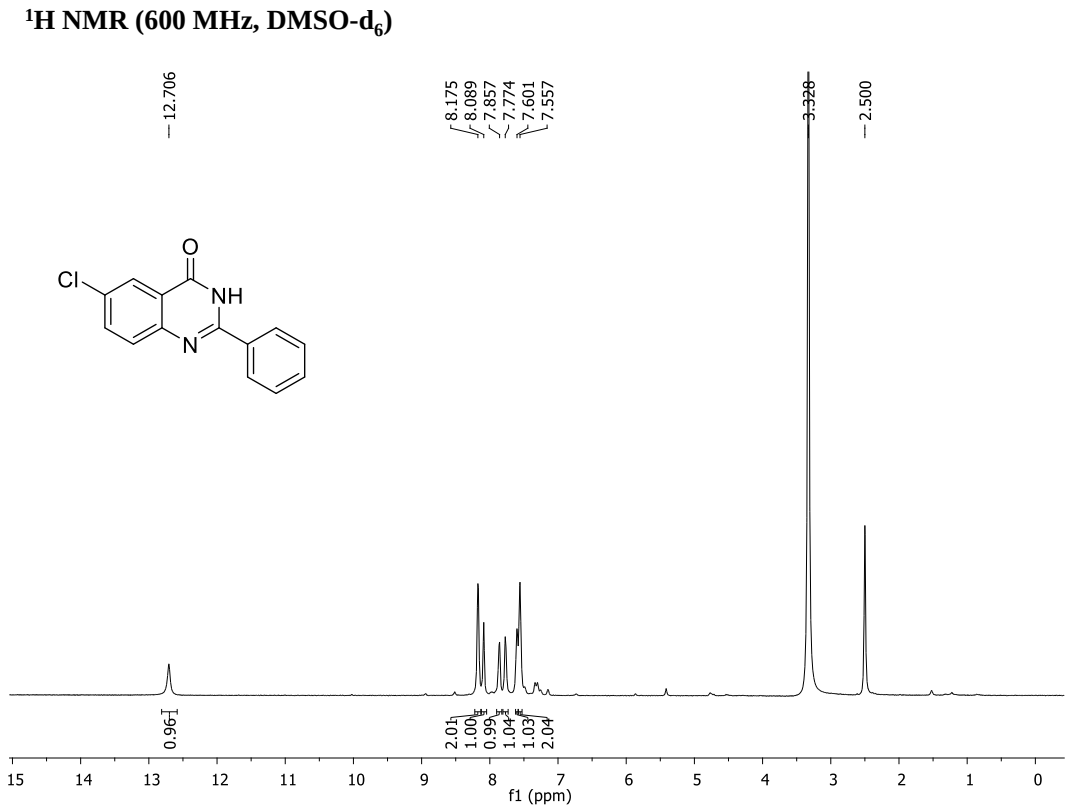


Figure S37. ^{1}H NMR spectrum of 6-Chloro-2-phenylquinazolin-4(3*H*)-one (**3ca**)

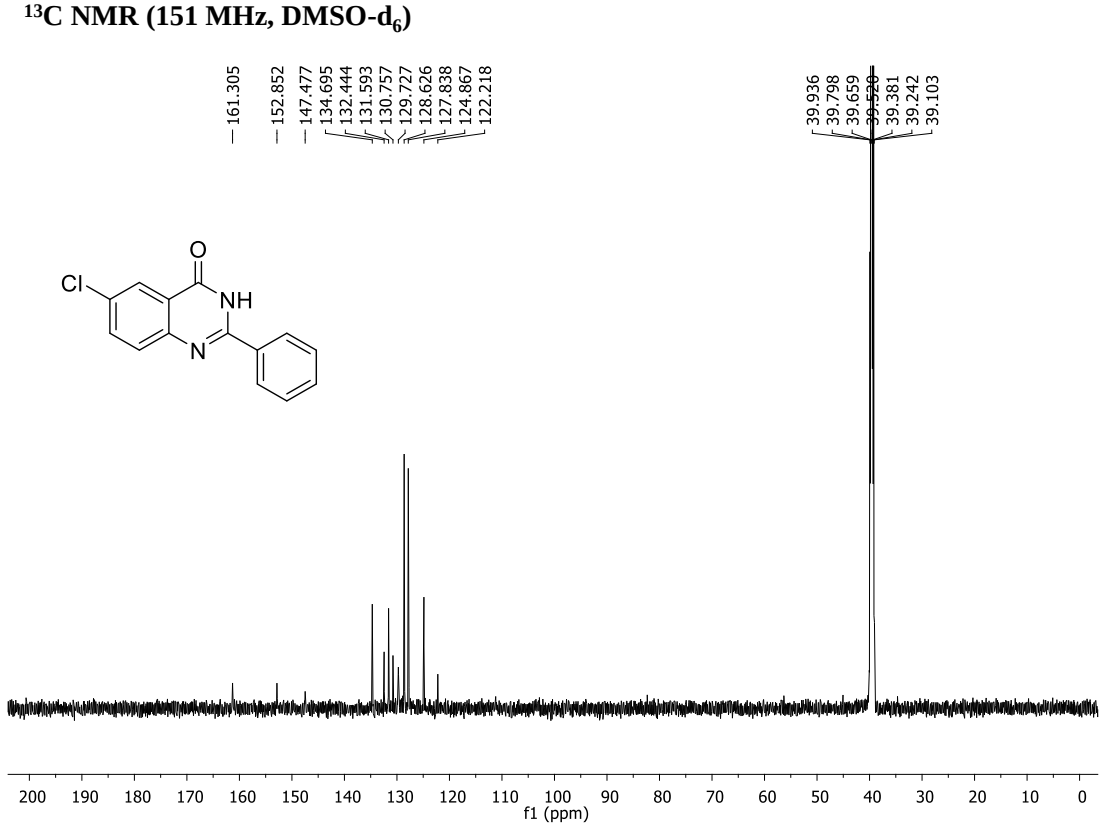


Figure S38. ^{13}C NMR spectrum of 6-Chloro-2-phenylquinazolin-4(3*H*)-one (**3ca**)

^{1}H NMR (600 MHz, DMSO-d$_6$)

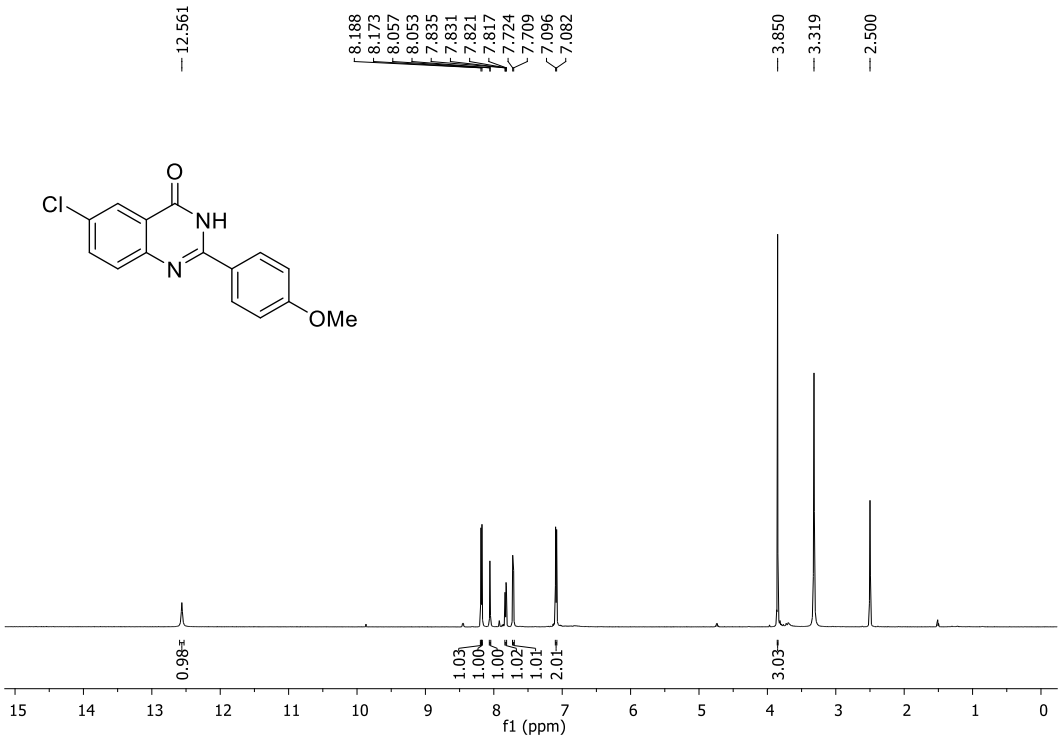


Figure S39. ^{1}H NMR spectrum of 6-Chloro-2-(4-methoxyphenyl)quinazolin-4(3*H*)-one (**3cb**)

^{13}C NMR (151 MHz, DMSO-d$_6$)

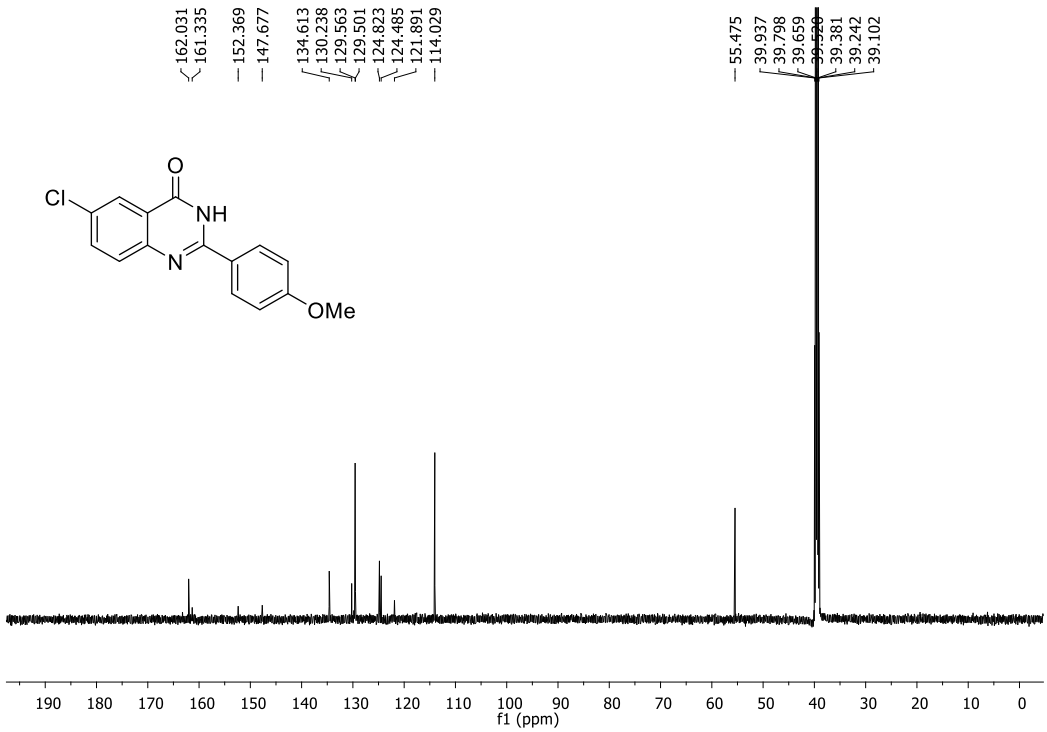


Figure S40. ^{13}C NMR spectrum of 6-Chloro-2-(4-methoxyphenyl)quinazolin-4(3*H*)-one (**3cb**)

^{1}H NMR (600 MHz, DMSO-d$_6$)

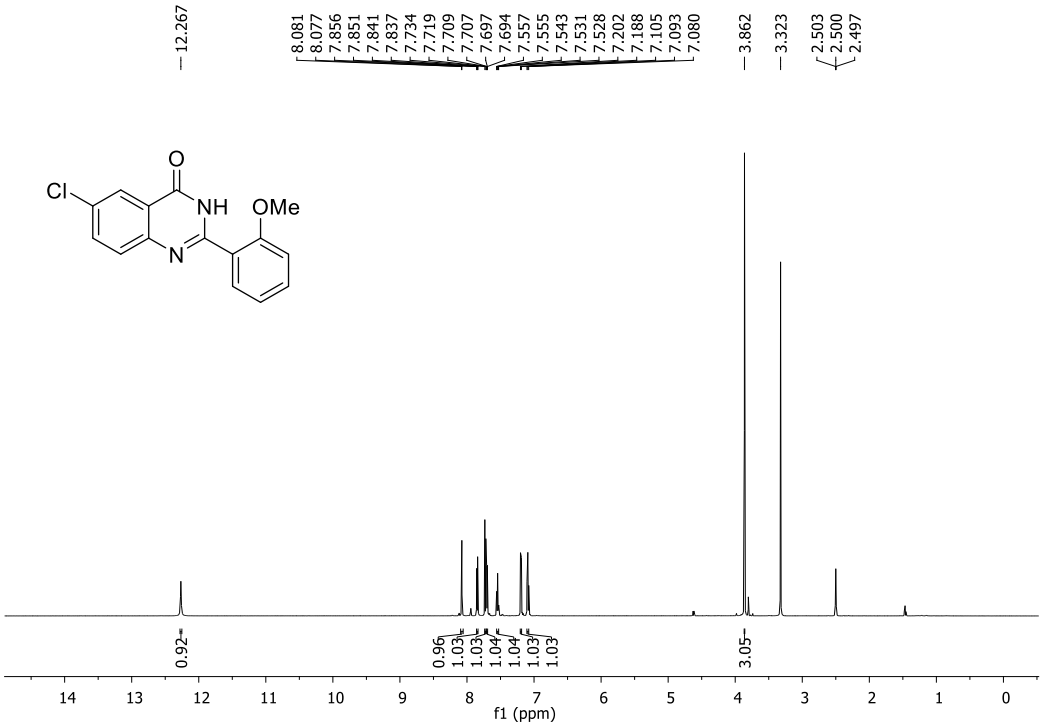


Figure S41. ^{1}H NMR spectrum of 6-Chloro-2-(2-methoxyphenyl)quinazolin-4(3*H*)-one (**3cc**)

^{13}C NMR (151 MHz, DMSO-d$_6$)

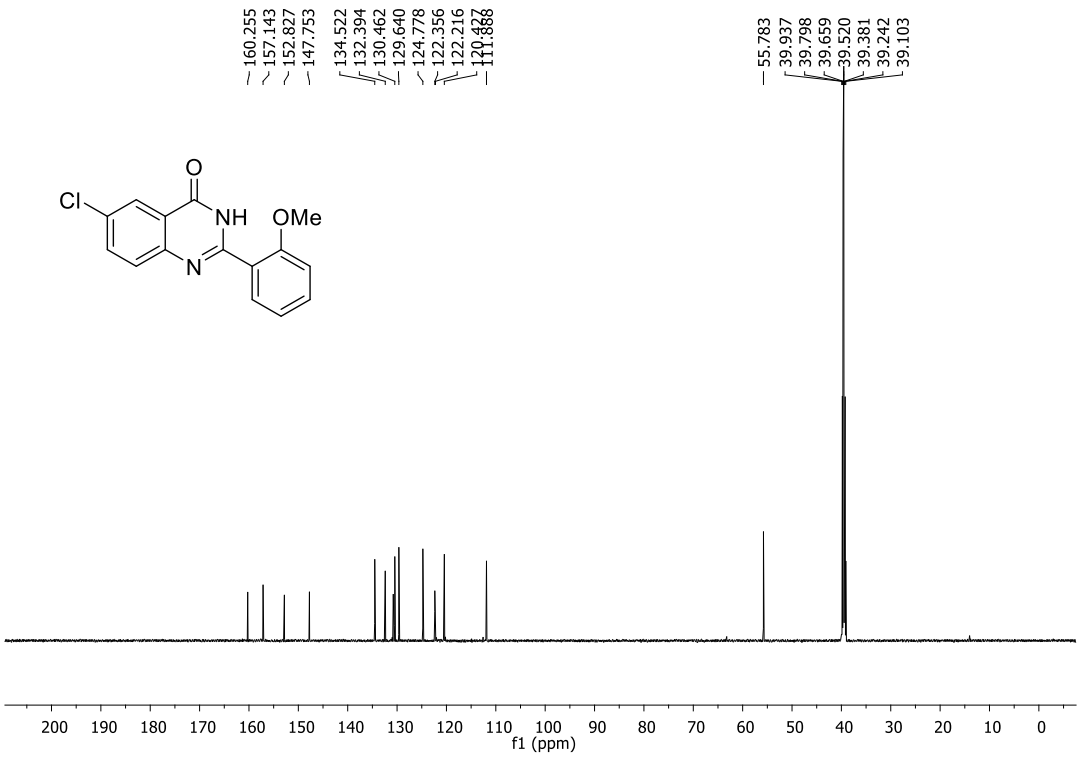


Figure S42. ^{13}C NMR spectrum of 6-Chloro-2-(2-methoxyphenyl)quinazolin-4(3*H*)-one (**3cc**)

^{1}H NMR (600 MHz, DMSO-d_6)

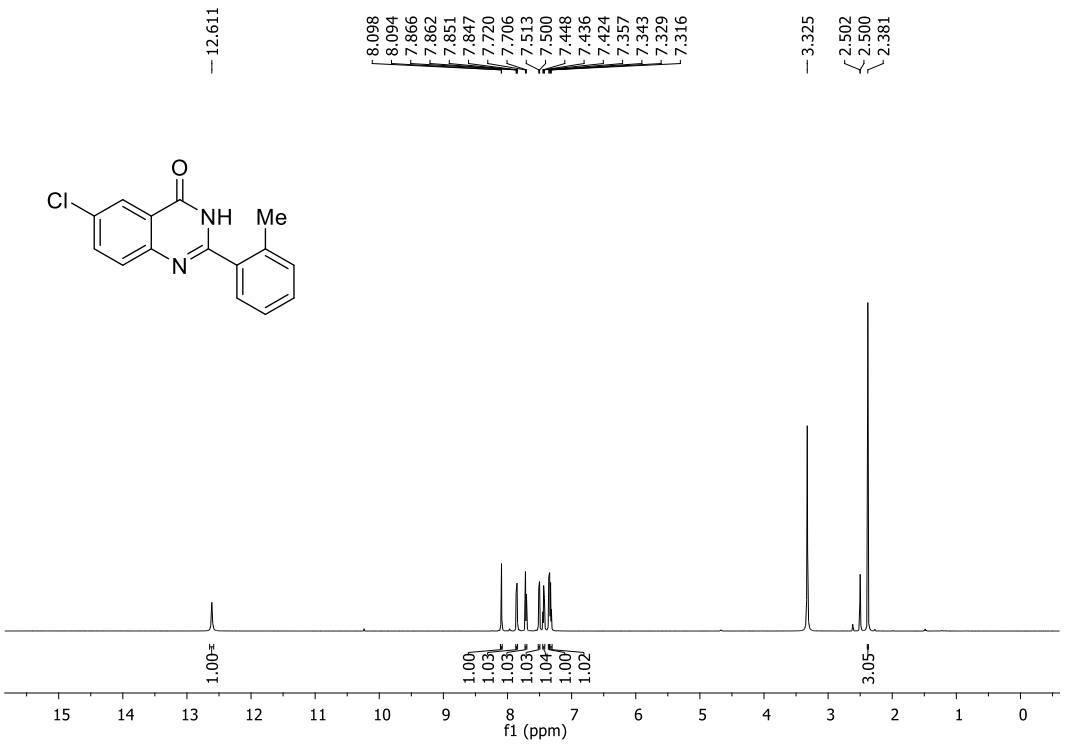


Figure S43. ^{1}H NMR spectrum of 6-Chloro-2-(o-tolyl)quinazolin-4(3*H*)-one (**3cd)**

^{13}C NMR (151 MHz, DMSO-d_6)

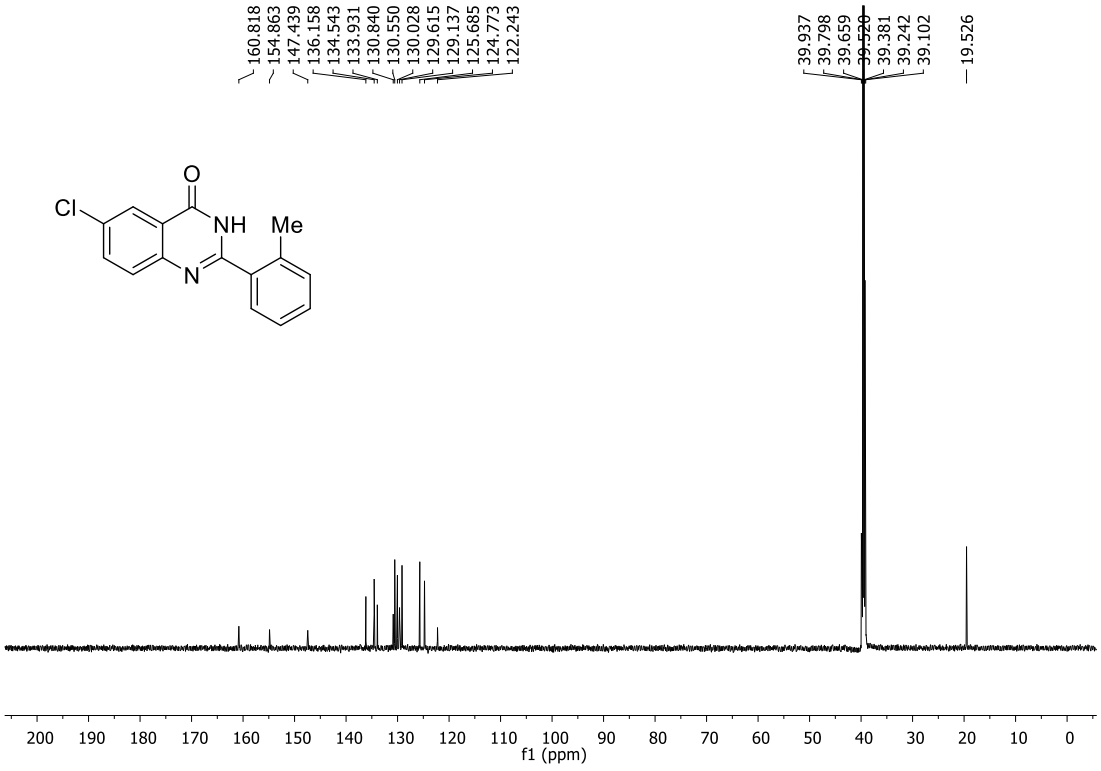


Figure S44. ^{13}C NMR spectrum of 6-Chloro-2-(o-tolyl)quinazolin-4(3*H*)-one (**3cd)**

^{1}H NMR (600 MHz, DMSO-d$_6$)

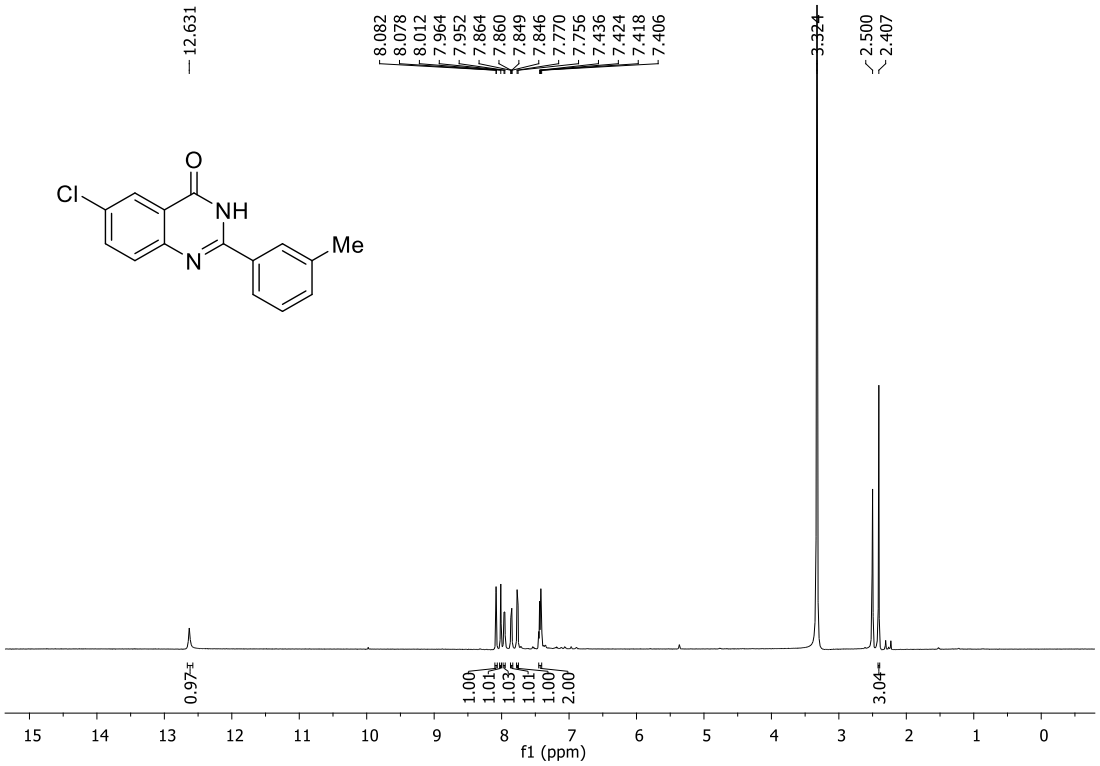


Figure S45. ^{1}H NMR spectrum of 6-Chloro-2-(m-tolyl)quinazolin-4(3*H*)-one (**3ce**)

^{13}C NMR (151 MHz, DMSO-d$_6$)

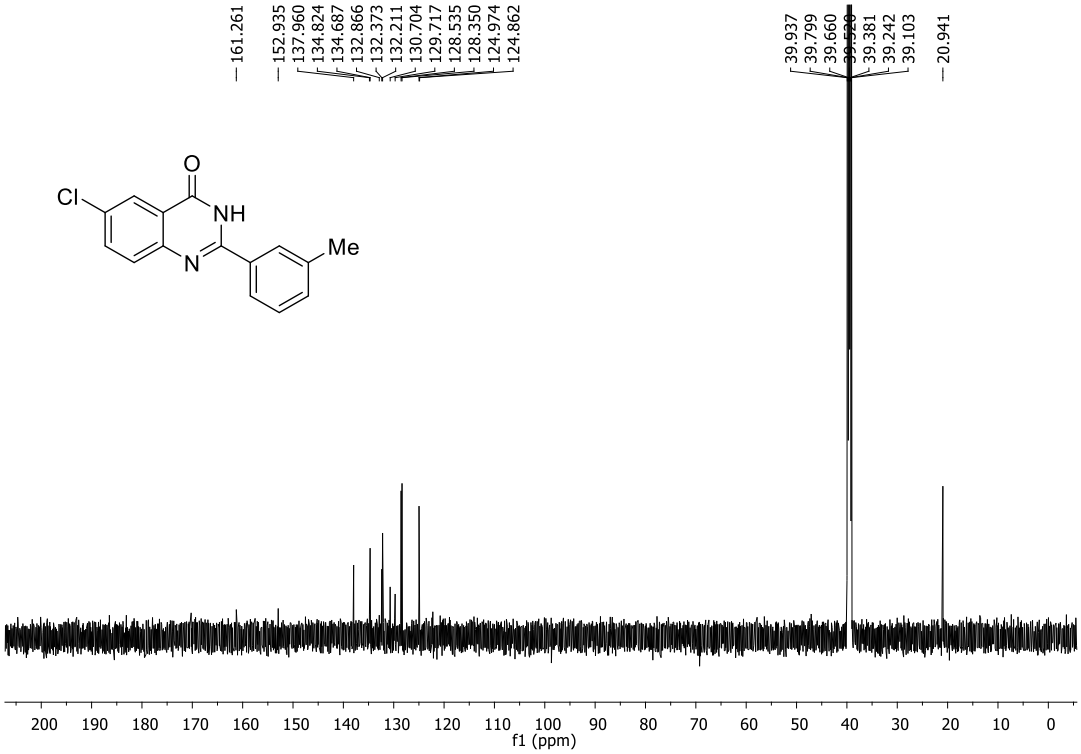


Figure S46. ^{13}C NMR spectrum of 6-Chloro-2-(m-tolyl)quinazolin-4(3*H*)-one (**3ce**)

^{1}H NMR (600 MHz, DMSO-d_6)

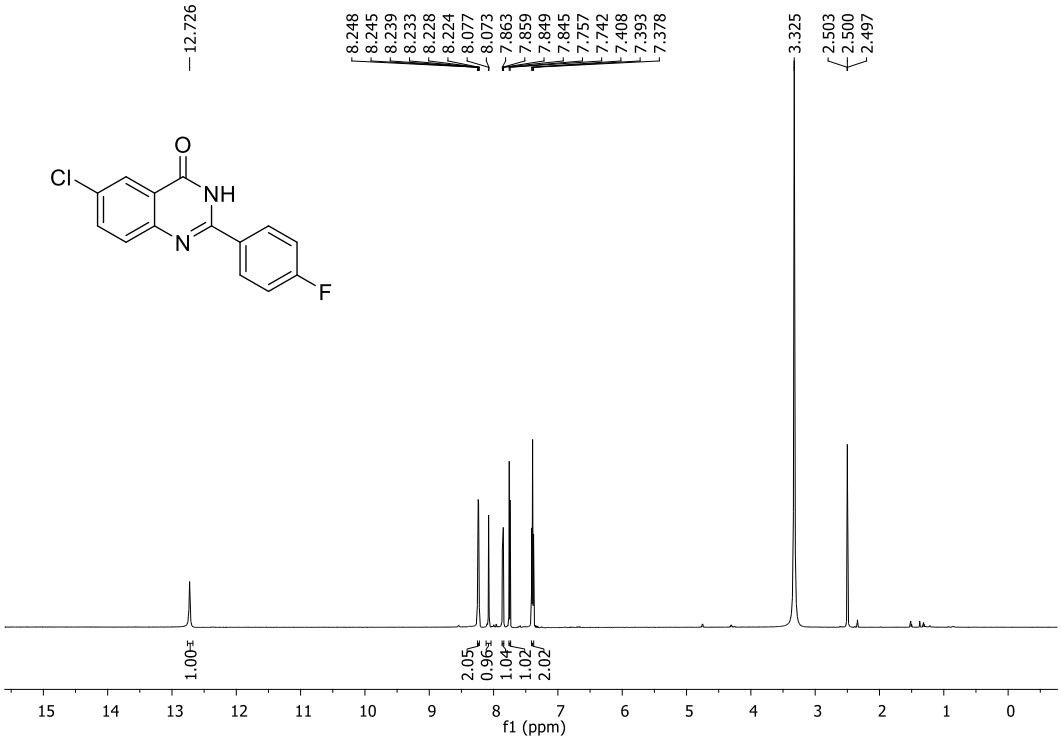


Figure S47. ^{1}H NMR spectrum of 6-Chloro-2-(4-fluorophenyl)quinazolin-4(3*H*)-one (**3cf)**

^{13}C NMR (151 MHz, DMSO-d_6)

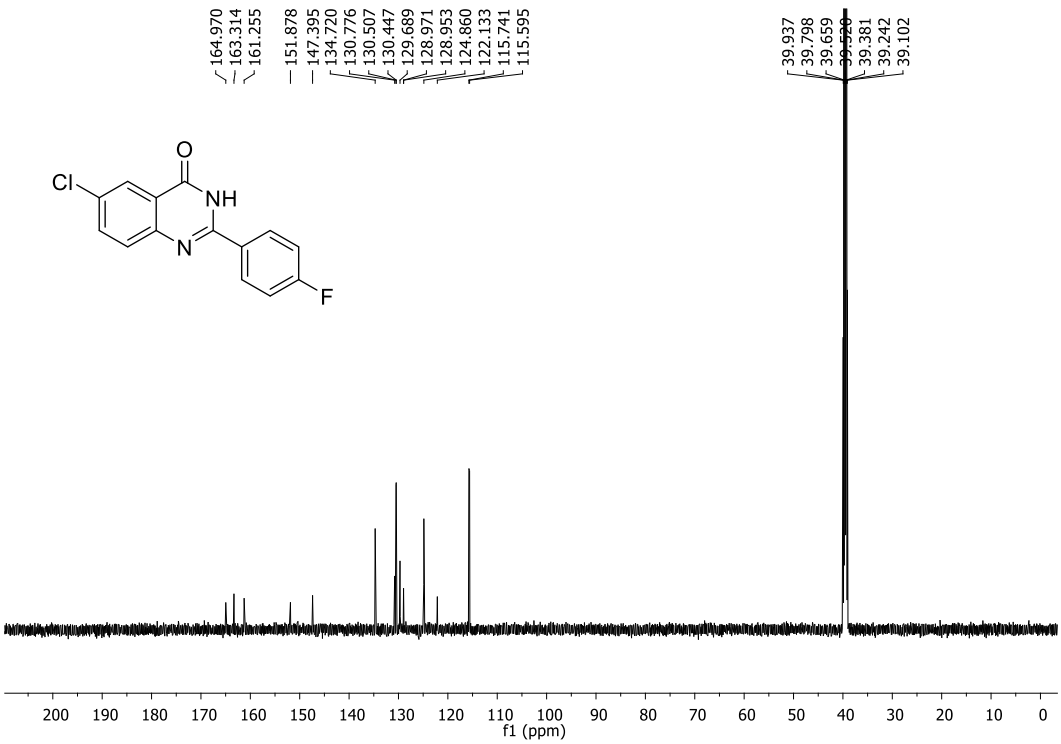


Figure S48. ^{13}C NMR spectrum of 6-Chloro-2-(4-fluorophenyl)quinazolin-4(3*H*)-one (**3cf)**

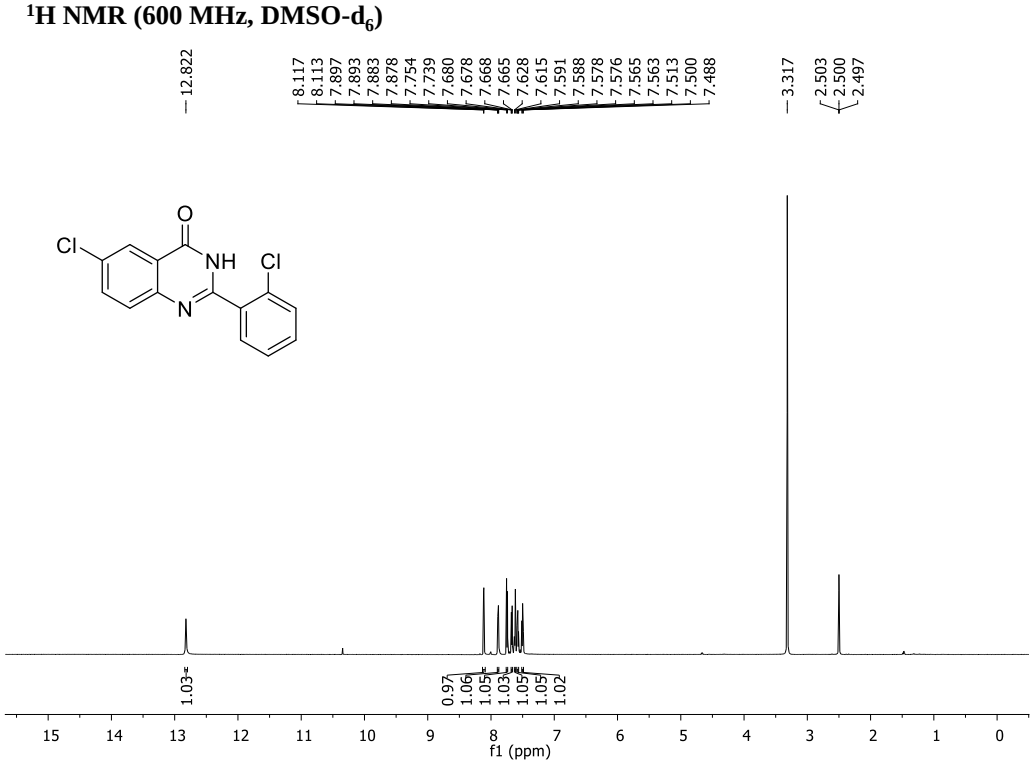


Figure S49. [1]H NMR spectrum of 6-Chloro-2-(2-chlorophenyl)quinazolin-4(3*H*)-one (**3cg)**

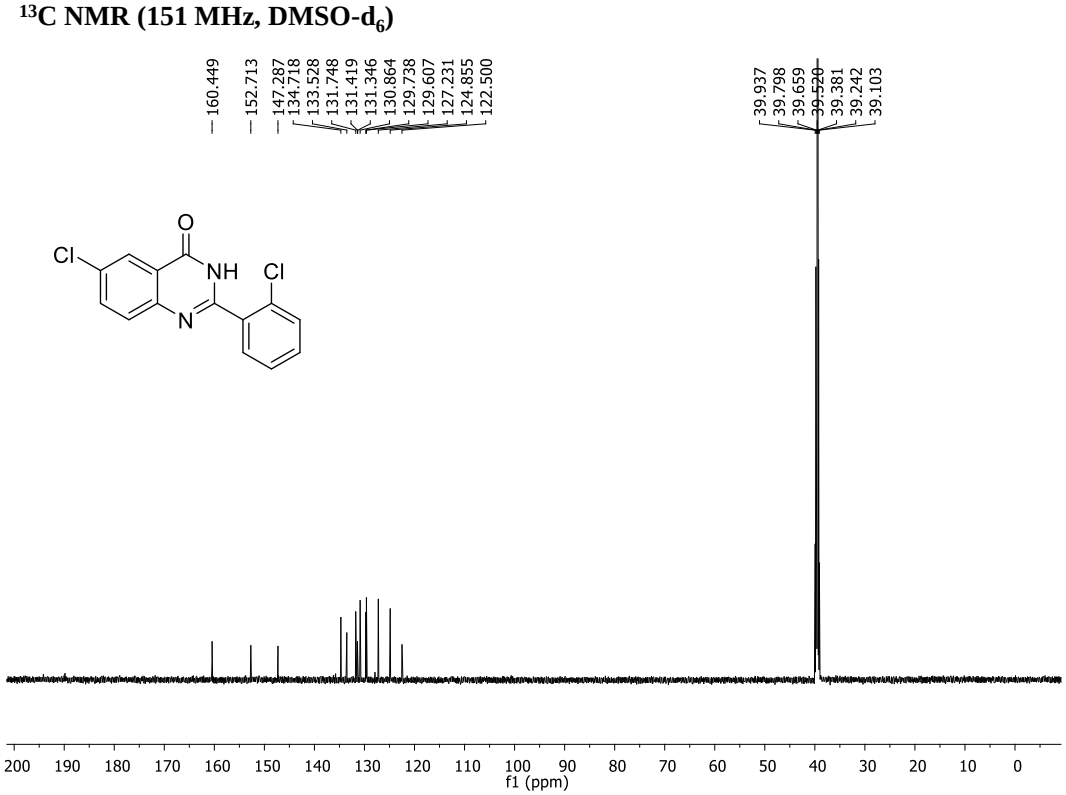


Figure S50. [13]C NMR spectrum of 6-Chloro-2-(2-chlorophenyl)quinazolin-4(3*H*)-one (**3cg)**

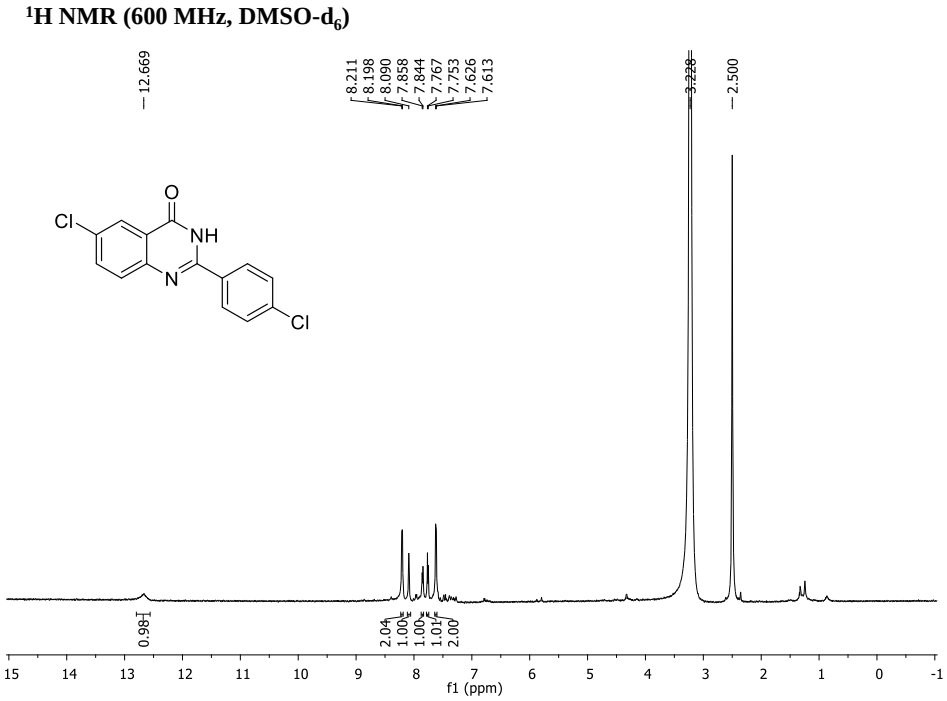


Figure S51. ^{1}H NMR spectrum of 6-Chloro-2-(4-chlorophenyl)quinazolin-4(3*H*)-one (**3ch)**

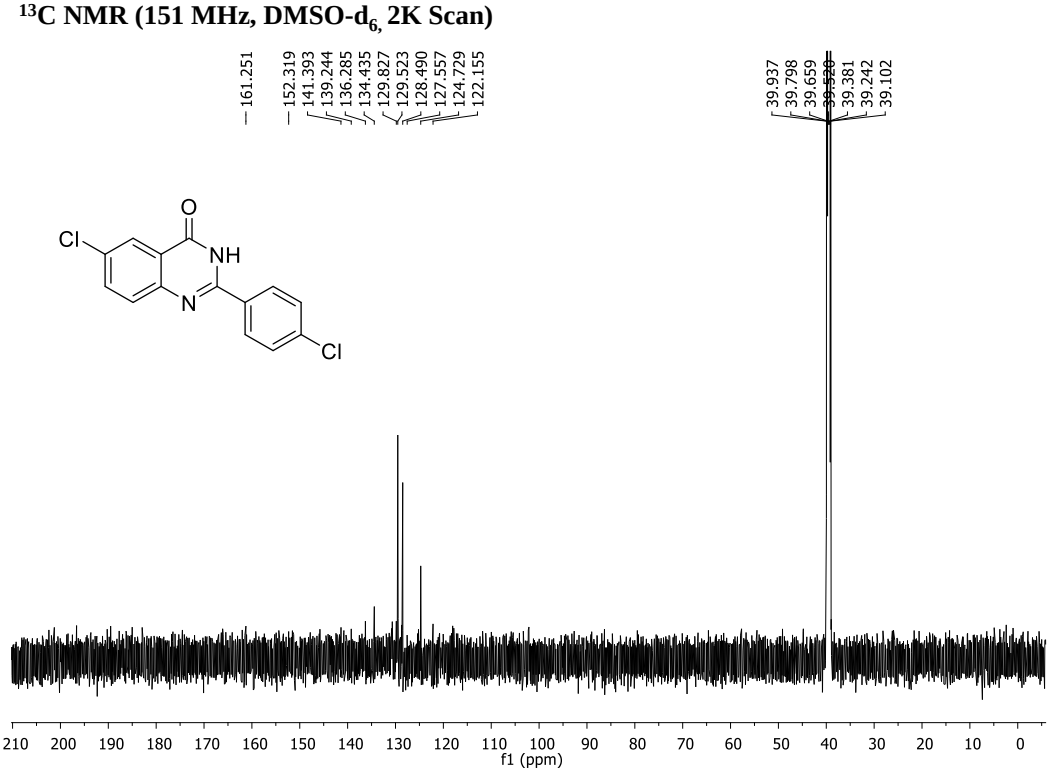


Figure S52. ^{13}C NMR spectrum of 6-Chloro-2-(4-chlorophenyl)quinazolin-4(3*H*)-one (**3ch)**

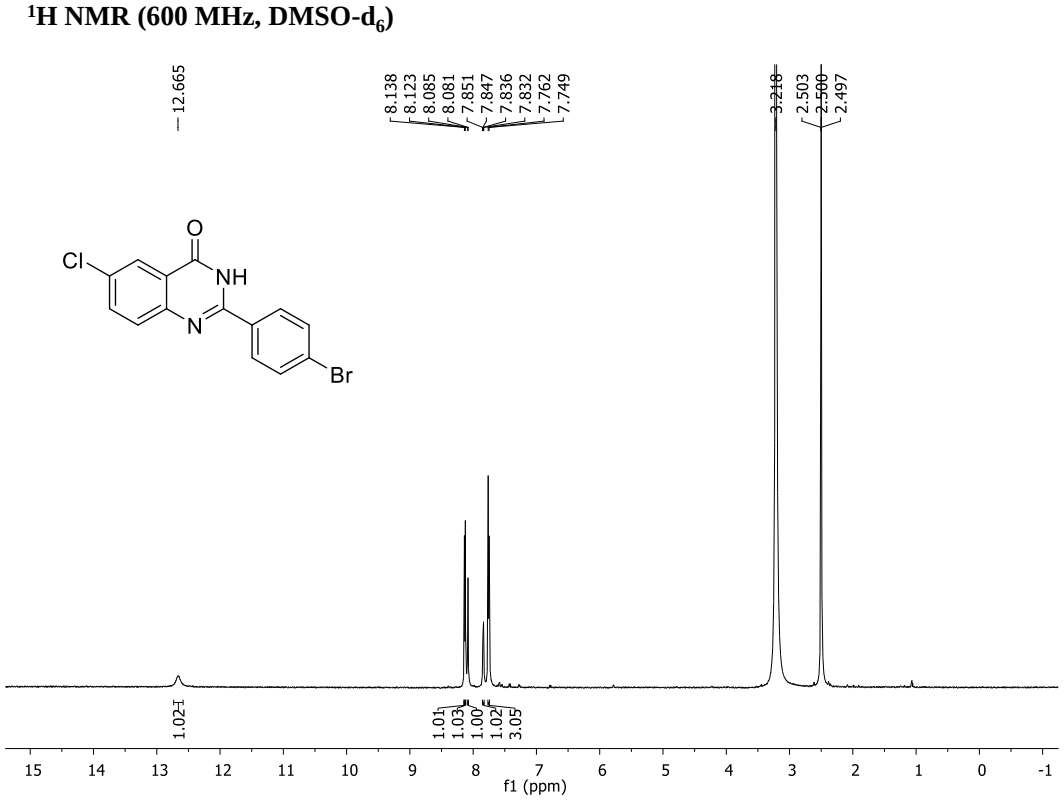


Figure S53. ^{1}H NMR spectrum of 2-(4-Bromophenyl)-6-chloroquinazolin-4(3*H*)-one (**3ci)**

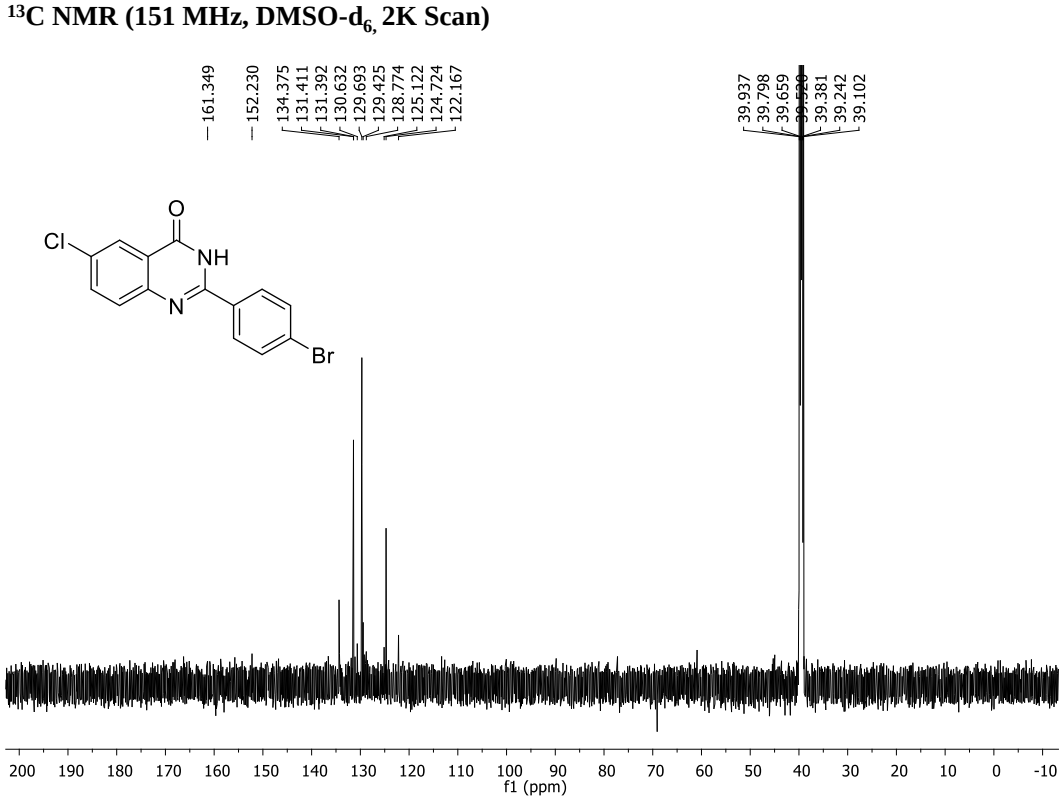


Figure S54. ^{13}C NMR spectrum of 2-(4-Bromophenyl)-6-chloroquinazolin-4(3*H*)-one (**3ci)**

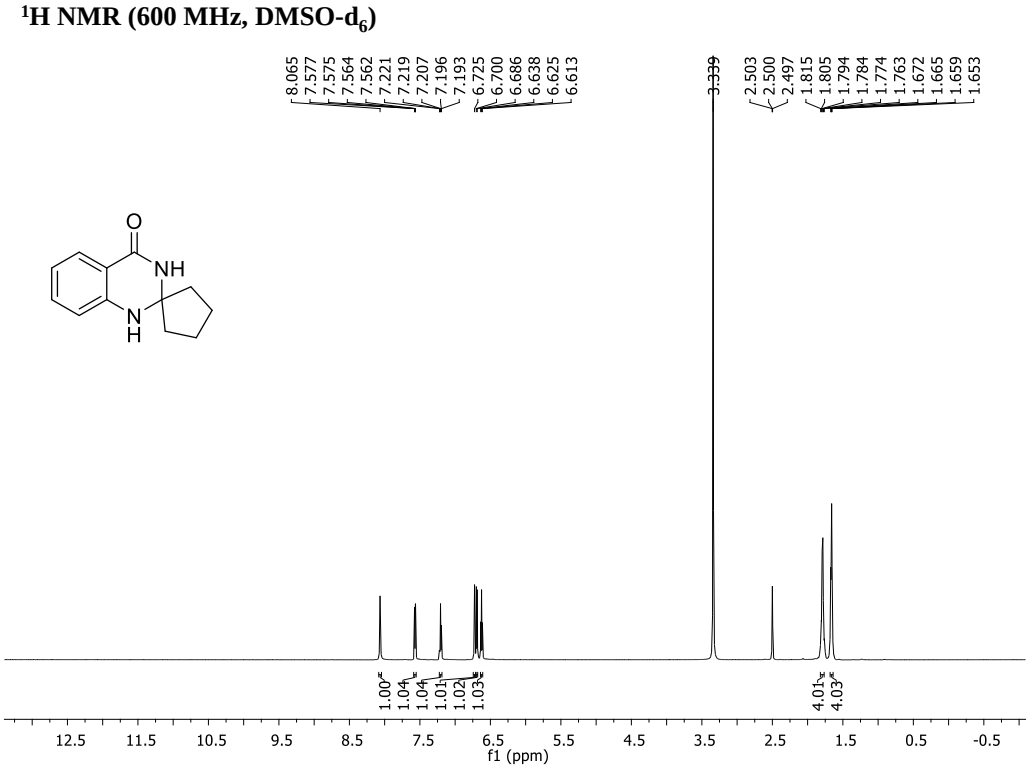


Figure S55. ^{1}H NMR spectrum of 1'*H*-spiro[cyclopentane-1,2'-quinazolin]-4'(3'*H*)-one (**3an**)

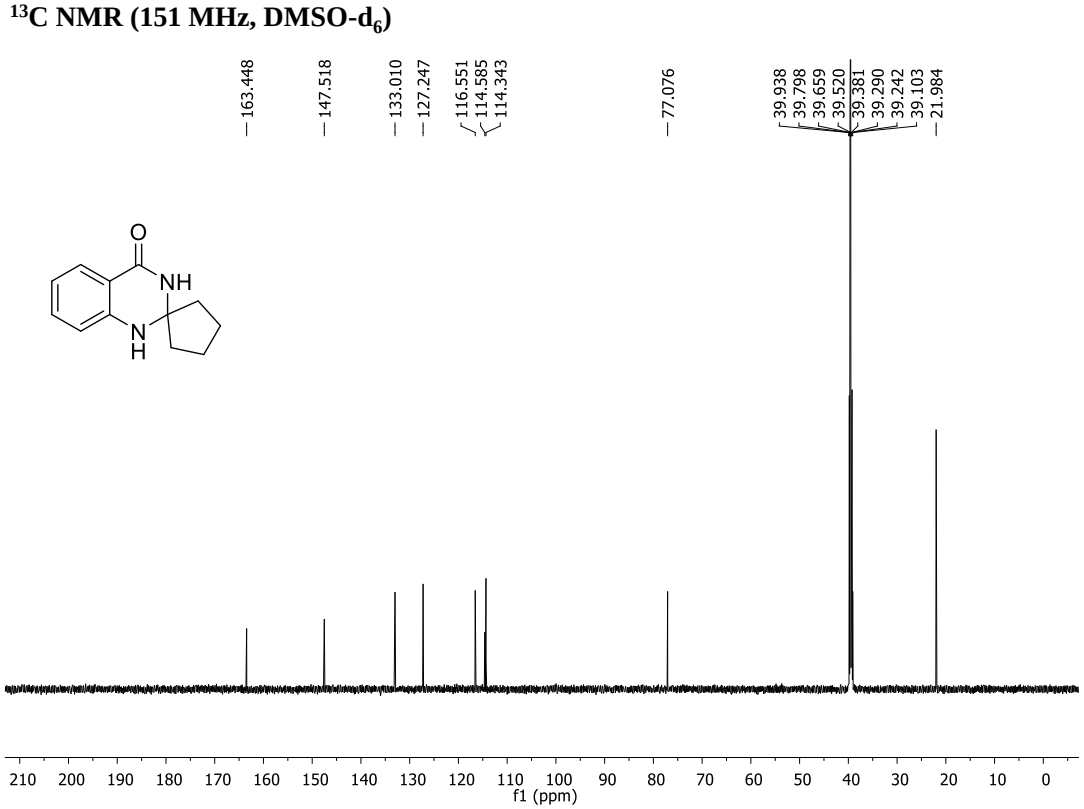


Figure S56. ^{13}C NMR spectrum of 1'*H*-spiro[cyclopentane-1,2'-quinazolin]-4'(3'*H*)-one (**3an**)

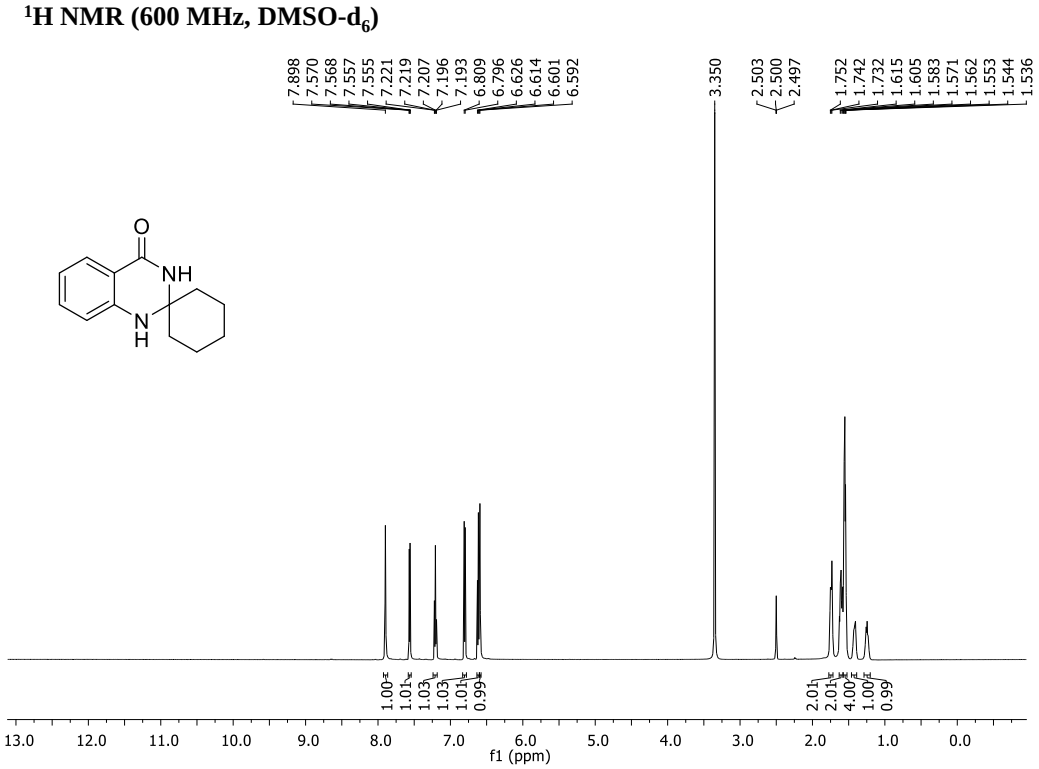


Figure S57. ^{1}H NMR spectrum of 1'*H*-spiro[cyclohexane-1,2'-quinazolin]-4'(3'*H*)-one (**3ao**)

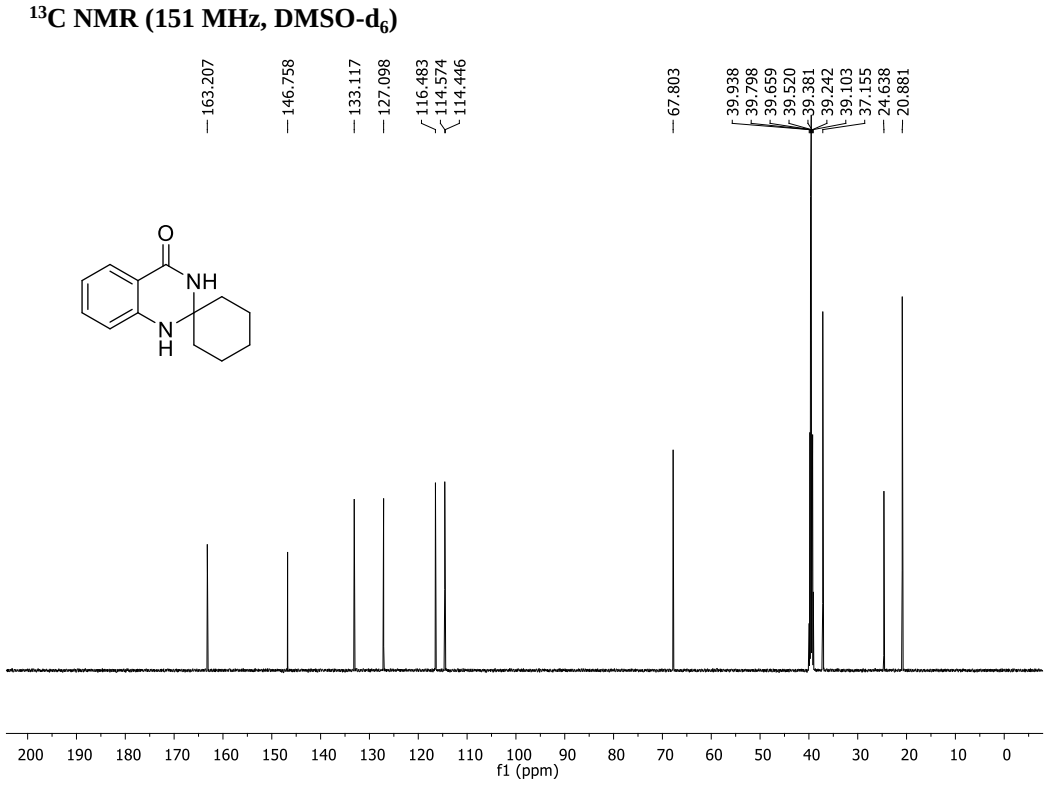


Figure S58. ^{13}C NMR spectrum of 1'*H*-spiro[cyclohexane-1,2'-quinazolin]-4'(3'*H*)-one (**3ao**)

^{1}H NMR (600 MHz, DMSO-d_6)

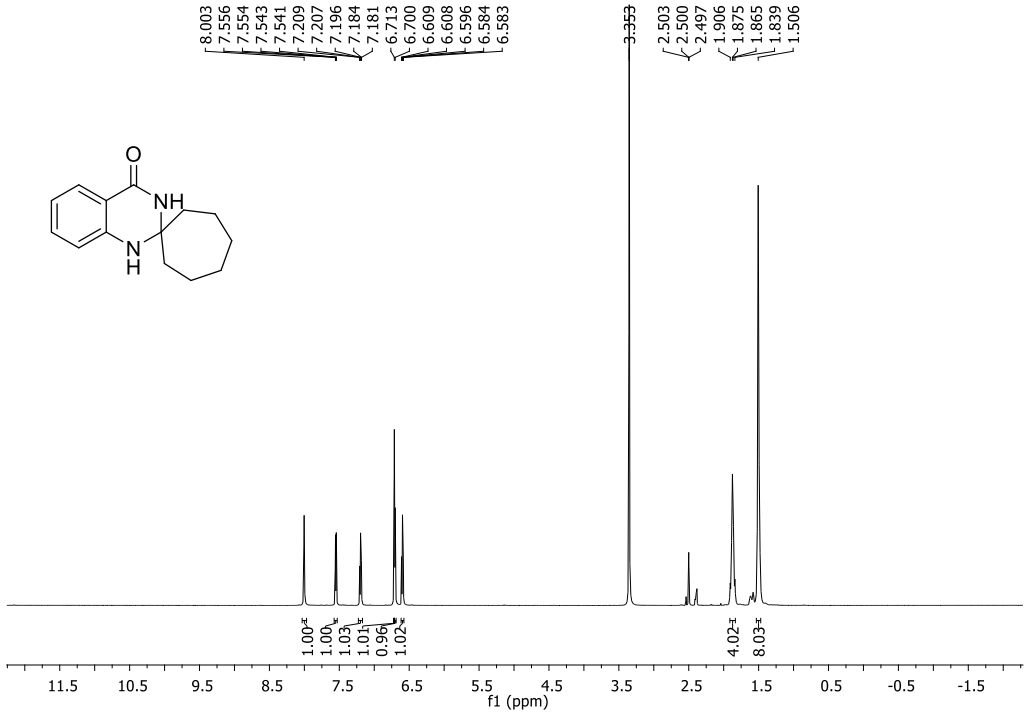


Figure S59. ^{1}H NMR spectrum of 1'*H*-spiro[cycloheptane-1,2'-quinazolin]-4'(3'*H*)-one **(3ap)**

^{13}C NMR (151 MHz, DMSO-d_6)

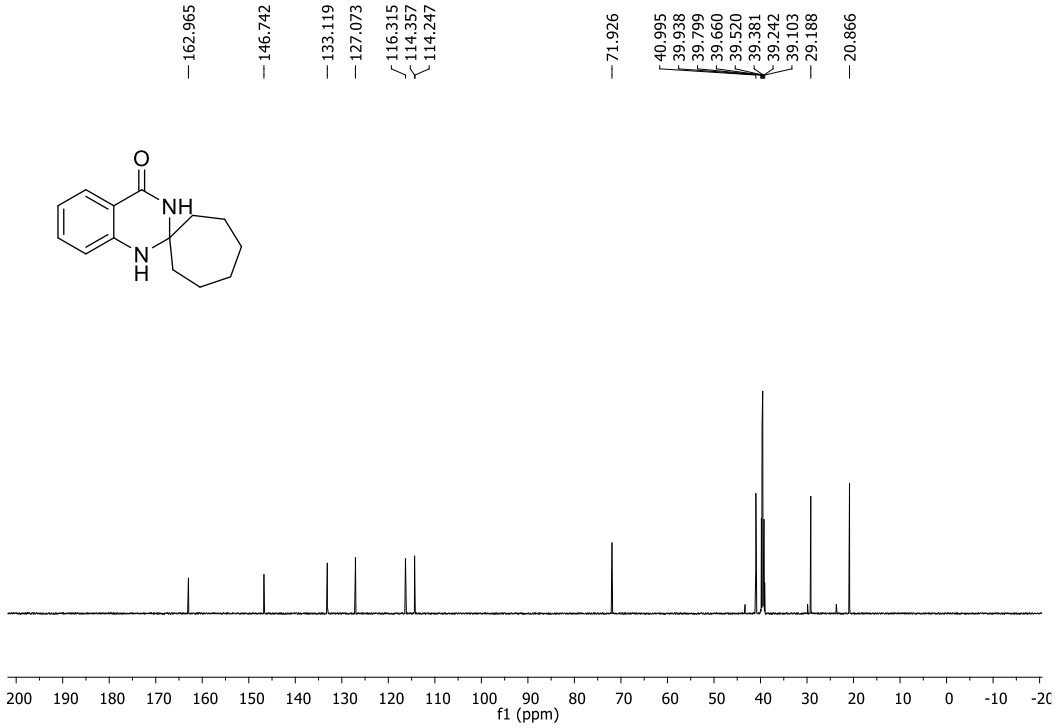


Figure S60. ^{13}C NMR spectrum of 1'*H*-spiro[cycloheptane-1,2'-quinazolin]-4'(3'*H*)-one **(3ap)**

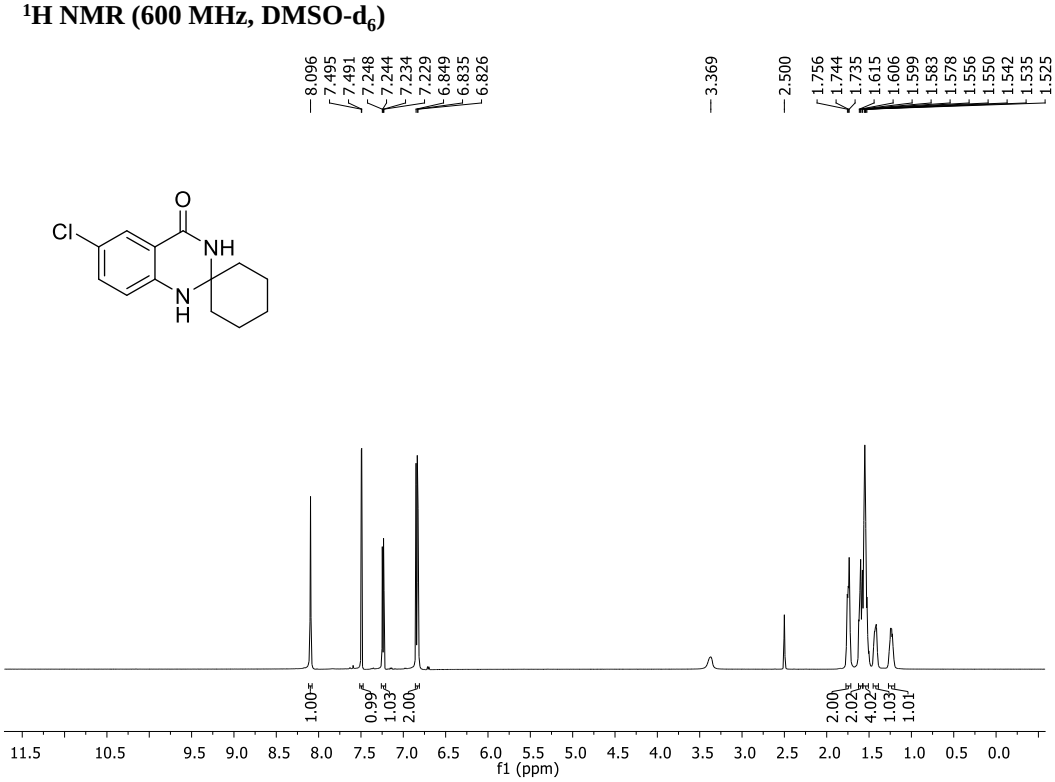


Figure S61. ^{1}H NMR spectrum of 6'-Chloro-1'*H*-spiro[cyclohexane-1,2'-quinazolin]-4'(3'*H*)-one (**3co**)

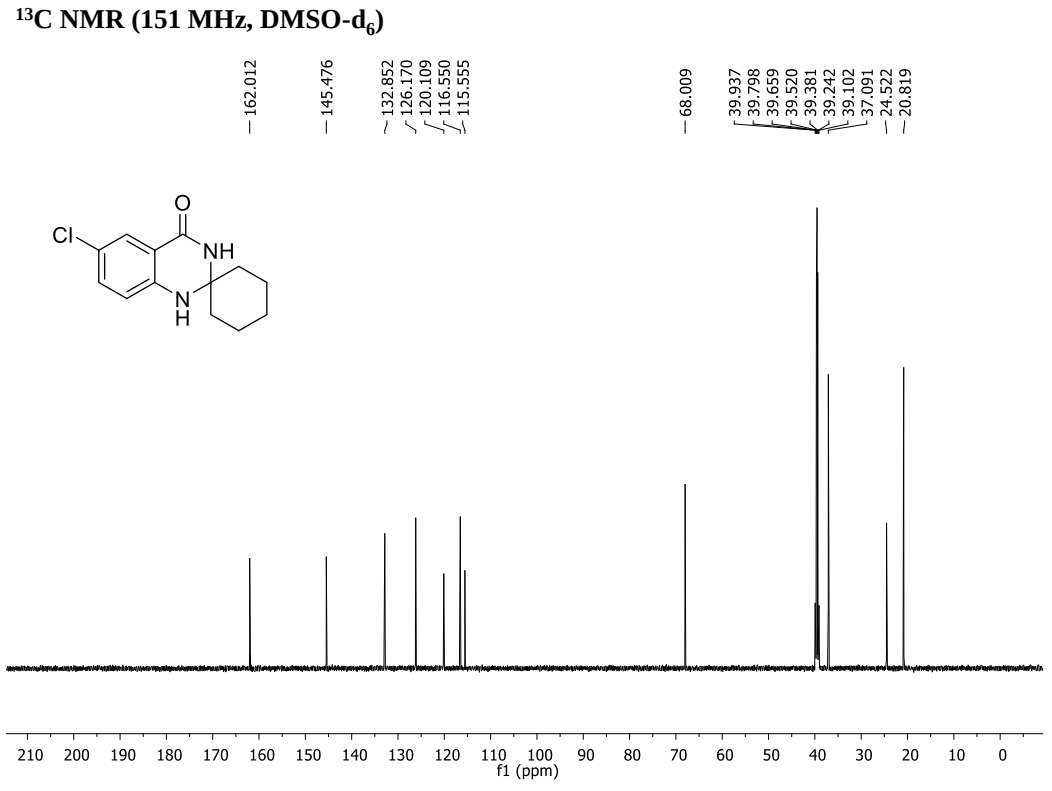
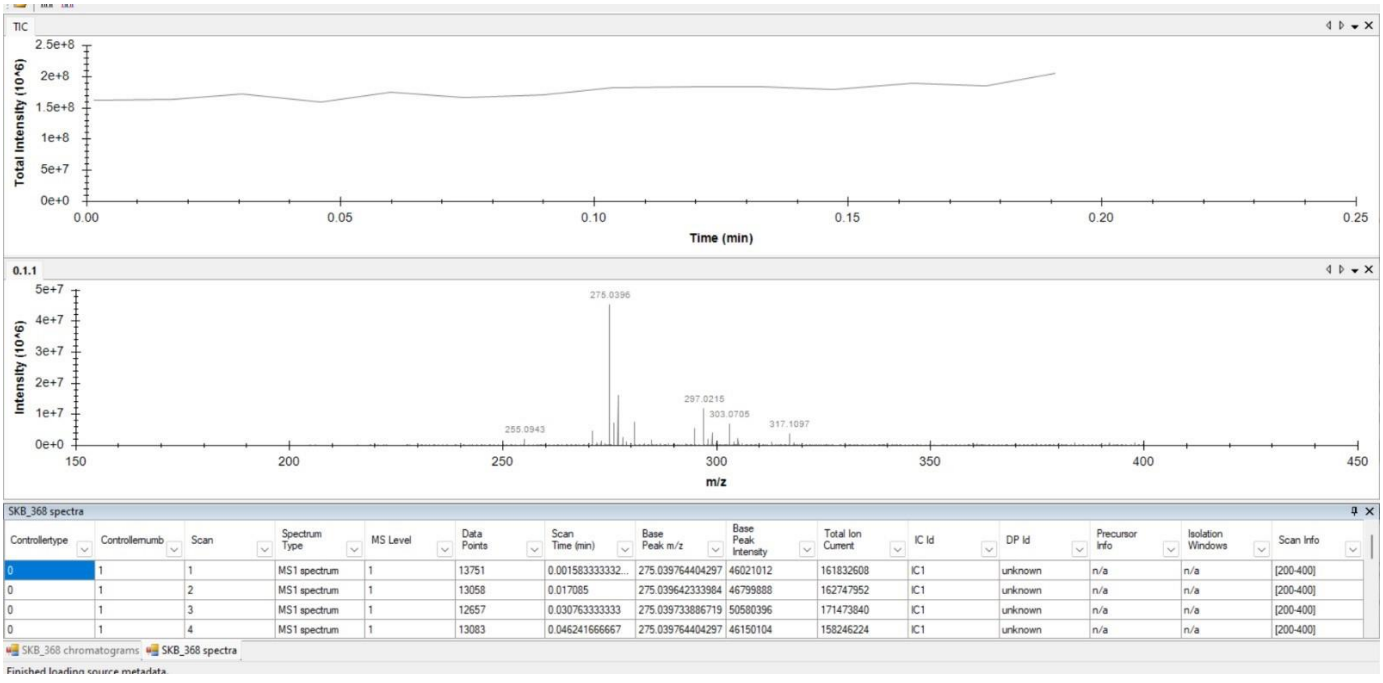


Figure S62. ^{13}C NMR spectrum of 6'-Chloro-1'*H*-spiro[cyclohexane-1,2'-quinazolin]-4'(3'*H*)-one (**3co**)

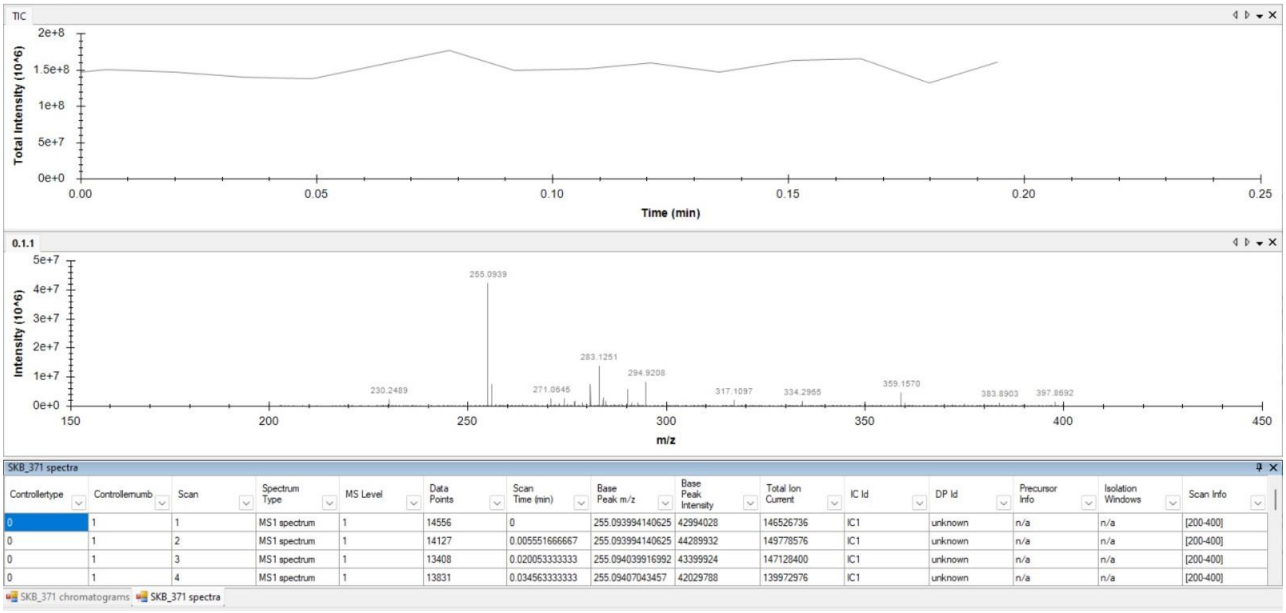
Controllertype	Controllernumb	Scan	Spectrum Type	MS Level	Data Points	Scan Time (min)	Base Peak m/z	Base Peak Intensity	Total Ion Current	IC Id	DP Id	Precursor Info	Isolation Windows	Scan Info
0	1	1	MS1 spectrum	1	16365	0.004565	317.110595703125	30749930	118582064	IC1	unknown	n/a	n/a	[200-400]
0	1	2	MS1 spectrum	1	16099	0.019055	317.110473632813	34781880	127736312	IC1	unknown	n/a	n/a	[200-400]
0	1	3	MS1 spectrum	1	16500	0.033555	317.110534667969	32435376	120971904	IC1	unknown	n/a	n/a	[200-400]
0	1	4	MS1 spectrum	1	17163	0.048055	317.110534667969	30770796	119169888	IC1	unknown	n/a	n/a	[200-400]

HRMS data for **3bj**: calculated for $C_{20}H_{14}FN_2O$: 317.1090 $[M+H]^+$; found: 317.1103.



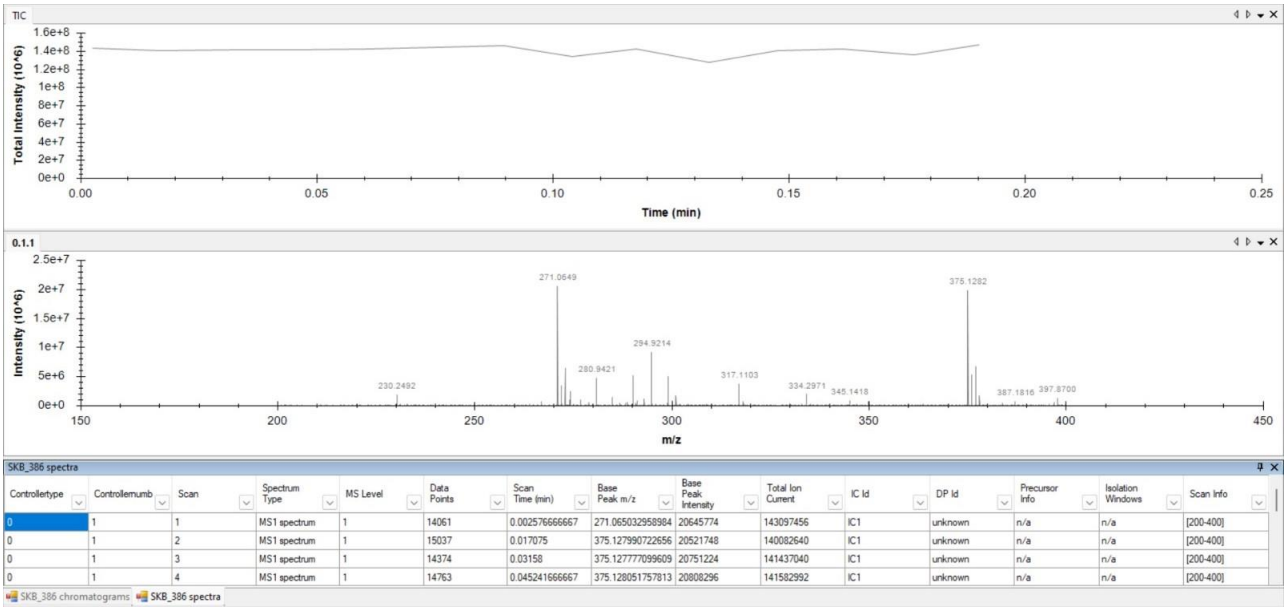
Controllertype	Controllernumb	Scan	Spectrum Type	MS Level	Data Points	Scan Time (min)	Base Peak m/z	Base Peak Intensity	Total Ion Current	IC Id	DP Id	Precursor Info	Isolation Windows	Scan Info
0	1	1	MS1 spectrum	1	13751	0.001583333332...	275.039764404297	46021012	161832608	IC1	unknown	n/a	n/a	[200-400]
0	1	2	MS1 spectrum	1	13058	0.017085	275.039642333984	46799888	162747952	IC1	unknown	n/a	n/a	[200-400]
0	1	3	MS1 spectrum	1	12657	0.030763333333	275.039733886719	50580396	171473840	IC1	unknown	n/a	n/a	[200-400]
0	1	4	MS1 spectrum	1	13083	0.046241666667	275.039764404297	46150104	158246224	IC1	unknown	n/a	n/a	[200-400]

HRMS data for **3bg**: calculated for $C_{14}H_9ClFN_2O$: 275.0387 $[M+H]^+$; found: 275.0396.



Controltype	Controlnumb	Scan	Spectrum Type	MS Level	Data Points	Scan Time (min)	Base Peak m/z	Base Peak Intensity	Total Ion Current	IC Id	DP Id	Precursor Info	Isolation Windows	Scan Info
0	1	1	MS1 spectrum	1	14556	0	255.093994140625	42994028	146526736	IC1	unknown	n/a	n/a	[200-400]
0	1	2	MS1 spectrum	1	14127	0.005551666667	255.093994140625	44289932	149778576	IC1	unknown	n/a	n/a	[200-400]
0	1	3	MS1 spectrum	1	13408	0.020053333333	255.094039916992	43399924	147128400	IC1	unknown	n/a	n/a	[200-400]
0	1	4	MS1 spectrum	1	13831	0.034563333333	255.09407043457	42029788	139972976	IC1	unknown	n/a	n/a	[200-400]

HRMS data for **3be**: calculated for $C_{15}H_{12}FN_2O$: 255.0928 $[M+H]^+$; found: 255.0939.



Controltype	Controlnumb	Scan	Spectrum Type	MS Level	Data Points	Scan Time (min)	Base Peak m/z	Base Peak Intensity	Total Ion Current	IC Id	DP Id	Precursor Info	Isolation Windows	Scan Info
0	1	1	MS1 spectrum	1	14061	0.002576666667	271.065032958984	20645774	143097456	IC1	unknown	n/a	n/a	[200-400]
0	1	2	MS1 spectrum	1	15037	0.017075	375.127990722656	20521748	140082640	IC1	unknown	n/a	n/a	[200-400]
0	1	3	MS1 spectrum	1	14374	0.03158	375.127777099609	20751224	141437040	IC1	unknown	n/a	n/a	[200-400]
0	1	4	MS1 spectrum	1	14763	0.045241666667	375.128051757813	20808296	141582992	IC1	unknown	n/a	n/a	[200-400]

HRMS data for **3ce**: calculated for $C_{15}H_{12}ClN_2O$: 271.0638 $[M+H]^+$; found: 271.0649.

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