

Photochemical dehydrogenation transformation to heterocycles facilitated by azo/hydrazo redox couple

Ayanangshu Biswas, Supriya Halder, Sourav Mandal, Rahul Singh and Debashis Adhikari*

Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Mohali, Sector-81,
Knowledge City, Manauli-140306, India. E-mail: adhikari@iisermohali.ac.in

Table of contents

Serial No	Content	Page
1.	General information	S2
2.	General Procedure for the synthesis BTAN catalyst	S3
3.	Complementary reaction optimisation data	S5
4.	General Procedure General procedure for the synthesis of quinazolinones	S6
5.	Mechanistic investigation a) Radical quenching with TEMPO b) EPR analysis of BTAN radical anion c) Cyclic voltammetry experiment for BTAN d) UV-Visible absorption of BTAN and BTAN radical anion e) Emission spectra of BTAN f) Fluorescence quenching experiment and Stern-Volmer plot g) Detection of H ₂ O ₂ during alcohol oxidation h) Trapping of intermediate H₂BTAN i) Radical clock experiment	S6
6.	E _{0,0} and excited state reduction potential calculations for BTAN	S16
7.	Mechanistic insight into the reaction	S17
8.	LUMO of BTAN molecule	S20
9.	Analytical data	S21
10.	¹ H and ¹³ C NMR spectra for synthesized compounds	S37
11.	References	S84

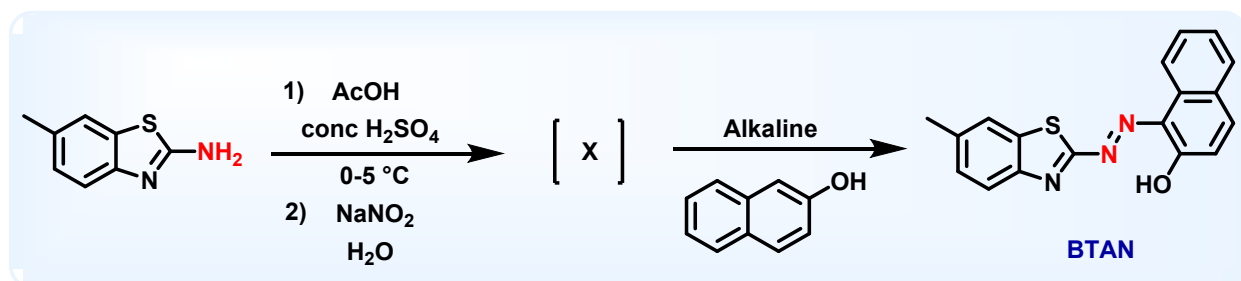
1. General Information:

Reagent Information. All starting compounds employed in this study were procured from commercial suppliers. Potassium *tert*-butoxide, potassium hydroxide, and sodium hydroxide were purchased from Avra Synthesis Pvt. Ltd., India. 2-aminobenzonitrile; β -Naphthol; and 5-Methyl benzothiazole were purchased from Sigma-Aldrich. These chemicals were used without further purification. All chemicals were used without further purification. Glassware were dried overnight at 160 °C. Solvents such as xylene, toluene, acetonitrile, THF were used as received from the suppliers (Finar Chemicals). For thin layer chromatography (TLC), aluminum foil coated with silica and fluorescent indicator 254 nm (from Merck) was used. Column chromatography was performed using SD Fine silica gel 60-120 mesh using a gradient of hexane and ethyl acetate/ diethyl ether as mobile phase.

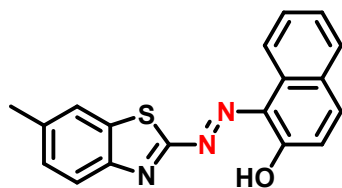
Analytical Information. All isolated compounds were characterized by ^1H NMR, ^{13}C NMR spectroscopy. ^1H NMR and ^{13}C NMR spectra were recorded on a 400 MHz Bruker Biospin Advance III FT-NMR spectrometer. NMR shifts are reported as delta (δ) units in parts per million (ppm), and coupling constants (J) are reported in Hertz (Hz). Chemical shifts (δ) are quoted to the nearest 0.01 ppm relative to the residual protons in DMSO- d_6 (δ 2.5 ppm). Carbon chemical shifts are internally referenced to the deuterated solvent signals in DMSO- d_6 (δ 39.5 ppm). Fluorescence quenching experiments of the **BTAN** Catalyst were carried out in a Cary Eclipse Fluorescence Spectrofluorometer. The X-band EPR spectrum was collected in a JEOL Model: JES-FA200 machine operating at a microwave frequency of 9.4 GHz, modulation frequency of 100 kHz, 5 mW power, along with 30 seconds of sweep time. Cyclic voltammetry was performed using an AUTOLAB potentiostat. IR spectra was collected in PerkinElmer Spectrum RX1 FT-IR Spectrometer. UV-Vis was recorded using Varian Cary 60 (Agilent Technologies) spectrophotometer. The total volume in the cuvette was fixed at 3 mL and a cuvette of path length 1 cm was used. The GC data were collected using SHIMADZU GC-2010 PLUS instrument. The photochemical reactions were conducted with two eplite 30 W (400-800 nm) white LED. The reaction tube was kept 7-8 cm away from the light source.

2. General synthetic procedure 1-((6-methylbenzo[d]thiazol-2-yl)diazenyl)naphthalen-2-ol (BTAN) catalyst ¹

2-Amino-6-methyl benzothiazole (2.0 mmol) were dissolved in acetic acid (7.6 mL) containing concentrated sulphuric acid (4 mL) and cooled to 0-5°C in an ice bath. The ice-cold solution of NaNO₂ (2.8 mmol, 194 mg) in water (0.5 mL) was added dropwise to the reaction mixture with constant stirring to obtain the diazonium salt. After complete addition the alkaline beta-naphthol (2.0 mmol, 0.288 g) solution was added dropwise to the ice-cold solution of diazonium salt to obtain dark reddish brown coloured azo compound which, upon addition of more alkaline beta-naphthol solution, become darkened. After complete addition, the reaction mixture was further stirred for 2 h and then filtered. The residue was washed multiple times with water, dried, and again washed with methanol multiple times and then crystallized in chloroform. The catalyst was characterised by ¹H, ¹³C NMR spectroscopies.



1-((6-methylbenzo[d]thiazol-2-yl)diazenyl)naphthalen-2-ol : Reddish brown solid, 389 mg, 61% yield. The NMR spectroscopic data is in agreement with the literature¹.



¹H NMR (400 MHz, CDCl₃) δ 15.36 (s, 1H), 8.43 (d, *J* = 8.1 Hz, 1H), 7.78 (d, *J* = 8.3 Hz, 1H), 7.72 (d, *J* = 9.5 Hz, 1H), 7.60 – 7.54 (m, 3H), 7.43 (t, *J* = 7.3 Hz, 1H), 7.24 (s, 1H), 6.81 (d, *J* = 9.5 Hz, 1H), 2.47 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 172.71, 168.72, 150.22, 142.50, 135.74, 133.14, 132.62, 131.69, 129.78, 129.07, 128.83, 128.23, 127.36, 124.34, 122.73, 122.48, 121.67, 21.76.

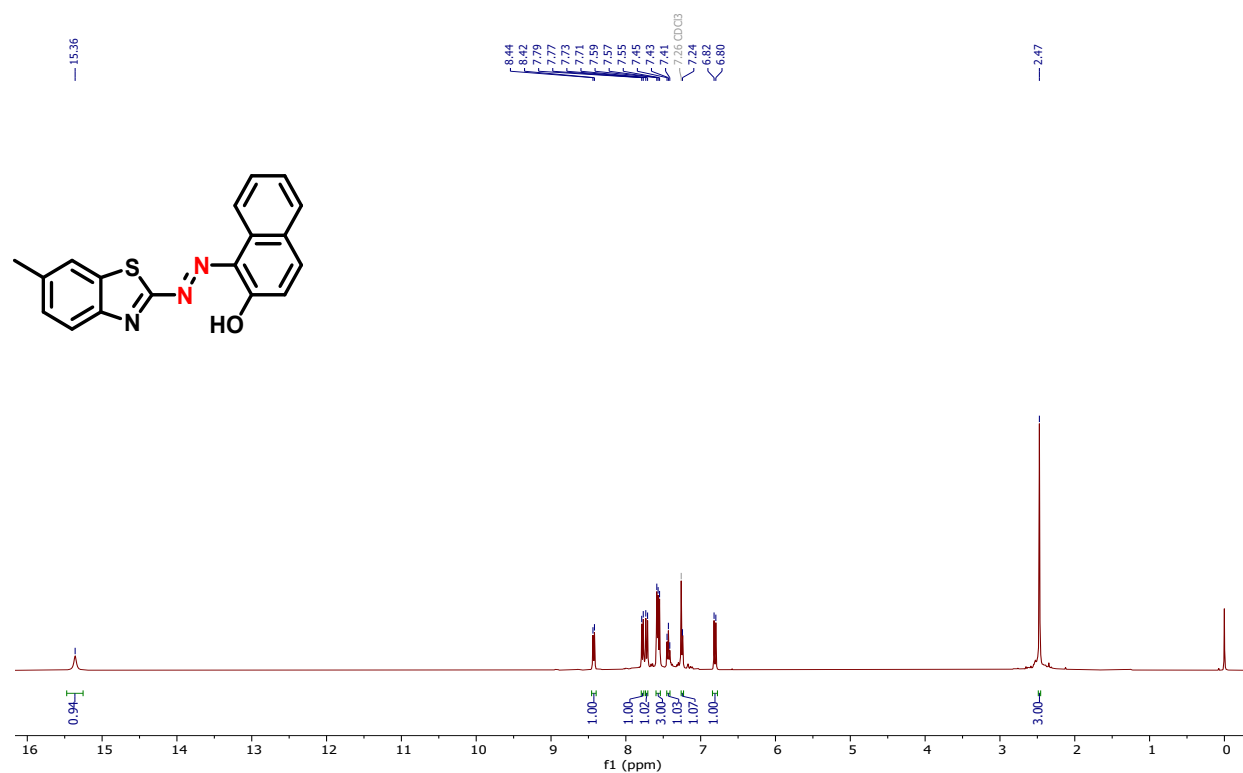


Figure S1: ¹H NMR spectrum (400 MHz) of BTAN in CDCl₃

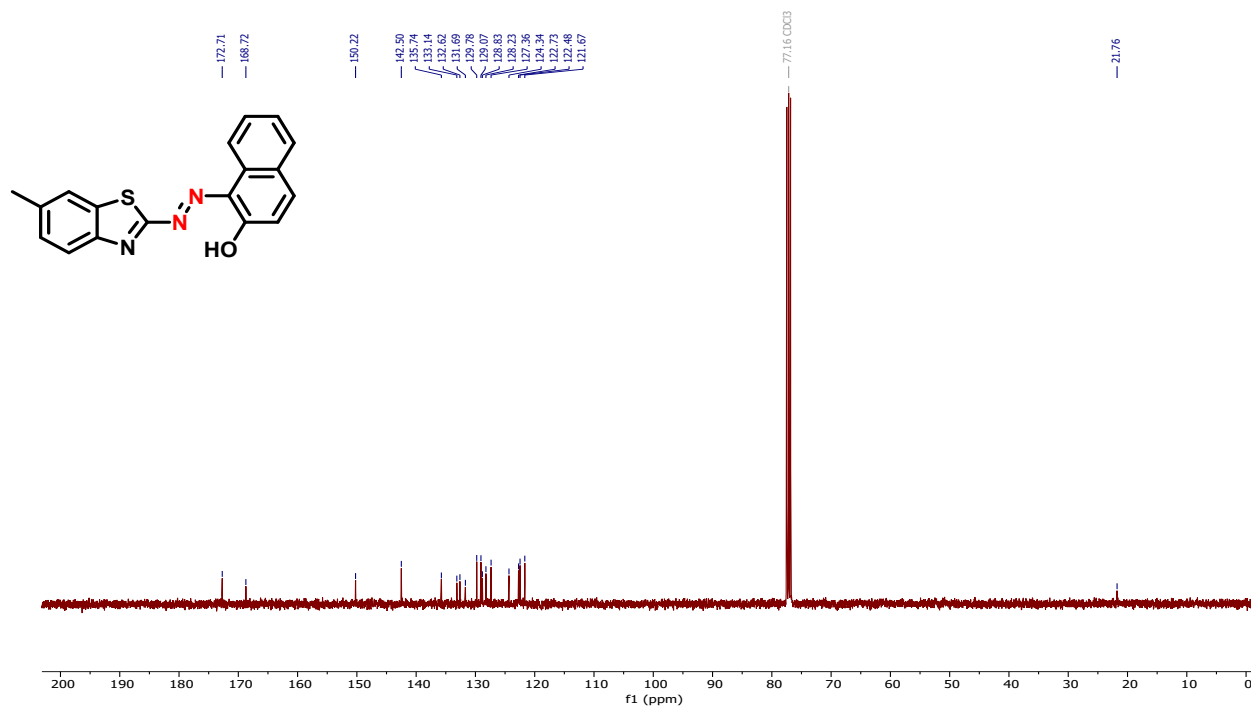
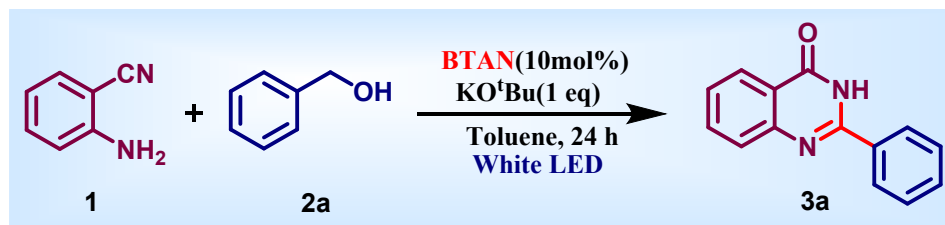


Figure S2: ¹³C NMR spectrum (100 MHz) of BTAN in CDCl₃

3. Reaction Optimization Data:

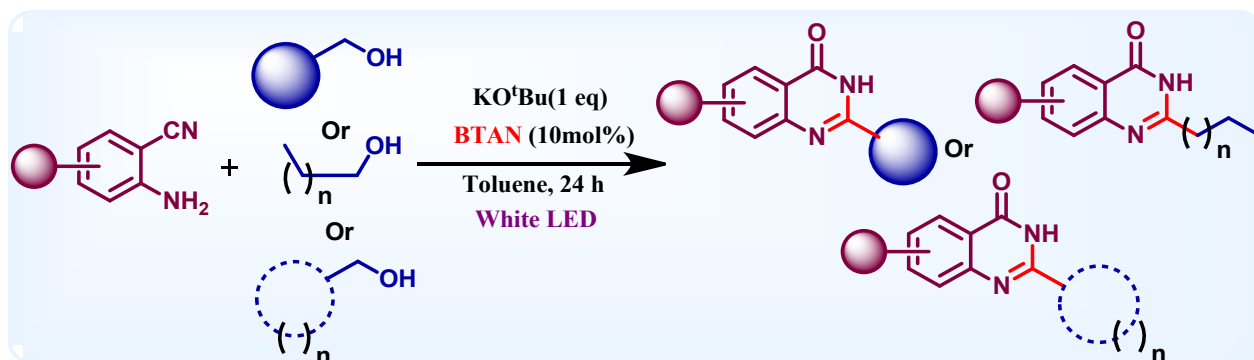


Entry	Catalyst (mol %)	Base (equiv.)	Time (hr)	Solvent	Yield (%)
1	5	KO ^t Bu (1)	24	Toluene	20
2	10	KO ^t Bu (1)	24	1,4-dioxane	23
3	10	KO ^t Bu (1)	24	Toluene	93
4	10	KO ^t Bu (0.5)	24	Toluene	31
5	10	KO ^t Bu (1)	16	Toluene	60
6	15	KO ^t Bu (1)	20	Toluene	82
7	10	NaOH (1)	24	Toluene	Trace
8	10	KOH (1)	24	Toluene	Trace
9	10	Et ₃ N (1)	24	Toluene	6
10	10	DIPEA (1)	24	Toluene	Trace
11	10	DABCO (1)	24	Toluene	9
12	10	KO ^t Bu (1)	24	Xylene	40
13	10	KO ^t Bu (1)	24	THF, MeCN	trace
14	-	KO ^t Bu (1)	24	Toluene	15
15	10	-	24	Toluene	n.r

* *Reaction conditions:* BTAN (x mol %, with respect to 2-amino benzo nitrile), 2-amino benzonitrile (0.5 mmol, 1 equiv), benzyl alcohol (1.2 equiv) base (y equiv), solvent (2 mL) in white LED, 24 h (isolated yield).

4. General procedure:

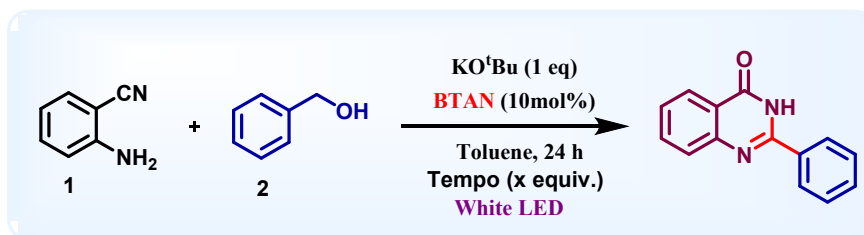
a) General procedure for the synthesis of Quinazolinones using benzylic and aliphatic alcohols with 2-aminobenzonitrile.



A 15 mL vial was charged with 10 mol% of **BTAN**, 0.5 mmol of 2-aminobenzonitrile, KO^tBu (0.5 mmol), and alcohol (0.75 mmol) in 2 mL toluene. The reaction mixture was stirred under two white light irradiation for 24 h in an open atmosphere. Upon completion of the reaction, work up was done using ethyl acetate and brine solution. Then the organic layer was collected, dried over MgSO₄, and concentrated *in vacuo*. The residue was purified by column chromatography using hexane/ethyl acetate (4:1) to (2:1) as eluent to afford pure products. The desired products were fully characterized by ¹H, ¹³C NMR spectroscopies.

5. Mechanistic investigation:

a) Procedure for radical quenching experiment:



In a typical reaction, a 15 mL vial was charged with **BTAN** (10 mol%), benzyl alcohol (0.75 mmol), 2-aminobenzonitrile (0.5 mmol), KO^tBu (0.5 mmol), and the varying equivalent of TEMPO dissolved in 2 mL toluene. The reaction mixture was stirred under white light irradiation

for 24 h in an open atmosphere, to maintain the identical conditions to the optimized protocol. The yield of the reaction decreased drastically with the addition of TEMPO, as probed by GC-MS analysis. On addition of 1 equivalent of TEMPO, complete quenching of the reaction occurs.

Product formation on varying equivalent TEMPO addition

Tempo (x Equiv.)	Product Formation
0.7	18%
1.0	0%

b) EPR analysis of BTAN radical anion:

In a solution of **BTAN** (0.03 mmol, 10 mg) in toluene, KO^tBu (0.15 mmol, 16 mg) was added. Under the dark condition, this solution is reddish in colour. Then the reaction mixture was irradiated with white light for 5 minutes which prompted a sharp colour change to deep violet. The X-band (9.4 GHz) EPR measurement of this solution was carried out at room temperature. A relatively broad signal at $g = 2.006$ was observed, which indicated the formation of a **BTAN** radical anion.

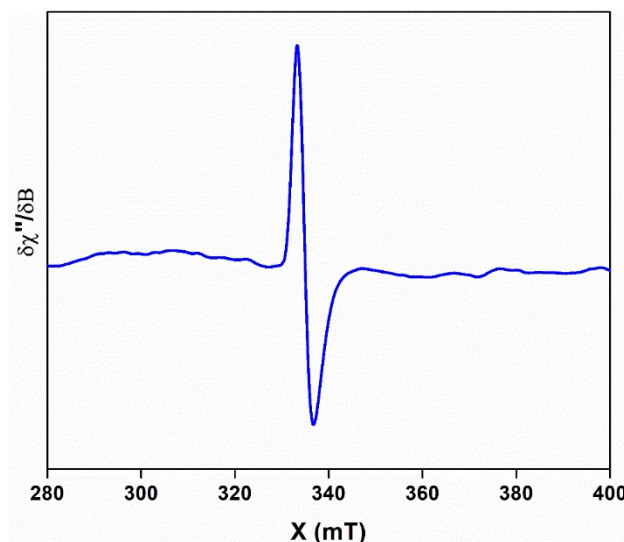


Figure S3a: X-band (9.4 GHz) EPR signal of **BTAN** radical anion obtained by adding KO^tBu and after shining visible light.

c) Cyclic voltammetry experiment for BTAN:

We attempted to evaluate the reduction potential of BTAN by cyclic voltammetry. BTAN (6.4 mg) was dissolved in 20 ml dry THF to prepare a 0.001 M solution. To this solution a 0.1 M (nBu₄N) PF₆ in THF was added as the supporting electrolyte. A three-electrode set-up was used to determine the reduction potential where glassy carbon was the working electrode, a Pt wire as the counter and Ag/AgCl containing 1M KCl solution as the reference electrode, respectively. The shown voltammogram was collected with a scan rate of 100 mV sec⁻¹. The first reduction wave was found at -0.75 V vs Ag/AgCl.

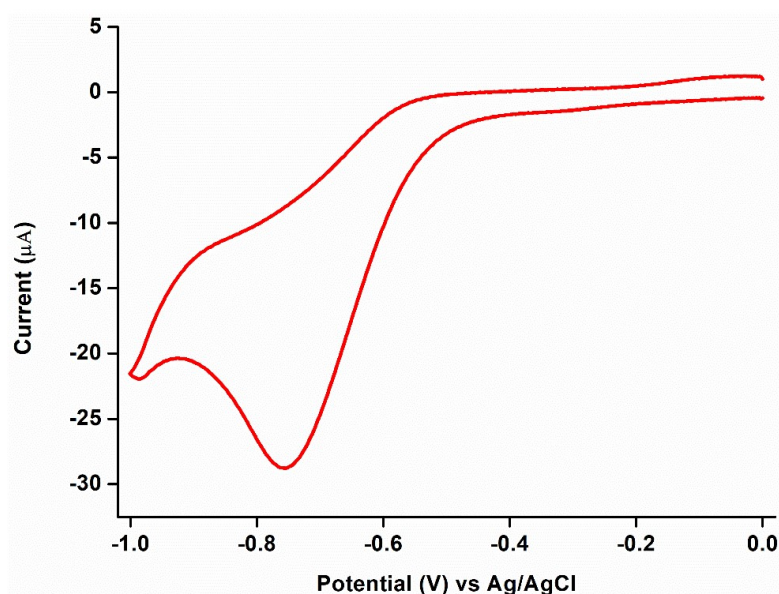


Figure S4: Cyclic voltammogram of BTAN

d) UV-Visible Spectrum:

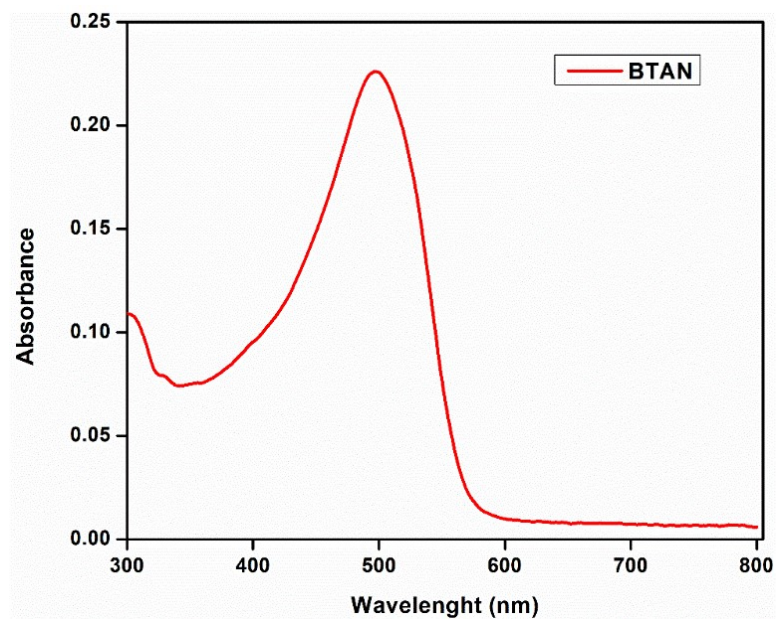


Figure S5: UV-visible spectra of **BTAN** in toluene (10^{-6} M)

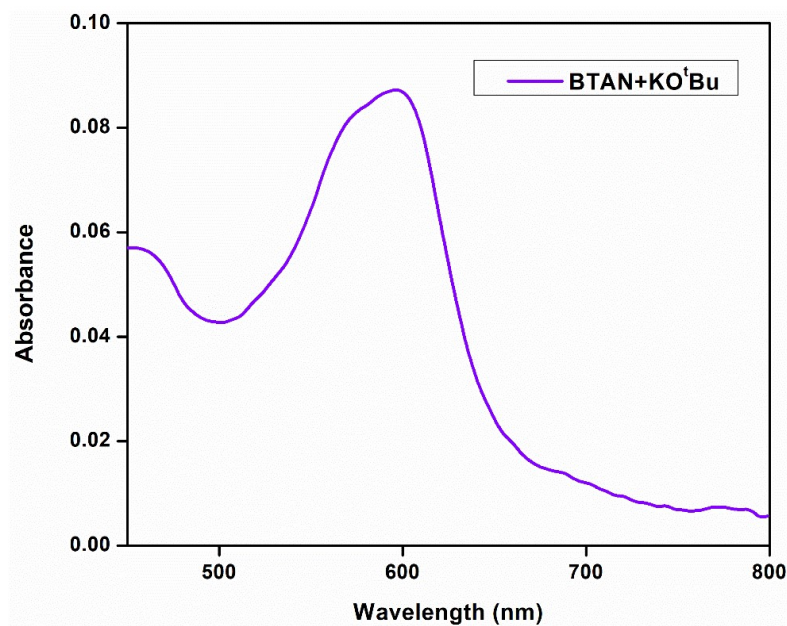


Figure S6: UV-visible spectra of **BTAN** in toluene (10^{-6} M) after adding KO^tBu .

e) Fluorescence spectra of BTAN:

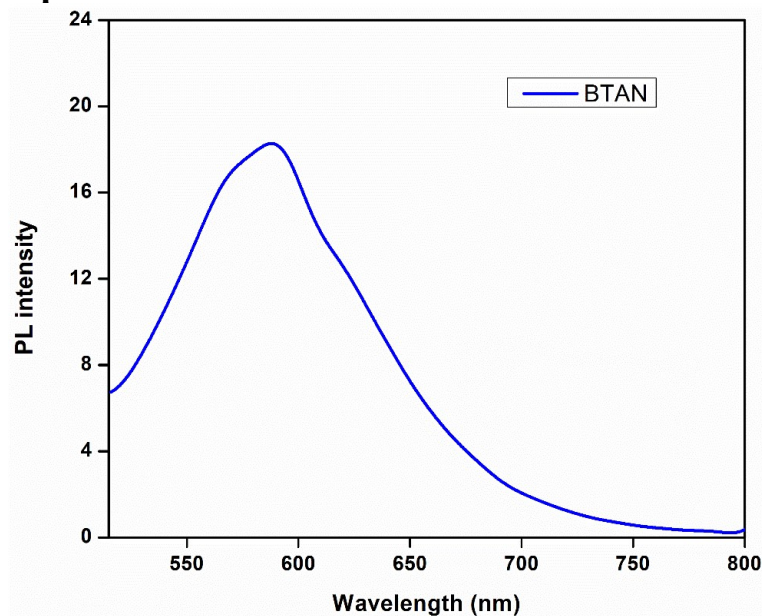


Figure S7: Fluorescence spectra of **BTAN** in toluene.

f) Fluorescence quenching experiment and Stern-Volmer plot:

In this experiment, measurements were carried out on a 10^{-4} M solution of BTAN in dry toluene with varying amount of KO^tBu in quartz cuvette. The sample solutions were previously degassed with argon. The solution was irradiated at 500 nm, and the emission intensity was examined at 590 nm. Plots were derived according to the Stern-Volmer equation and K_{SV} was calculated. Stern-Volmer equation is the following

$$I_0/I = 1 + K_{SV}[Q]$$

Where I_0 is the fluorescence intensity without the quencher, I is the intensity in the presence of the quencher, $[Q]$ is the concentration of added quencher and K_{SV} is the Stern-Volmer quenching constant.

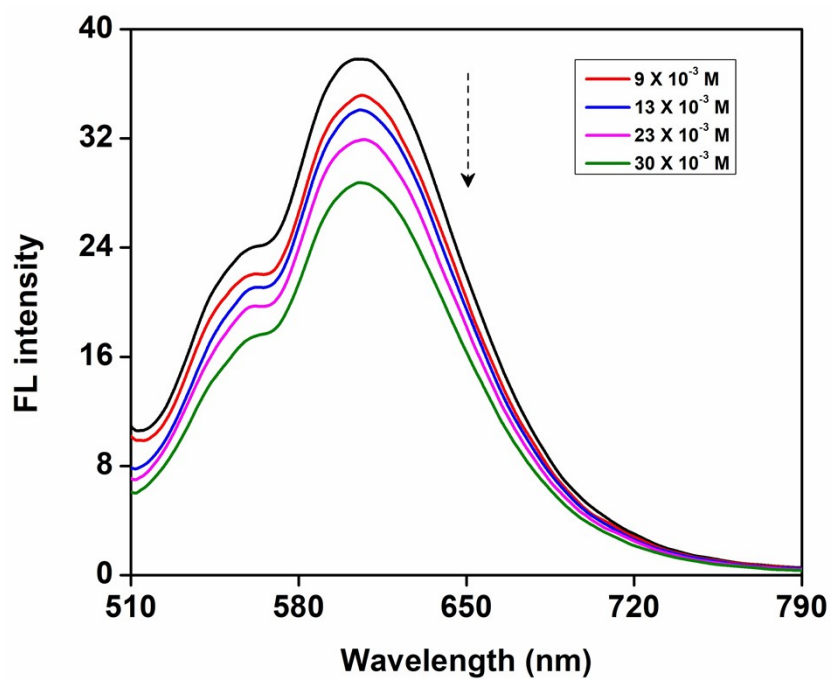


Figure S8: Emission spectra of **BTAN** in toluene with varying amounts **KO^tBu** added as quencher

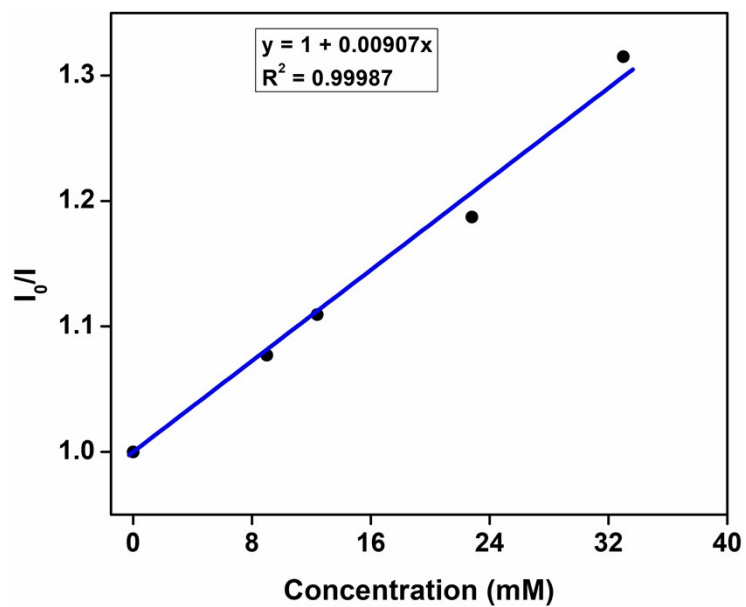


Figure S9: Stern-Volmer quenching of **BTAN** showing a linear correlation with increasing quencher (**KO^tBu**) concentration.

g) Detection of H₂O₂ during alcohol oxidation:

For oxidation of alcohols, presence of H₂O₂ in the reaction mixture was analyzed by UV–Vis spectroscopy² using the iodometric assay based on peak of I₃[−] at $\lambda_{\text{max}} = 345 \text{ nm}$; $\epsilon = 26\,000 \text{ M}^{-1} \text{ cm}^{-1}$ upon reaction with KI. In a typical reaction 5 mL vial was charged with benzyl alcohol (1 mmol), KO^tBu (1 mmol), **BTAN** (10 mol%) in 5 mL dry toluene and was closed with rubber septum. The resulting solution was purged with O₂. The reaction mixture was stirred for 6 h under white light. To the reaction mixture, 10 mL of water + 10 mL of DCM was added. The aqueous part was then separated. To the separated aqueous layer, dilute H₂SO₄ (pH = 2) added to stop further oxidation. Then, 1 mL of a 10% solution of KI and a few drops of a 3% solution of ammoniummolybdate was added. The produced H₂O₂ oxidizes I[−] to I₂, which reacts with an excess of I[−] to form I₃[−]. The chemical reactions are as follows⁶

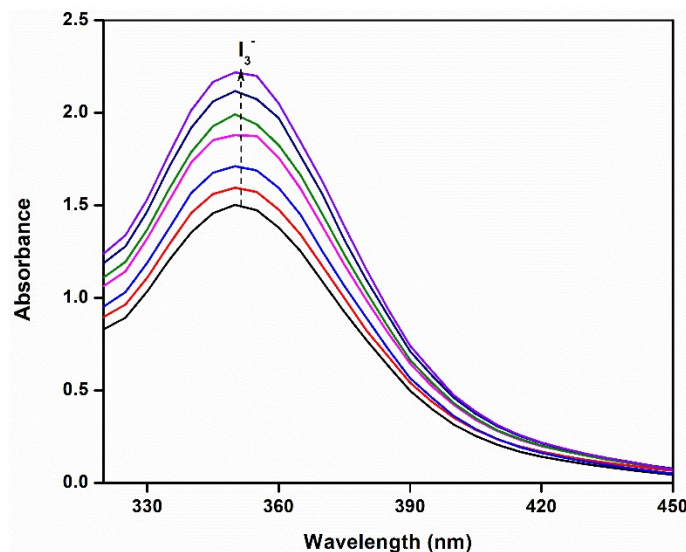
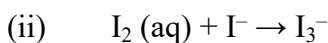
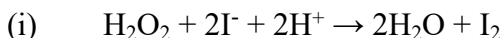


Figure S10: UV-Visible spectrum of I₃[−] ion formation in presence of H₂O₂. Absorption spectral changes during formation of I[−] in presence of H₂O₂.

h) Trapping of intermediate H₂-BTAN

In a 25 mL Schlenk flask, 0.5 mmol of BTAN was suspended in THF solution of 0.6 mmol benzyl alcohol and 0.5 mmol KO^tBu and maintained under nitrogen atmosphere through multiple times vacuum-nitrogen cycle. The solution was irradiated under white LED for 12 h. The colour of the solution became black from maroon after the reaction. The reaction mixture was worked up with ethyl acetate and brine solution and the organic part was dried in vacuo and the residue was washed with dry hexane (5 mL × 3 times). The precipitate was dried, collected and was characterized by IR spectroscopies.

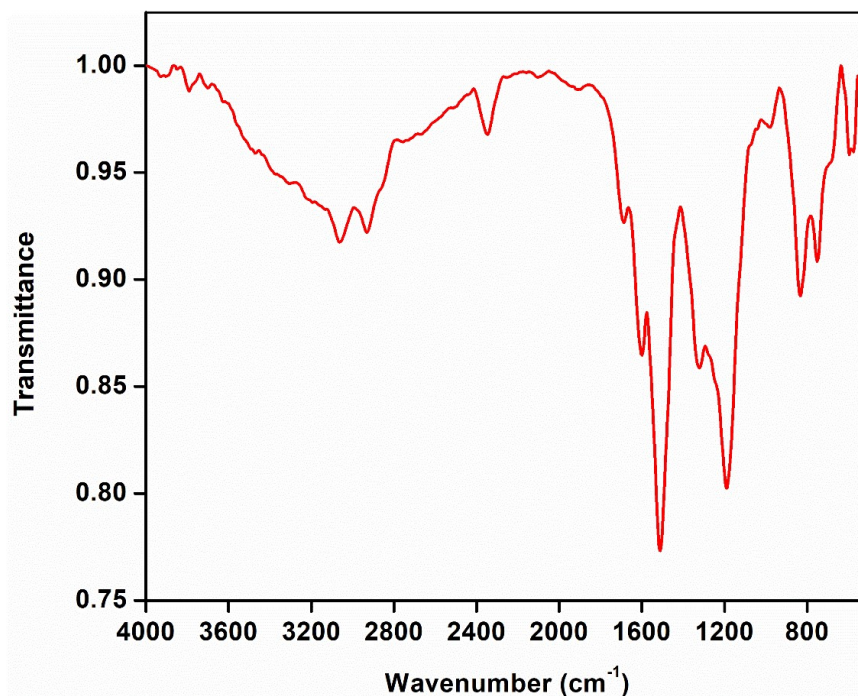
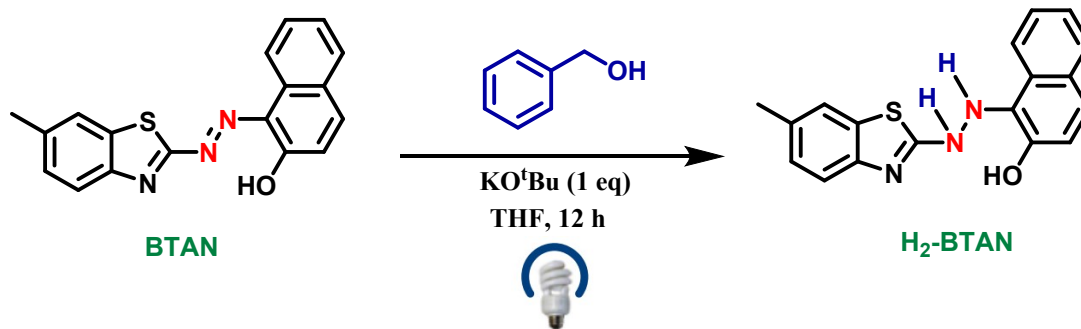


Figure S11: IR spectrum of **BTAN**.

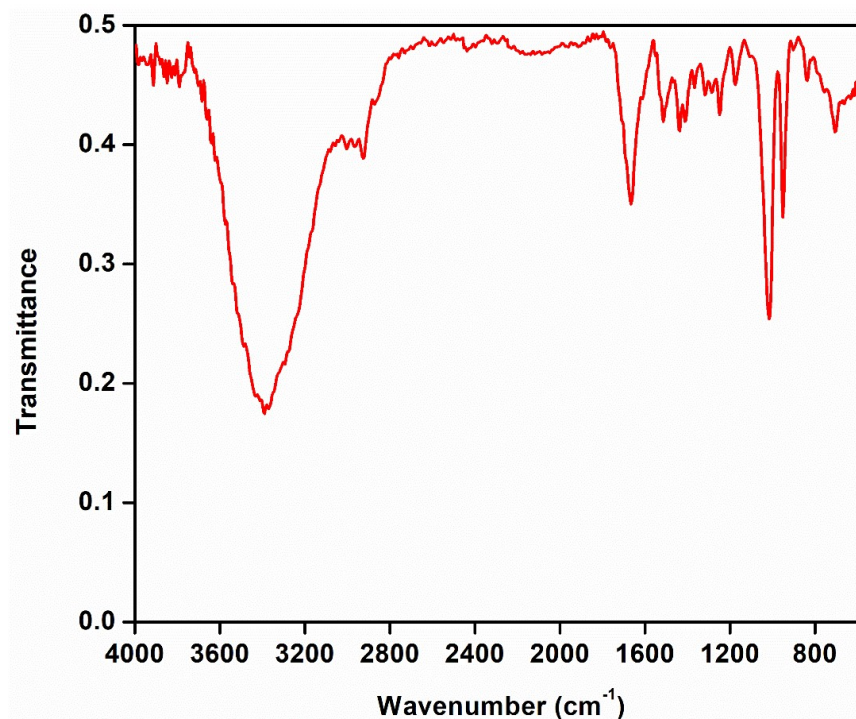
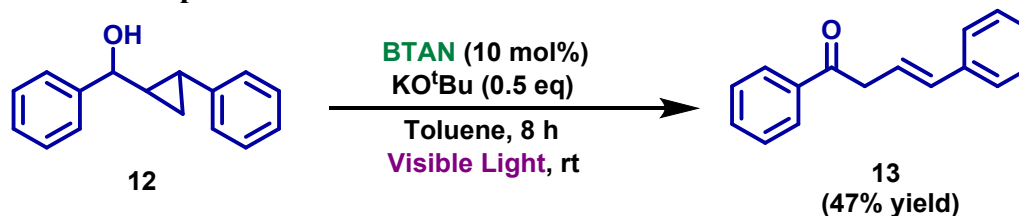
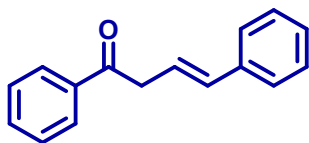


Figure S12: IR spectrum of **H₂-BTAN**.

j) **Radical clock experiment:**



In a typical reaction 10 mL vial was charged with **BTAN** (10 mol%), **KO^tBu** (0.5 mmol), phenyl-(2- phenylcyclopropyl) methanol (1 mmol) in 3 mL toluene. The reaction mixture was stirred for 8 h under white light. The ring opened product was obtained in 47% yield and was characterized by ¹H NMR spectroscopy.



(E)-1,4-diphenylbut-3-en-1-one: ^1H NMR (400 MHz, Chloroform- d) δ 8.05 (d, $J = 7.5$ Hz, 2H), 7.62 (t, $J = 7.4$ Hz, 1H), 7.52 (t, $J = 7.6$ Hz, 2H), 7.43 (d, $J = 7.4$ Hz, 2H), 7.33 (d, $J = 7.7$ Hz, 2H), 7.27 (d, $J = 8.0$ Hz, 1H), 6.64 – 6.48 (m, 2H), 3.96 (s, 2H).

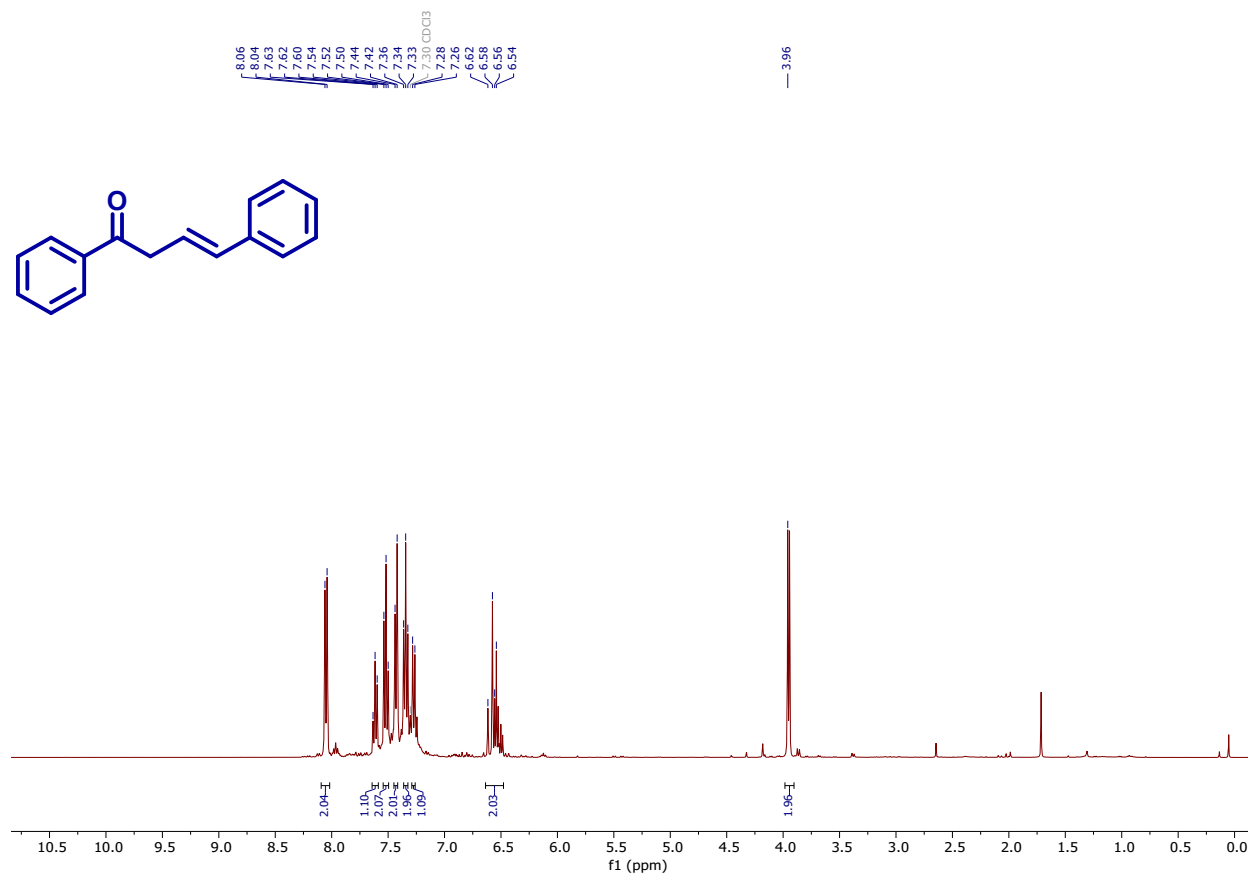


Figure S13: ^1H NMR(100 MHz) spectrum of ring opened product in CDCl_3

6. $E_{0,0}$ and excited state oxidation potential calculations for BTAN

The average of absorption maxima and corresponding emission was found to be 545 nm.

$E_{0,0}$ calculated by the following equation $E_{0,0} = 1240/\lambda$ Corresponding to the $E_{0,0}$ to be 2.275 V.

The ground state reduction potential of BTAN is -0.753 V vs Ag/AgCl. The excited state oxidation potential (E^*_{ox}) was calculated as:

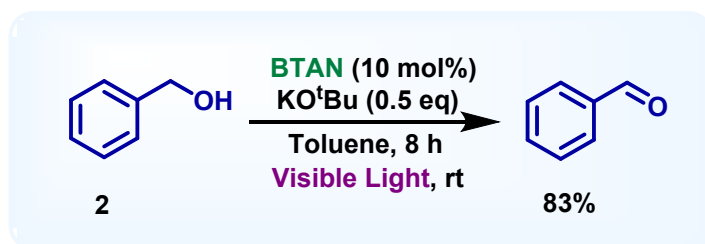
$$E^*_{red} = E_{red} + E_{0,0}$$

$$E^*_{red} = -0.753 + 2.275 = 1.52 \text{ V vs Ag/AgCl}$$

$$= 1.52 - 0.046 = 1.48 \text{ V vs SCE}$$

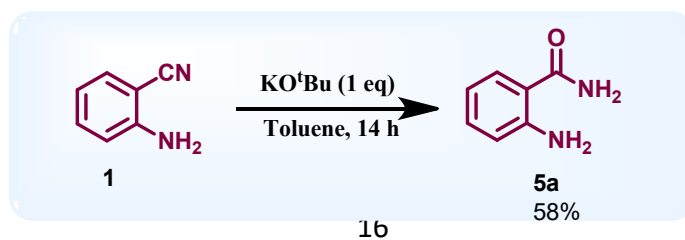
7. Mechanistic insight into the reaction:

a) Photo catalysed alcohol dehydrogenation:



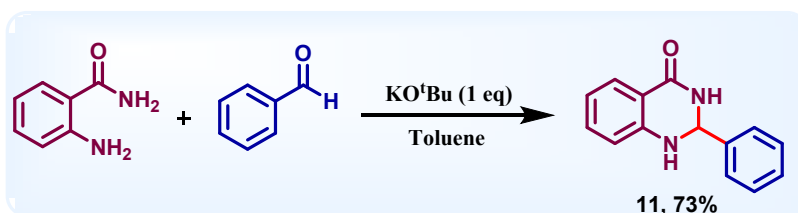
A 10 mL vial was charged with 10 mol% of **BTAN**, KO^tBu (0.5 mmol), and benzyl alcohol (0.5 mmol) in 2 mL toluene. The reaction mixture was stirred under two white light irradiation for 8 h in an open atmosphere. Upon completion of the reaction, work up was done using ethyl acetate and brine. Then the organic layer was collected and then submitted to ¹H NMR. By analysing the ¹H NMR data, it is found that 82% of benzaldehyde is forming within 8 h under photochemical condition.

b) KO^tBu mediated hydration of *O*-aminobenzonitrile (1):



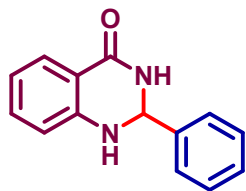
A 10 mL glass vial was charged with 0.5 mmol of 2-aminobenzonitrile and KO^tBu (0.5 mmol) in 2 mL toluene. The reaction mixture was stirred in an open atmosphere for 14 h. Upon completion, the reaction mixture was extracted with ethyl acetate and brine. Organic layers were collected, dried and evaporated *in vacuo*. Then the residue was purified by column chromatography on silica gel using hexane and ethyl acetate as eluent (3:2), giving 58% isolated yield of 2-aminobenzamide (5a).

c) Synthesis of the intermediate 2-phenyl-2,3-dihydroquinazolin-4(1H)-one:



A 10 mL vial was charged with 0.5 mmol of 2-aminobenzamide (5a) and KO^tBu (0.5 mmol) in 2 mL toluene. The reaction mixture was stirred in an open atmosphere for 12 h. Upon completion, the reaction mixture was extracted with ethyl acetate and evaporated *in vacuo*. Then the resultant residue was purified by column chromatography using silica employing ethyl acetate in hexane (3:2) as an eluent. It was found that 55% of the intermediate product **6a** was isolated which is forming by the action of base without the catalyst BTAN or light. **6a** were fully characterized by ¹H and ¹³C NMR spectroscopies

2-phenyl-2,3-dihydroquinazolin-4(1H)-one: eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature⁵.



¹H NMR (400 MHz, DMSO-*d*₆) δ 8.34 (s, 1H), 7.64 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.55 – 7.49 (m, 2H), 7.44 – 7.32 (m, 3H), 7.30 – 7.22 (m, 1H), 7.15 (s, 1H), 6.78 (dd, *J* = 8.2, 1.0 Hz, 1H), 6.69 (td, *J* = 7.5, 1.1 Hz, 1H), 5.80 – 5.75 (m, 1H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 163.70, 147.94, 141.66, 133.39, 128.53, 128.39, 127.43, 126.94, 117.19, 115.00, 114.47, 66.64.

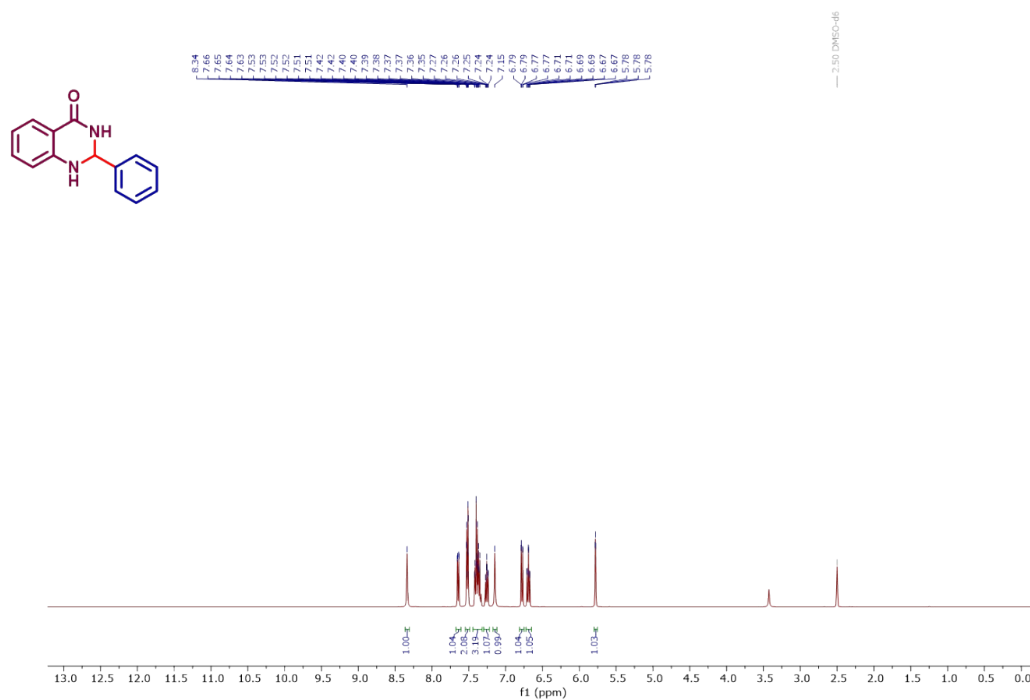


Figure S14: ¹H NMR spectrum (400 MHz) of 2-phenyl-2,3-dihydroquinazolin-4(1H)-one in DMSO-d₆

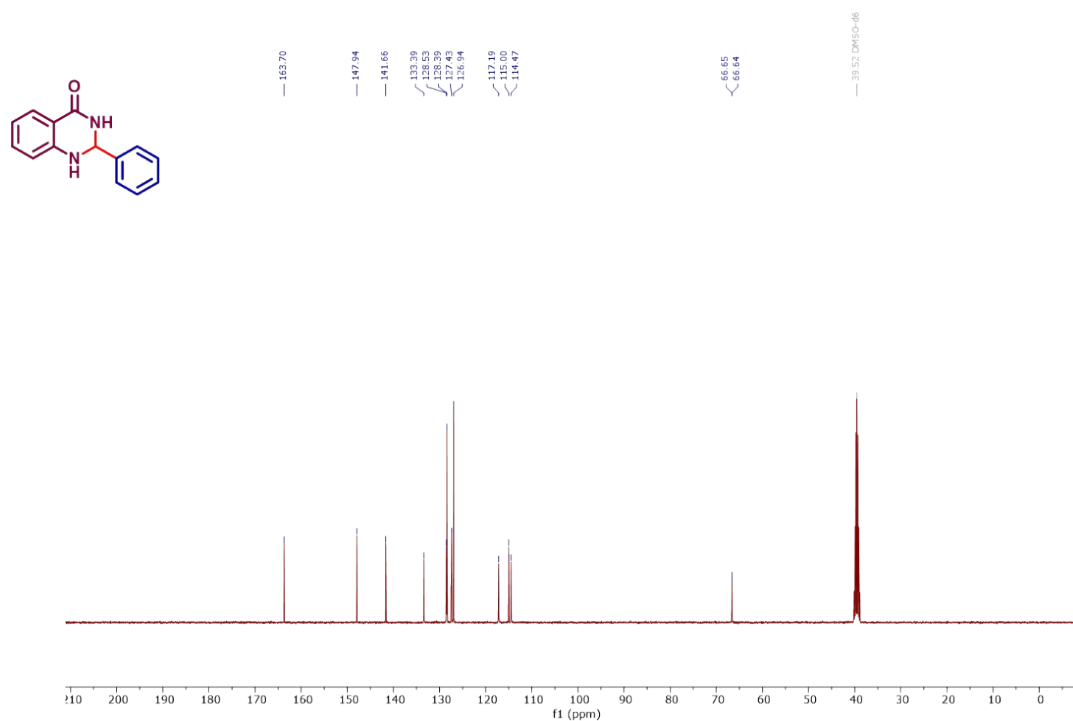
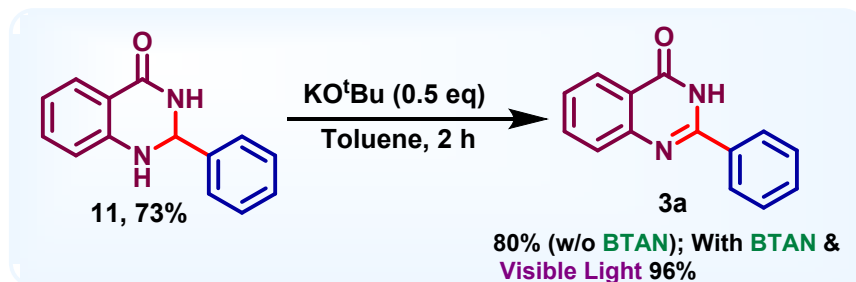


Figure S15: ^{13}C NMR spectrum (100 MHz) of 2-phenyl-2,3-dihydroquinazolin-4(1H)-one in DMSO- d_6

d) BTAN catalysed dehydrogenation of intermediate 2-phenyl-2,3-dihydroquinazolin-4(1H)-one:



A 10 mL vial tube was charged with 0.5 mmol of 2-phenyl-2,3-dihydroquinazolin-4(1H)-one (**6a**), 10 mol% of catalyst **BTAN** and KO^tBu (0.5 mmol) in 2 mL toluene. The reaction mixture was stirred under white light irradiation in an open atmosphere for 2 h. Upon completion, the reaction mixture was extracted with ethyl acetate and evaporated *in vacuo*. Then the resultant residue was purified by column chromatography using silica employing ethyl acetate in hexane (1:3) to isolate 96% yield of desired product **3a**. However, a control reaction in absence of BTAN (keeping other conditions identical) affords 80% of **3a**. This observation suggests the amination is prone to aerobic oxidation likely due to attaining aromatic character in it. The catalyst BTAN makes the conversion exclusive.

KIE measurement:

Pseudo-first-order rate constants were calculated for benzyl alcohol and deuterated-benzyl alcohol using conc. 0.05 M, 0.1 M, 0.15 M, and 0.2 M. KIE was obtained by taking the ratio $k_{\text{obs}}^{\text{H}}/k_{\text{obs}}^{\text{D}}$

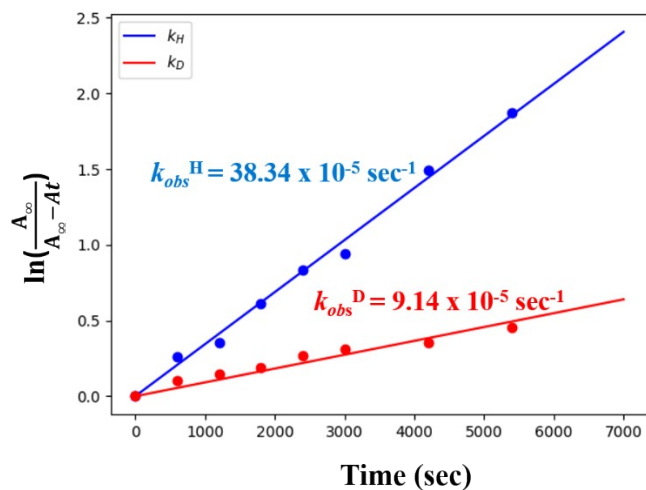


Figure S16: Product formation plot for PhCD₂OH and PhCH₂OH.

8. LUMO of BTAN Molecule:

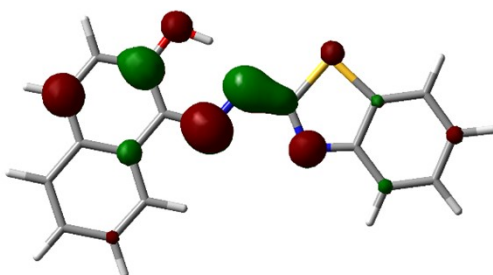
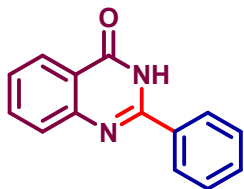


Figure S17: LUMO of the BTAN molecule. The LUMO largely resides on the azo-motif (B3LYP/6-31G* level of theory).

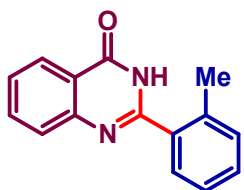
Analytical Data:

2-phenylquinazolin-4(3*H*)-one (3a): (yield: 103 mg, 93%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature².



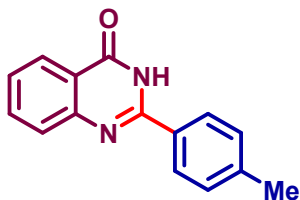
¹H NMR (400 MHz, DMSO-*d*₆): δ 12.55 (brs, 1H, NH), 8.20 - 8.15 (m, 3H), 7.82 (t, *J* = 8.0 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.60 – 7.49 (m, 4H). **¹³C{¹H} NMR** (100 MHz, DMSO-*d*₆): δ 162.3, 152.3, 148.8, 134.6, 132.7, 131.4, 128.6, 127.8, 127.5, 126.6, 125.9, 121.0 ppm.

2-(o-tolyl)quinazolin-4(3*H*)-one (3b): (yield: 96 mg, 81%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature².



¹H NMR (400 MHz, DMSO-*d*₆): δ 12.45 (brs, 1H, NH), 8.17 (d, *J* = 8.0 Hz, 1H), 7.84 (t, *J* = 8.0 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.56 – 7.49 (m, 2H), 7.43 (t, *J* = 8.0 Hz, 1H), 7.36 – 7.31 (m, 2H), 2.38 (s, 3H). **¹³C{¹H} NMR** (100 MHz, DMSO-*d*₆): δ 162.8, 154.4, 148.8, 136.1, 134.5, 134.3, 130.6, 129.9, 129.2, 127.4, 126.7, 125.8, 125.7, 121.0, 19.6 ppm.

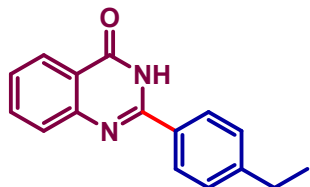
2-(p-tolyl)quinazolin-4(3*H*)-one (3c): (yield: 99 mg, 84%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature².



¹H NMR (400 MHz, DMSO-*d*₆): δ 12.44 (brs, 1H, NH), 8.11 (d, *J* = 8.0 Hz, 1H), 8.07- 8.04 (m, 2H), 7.82 (t, *J* = 8.0 Hz, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.51 (t, *J* = 8.0 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 2H), 2.37 (s, 3H). **¹³C{¹H} NMR** (100 MHz, DMSO-*d*₆): δ 162.7, 152.7, 148.8, 141.9, 135.0, 130.1, 129.5, 127.9, 126.8, 126.1, 121.0, 21.2 ppm.

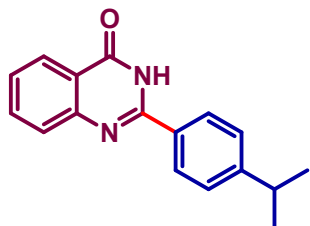
2-(4-ethylphenyl) quinazolin-4(3*H*)-one (3d): (yield: 102 mg, 82%), eluent: hexane/EtOAc.

The NMR spectroscopic data is in agreement with the literature³.



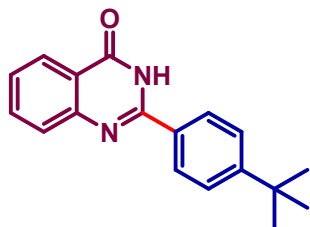
¹H NMR (400 MHz, DMSO-*d*₆): δ 12.46 (brs, 1H, NH), 8.14 (d, *J* = 8.0 Hz, 1H), 8.09 (d, *J* = 8.0 Hz, 2H), 7.83 (t, *J* = 8.0 Hz, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.51 (t, *J* = 8.0 Hz, 1H), 7.38 (d, *J* = 8.0 Hz, 2H), 2.68 (q, *J* = 8.0 Hz, 2H), 1.21 (t, *J* = 8.0 Hz, 3H). **¹³C{¹H} NMR** (100 MHz, DMSO-*d*₆): δ 162.5, 152.5, 149.0, 147.9, 134.9, 130.3, 128.3, 128.0, 127.6, 126.7, 126.1, 121.0, 28.2, 15.5 ppm.

2-(4-isopropylphenyl) quinazolin-4(3*H*)-one (3e): (yield: 103 mg, 78%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature³.



¹H NMR (400 MHz, DMSO-*d*₆): δ 12.46 (brs, 1H, NH), 8.14 (d, *J* = 8.0 Hz, 1H), 8.09 (d, *J* = 8.0 Hz, 2H), 7.82 (t, *J* = 8.0 Hz, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.50 (t, *J* = 8.0 Hz, 1H), 7.40 (d, *J* = 12.0 Hz, 2H), 2.96 (m, 1H), 1.22 (d, *J* = 4.0 Hz, 6H). **¹³C{¹H} NMR** (100 MHz, DMSO-*d*₆): δ 162.5, 152.5, 152.4, 149.0, 134.9, 130.5, 128.0, 127.6, 126.8, 126.7, 126.0, 121.0, 33.6, 23.8 ppm.

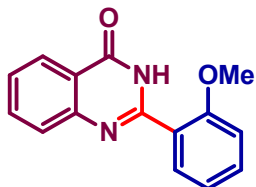
2-(4-(tert-butyl) phenyl) quinazolin-4(3*H*)-one (3f): (yield: 111 mg, 80%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature⁵.



¹H NMR (400 MHz, DMSO-*d*₆): δ 12.46 (brs, 1H, NH), 8.14 (d, *J* = 8.0 Hz, 1H), 8.10 (d, *J* = 8.0 Hz, 2H), 7.82 (t, *J* = 8.0 Hz, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.55 (d, *J* = 8.0 Hz, 2H), 7.51 (t, *J* = 8.0 Hz, 1H), 1.31 (s, 9H). **¹³C{¹H} NMR** (100 MHz, DMSO-*d*₆): δ 162.5, 154.6, 134.9, 130.1, 127.8, 126.7, 126.1, 125.7, 121.0, 34.9, 31.1 ppm.

2-(2-methoxyphenyl)quinazolin-4(3H)-one (3g): (yield: 117 mg, 93%), eluent: hexane/EtOAc.

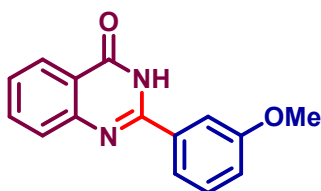
The NMR spectroscopic data is in agreement with the literature⁵.



¹H NMR (400 MHz, DMSO-*d*₆): δ 12.11 (brs, 1H, NH), 8.15 (d, *J* = 8.0 Hz, 1H), 7.83 (t, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 8.0 Hz, 2H), 7.56 – 7.51 (m, 2H), 7.19 (d, *J* = 8.0 Hz, 1H), 7.09 (t, *J* = 8.0 Hz, 1H), 3.86 (s, 3H). ¹³C{¹H} NMR (100 MHz, DMSO-*d*₆): δ 161.3, 157.2, 152.4, 149.1, 134.5, 132.2, 130.5, 127.4, 126.6, 125.8, 122.7, 121.0, 120.5, 111.9, 55.8 ppm.

2-(3-methoxyphenyl)quinazolin-4(3H)-one (3h): (yield: 94 mg, 75%), eluent: hexane/EtOAc.

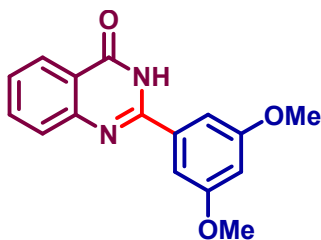
The NMR spectroscopic data is in agreement with the literature⁵.



¹H NMR (400 MHz, DMSO-*d*₆): δ 12.54 (brs, 1H, NH), 8.15 (d, *J* = 8.0 Hz, 1H), 7.84 (t, *J* = 8.0 Hz, 1H), 7.79- 7.73 (m, 3H), 7.53 (t, *J* = 8.0 Hz, 1H), 7.46 (t, *J* = 8.0 Hz, 1H), 7.15 (d, *J* = 8.0 Hz, 1H), 3.86 (s, 3H). ¹³C{¹H} NMR (100 MHz, DMSO-*d*₆): δ 162.5, 159.4, 152.2, 134.8, 134.1, 129.9, 127.6, 126.0, 121.1, 120.2, 117.7, 112.6, 55.5 ppm.

2-(3,5-dimethoxyphenyl)quinazolin-4(3H)-one (3i): (yield: 95 mg, 67%), eluent:

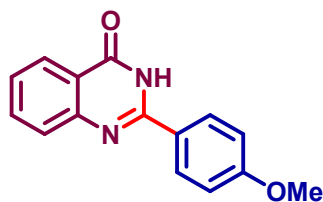
hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature³.



¹H NMR (400 MHz, DMSO-*d*₆): δ 12.45 (brs, 1H, NH), 8.13 (d, *J* = 8.0 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.84- 7.80 (m, 2H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.49 (t, *J* = 8.0 Hz, 1H), 7.12 (d, *J* = 8.0 Hz, 1H), 3.88 (s, 3H), 3.84 (s, 3H). ¹³C{¹H} NMR (100 MHz, DMSO-*d*₆): δ 162.3, 151.9, 149.0, 148.6, 134.7, 127.4, 126.3, 125.9, 124.8, 121.2, 120.9, 111.4, 110.7, 55.8 ppm.

2-(4-methoxyphenyl)quinazolin-4(3H)-one (3j): (yield: 91 mg, 72%), eluent: hexane/EtOAc.

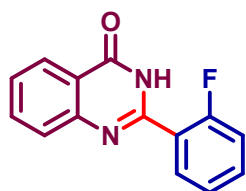
The NMR spectroscopic data is in agreement with the literature².



¹H NMR (400 MHz, DMSO-*d*₆): δ 12.54 (brs, 1H, NH), 8.15 (d, *J* = 8.0 Hz, 1H), 7.84 (t, *J* = 8.0 Hz, 1H), 7.79- 7.73 (m, 3H), 7.53 (t, *J* = 8.0 Hz, 1H), 7.46 (t, *J* = 8.0 Hz, 1H), 7.15 (d, *J* = 8.0 Hz, 1H), 3.86 (s, 3H). ¹³C{¹H} NMR (100 MHz, DMSO-*d*₆): δ 162.2, 161.8, 152.6, 149.7, 135.0, 129.8, 126.6, 126.2, 125.0, 120.9, 114.3, 55.8 ppm.

2-(2-fluorophenyl)quinazolin-4(3H)-one (3k): (yield: 103 mg, 86%), eluent: hexane/EtOAc.

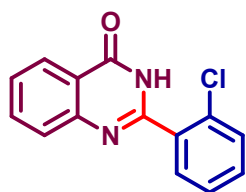
The NMR spectroscopic data is in agreement with the literature².



¹H NMR (400 MHz, DMSO-*d*₆): δ 12.59 (brs, 1H, NH), 8.17 (d, *J* = 8.0 Hz, 1H), 7.85 (t, *J* = 8.0 Hz, 1H), 7.78 (t, *J* = 8.0 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.65 - 7.54 (m, 2H), 7.41 – 7.33 (m, 2H). ¹³C{¹H} NMR (100 MHz, DMSO-*d*₆): δ 161.6, 160.9, 158.4, 150.1, 148.8, 134.8, 133.0, 132.9, 131.2, 131.1, 127.6, 127.2, 126.0, 124.8, 124.7, 122.4, 122.3, 121.2, 116.4, 116.2. ppm.

2-(2-chlorophenyl)quinazolin-4(3H)-one (3l): (yield: 102 mg, 80%), eluent: hexane/EtOAc.

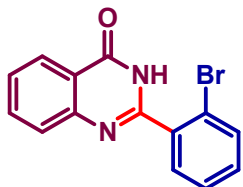
The NMR spectroscopic data is in agreement with the literature².



¹H NMR (400 MHz, DMSO-*d*₆): δ 12.65 (brs, 1H, NH), 8.18 (d, *J* = 8.0 Hz, 1H), 7.86 (t, *J* = 8.0 Hz, 1H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.62 (d, *J* = 8.0 Hz, 1H), 7.57 (t, *J* = 8.0 Hz, 2H), 7.50 (t, *J* = 8.0 Hz, 1H). ¹³C{¹H} NMR (100 MHz, DMSO-*d*₆): δ 161.5, 152.3, 148.6, 134.6, 133.8, 131.7, 131.5, 130.9, 129.6, 127.5, 127.3, 127.1, 125.9, 121.3 ppm.

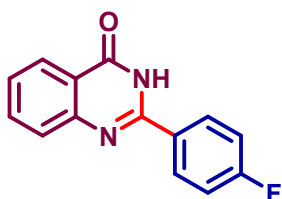
2-(2-bromophenyl)quinazolin-4(3H)-one (3m): (yield: 112 mg, 75%), eluent: hexane/EtOAc.

The NMR spectroscopic data is in agreement with the literature².



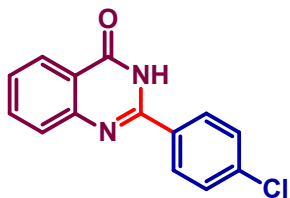
¹H NMR (400 MHz, DMSO-*d*₆): δ 12.65 (brs, 1H, NH), 8.18 (d, *J* = 8.0 Hz, 1H), 7.86 (t, *J* = 8.0 Hz, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.63 – 7.55 (m, 3H), 7.50 (t, *J* = 8.0 Hz, 1H). **¹³C{¹H} NMR** (100 MHz, DMSO-*d*₆): δ 161.4, 152.3, 148.6, 134.6, 133.8, 131.7, 131.5, 130.9, 129.6, 127.5, 127.2, 127.1, 125.9, 121.2 ppm.

2-(4-fluorophenyl)quinazolin-4(3H)-one (3n): (yield: 82 mg, 68%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature².



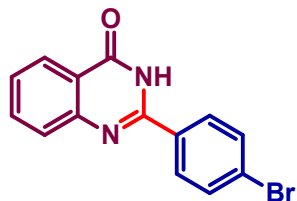
¹H NMR (400 MHz, DMSO-*d*₆): δ 12.58 (brs, 1H, NH), 8.27- 8.23 (m, 2H), 8.15 (d, *J* = 8.0 Hz, 1H), 7.84 (t, *J* = 8.0 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.52 (t, *J* = 8.0 Hz, 1H), 7.40 (t, *J* = 8.0 Hz, 2H). **¹³C{¹H} NMR** (100 MHz, DMSO-*d*₆): δ 165.3, 162.6, 162.2 (d, ¹*J*_{C-F} = 248 Hz), 151.4, 148.6, 134.7, 130.4, 130.3, 129.3, 129.2, 127.5, 126.7, 125.9, 120.9, 115.8, 115.6 ppm.

2-(4-chlorophenyl)quinazolin-4(3H)-one (3o): (yield: 83 mg, 65%), eluent: hexane. The NMR spectroscopic data is in agreement with the literature².



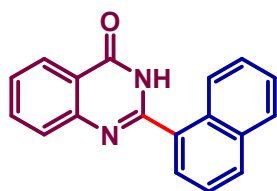
¹H NMR (400 MHz, DMSO-*d*₆): δ 12.63 (brs, 1H, NH), 8.20 (d, *J* = 8.0 Hz, 2H), 8.16 (d, *J* = 8.0 Hz, 1H), 7.85 (t, *J* = 8.0 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.63 (d, *J* = 8.0 Hz, 2H), 7.54 (t, *J* = 8.0 Hz, 1H). **¹³C{¹H} NMR** (100 MHz, DMSO-*d*₆): δ 162.2, 151.4, 148.6, 136.3, 134.7, 131.6, 129.7, 128.7, 127.6, 126.8, 125.9, 121.0 ppm.

2-(4-bromophenyl)quinazolin-4(3H)-one (3p): (yield: 91 mg, 61%), eluent: hexane. The NMR spectroscopic data is in agreement with the literature².



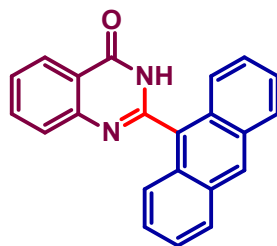
¹H NMR (400 MHz, DMSO-*d*₆): δ 12.61 (brs, 1H, NH), 8.16 (t, *J* = 8.0 Hz, 1H), 8.11 (d, *J* = 8.0 Hz, 2H), 7.85 (t, *J* = 8.0 Hz, 1H), 7.75 (t, *J* = 8.0 Hz, 3H), 7.54 (t, *J* = 8.0 Hz, 1H). **¹³C{¹H}** **NMR** (100 MHz, DMSO-*d*₆): δ 162.4, 151.6, 148.7, 136.5, 134.9, 131.7, 129.8, 128.9, 127.7, 127.0, 126.0, 121.1 ppm.

2-(naphthalen-1-yl)quinazolin-4(3H)-one (3q): (yield: 95 mg, 70%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature³.



¹H NMR (400 MHz, DMSO-*d*₆): δ 12.68 (brs, 1H, NH), 8.21 (d, *J* = 8.0 Hz, 1H), 8.13 (t, *J* = 8.0 Hz, 2H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.87 (t, *J* = 8.0 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.66- 7.56 (m, 4H). **¹³C{¹H}** **NMR** (100 MHz, DMSO-*d*₆): δ 162.0, 153.7, 148.7, 134.6, 133.2, 131.8, 130.4, 130.3, 128.4, 127.7, 127.5, 127.1, 126.9, 126.4, 125.9, 125.3, 125.1, 121.3 ppm.

2-(anthracen-9-yl)quinazolin-4(3H)-one (3r): (yield: 118 mg, 73%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature².

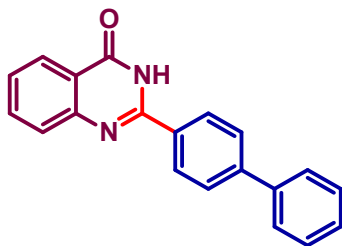


¹H NMR (400 MHz, DMSO-*d*₆): δ 12.86 (brs, 1H, NH), 8.83 (s, 1H), 8.32 (d, *J* = 8.0 Hz, 1H), 8.21 (d, *J* = 8.0 Hz, 2H), 7.91 (t, *J* = 8.0 Hz, 1H), 7.81 (d, *J* = 8.0 Hz, 2H), 7.77 (d, *J* = 8.0 Hz,

1H), 7.65 (t, J = 8.0 Hz, 1H), 7.61- 7.52 (m, 4H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6): δ 161.8, 153.1, 148.9, 134.6, 130.6, 129.1, 128.8, 128.6, 127.6, 127.1, 126.1, 125.7, 125.1, 121.7 ppm.

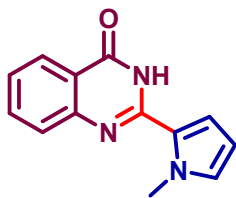
2-([1,1'-biphenyl]-4-yl)quinazolin-4(3H)-one (3s): (yield: 98 mg, 66%), eluent: hexane/EtOAc.

The NMR spectroscopic data is in agreement with the literature².



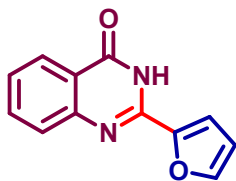
^1H NMR (400 MHz, DMSO- d_6): δ 12.60 (brs, 1H, NH), 8.30 (d, J = 8.0 Hz, 2H), 8.17 (d, J = 8.0 Hz, 1H), 7.87 (d, J = 8.0 Hz, 3H), 7.77 (t, J = 8.0 Hz, 3H), 7.55- 7.50 (m, 3H). 7.44 (d, J = 8.0 Hz, 1H), $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6): δ 162.4, 142.9, 139.0, 134.8, 131.6, 129.2, 128.5, 128.3, 126.9, 126.8, 126.7, 126.0 ppm.

2-(1-methyl-1H-pyrrol-2-yl)quinazolin-4(3H)-one (3t): (yield: 89 mg, 79%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature³.



^1H NMR (400 MHz, DMSO- d_6): δ 12.06 (brs, 1H, NH), 8.09 (d, J = 8.0 Hz, 1H), 7.77 (t, J = 8.0 Hz, 1H), 7.62 (d, J = 8.0 Hz, 1H), 7.43 (t, J = 8.0 Hz, 1H), 7.22 (d, J = 4.0 Hz, 1H), 7.10 (s, 1H), 6.16- 6.14 (m, 1H), 4.07 (s, 3H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6): δ 162.0, 148.8, 146.8, 134.5, 130.2, 127.1, 125.8, 125.7, 124.0, 120.4, 114.9, 107.7, 37.6 ppm.

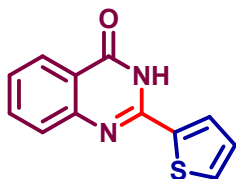
2-(furan-2-yl)quinazolin-4(3H)-one (3u): (yield: 86 mg, 81%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature⁵.



^1H NMR (400 MHz, DMSO- d_6): δ 12.52 (brs, 1H, NH), 8.12 (d, J = 8.0 Hz, 2H), 8.01 (s, 1H), 7.82 (t, J = 8.0 Hz, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.63 (d, J = 4.0 Hz, 1H), 7.50 (t, J = 8.0 Hz,

1H), 6.76- 6.75 (m, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6): δ 161.6, 148.7, 146.7, 146.1, 144.0, 134.7, 127.3, 126.5, 126.0, 121.2, 114.5, 112.6 ppm.

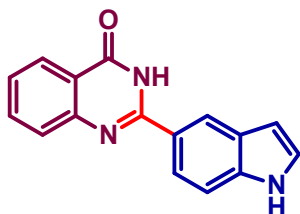
2-(thiophen-2-yl)quinazolin-4(3H)-one (3v): (yield: 78 mg, 68%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature⁴.



^1H NMR (400 MHz, DMSO- d_6): δ 12.44 (brs, 1H, NH), 8.53 (s, 1H), 8.12 (d, J = 8.0 Hz, 1H), 7.85- 7.80 (m, 2H), 7.69 (d, J = 8.0 Hz, 2H), 7.50 (t, J = 8.0 Hz, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6): δ 162.1, 148.9, 148.3, 135.4, 134.7, 128.7, 127.4, 127.3, 127.1, 126.4, 125.9, 121.0 ppm.

2-(1H-indol-5-yl)quinazolin-4(3H)-one (3w): (yield: 103 mg, 79%), eluent: hexane/EtOAc.

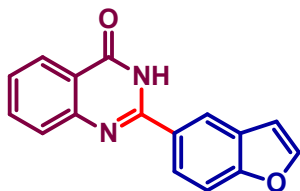
The NMR spectroscopic data is in agreement with the literature³.



^1H NMR (400 MHz, DMSO- d_6): δ 11.64 (brs, 1H, NH), 8.41 (s, 1H), 8.19 (t, J = 8.0 Hz, 1H), 7.93 (d, J = 8.0 Hz, 1H), 7.83 (t, J = 8.0 Hz, 2H), 7.69 – 7.60 (m, 3H), 7.57 (s, 1H), 6.68 (s, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6): δ 161.1, 159.8, 156.7, 138.5, 135.6, 130.0, 127.4, 126.4, 122.3, 121.5, 119.7, 112.0, 102.8 ppm.

2-(benzofuran-5-yl)quinazolin-4(3H)-one (3x): (yield: 106 mg, 81%), eluent: hexane/EtOAc.

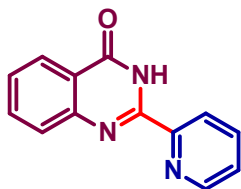
The NMR spectroscopic data is in agreement with the literature³.



^1H NMR (400 MHz, DMSO- d_6): δ 12.70 (brs, 1H, NH), 10.11 (s, 1H), 8.37 (d, J = 8.0 Hz, 2H), 8.17 (d, J = 8.0 Hz, 1H), 8.06 (d, J = 8.0 Hz, 2H), 7.87 (t, J = 8.0 Hz, 1H), 7.78 (d, J = 8.0 Hz,

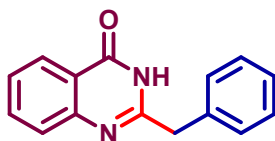
1H), 7.56 (t, J = 8.0 Hz, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6): δ 192.9, 162.2, 151.5, 148.5, 137.8, 134.8, 129.6, 128.6, 127.2, 126.0, 121.2 ppm.

2-(pyridin-2-yl)quinazolin-4(3H)-one (3y): (yield: 80 mg, 72%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature².



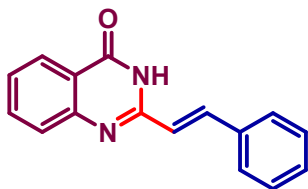
^1H NMR (400 MHz, DMSO- d_6): δ 11.86 (brs, 1H, NH), 8.77 (d, J = 4.0 Hz, 1H), 8.46 (d, J = 8.0 Hz, 1H), 8.19 (d, J = 8.0 Hz, 1H), 8.08 (t, J = 8.0 Hz, 1H), 7.88 (t, J = 8.0 Hz, 1H), 7.81 (d, J = 8.0 Hz, 1H), 7.68 – 7.65 (m, 1H), 7.58 (t, J = 8.0 Hz, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6): δ 160.8, 150.0, 149.0, 148.8, 148.5, 138.1, 134.8, 127.8, 127.4, 126.6, 126.2, 122.2, 122.1 ppm.

2-benzylquinazolin-4(3H)-one (3z): (yield: 92 mg, 78%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature⁵.



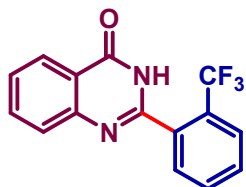
^1H NMR (400 MHz, DMSO- d_6): δ 12.42 (brs, 1H, NH), 8.07 (d, J = 8.0 Hz, 1H), 7.77 (t, J = 8.0 Hz, 1H), 7.60 (d, J = 8.0 Hz, 1H), 7.46 (t, J = 8.0 Hz, 1H), 7.38 (d, J = 8.0 Hz, 2H), 7.32 (t, J = 8.0 Hz, 2H), 7.23 (t, J = 8.0 Hz, 1H), 3.93 (s, 2H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6): δ 162.0, 156.1, 149.0, 136.6, 134.6, 129.0, 128.6, 127.0, 126.9, 126.4, 125.8, 120.8, 48.9 ppm.

(E)-2-styrylquinazolin-4(3H)-one (3za): (yield: 105 mg, 85%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature⁵.



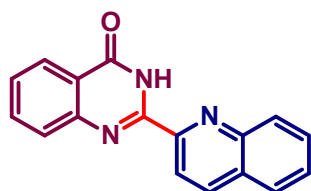
^1H NMR (400 MHz, DMSO- d_6): δ 12.34 (brs, 1H, NH), 8.10 (d, J = 8.0 Hz, 1H), 7.94 (t, J = 16.0 Hz, 1H), 8.00 (t, J = 8.0 Hz, 1H), 7.67 (t, J = 6.0 Hz, 3H), 7.49 - 7.39 (m, 4H), 7.00 (d, J = 16.0 Hz, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6): δ 161.9, 151.5, 149.1, 138.4, 135.1, 134.7, 129.9, 129.2, 127.8, 127.2, 126.4, 126.0, 121.2, 121.1 ppm.

2-(2-(trifluoromethyl)phenyl)quinazolin-4(3H)-one (3zb): (yield: 102 mg, 70%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature³.



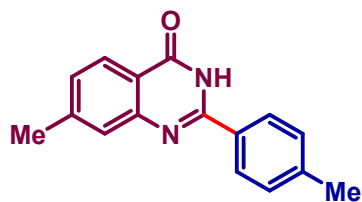
¹H NMR (400 MHz, DMSO-*d*₆): δ 12.70 (brs, 1H, NH), 8.18 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.87- 7.74 (m, 4H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.58 (t, *J* = 8.0 Hz, 1H). ¹³C{¹H} NMR (100 MHz, DMSO-*d*₆): δ 161.6, 152.6, 148.5, 134.9, 133.1, 132.6, 130.8, 130.7, 127.6, 127.4 (q, ²*J*_{C-F} = 31 Hz), 126.6 (q, ³*J*_{C-F} = 4.0 Hz), 126.0, 125.3, 122.6 (q, ¹*J*_{C-F} = 272.1 Hz), 121.3 ppm.

2-(quinolin-2-yl)quinazolin-4(3H)-one (3zc): (yield: 111 mg, 81%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature⁵.



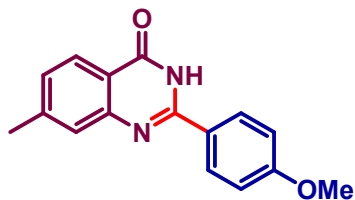
¹H NMR (400 MHz, CDCl₃) δ 11.22 (brs, 1H, NH), 8.62 (d, *J* = 8.6 Hz, 1H), 8.37 – 8.31 (m, 2H), 8.13 (d, *J* = 8.5 Hz, 1H), 7.89 – 7.84 (m, 2H), 7.82 – 7.76 (m, 2H), 7.62 (t, *J* = 7.5 Hz, 1H), 7.55 – 7.50 (m, 1H). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 161.6, 149.2, 149.0, 148.1, 146.9, 137.7, 134.7, 130.6, 129.4, 128.3, 127.7, 122.7, 118.5 ppm.

7-methyl-2-(p-tolyl) quinazolin-4(3H)-one (6a): (yield: 91 mg, 73%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature³.



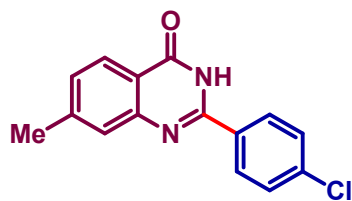
¹H NMR (400 MHz, DMSO-*d*₆): δ 12.36 (brs, 1H, NH), 8.06 (d, *J* = 8.0 Hz, 2H), 8.02 (d, *J* = 8.6 Hz, 1H), 7.53 (s, 1H), 7.34 (t, *J* = 8.5 Hz, 3H), 2.46 (s, 3H), 2.38 (s, 3H). ¹³C{¹H} NMR (100 MHz, DMSO-*d*₆): δ 162.3, 152.1, 149.0, 145.2, 141.6, 130.1, 129.3, 128.0, 127.8, 126.9, 125.8, 118.5, 21.5, 21.1 ppm.

2-(4-methoxyphenyl)-7-methylquinazolin-4(3H)-one (6b): (yield: 108 mg, 81%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature³.



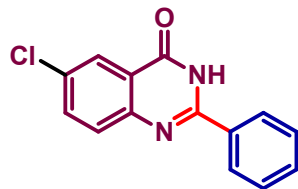
¹H NMR (400 MHz, DMSO-*d*₆): δ 12.31 (brs, 1H, NH), 8.16 (d, *J* = 8.5 Hz, 2H), 8.00 (d, *J* = 8.6 Hz, 1H), 7.51 (s, 1H), 7.30 (d, *J* = 8.3 Hz, 1H), 7.08 (d, *J* = 8.0 Hz, 2H), 3.84 (s, 3H), 2.45 (s, 3H). **¹³C{¹H} NMR** (100 MHz, DMSO-*d*₆): δ 161.9, 151.9, 149.3, 145.1, 129.5, 127.7, 127.0, 125.8, 124.9, 118.3, 114.0, 55.6, 21.4 ppm.

2-(4-chlorophenyl)-7-methylquinazolin-4(3H)-one (6c): (yield: 113 mg, 84%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature³.



¹H NMR (400 MHz, DMSO-*d*₆): δ 12.44 (brs, 1H, NH), 8.13 (d, *J* = 8.0 Hz, 2H), 8.03 (d, *J* = 8.0 Hz, 1H), 7.60- 7.52 (m, 3H), 7.35 (d, *J* = 8.0 Hz, 1H), 2.46 (s, 3H). **¹³C{¹H} NMR** (100 MHz, DMSO-*d*₆): δ 162.5, 152.5, 149.1, 145.5, 133.0, 131.7, 128.9, 128.4, 127.9, 127.4, 126.0, 118.7, 21.6 ppm.

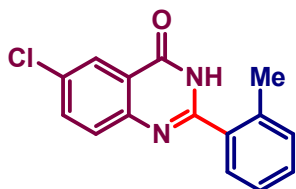
6-chloro-2-phenylquinazolin-4(3H)-one (7a): (yield: 113 mg, 88%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature⁵.



¹H NMR (400 MHz, DMSO-*d*₆): δ 12.73 (brs, 1H, NH), 8.17 (d, *J* = 8.0 Hz, 2H), 8.09 (d, *J* = 4.0 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.61 – 7.55 (m, 3H). **¹³C{¹H} NMR** (100 MHz, DMSO-*d*₆): δ 161.6, 151.6, 147.5, 134.8, 133.5, 131.7, 130.8, 129.8, 128.7, 127.9, 124.9, 122.3, 120.5 ppm.

6-chloro-2-(o-tolyl)quinazolin-4(3H)-one (7b): (yield: 93 mg, 69%), eluent: hexane/EtOAc.

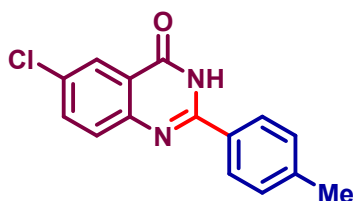
The NMR spectroscopic data is in agreement with the literature³.



¹H NMR (400 MHz, DMSO-*d*₆): δ 12.84 (brs, 1H, NH), 8.11 (s, 1H), 7.89- 7.86 (m, 1H), 7.74 (d, *J* = 12.0 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.62 (d, *J* = 8.0 Hz, 1H), 7.57 (t, *J* = 8.0 Hz, 1H), 7.50 (t, *J* = 8.0 Hz, 1H). **¹³C{¹H} NMR** (100 MHz, DMSO-*d*₆): δ 161.0, 155.0, 136.3, 134.7, 134.0, 131.0, 130.7, 130.2, 129.7, 129.3, 125.8, 124.9, 122.3, 19.7 ppm.

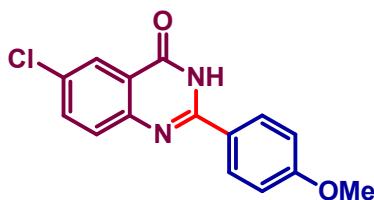
6-chloro-2-(p-tolyl)quinazolin-4(3H)-one (7c): (yield: 105 mg, 78%), eluent: hexane/EtOAc.

The NMR spectroscopic data is in agreement with the literature³.



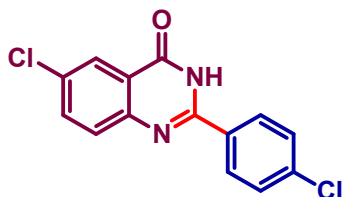
¹H NMR (400 MHz, DMSO-*d*₆): δ 12.62 (brs, 1H, NH), 8.09 (d, *J* = 8.0 Hz, 1H), 7.88- 7.85 (m, 1H), 7.72 (d, *J* = 12.0 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.44 (t, *J* = 8.0 Hz, 1H), 7.36- 7.31 (m, 2H), 2.37 (s, 3H). **¹³C{¹H} NMR** (100 MHz, DMSO-*d*₆): δ 161.0, 155.0, 136.3, 134.7, 134.0, 131.0, 130.7, 130.2, 129.7, 129.3, 125.8, 124.9, 122.3, 19.7 ppm.

6-chloro-2-(4-methoxyphenyl)quinazolin-4(3H)-one (7d): (yield: 100 mg, 70%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature³



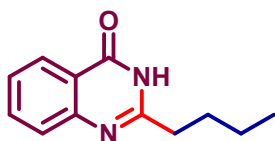
¹H NMR (400 MHz, DMSO-*d*₆): δ 12.59 (brs, 1H, NH), 8.18 (d, *J* = 8.0 Hz, 2H), 8.06 (s, 1H), 7.85- 7.82 (m, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.09 (d, *J* = 8.0 Hz, 2H), 3.85 (s, 3H). **¹³C{¹H} NMR** (100 MHz, DMSO-*d*₆): δ 162.1, 161.4, 152.4, 147.7, 134.7, 130.3, 129.6, 124.9, 124.5, 121.9, 114.1, 55.5 ppm.

6-chloro-2-(4-chlorophenyl)quinazolin-4(3H)-one (7e): (yield: 93 mg, 64%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature³



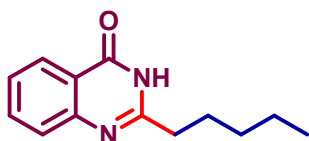
¹H NMR (400 MHz, DMSO-*d*₆): δ 12.84 (brs, 1H, NH), 8.12 (d, *J* = 4.0 Hz, 1H), 7.91- 7.88 (m, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.69- 7.66 (m, 1H), 7.64- 7.61 (m, 1H), 7.60- 7.56 (m, 1H), 7.52- 7.48 (m, 1H). **¹³C{¹H} NMR** (100 MHz, DMSO-*d*₆): δ 160.5, 152.8, 147.3, 134.8, 133.6, 131.8, 131.4, 130.9, 129.8, 129.7, 127.3, 124.9 ppm.

2-butylquinazolin-4(3H)-one (9a): (yield: 83 mg, 82%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature⁵.



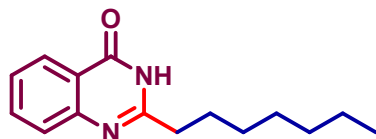
¹H NMR (400 MHz, DMSO-*d*₆): δ 12.17 (brs, 1H, NH), 8.07 (d, *J* = 8.0 Hz, 1H), 7.76 (t, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.44 (t, *J* = 8.0 Hz, 1H), 2.59 (t, *J* = 8.0 Hz, 2H), 1.73- 1.66 (m, 2H), 1.38- 1.29 (m, 2H), 0.89 (t, *J* = 8.0 Hz, 3H). **¹³C{¹H} NMR** (100 MHz, DMSO-*d*₆): δ 161.9, 157.5, 149.0, 134.3, 126.8, 125.9, 125.7, 120.8, 34.2, 28.9, 21.7, 13.7 ppm.

2-pentylquinazolin-4(3H)-one (9b): (yield: 84 mg, 78%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature⁵.



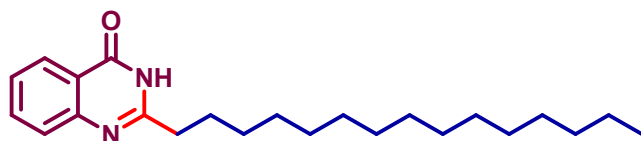
¹H NMR (400 MHz, DMSO-*d*₆): δ 12.18 (brs, 1H, NH), 8.06 (d, *J* = 8.0 Hz, 1H), 7.76 (t, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.45 (t, *J* = 8.0 Hz, 1H), 2.57 (t, *J* = 8.0 Hz, 2H), 1.72- 1.65 (m, 2H), 1.30- 1.25 (m, 4H), 0.83 (t, *J* = 8.0 Hz, 3H). **¹³C{¹H} NMR** (100 MHz, DMSO-*d*₆): δ 162.4, 158.2, 149.2, 135.0, 127.1, 126.6, 126.1, 121.0, 34.9, 31.1, 27.0, 22.2, 14.2 ppm.

2-heptylquinazolin-4(3H)-one (9c): (yield: 98 mg, 80%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature⁴.



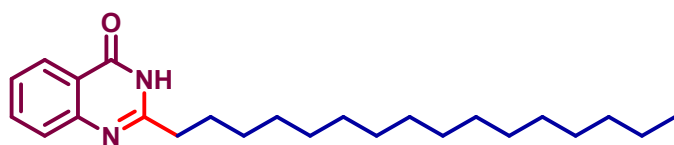
¹H NMR (400 MHz, DMSO-*d*₆): δ 12.17 (brs, 1H, NH), 8.07 (d, *J* = 8.0 Hz, 1H), 7.76 (t, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.45 (t, *J* = 8.0 Hz, 1H), 2.58 (t, *J* = 8.0 Hz, 2H), 1.73- 1.66 (m, 2H), 1.31- 1.21 (m, 8H), 0.83 (t, *J* = 8.0 Hz, 3H). **¹³C{¹H} NMR** (100 MHz, DMSO-*d*₆): δ 162.1, 157.5, 149.1, 134.6, 126.9, 126.2, 125.9, 120.9, 34.7, 31.3, 28.6, 28.5, 27.0, 22.2, 14.1 ppm.

2-pentadecylquinazolin-4(3H)-one (9d): (yield: 155 mg, 87%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature³.



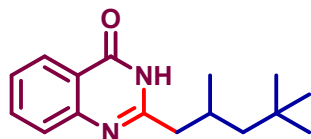
¹H NMR (400 MHz, CDCl₃): δ 11.31 (brs, 1H, NH), 8.28 (d, *J* = 8.0 Hz, 1H), 7.77 (t, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.46 (t, *J* = 8.0 Hz, 1H), 2.77 (t, *J* = 8.0 Hz, 2H), 1.91- 1.83 (m, 2H), 1.49- 1.42 (m, 2H), 1.38- 1.24 (m, 22H), 0.87 (t, *J* = 8.0 Hz, 3H). **¹³C{¹H} NMR** (100 MHz, CDCl₃): δ 164.0, 156.9, 149.6, 134.9, 127.4, 126.5, 126.4, 120.7, 36.2, 32.1, 29.9, 28.8, 29.6, 29.5, 29.4, 29.3, 27.7, 22.8, 14.3. ppm.

2-hexadecylquinazolin-4(3H)-one (9e): (yield: 167 mg, 90%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature³.



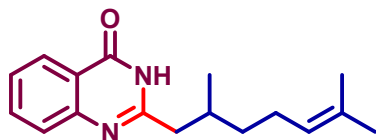
¹H NMR (400 MHz, CDCl₃): δ 11.7 (brs, 1H, NH), 8.29 (d, *J* = 8.0 Hz, 1H), 7.77 (t, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.46 (t, *J* = 6.0 Hz, 1H), 2.79 (t, *J* = 8.0 Hz, 2H), 1.92- 1.84 (m, 2H), 1.49- 1.42 (m, 2H), 1.38- 1.23 (m, 26H), 0.87 (t, *J* = 8.0 Hz, 3H). **¹³C{¹H} NMR** (100 MHz, CDCl₃): δ 164.3, 157.1, 149.6, 134.9, 127.4, 126.5, 126.4, 120.7, 36.2, 32.1, 29.9, 29.8, 28.8, 29.6, 29.5, 29.4, 29.4, 27.7, 22.8, 14.3. ppm.

2-(2,4,4-trimethylpentyl)quinazolin-4(3H)-one (9f): (yield: 111 mg, 86%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature³.



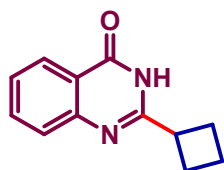
¹H NMR (400 MHz, DMSO-*d*₆): δ 12.22 (brs, 1H, NH), 8.06 (d, *J* = 8.0 Hz, 1H), 7.76 (t, *J* = 8.0 Hz, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.44 (t, *J* = 8.0 Hz, 1H), 2.53 – 2.48 (m, 1H), 2.41 (dd, *J* = 13.5, 7.6 Hz, 1H), 2.13 – 2.04 (m, 1H), 1.29 (dd, *J* = 14, 3.2 Hz, 1H), 1.06 (dd, *J* = 13.9, 6.8 Hz, 1H), 0.91 (d, *J* = 8.0 Hz, 3H), 0.78 (s, 1H). **¹³C{¹H} NMR** (100 MHz, DMSO-*d*₆): δ 162.4, 157.2, 149.0, 134.9, 127.1, 126.5, 126.1, 120.9, 50.0, 44.1, 31.1, 30.1, 28.8, 22.9 ppm.

2-(2,6-dimethylhept-5-en-1-yl)quinazolin-4(3H)-one (9g): (yield: 104 mg, 77%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature.



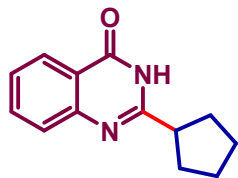
¹H NMR (400 MHz, DMSO-*d*₆) δ 7.87 (s, 1H), 7.57 (d, *J* = 9.3 Hz, 1H), 7.22 (t, *J* = 8.5 Hz, 1H), 6.75 (d, *J* = 9.2 Hz, 1H), 6.65 (t, *J* = 8.0 Hz, 1H), 6.56 (s, 1H), 5.07 (p, *J* = 5.8, 5.2 Hz, 1H), 4.75 – 4.66 (m, 1H), 1.92 (dq, *J* = 15.1, 7.2 Hz, 2H), 1.63 (s, 3H), 1.52 (s, 3H), 1.36 – 1.12 (m, 3H), 0.88 (d, *J* = 6.3 Hz, 3H). **¹³C NMR** (101 MHz, DMSO) δ 163.80, 148.19, 133.04, 130.52, 127.34, 124.53, 116.91, 115.19, 114.57, 62.55, 42.47, 37.07, 27.18, 25.53, 24.80, 19.39, 17.51.

2-cyclobutylquinazolin-4(3H)-one (9h): (yield: 85 mg, 85%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature³.



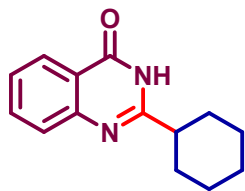
¹H NMR (400 MHz, DMSO-*d*₆): δ 12.05 (brs, 1H, NH), 8.07 (d, *J* = 8.0 Hz, 1H), 7.76 (t, *J* = 8.0 Hz, 1H), 7.63 (d, *J* = 8.0 Hz, 1H), 7.44 (t, *J* = 8.0 Hz, 1H), 3.50 (t, *J* = 8.6 Hz, 1H), 2.44- 2.34 (m, 2H), 2.27- 2.19 (m, 2H), 2.03- 1.91 (m, 1H), 1.86- 1.78 (m, 1H). **¹³C{¹H} NMR** (100 MHz, DMSO-*d*₆): δ 162.0, 159.2, 149.0, 134.4, 127.0, 126.1, 125.8, 121.0, 38.1, 25.9, 17.6 ppm.

2-cyclopentylquinazolin-4(3H)-one (9i): (yield: 85 mg, 79%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature³.



¹H NMR (400 MHz, DMSO-*d*₆): δ 12.12 (brs, 1H, NH), 8.06 (d, *J* = 8.0 Hz, 1H), 7.76 (t, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.45 (t, *J* = 8.0 Hz, 1H), 3.05- 2.97 (m, 1H), 2.01- 1.93 (m, 2H), 1.89- 1.81 (m, 2H), 1.77- 1.67 (m, 2H), 1.63- 1.56 (m, 2H). **¹³C{¹H} NMR** (100 MHz, DMSO-*d*₆): δ 162.4, 160.8, 149.1, 134.8, 127.2, 126.4, 126.1, 121.1, 44.2, 31.2, 25.7 ppm.

2-cyclopentylquinazolin-4(3*H*)-one (9j): (yield: 86 mg, 75%), eluent: hexane/EtOAc. The NMR spectroscopic data is in agreement with the literature⁴.



¹H NMR (400 MHz, DMSO-*d*₆): δ 12.12 (brs, 1H, NH), 8.06 (d, *J* = 8.0 Hz, 1H), 7.76 (t, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.45 (t, *J* = 8.0 Hz, 1H), 3.05- 2.97 (m, 1H), 2.01- 1.93 (m, 2H), 1.89- 1.81 (m, 2H), 1.77- 1.67 (m, 2H), 1.63- 1.56 (m, 2H). **¹³C{¹H} NMR** (100 MHz, DMSO-*d*₆): δ 162.4, 160.8, 149.1, 134.8, 127.2, 126.4, 126.1, 121.1, 44.2, 31.2, 25.7 ppm.

10. ^1H and ^{13}C NMR spectra for synthesized compounds:

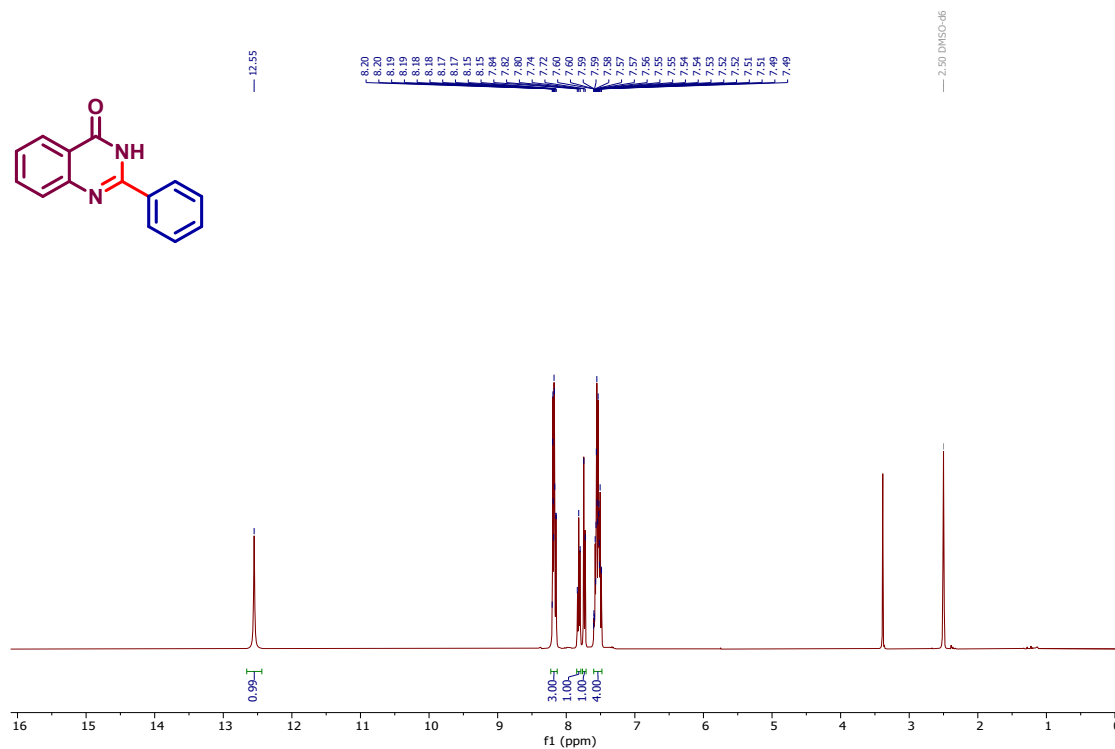


Figure S18: ^1H NMR spectrum (400 MHz) of 3a in DMSO-d_6

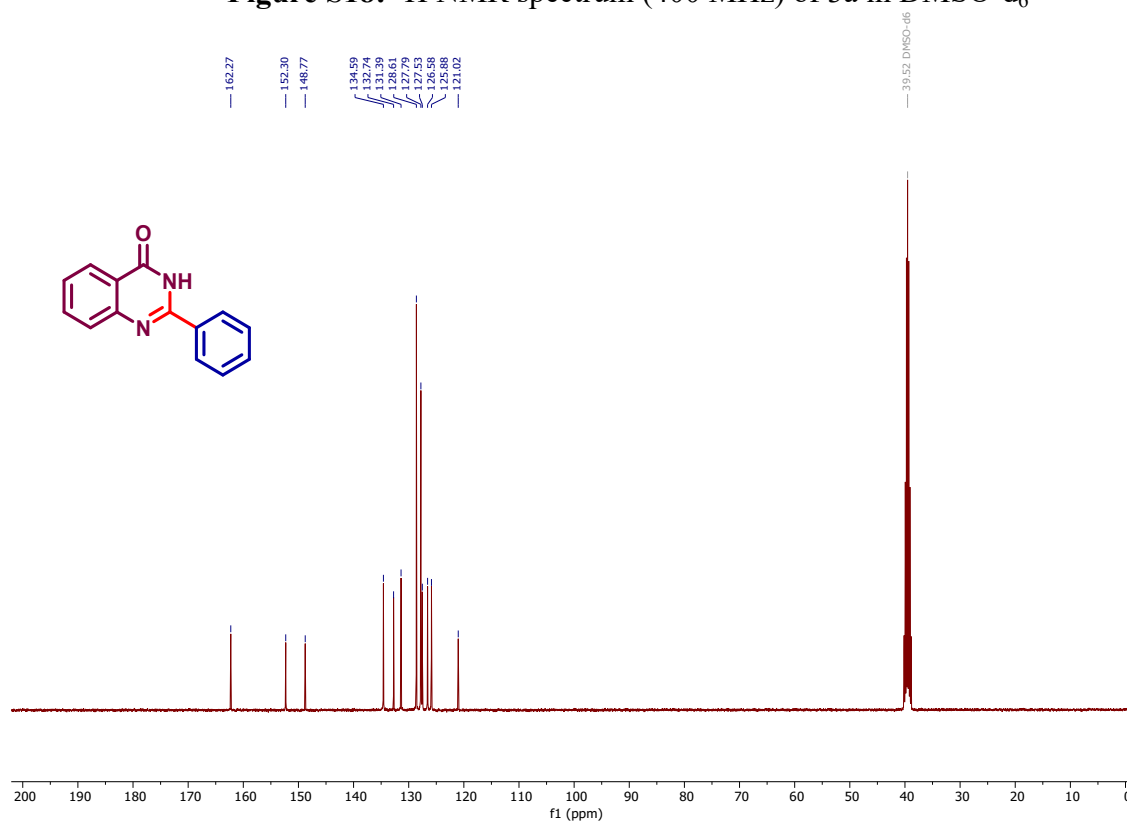


Figure S19: ^{13}C NMR spectrum (100 MHz) of 3a in DMSO-d_6

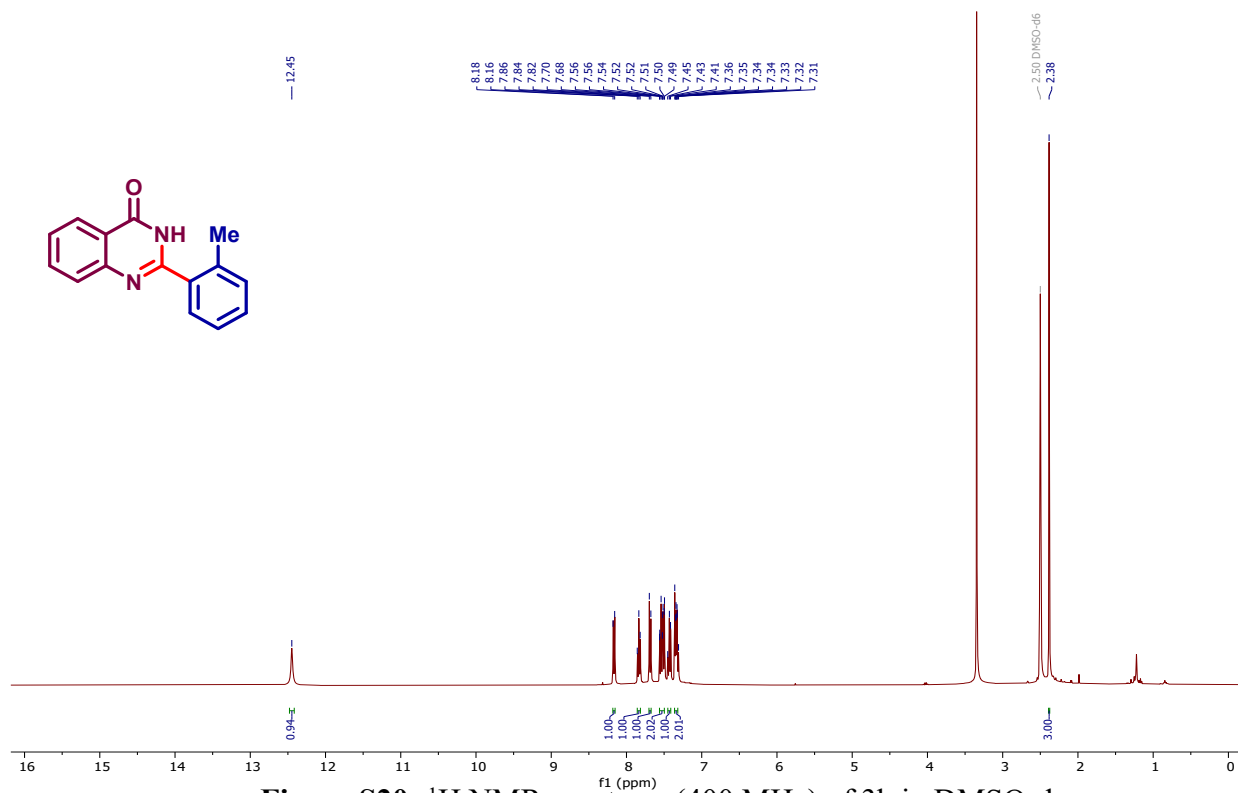


Figure S20: ¹H NMR spectrum (400 MHz) of 3b in DMSO-d₆

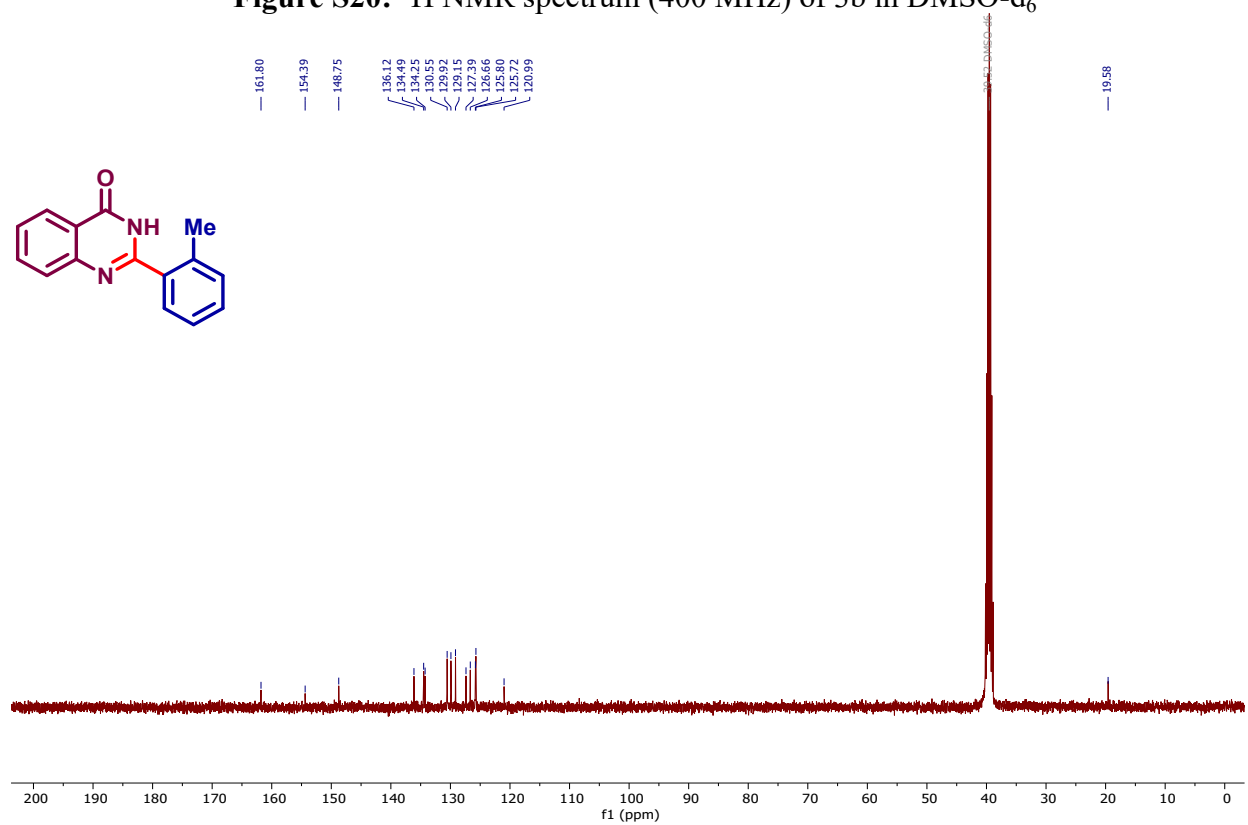


Figure S21: ¹³C NMR spectrum (100 MHz) of 3b in DMSO-d₆

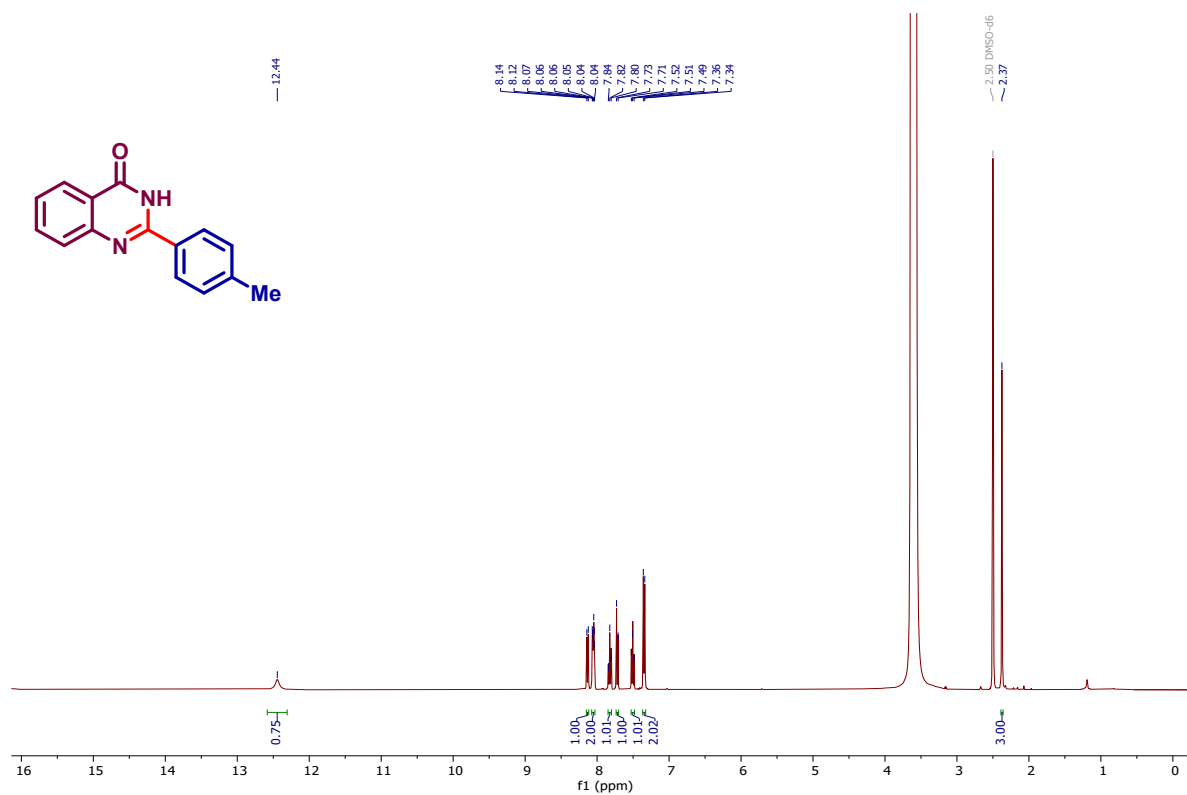


Figure S22: ¹H NMR spectrum (400 MHz) of 3c in DMSO-d₆

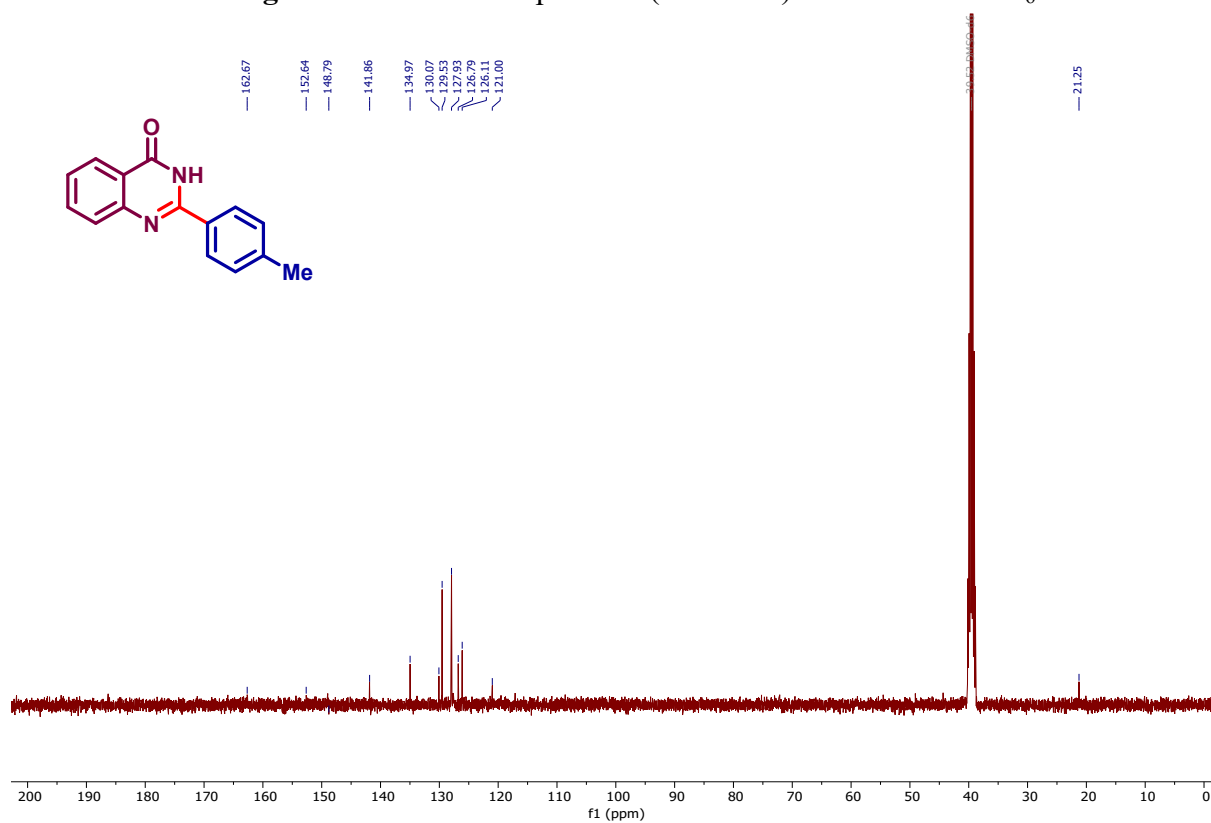


Figure S23: ¹³C NMR spectrum (100 MHz) of 3c in DMSO-d₆

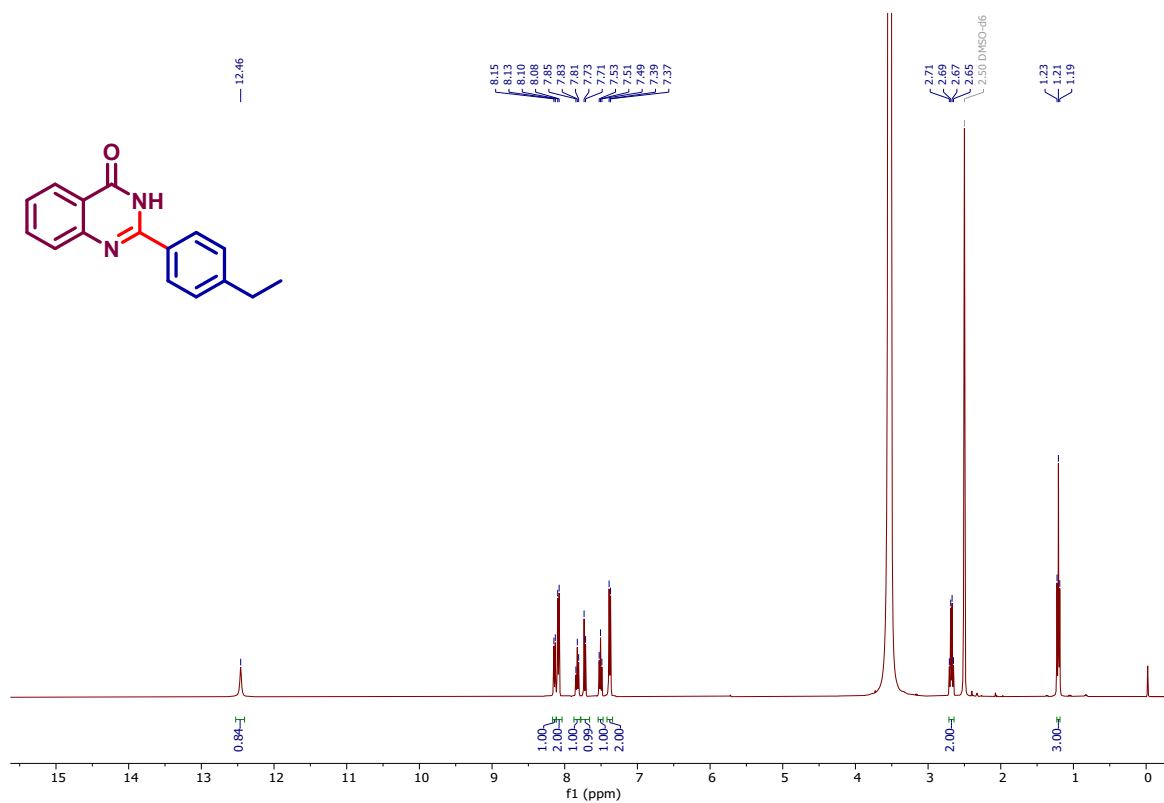


Figure S24: ¹H NMR spectrum (400 MHz) of 3d in DMSO-d₆

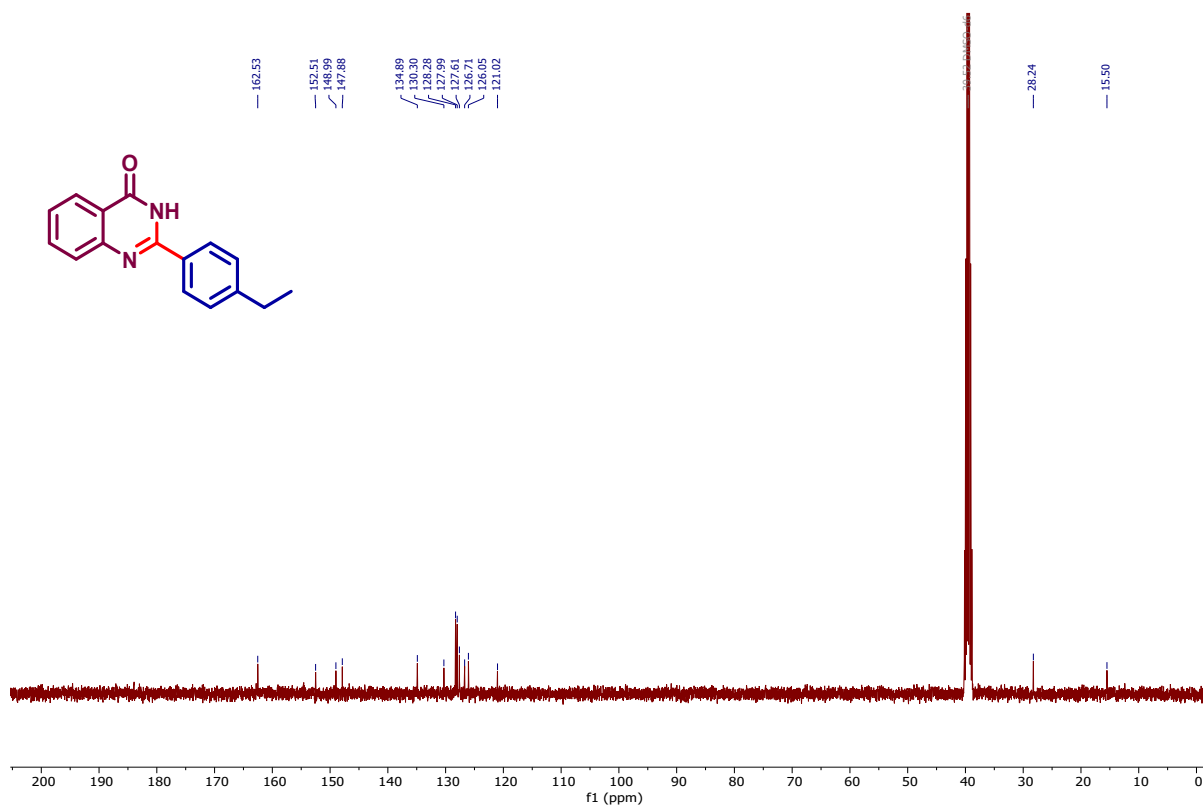


Figure S25: ¹³C NMR spectrum (100 MHz) of 3d in DMSO-d₆

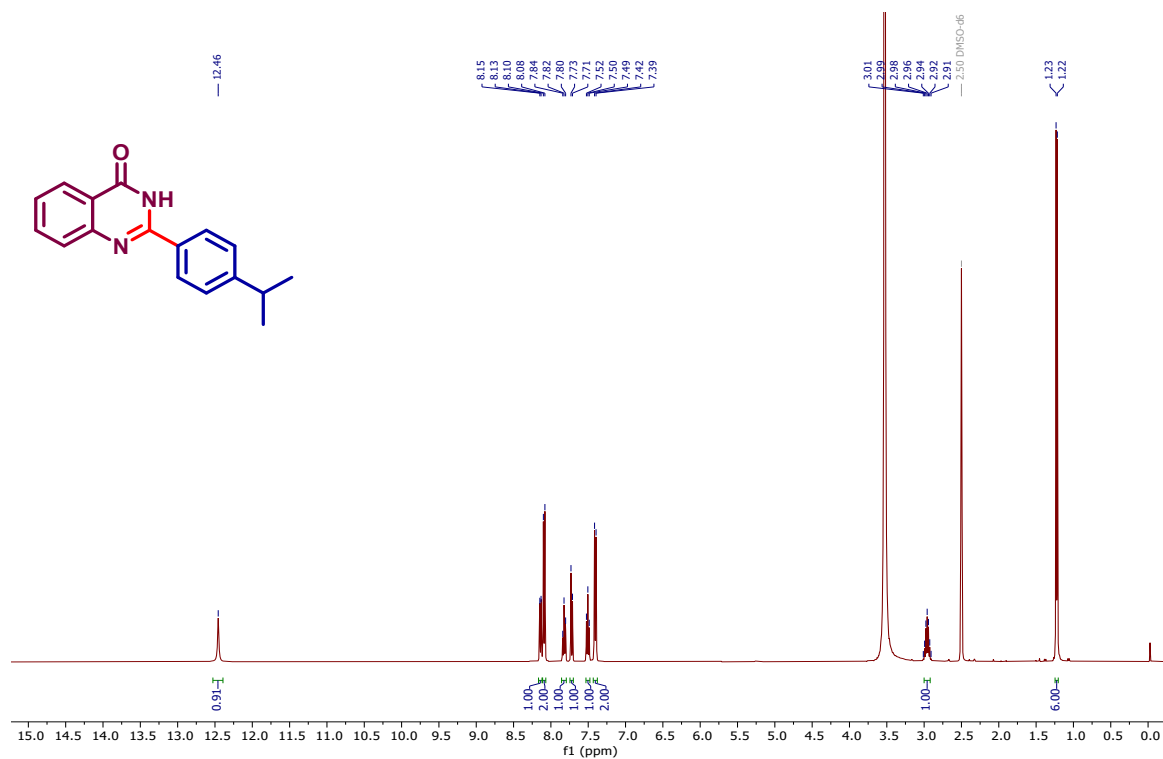


Figure S26: ¹H NMR spectrum (400 MHz) of 3e in DMSO-d₆

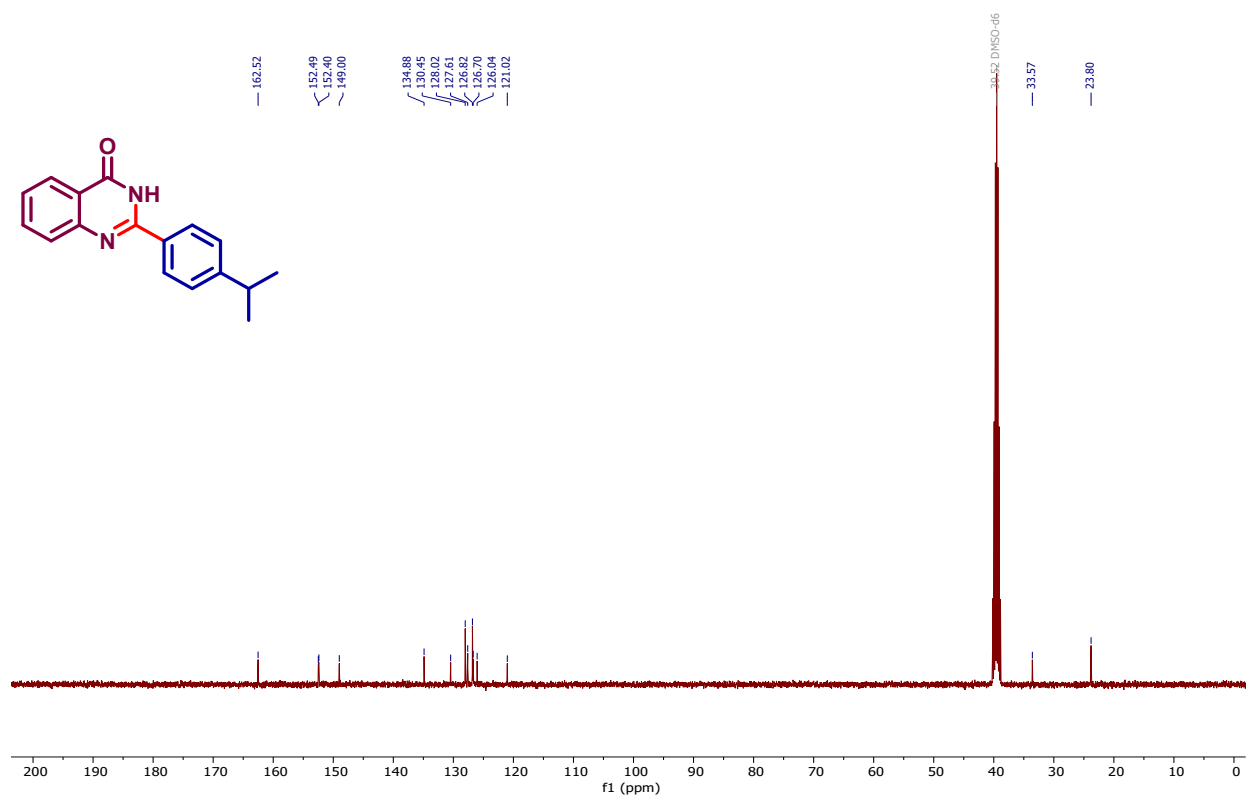


Figure S27: ¹³C NMR spectrum (100 MHz) of 3e in DMSO-d₆

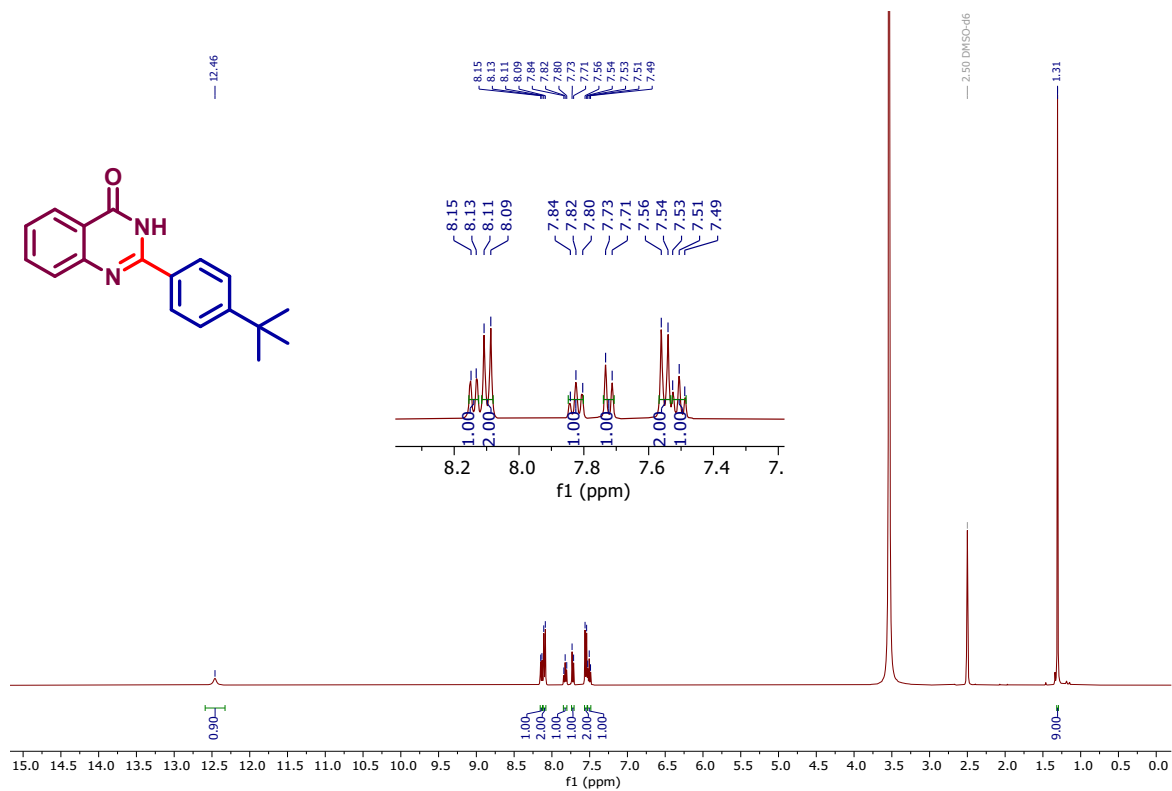


Figure S28: ¹H NMR spectrum (400 MHz) of 3f in DMSO-d₆

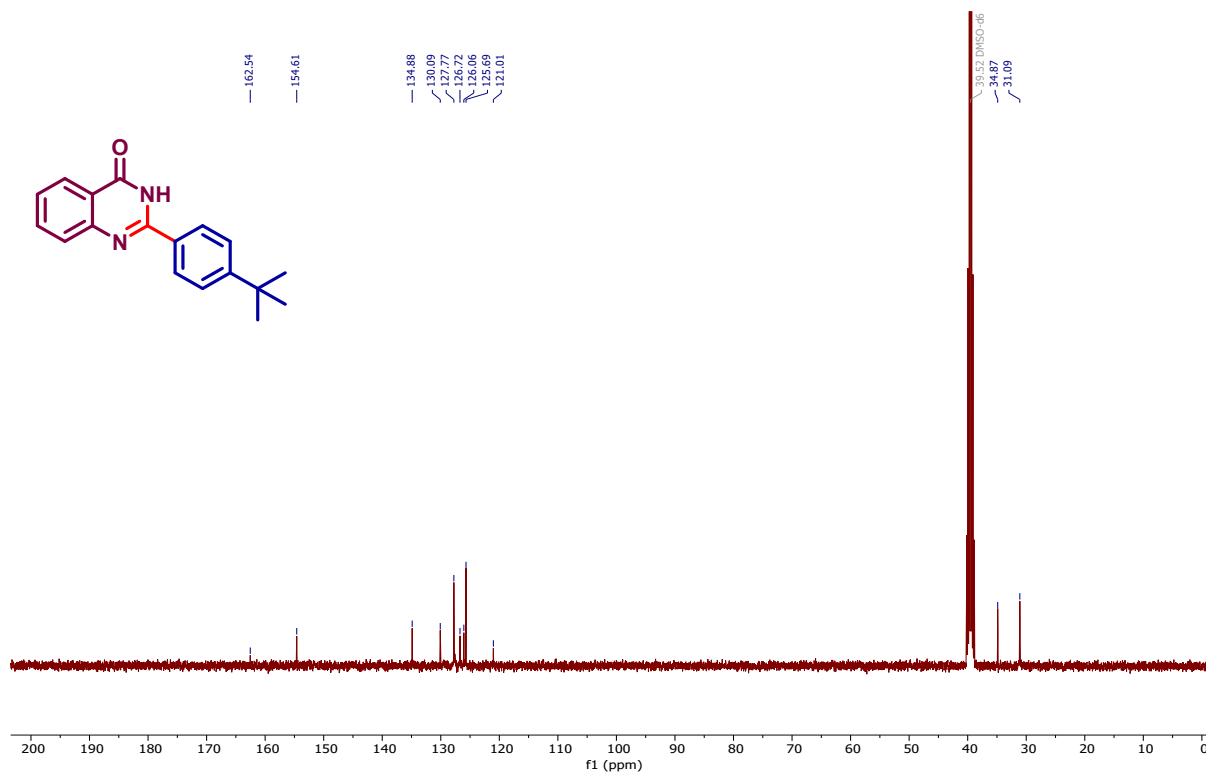


Figure S29: ¹³C NMR spectrum (100 MHz) of 3f in DMSO-d₆

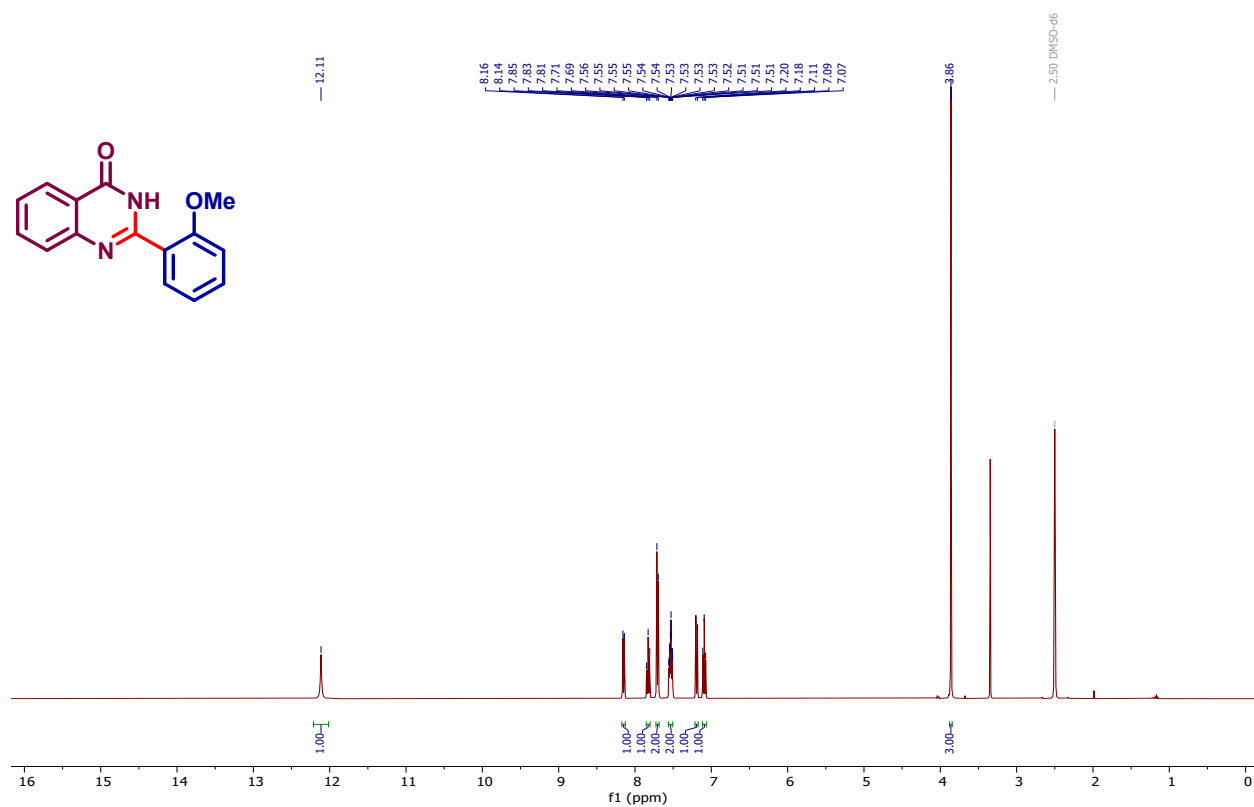


Figure S30: ¹H NMR spectrum (400 MHz) of 3g in DMSO-d₆

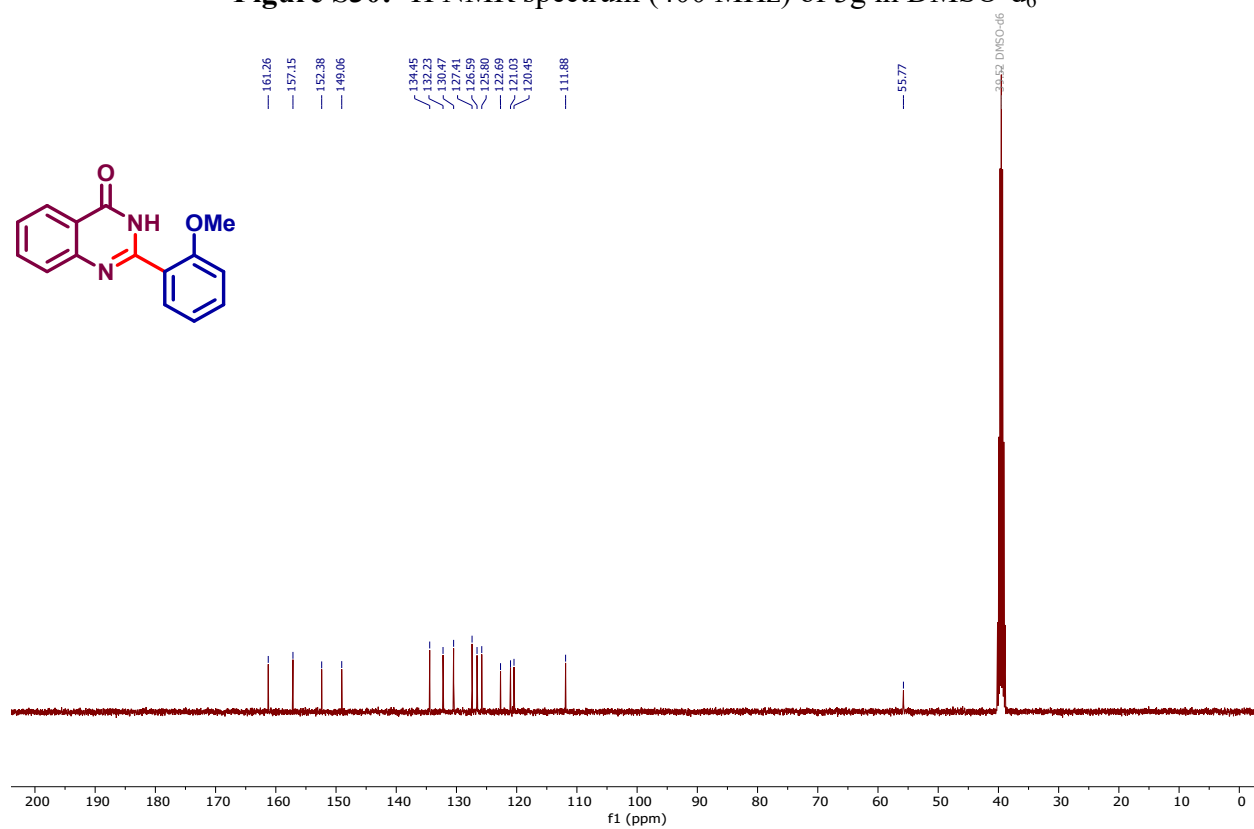


Figure S31: ¹³C NMR spectrum (100 MHz) of 3g in DMSO-d₆

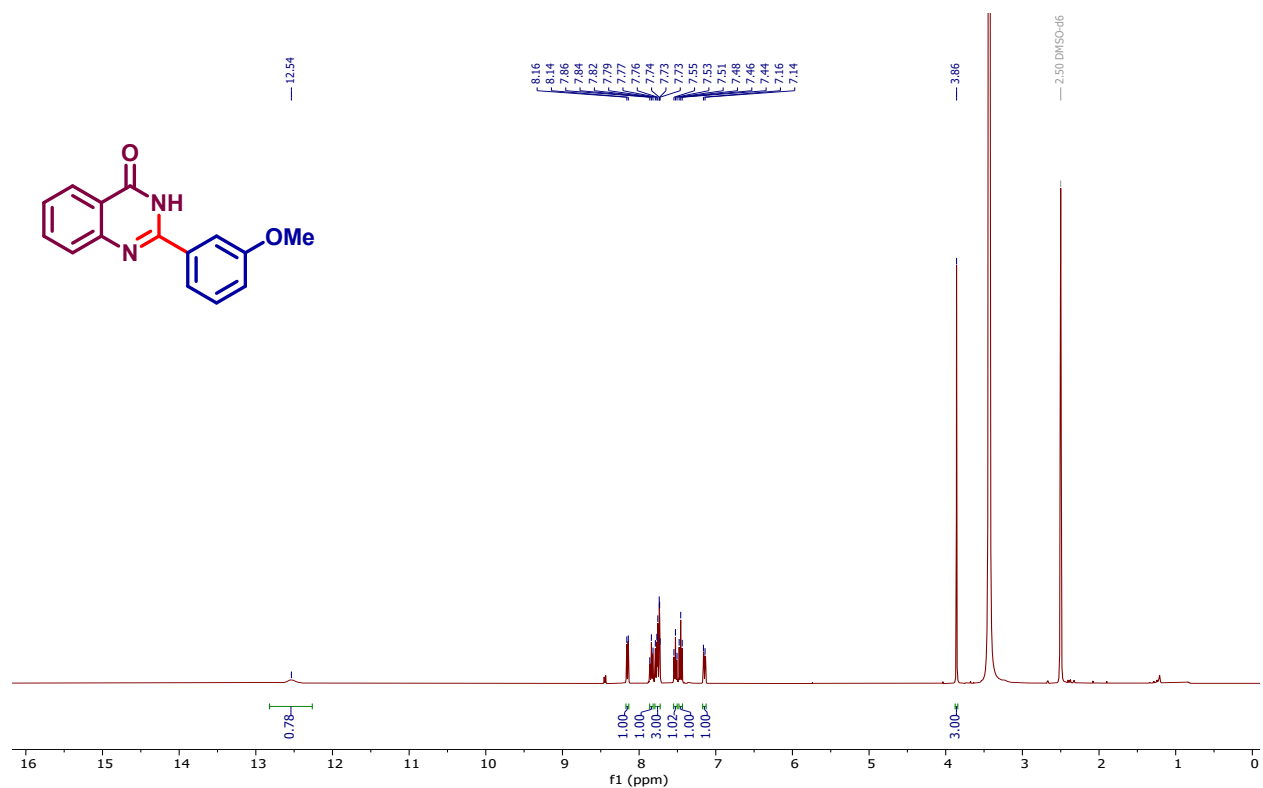


Figure S32: ¹H NMR spectrum (400 MHz) of 3h in DMSO-d₆

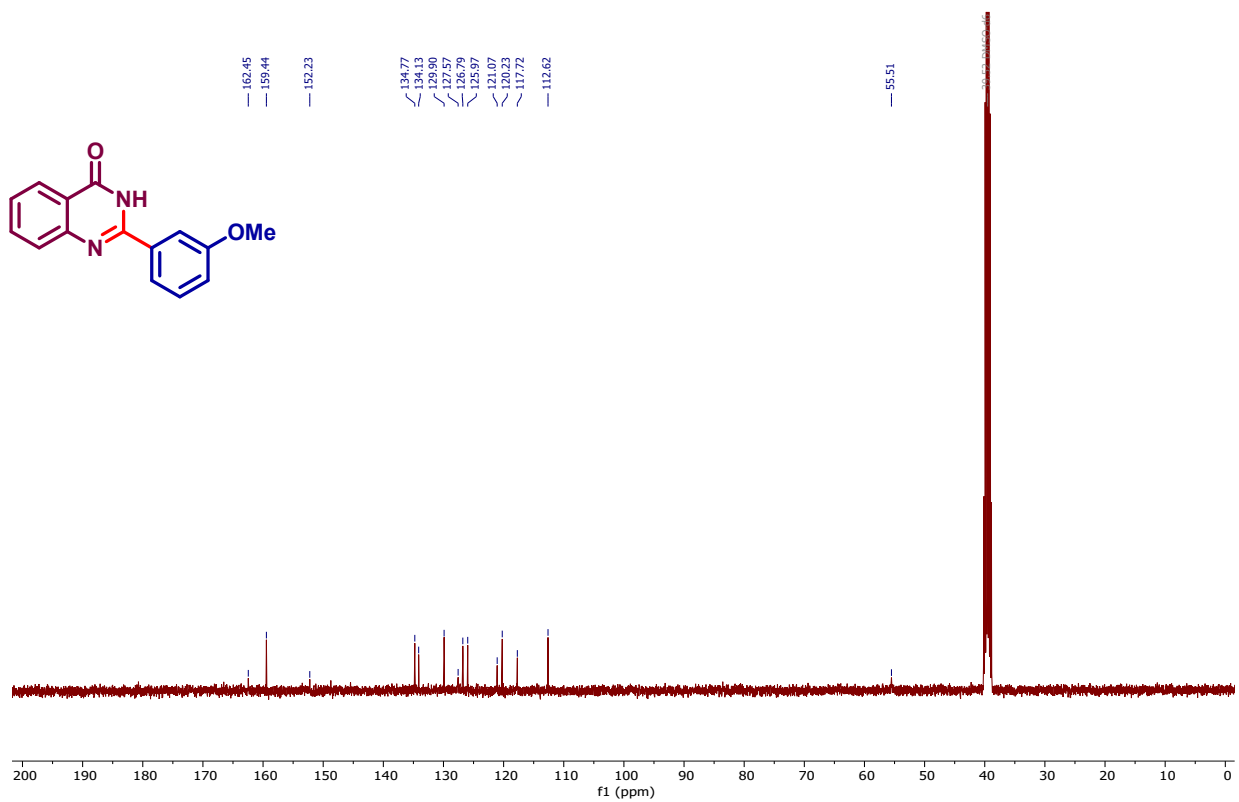


Figure S33: ¹³C NMR spectrum (100 MHz) of 3h in DMSO-d₆

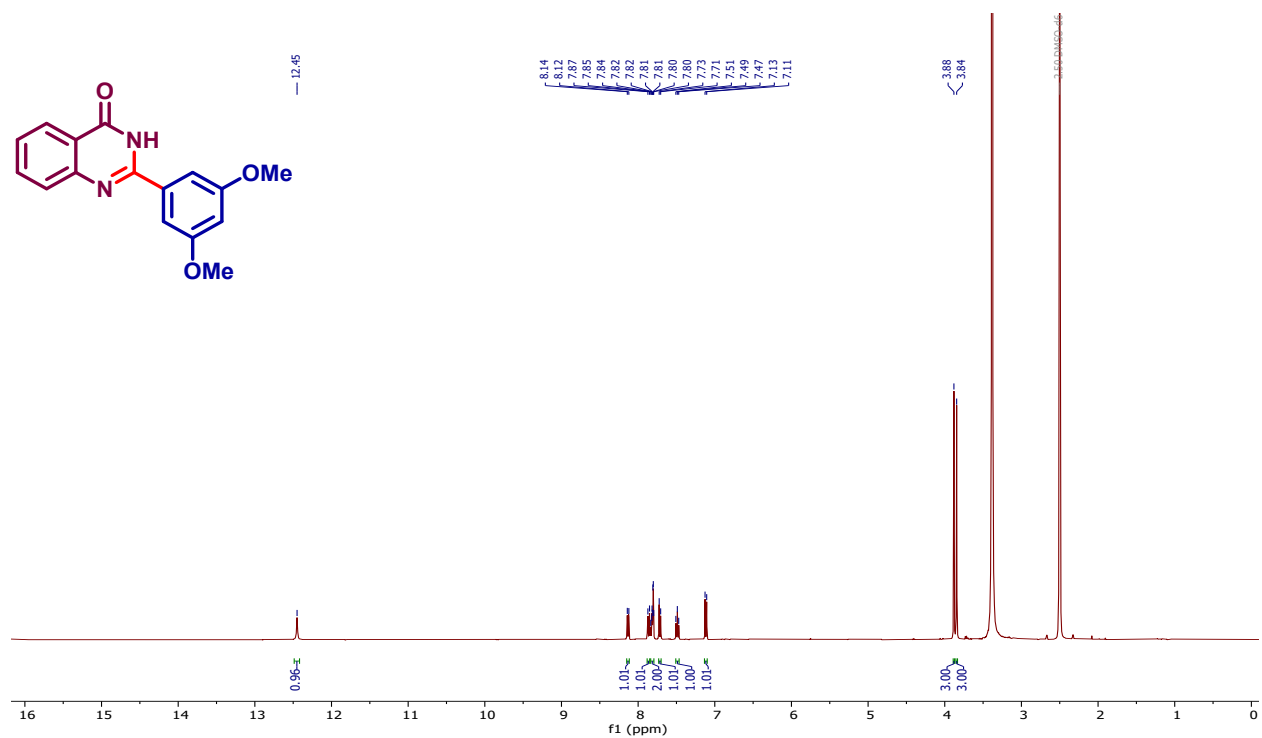


Figure S34: ¹H NMR spectrum (400 MHz) of 3i in DMSO-d₆

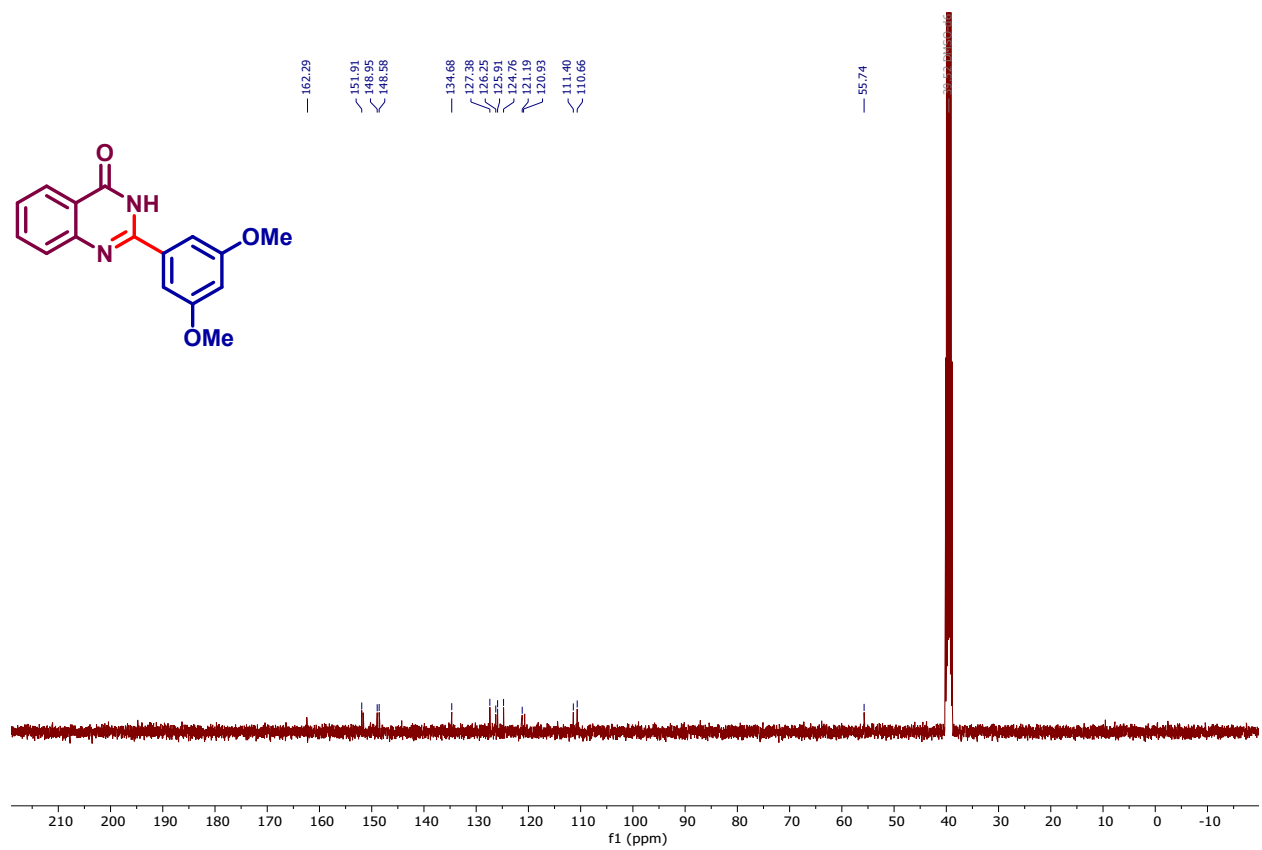


Figure S35: ¹³C NMR spectrum (100 MHz) of 3i in DMSO-d₆

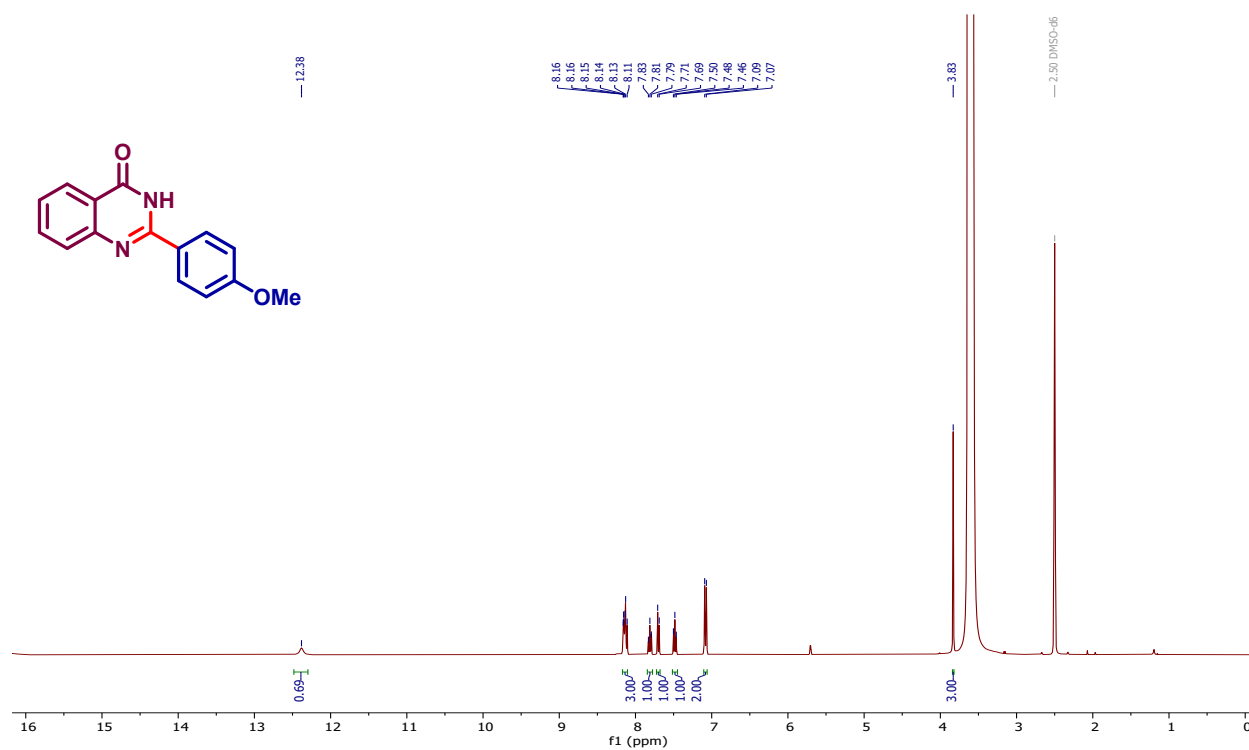


Figure S36: ¹H NMR spectrum (400 MHz) of 3j in DMSO-d₆

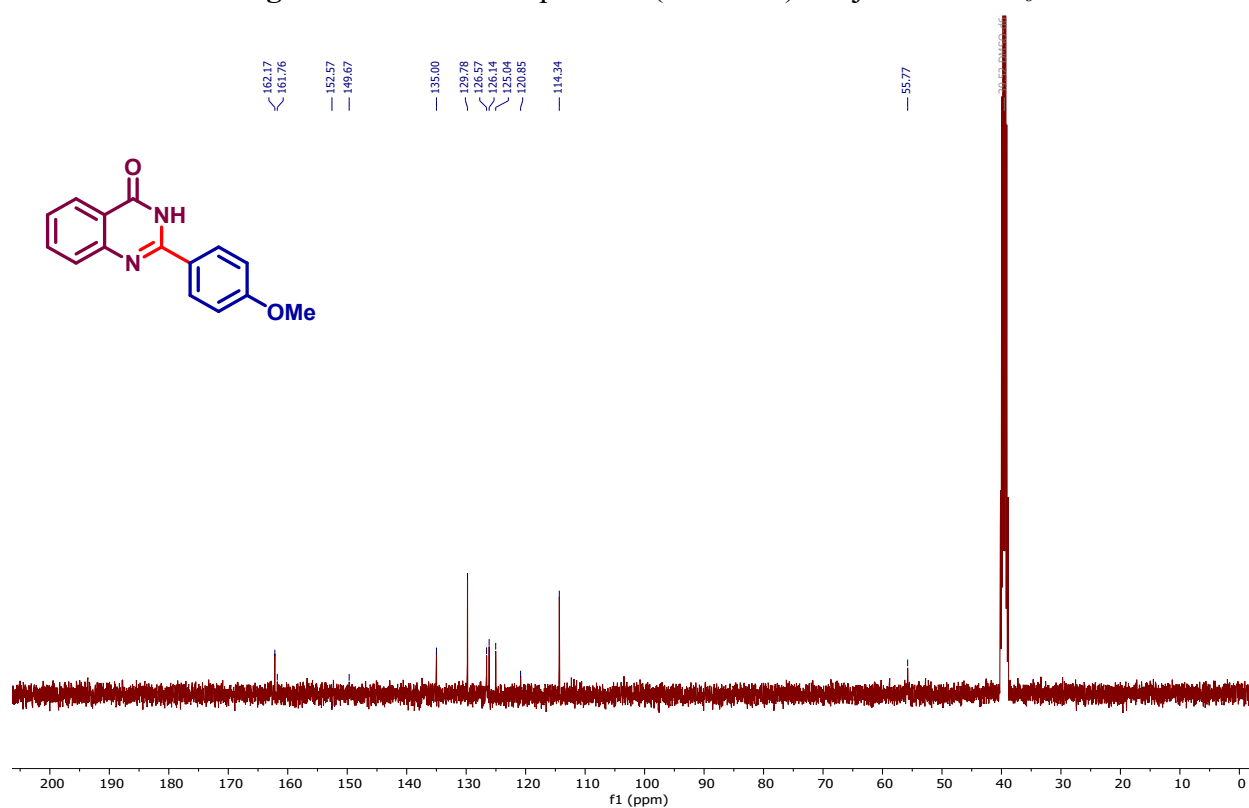


Figure S37: ¹³C NMR spectrum (100 MHz) of 3j in DMSO-d₆

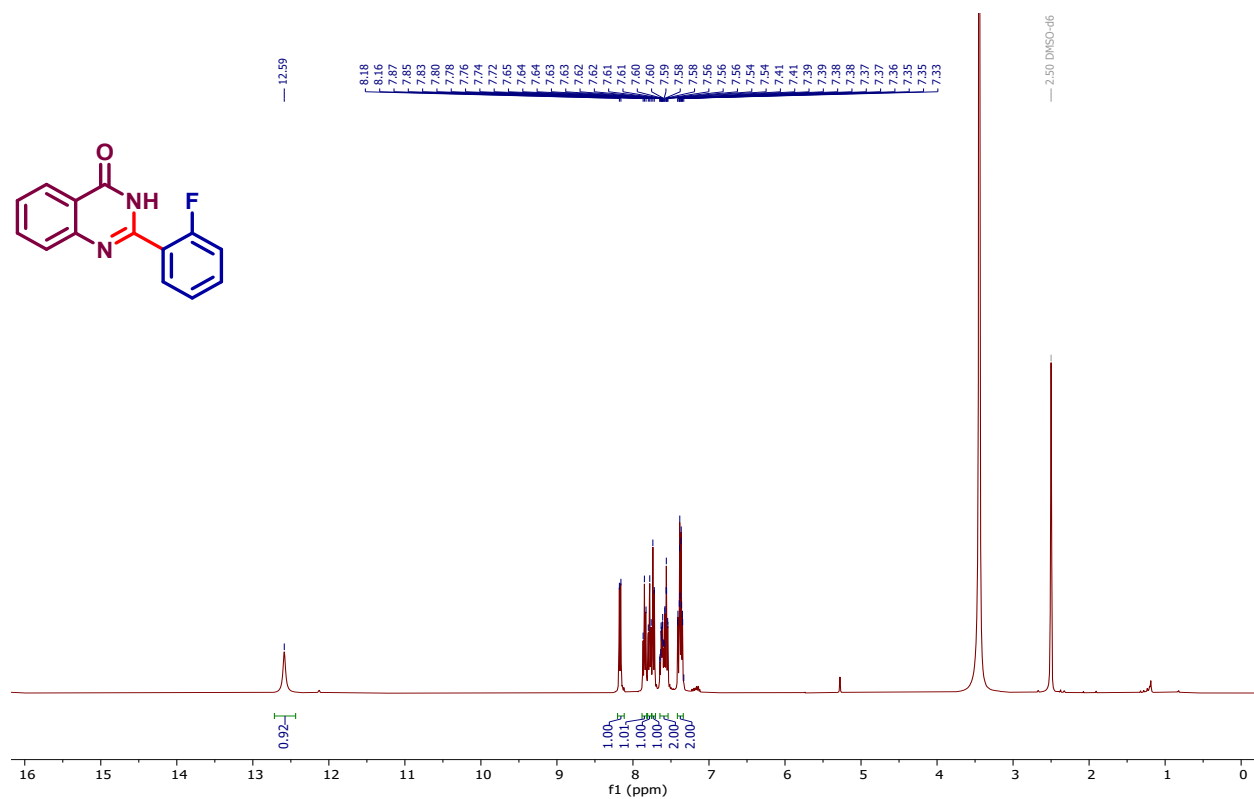


Figure S38: ¹H NMR spectrum (400 MHz) of 3k in DMSO-d₆

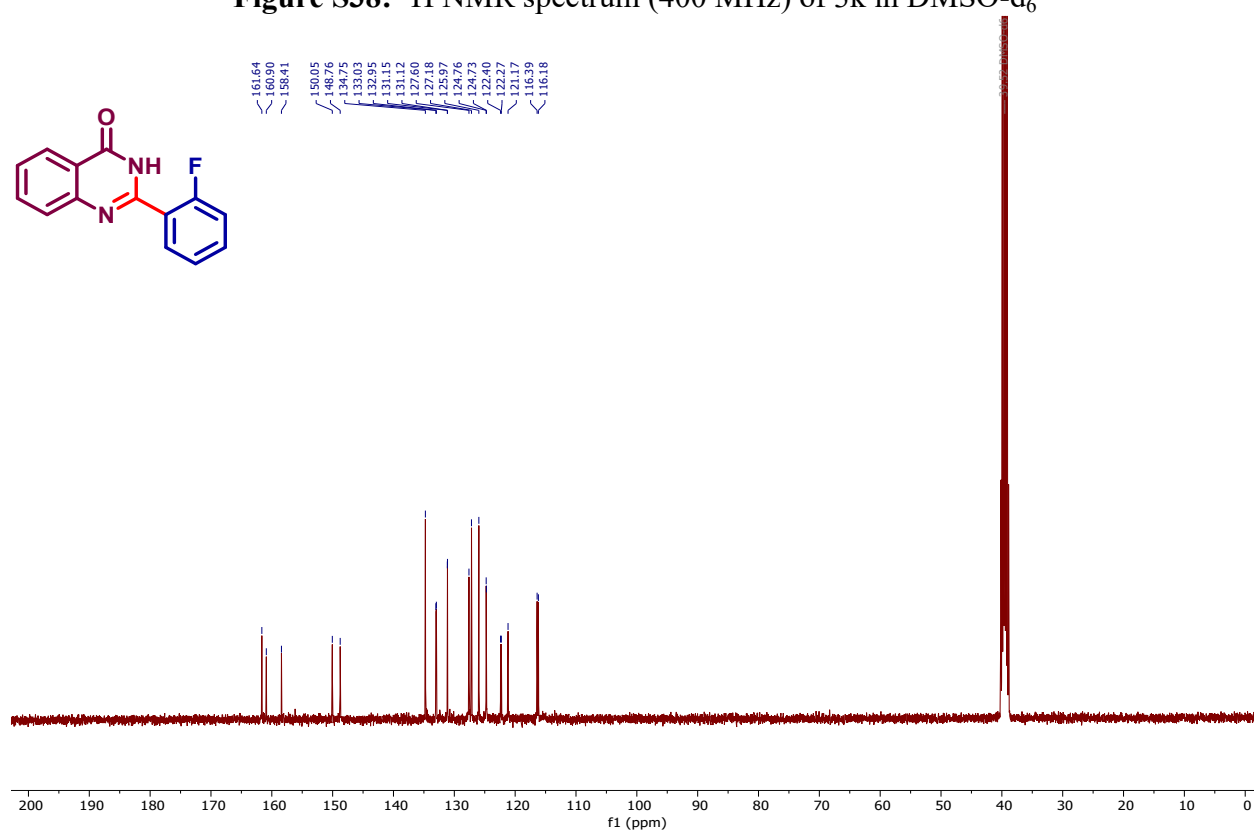


Figure S39: ¹³C NMR spectrum (100 MHz) of 3k in DMSO-d₆

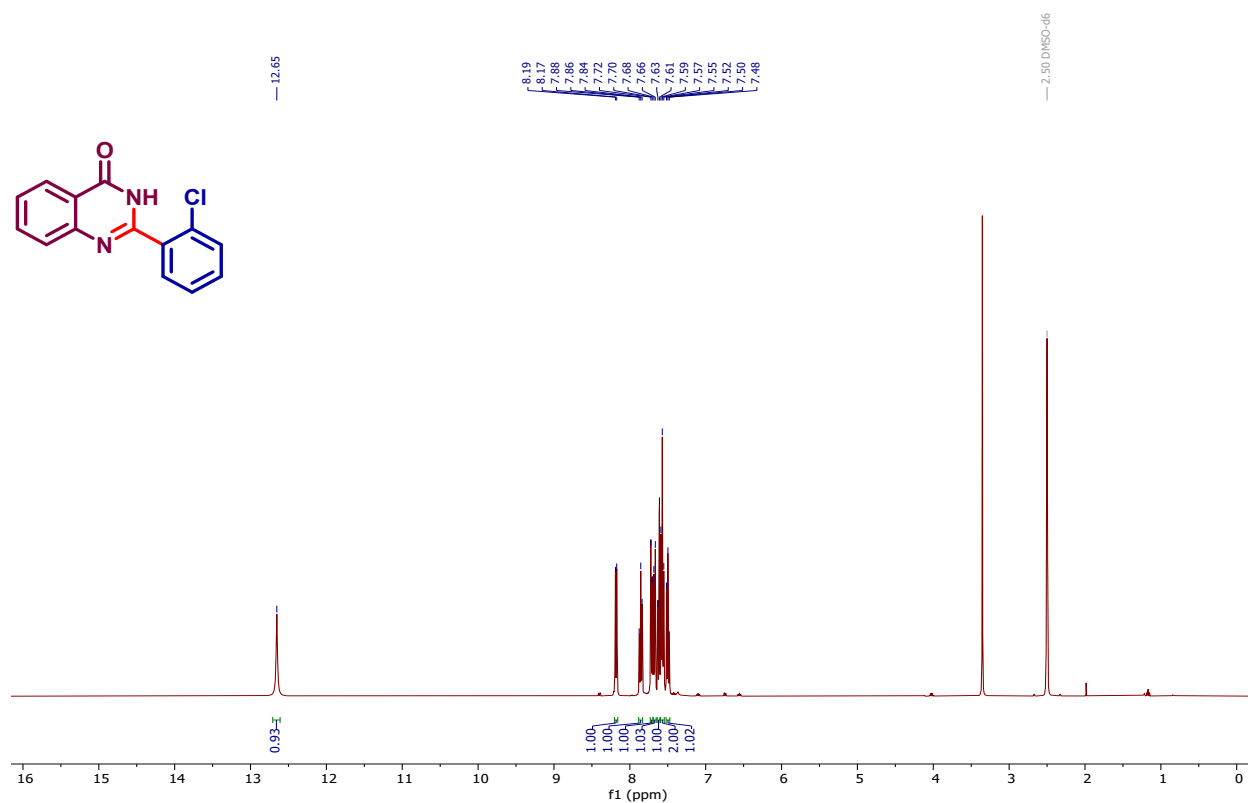


Figure S40: ¹H NMR spectrum (400 MHz) of 3l in DMSO-d₆

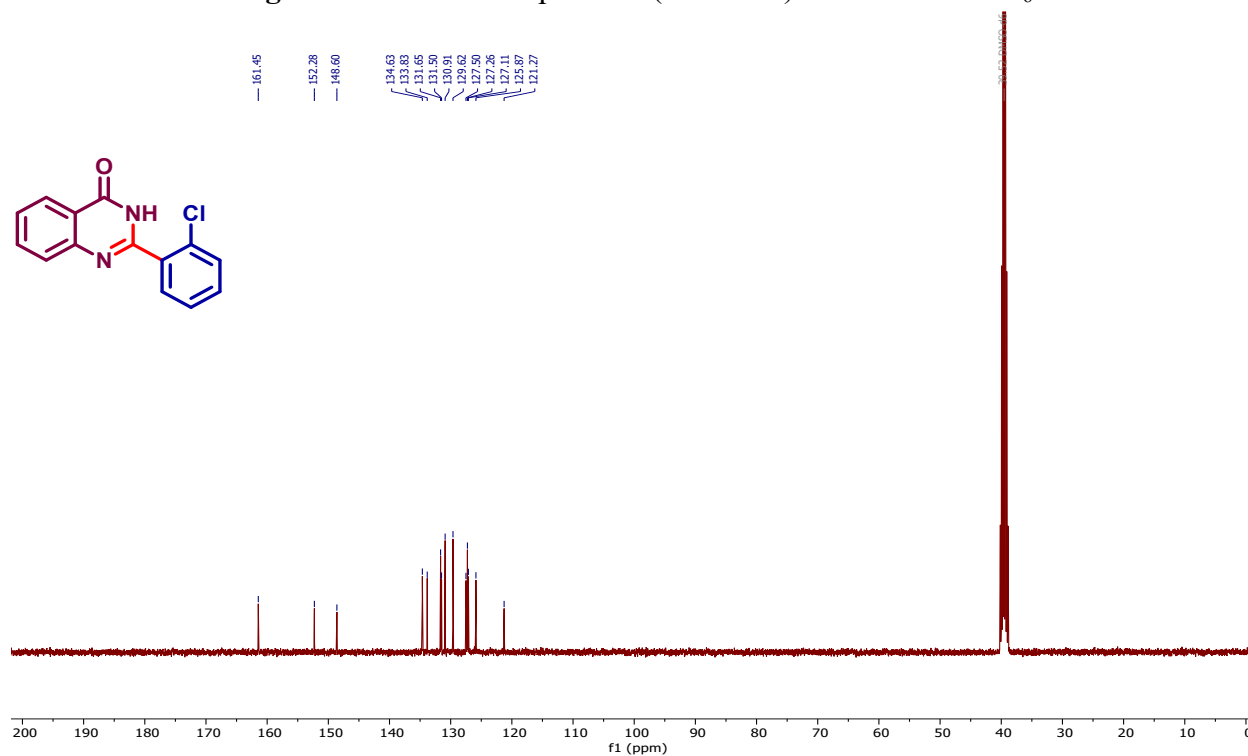


Figure S41: ¹³C NMR spectrum (100 MHz) of 3l in DMSO-d₆

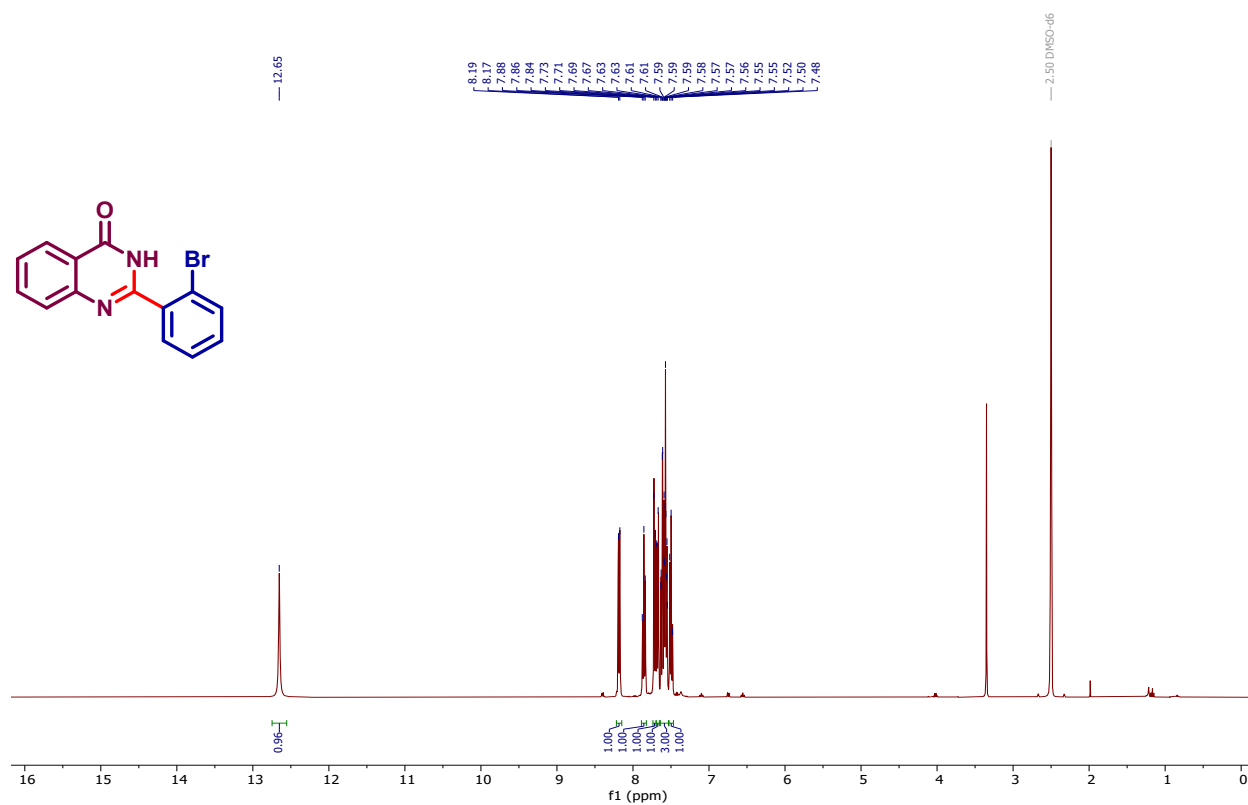


Figure S42: ^1H NMR spectrum (400 MHz) of 3m in DMSO-d_6

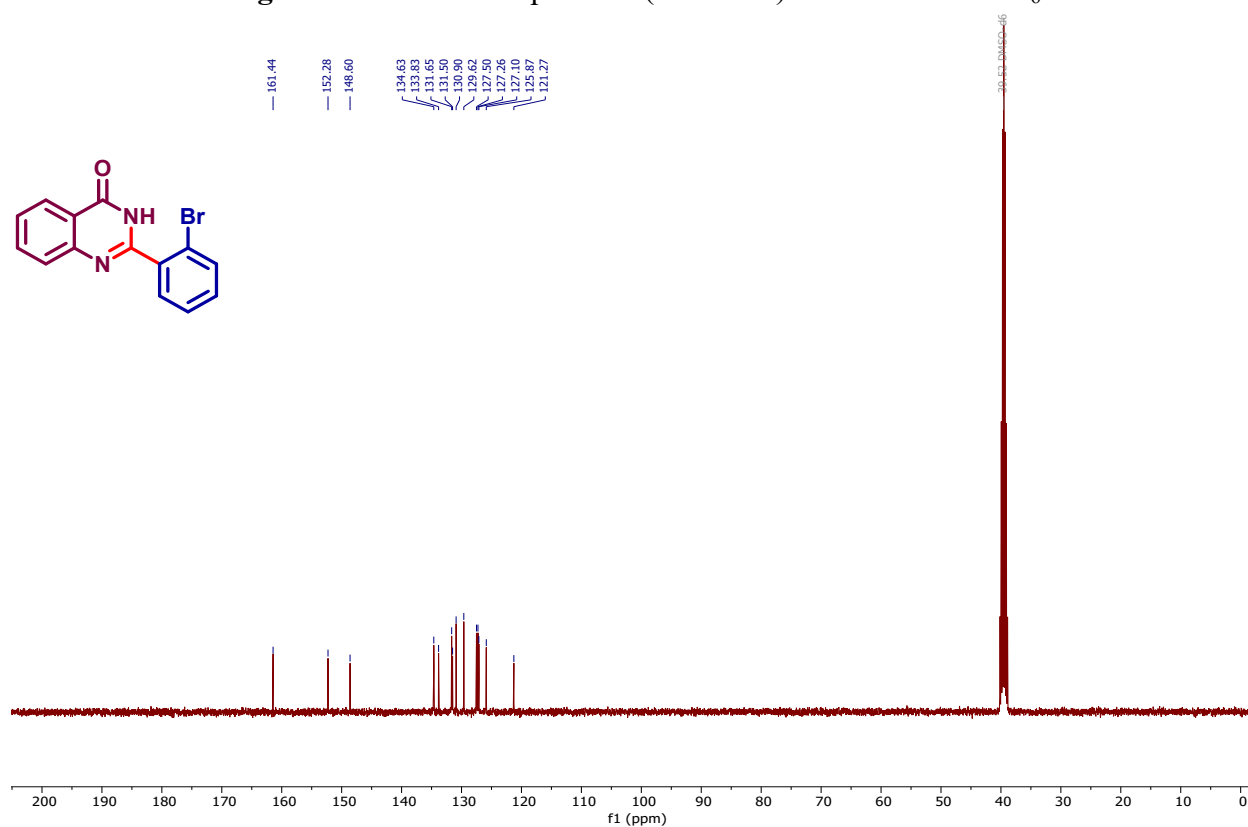


Figure S43: ^{13}C NMR spectrum (100 MHz) of 3m in DMSO-d_6

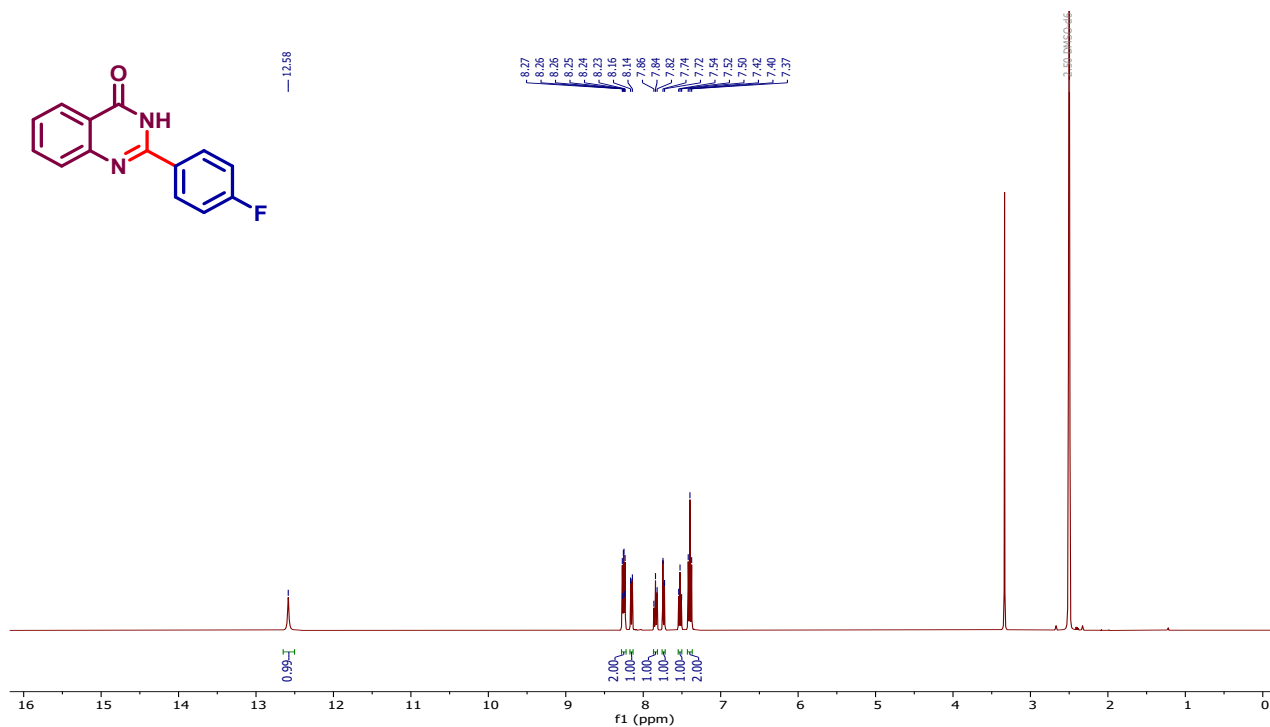


Figure S44: ¹H NMR spectrum (400 MHz) of 3n in DMSO-d₆

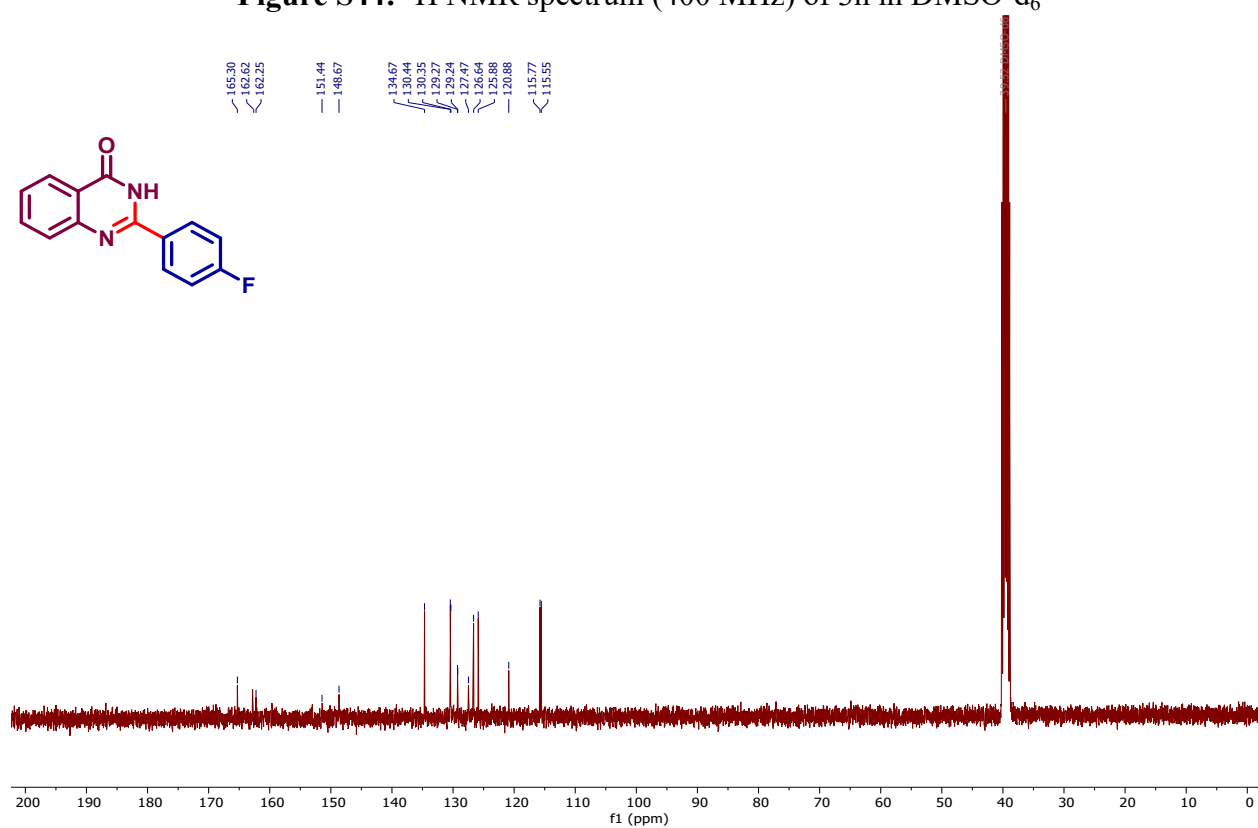


Figure S45: ¹³C NMR spectrum (100 MHz) of 3n in DMSO-d₆

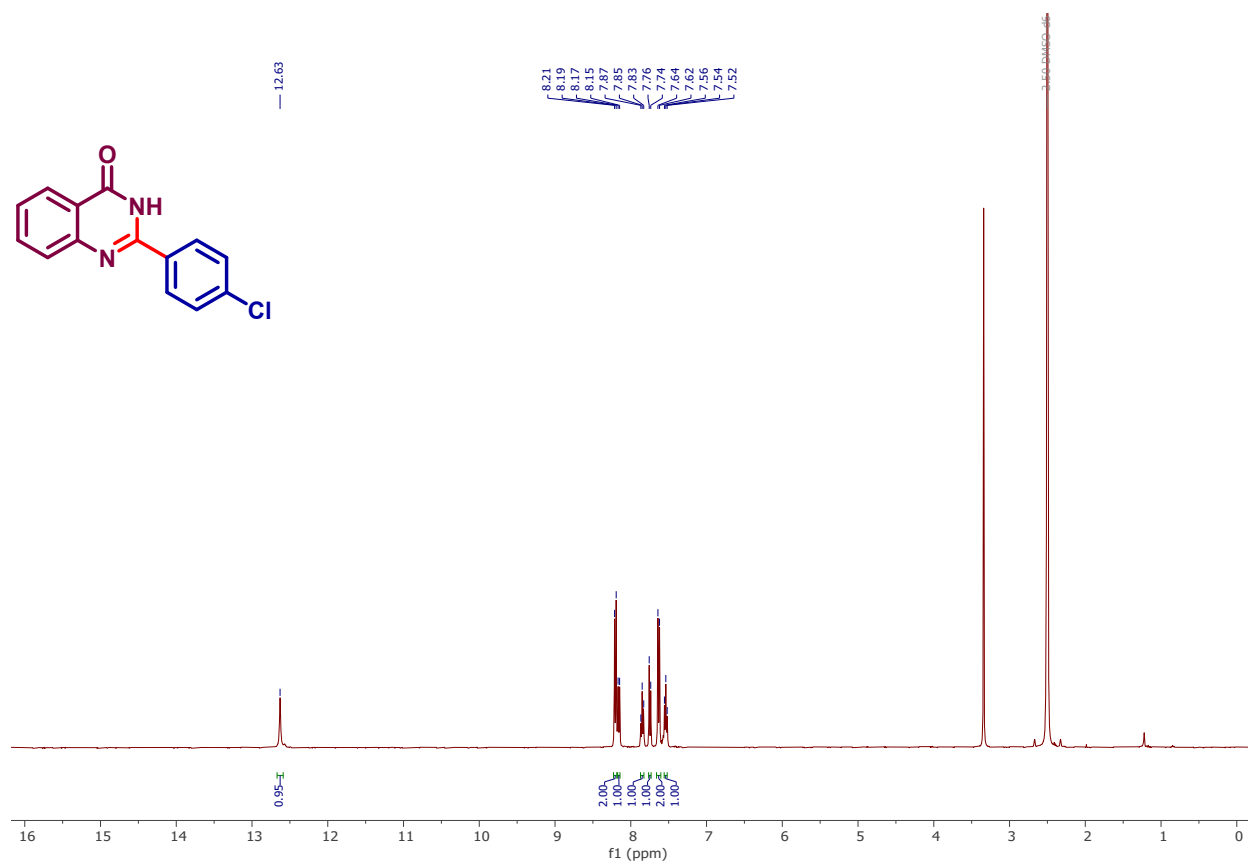


Figure S46: ¹H NMR spectrum (400 MHz) of 3o in DMSO-d₆

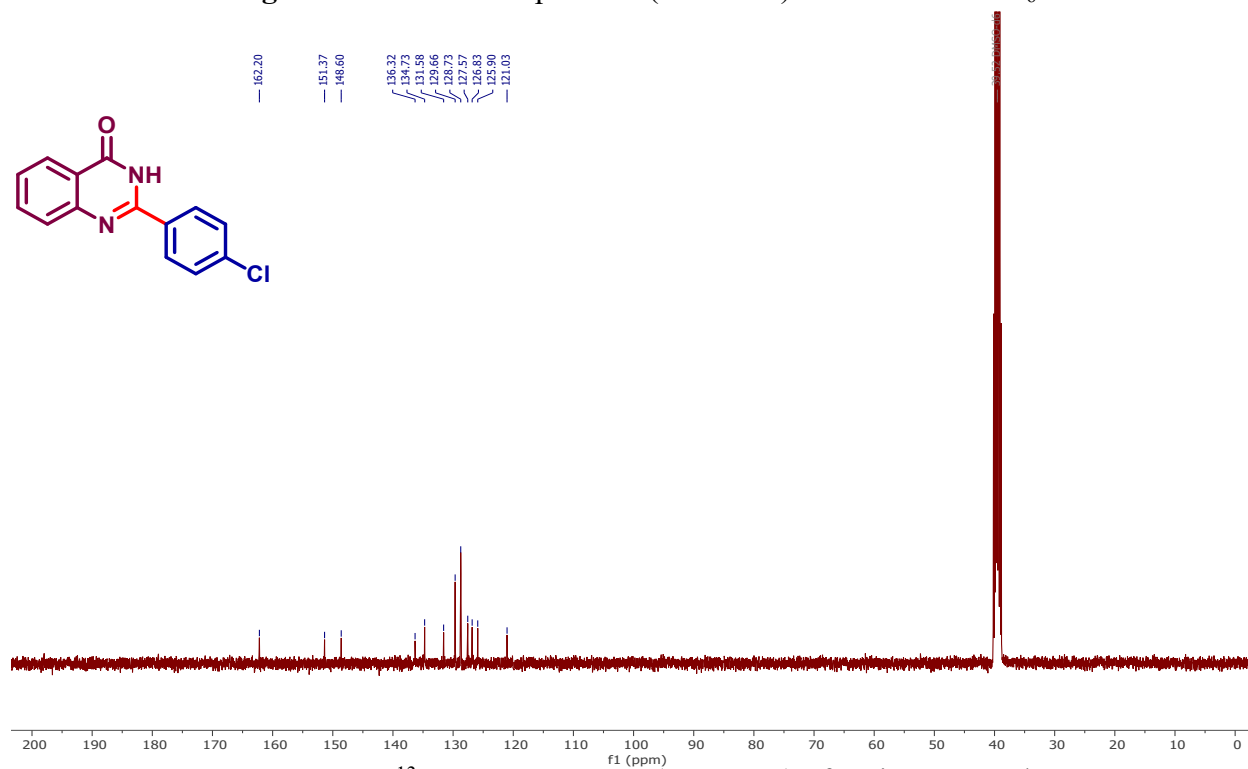


Figure S47: ¹³C NMR spectrum (100 MHz) of 3o in DMSO-d₆

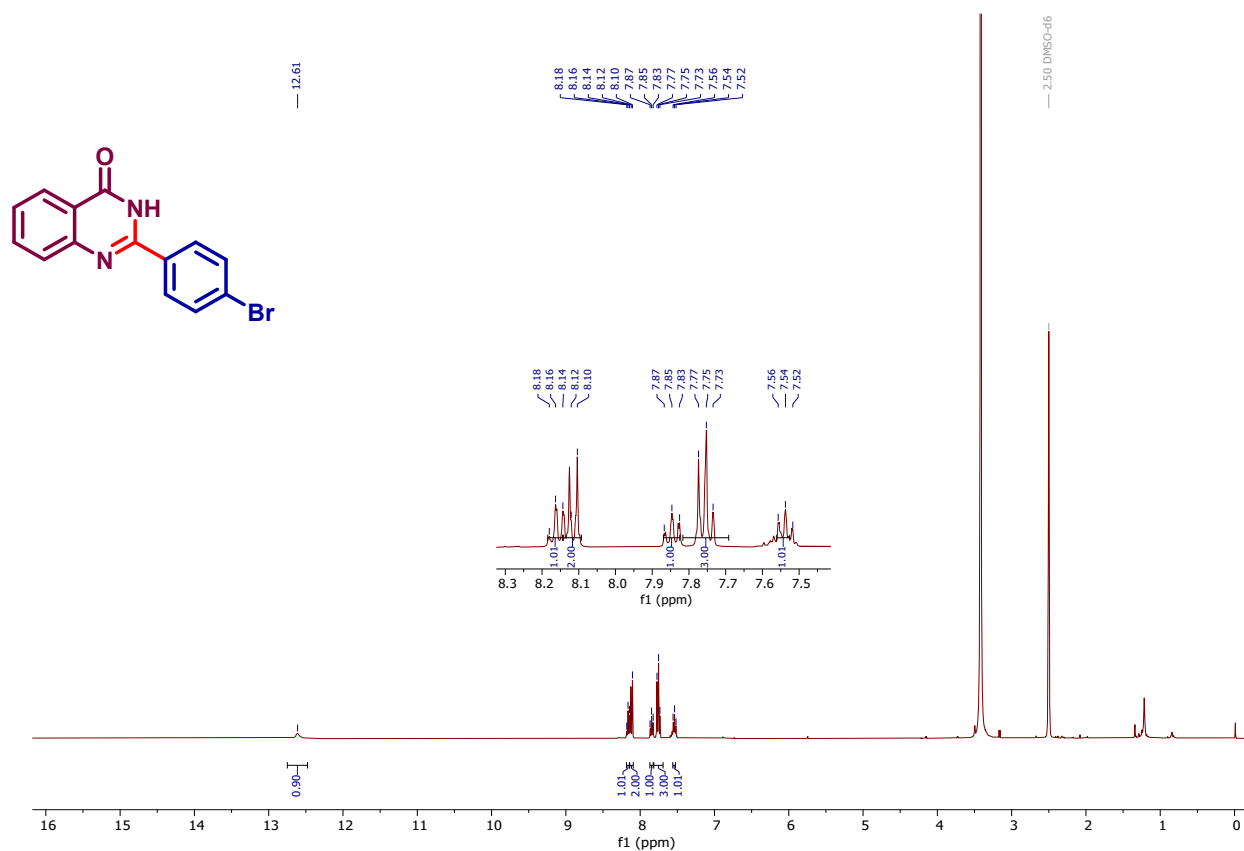


Figure S48: ¹H NMR spectrum (400 MHz) of 3p in DMSO-d₆

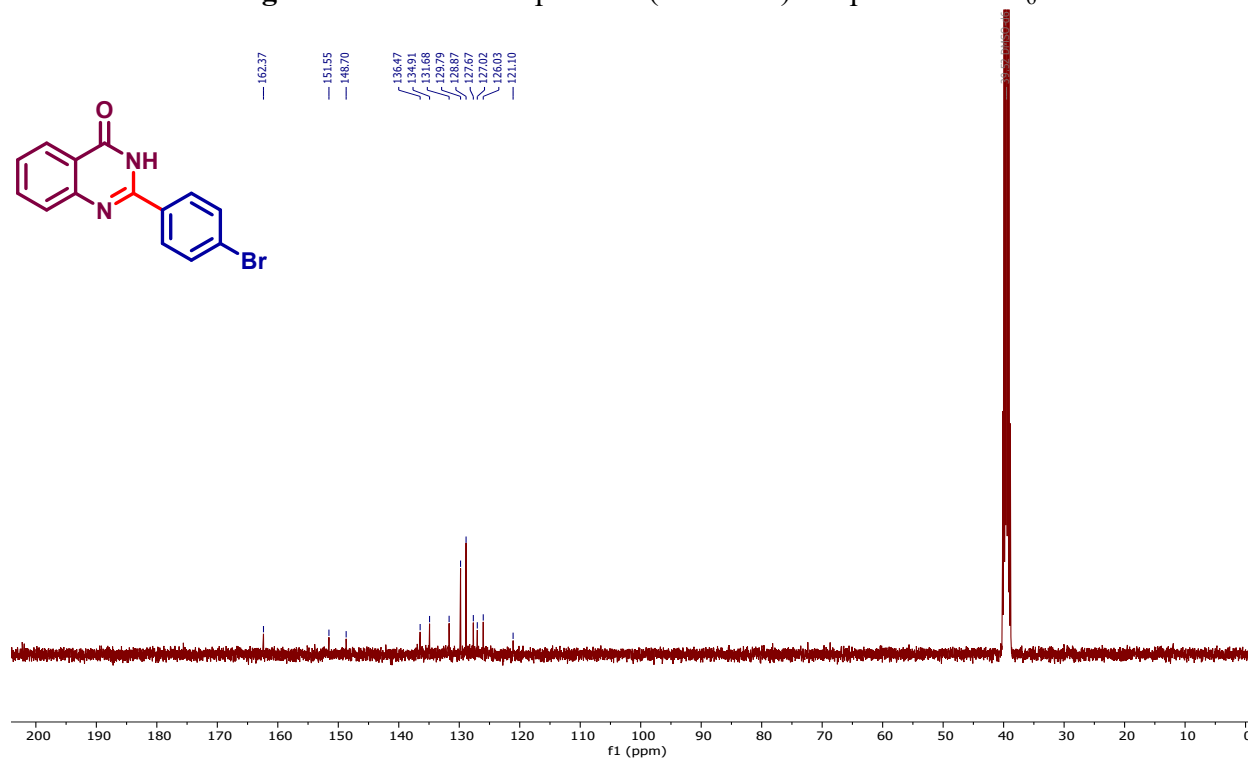


Figure S49: ¹³C NMR spectrum (100 MHz) of 3p in DMSO-d₆

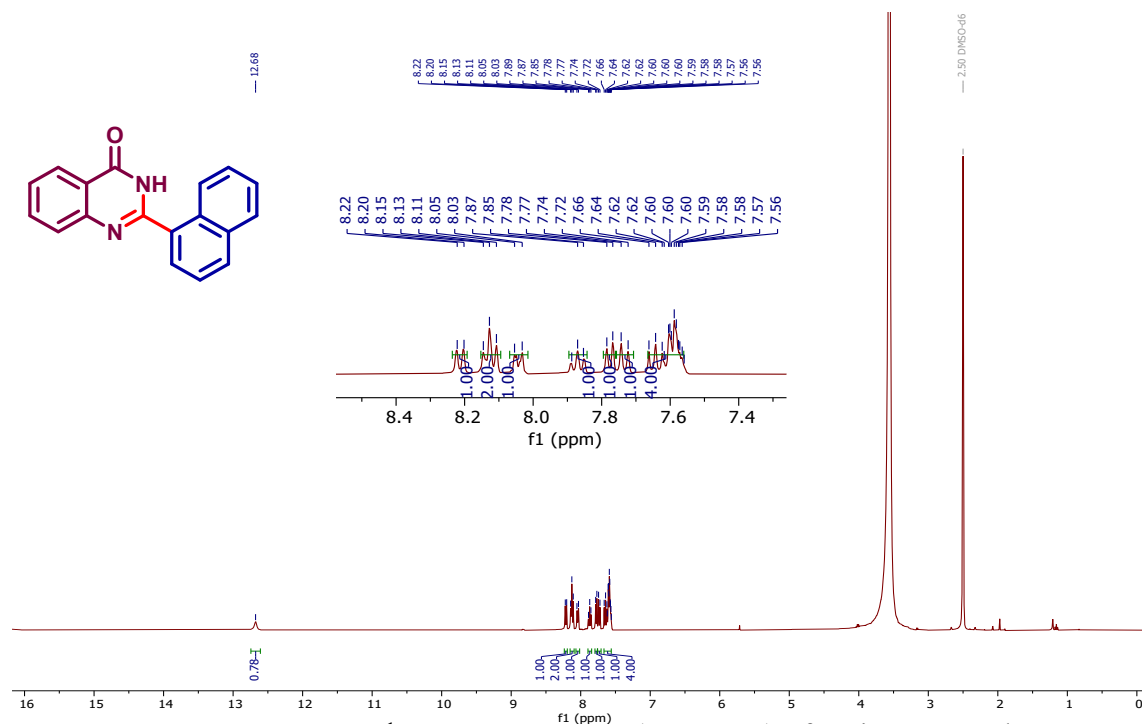


Figure S50: ¹H NMR spectrum (400 MHz) of 3q in DMSO-d₆

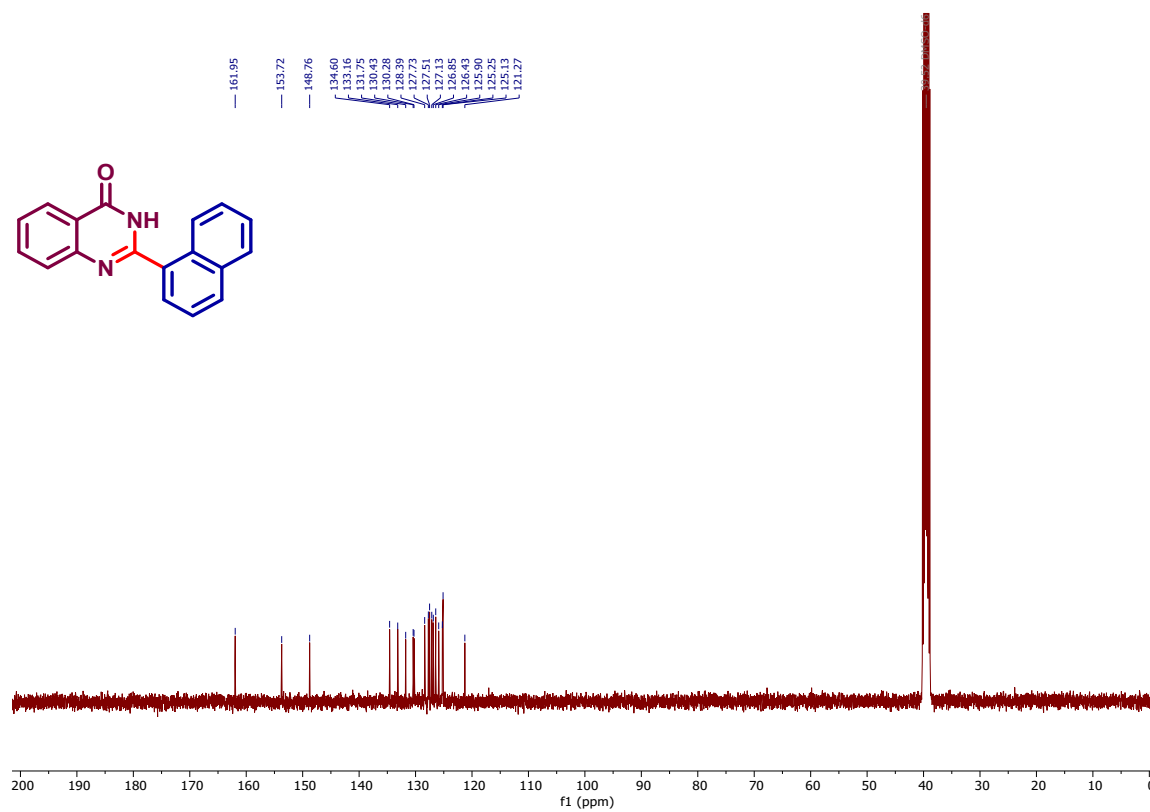


Figure S51: ¹³C NMR spectrum (100 MHz) of 3q in DMSO-d₆

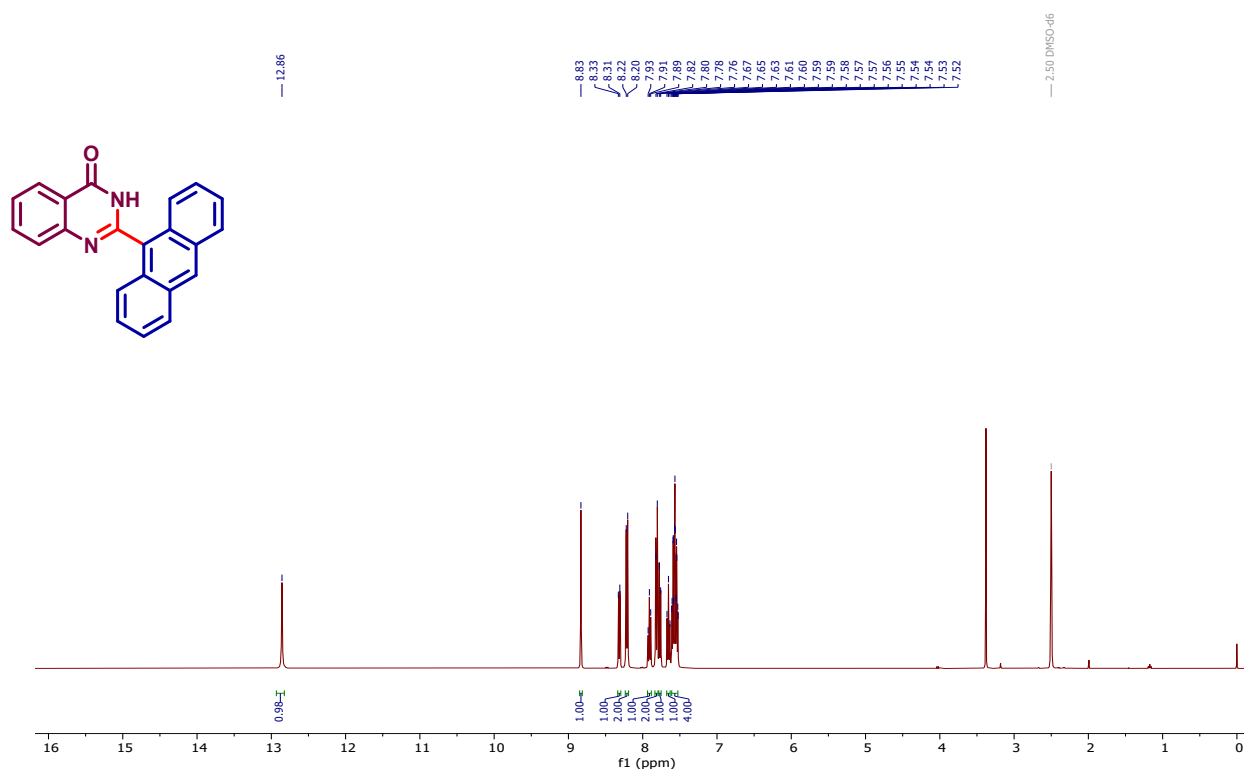


Figure S52: ¹H NMR spectrum (400 MHz) of 3r in DMSO-d₆

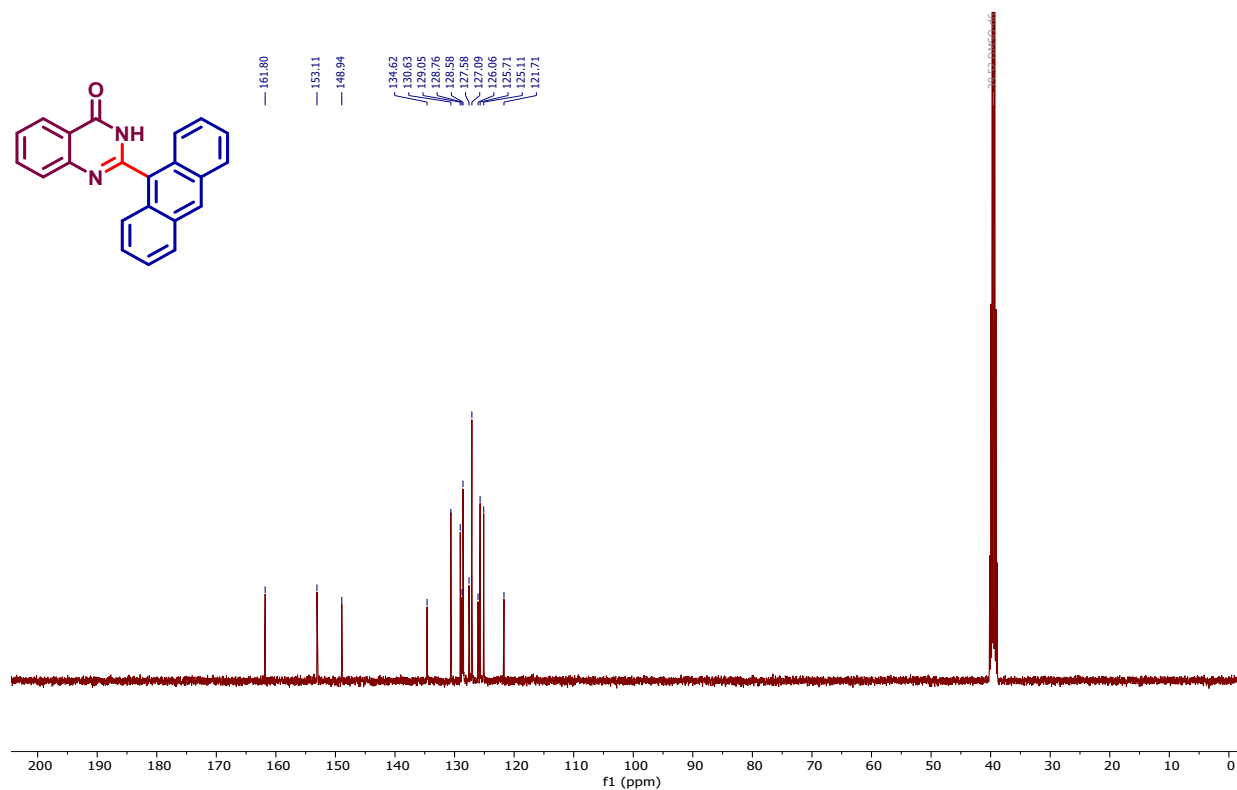


Figure S53: ¹³C NMR spectrum (100 MHz) of 3r in DMSO-d₆

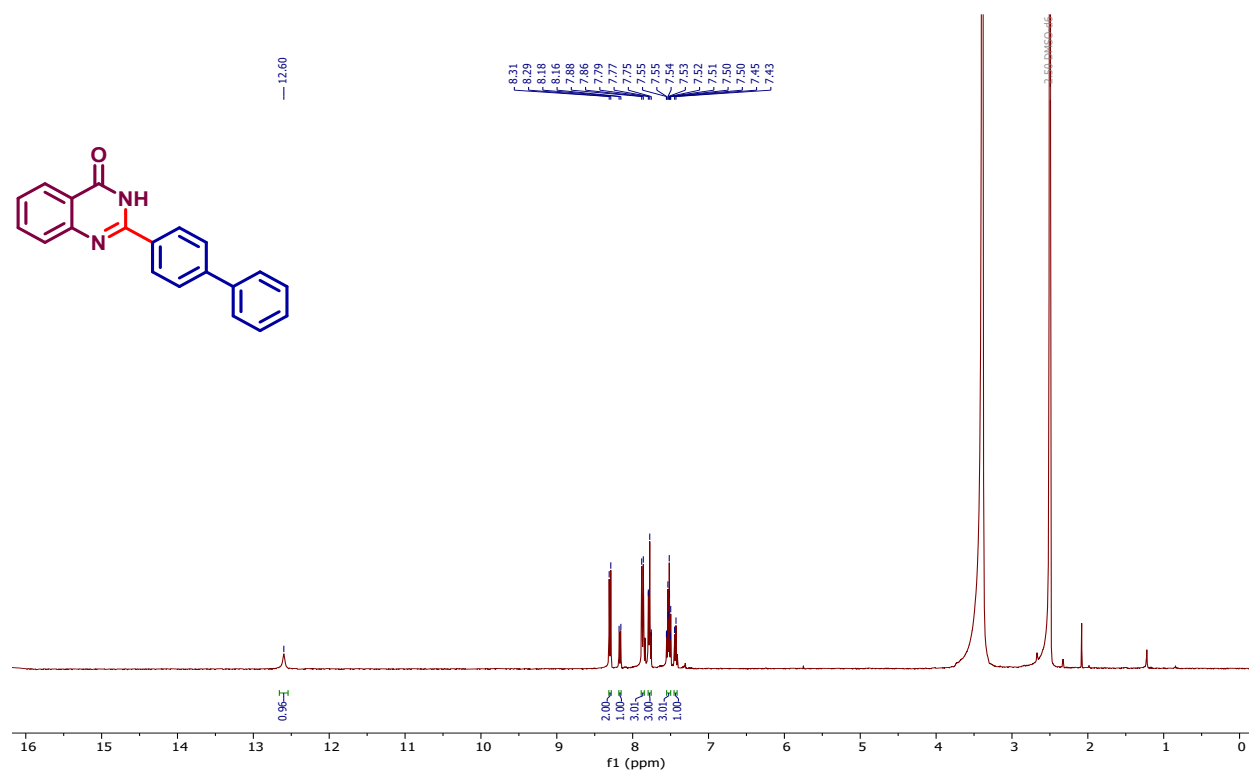


Figure S54: ¹H NMR spectrum (400 MHz) of 3s in DMSO-d₆

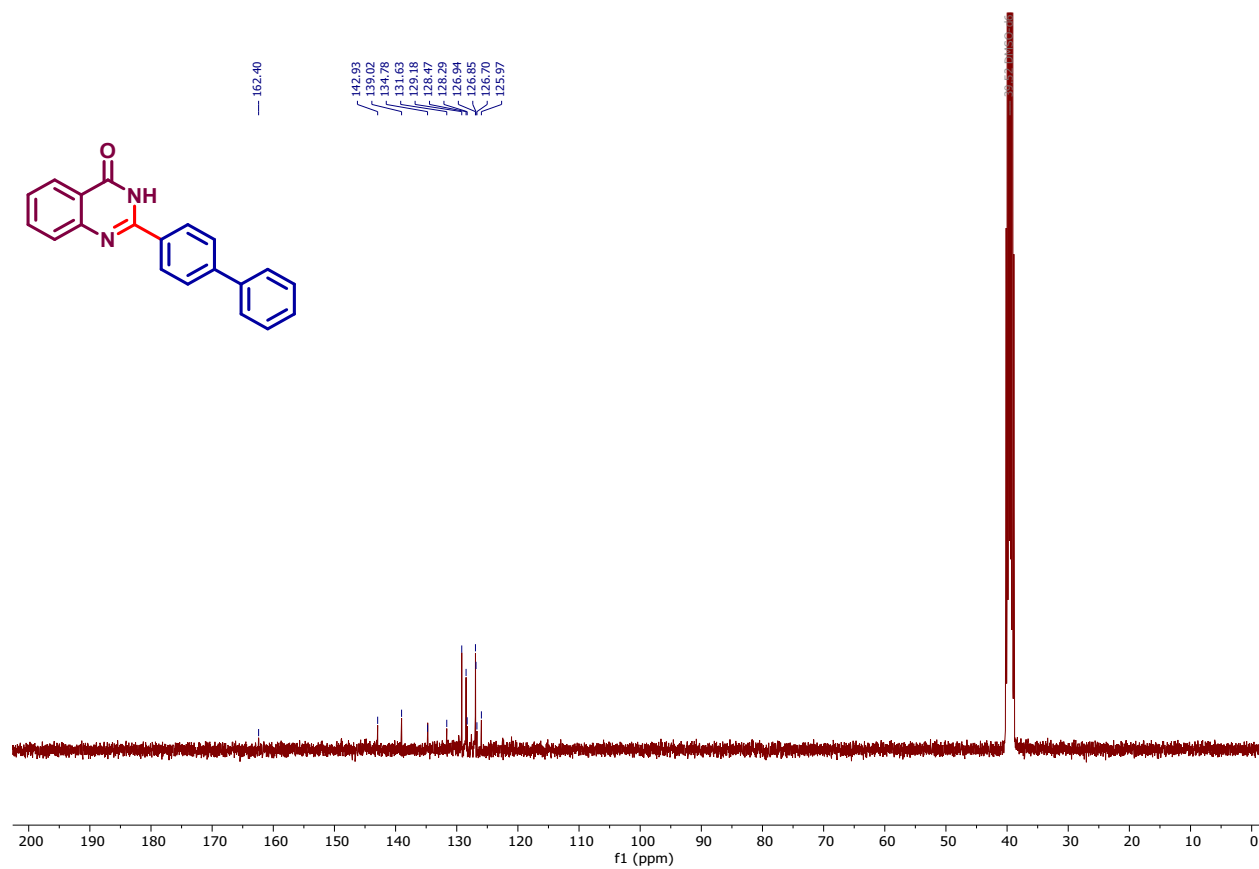


Figure S55: ¹³C NMR spectrum (100 MHz) of 3s in DMSO-d₆

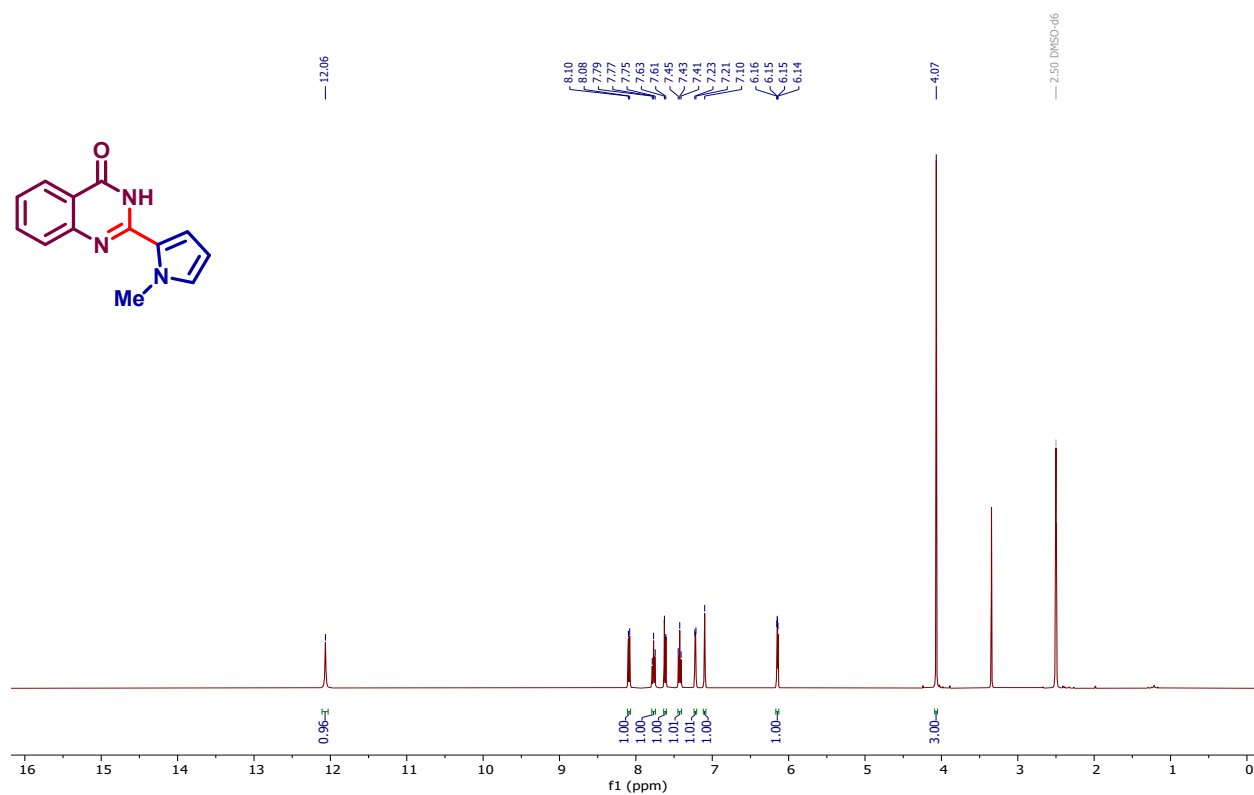


Figure S56: ¹H NMR spectrum (400 MHz) of 3t in DMSO-d₆

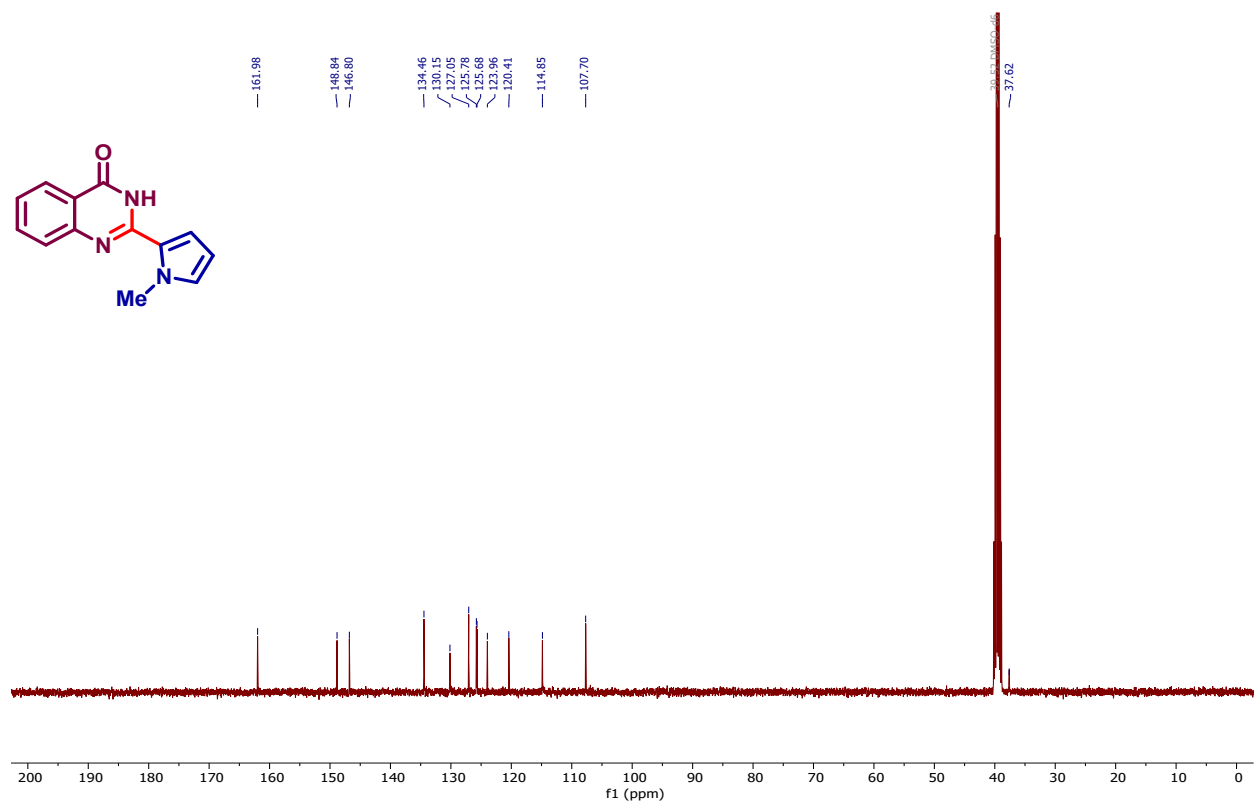


Figure S57: ¹³C NMR spectrum (100 MHz) of 3t in DMSO-d₆

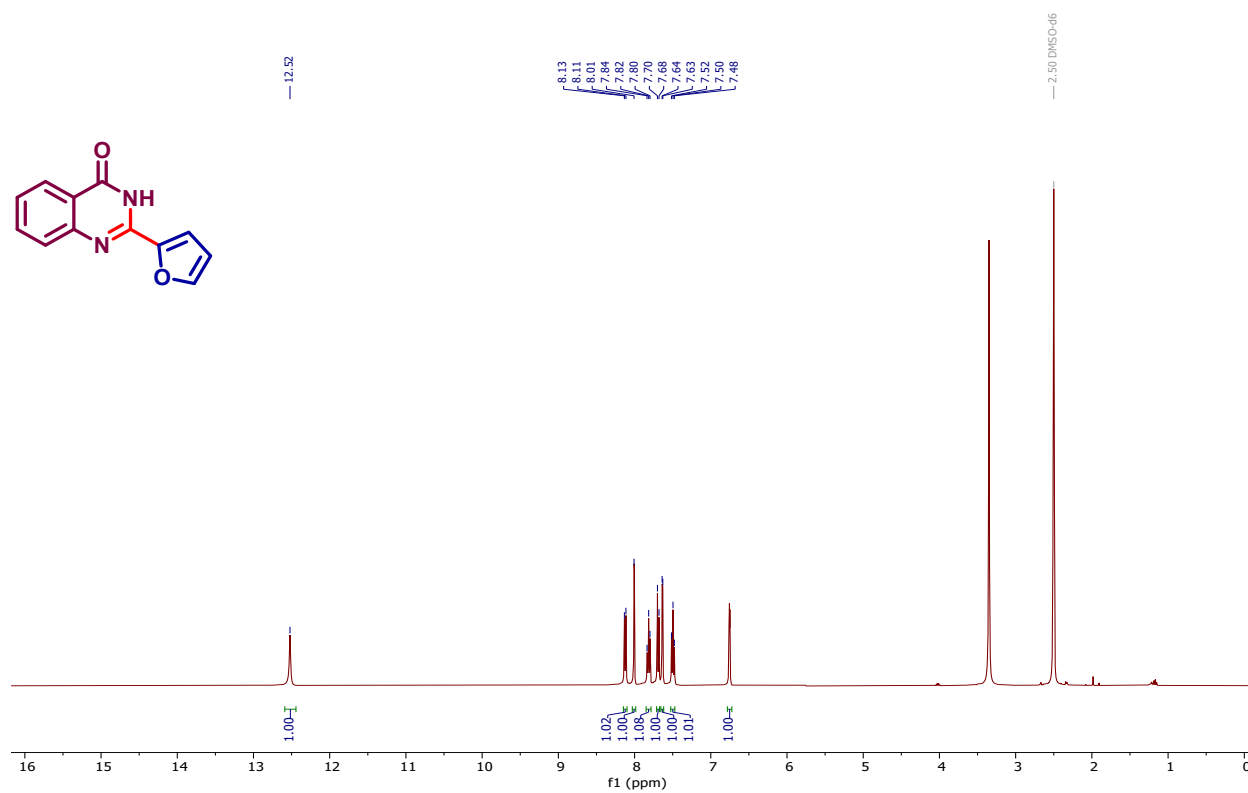


Figure S58: ¹H NMR spectrum (400 MHz) of 3u in DMSO-d₆

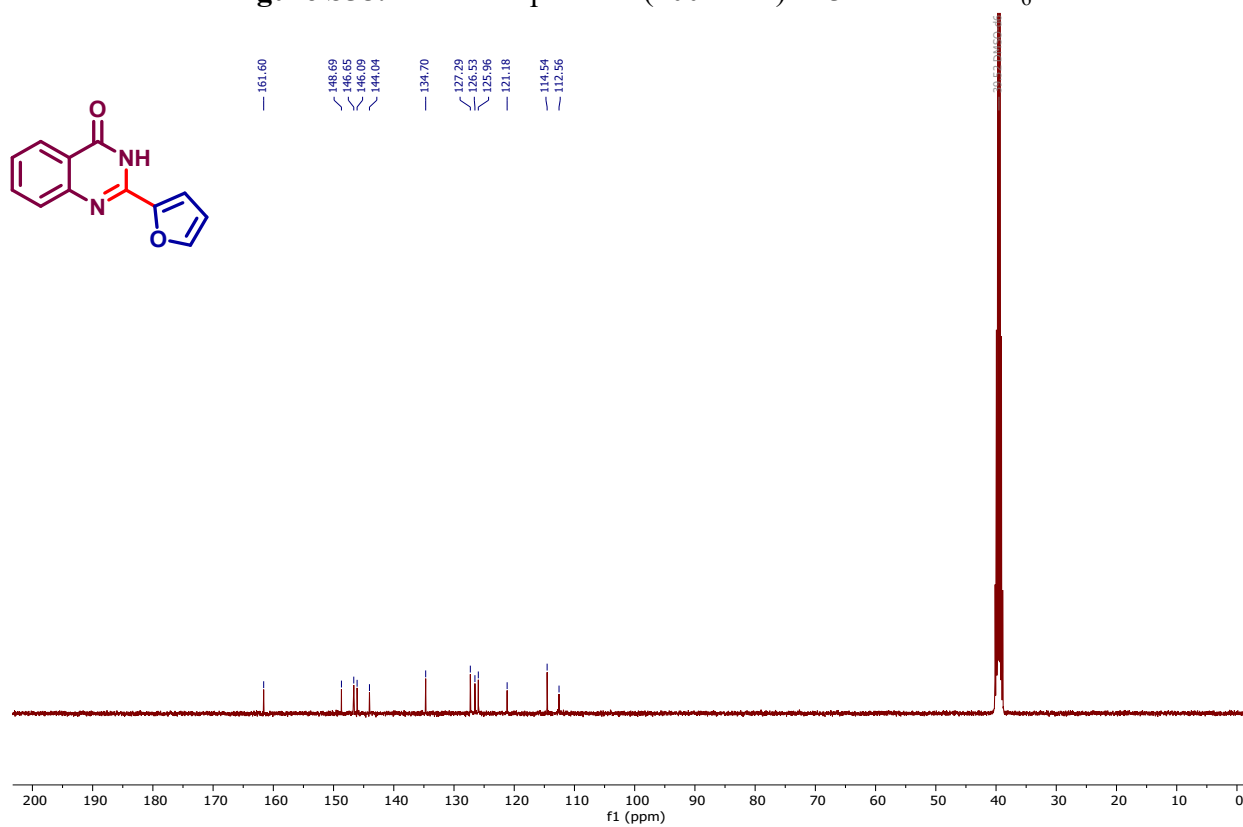
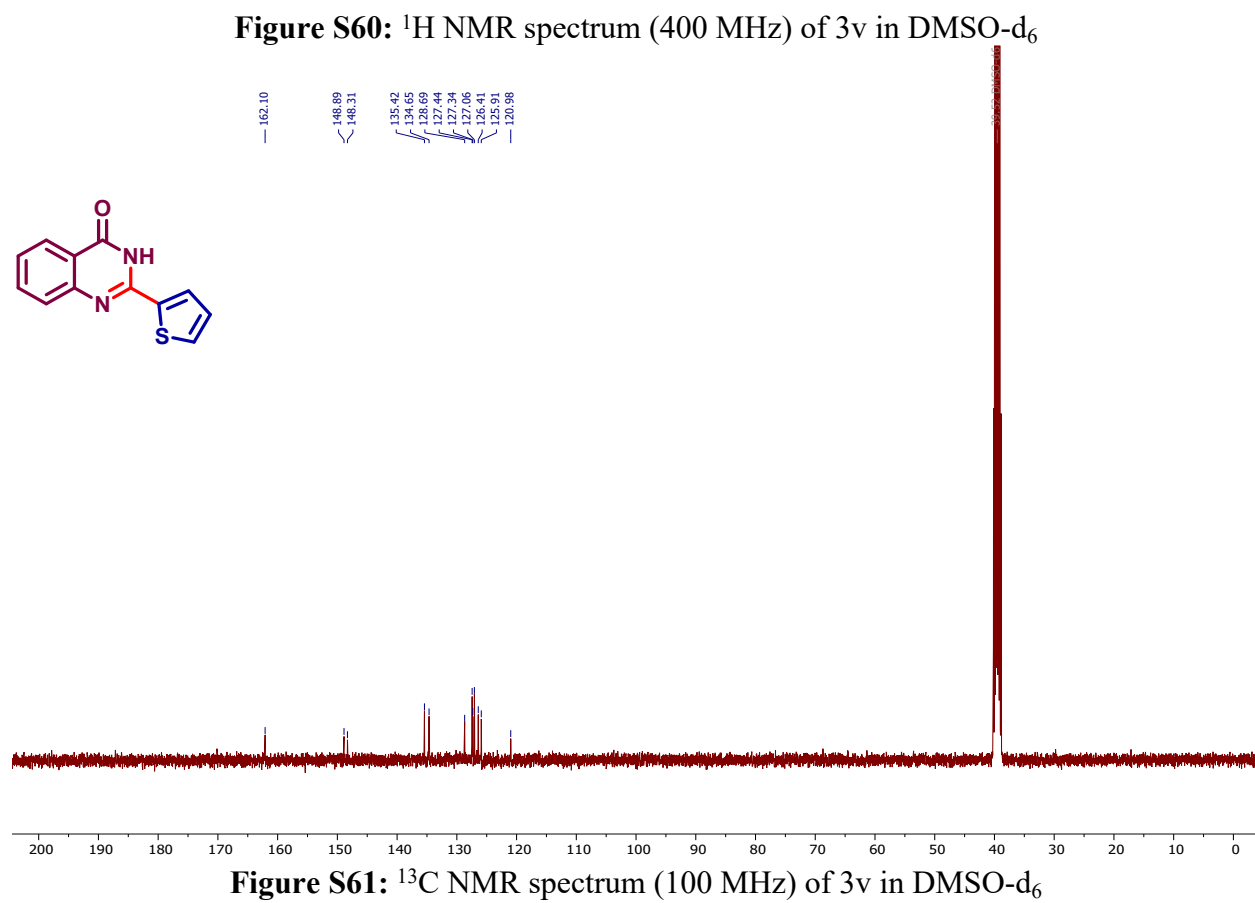
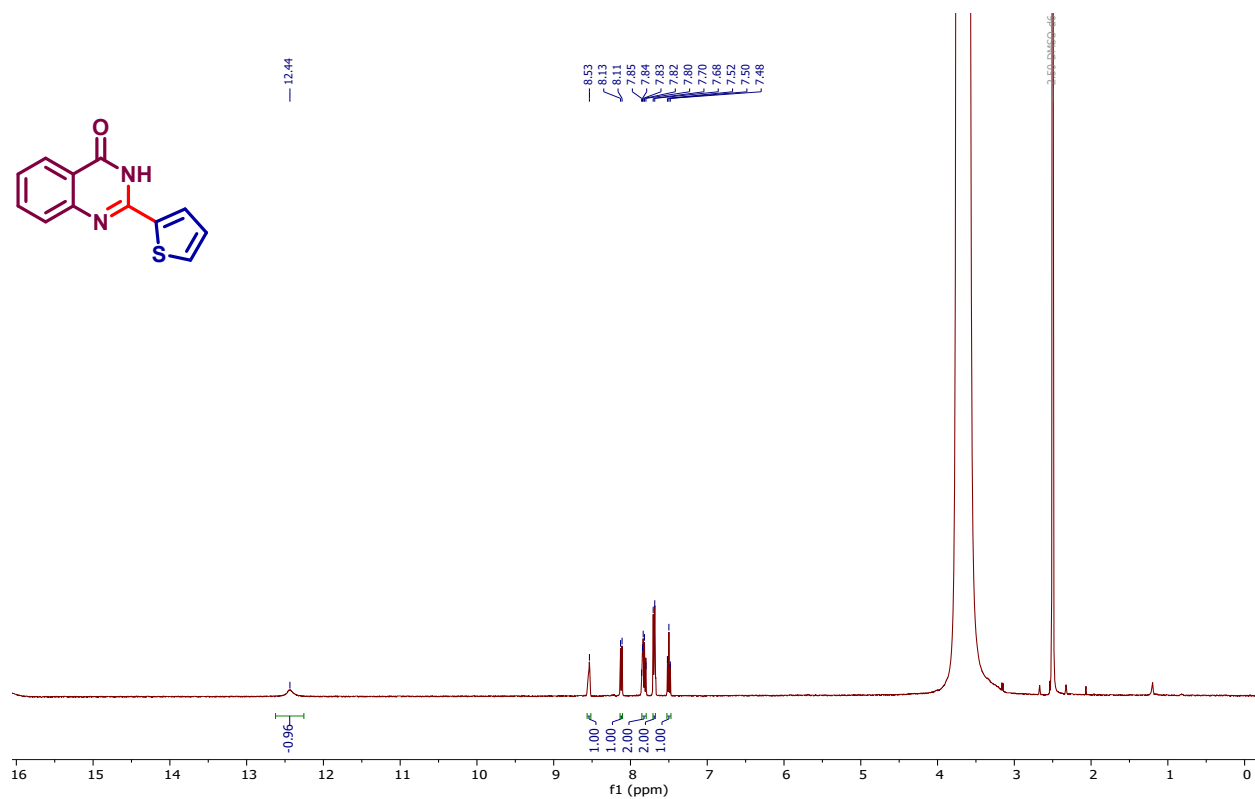


Figure S59: ¹³C NMR spectrum (100 MHz) of 3u in DMSO-d₆



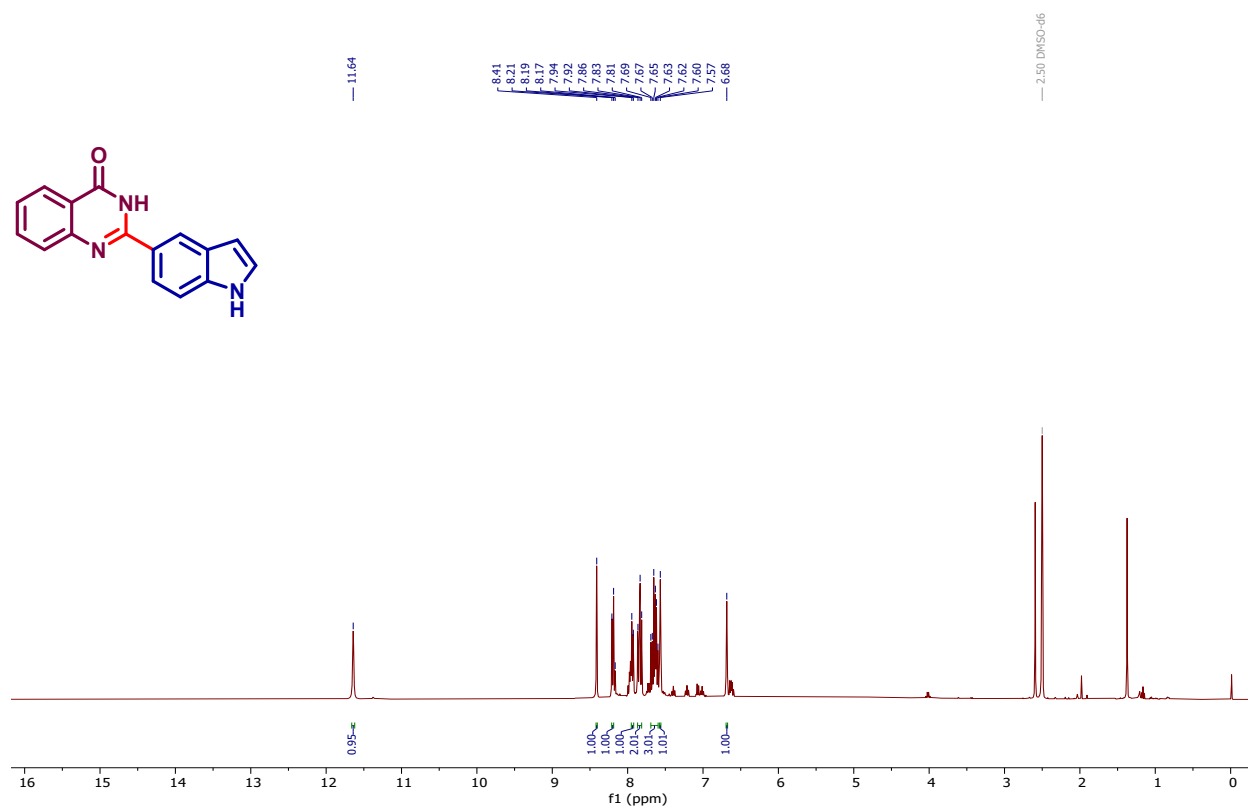


Figure S62: ¹H NMR spectrum (400 MHz) of 3w in DMSO-d₆

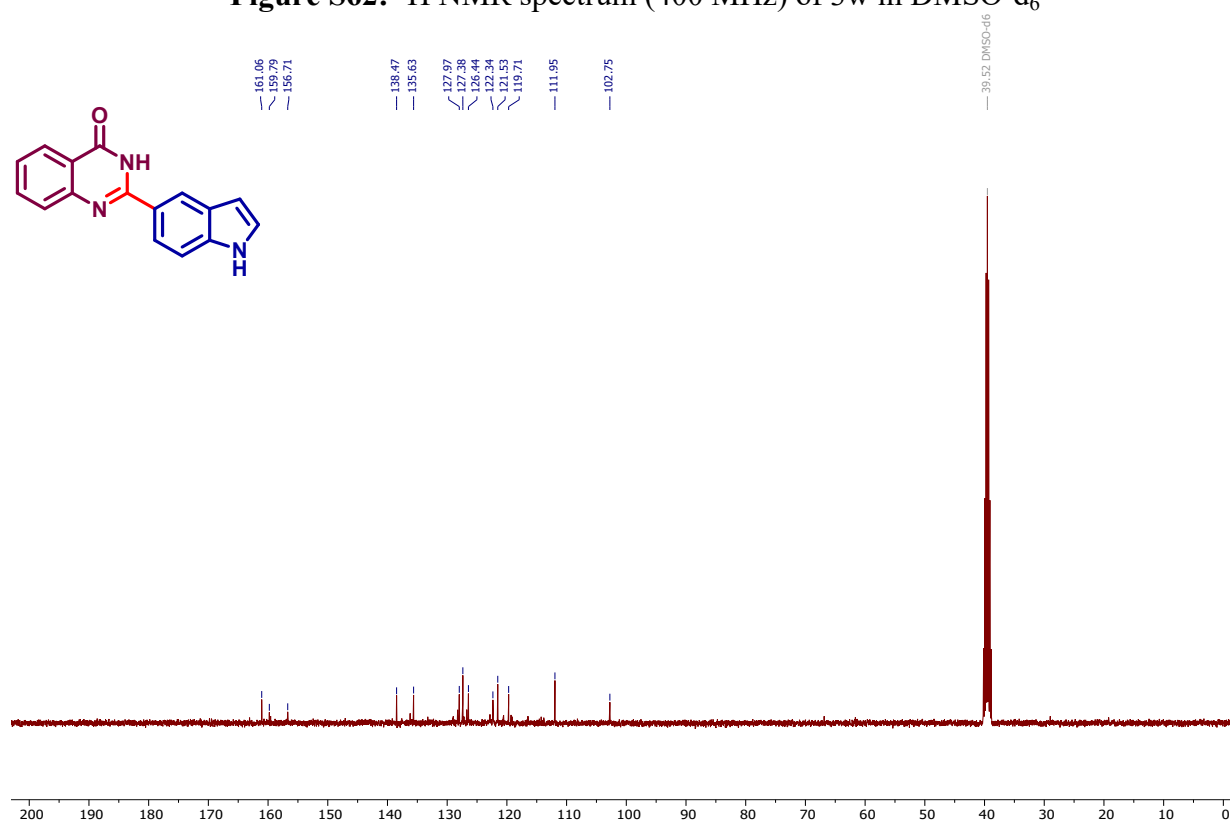


Figure S63: ¹³C NMR spectrum (100 MHz) of 3w in DMSO-d₆

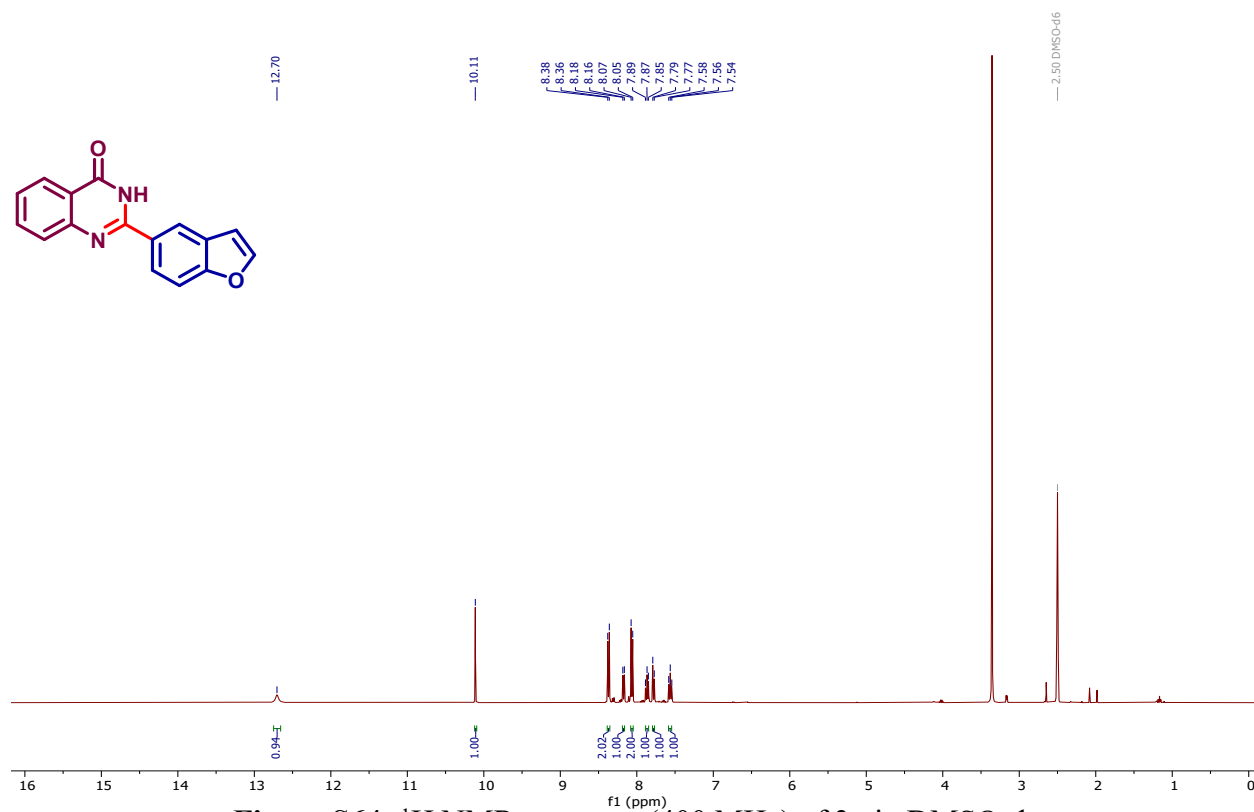


Figure S64: ¹H NMR spectrum (400 MHz) of 3x in DMSO-d₆

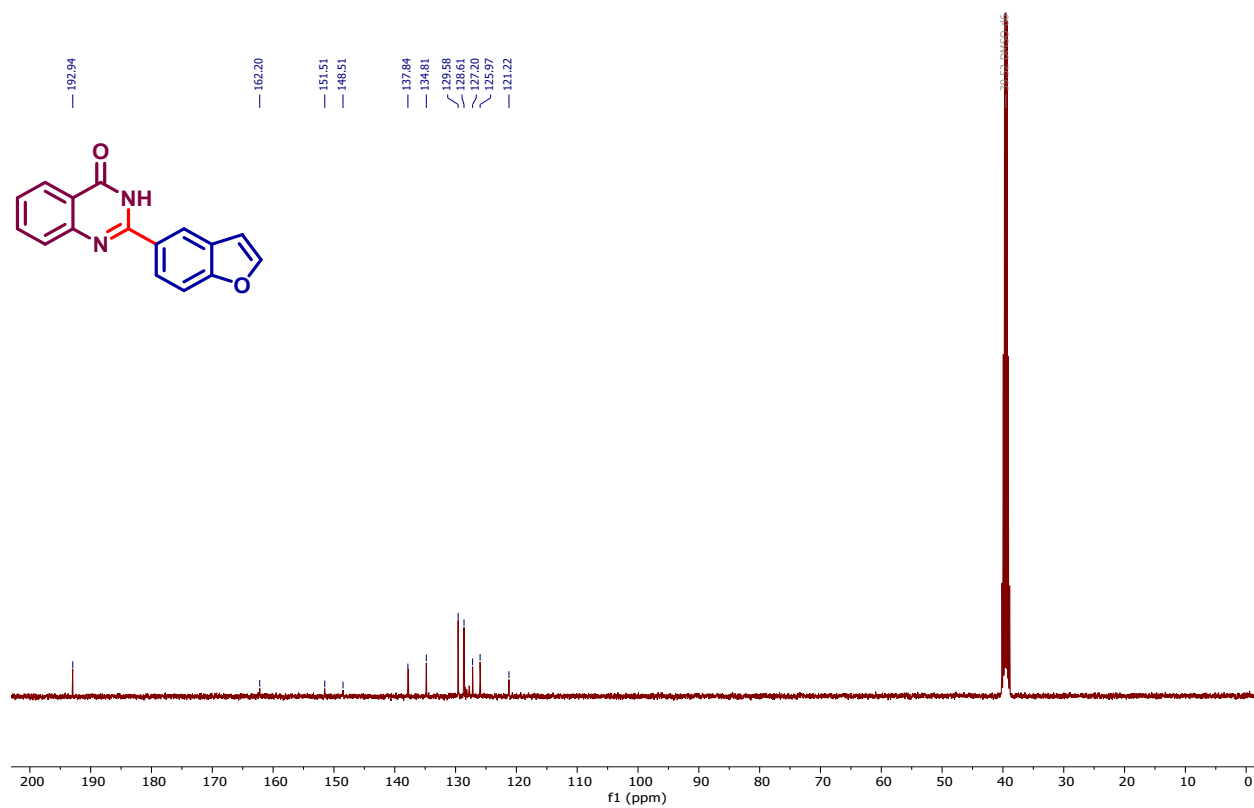


Figure S65: ¹³C NMR spectrum (100 MHz) of 3x in DMSO-d₆

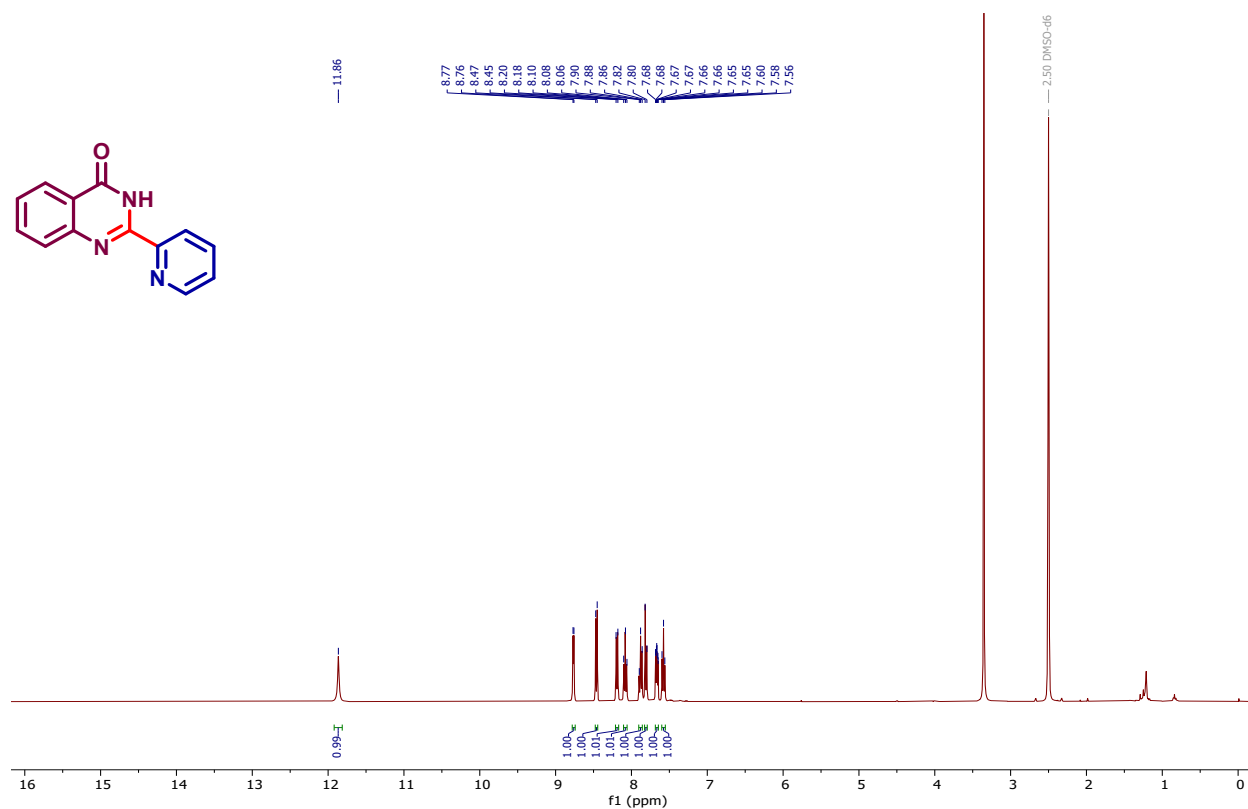


Figure S66: ¹H NMR spectrum (400 MHz) of 3y in DMSO-d₆

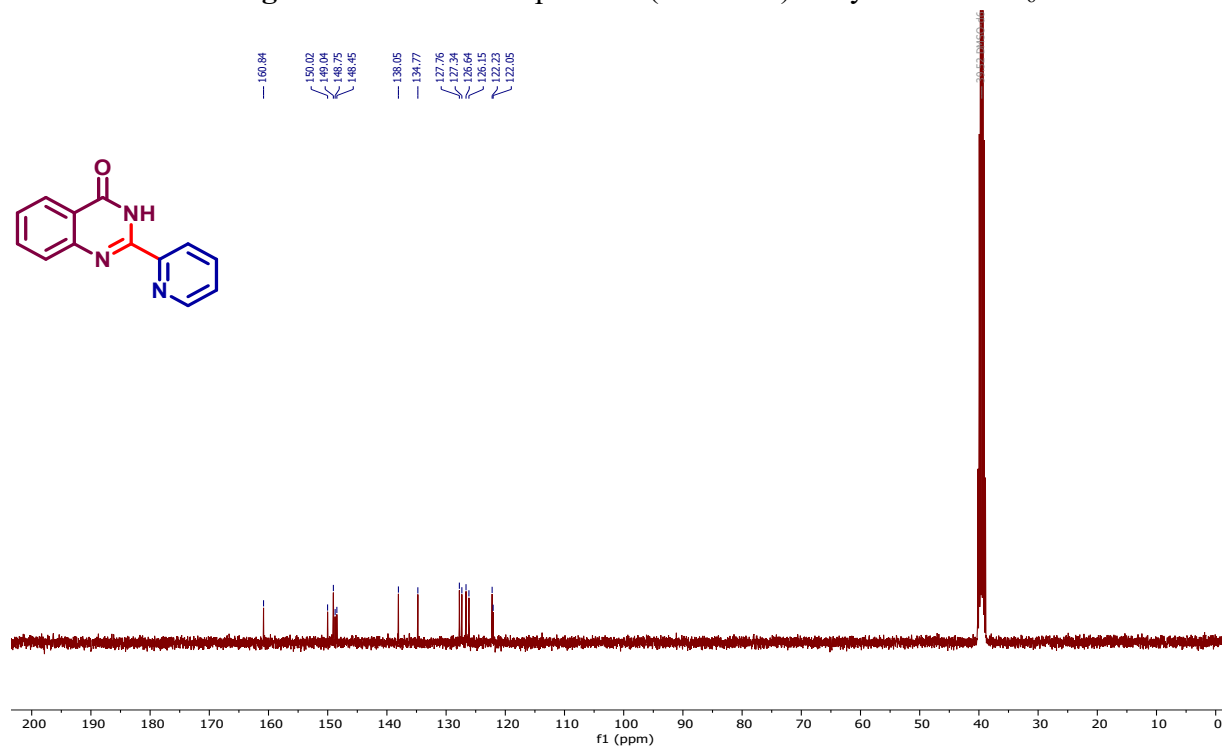


Figure S67: ¹³C NMR spectrum (100 MHz) of 3y in DMSO-d₆

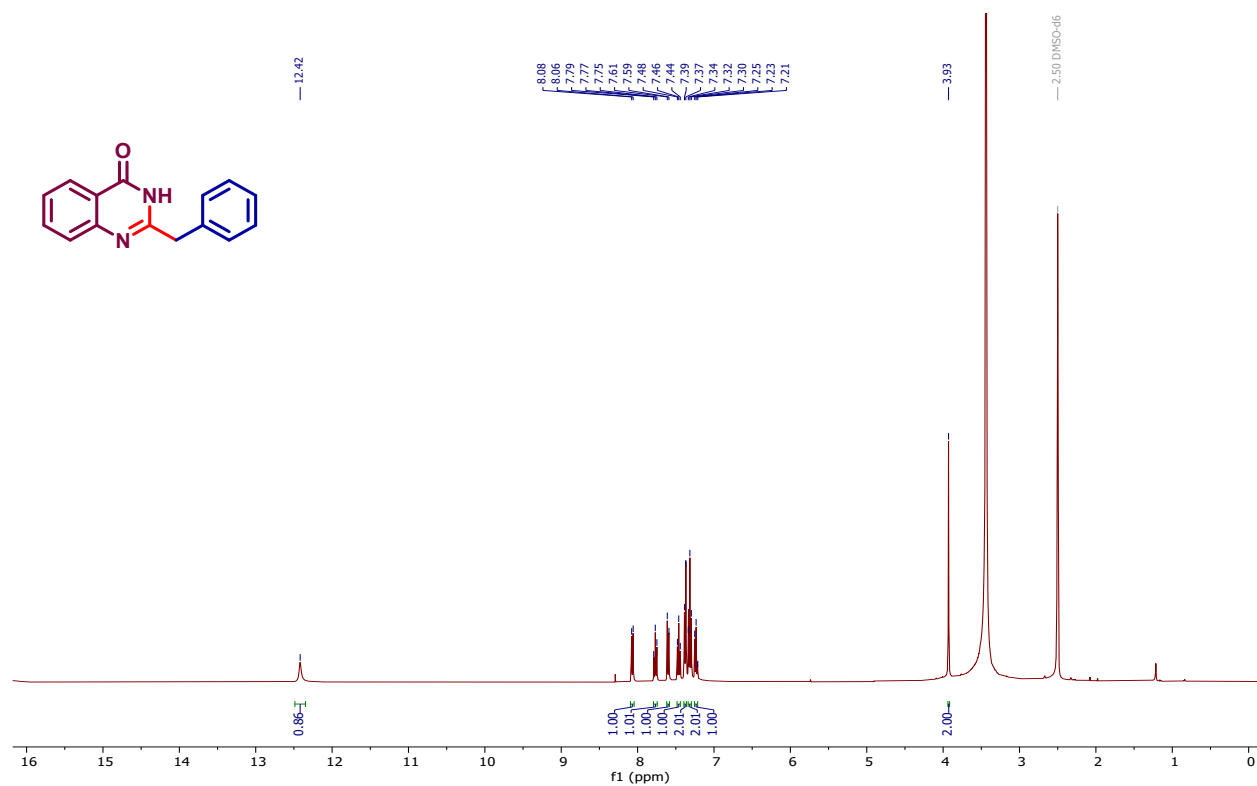


Figure S68: ¹H NMR spectrum (400 MHz) of 3z in DMSO-d₆

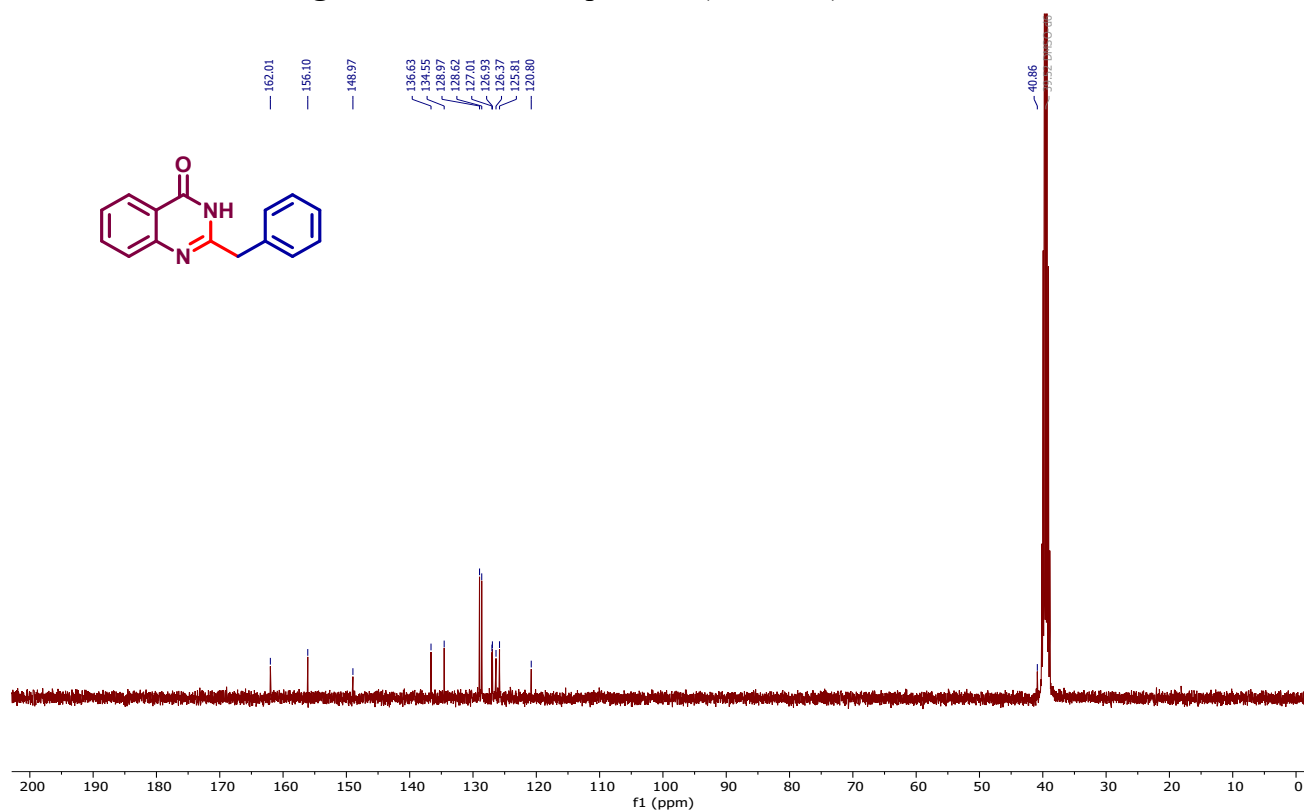


Figure S69: ¹³C NMR spectrum (100 MHz) of 3z in DMSO-d₆

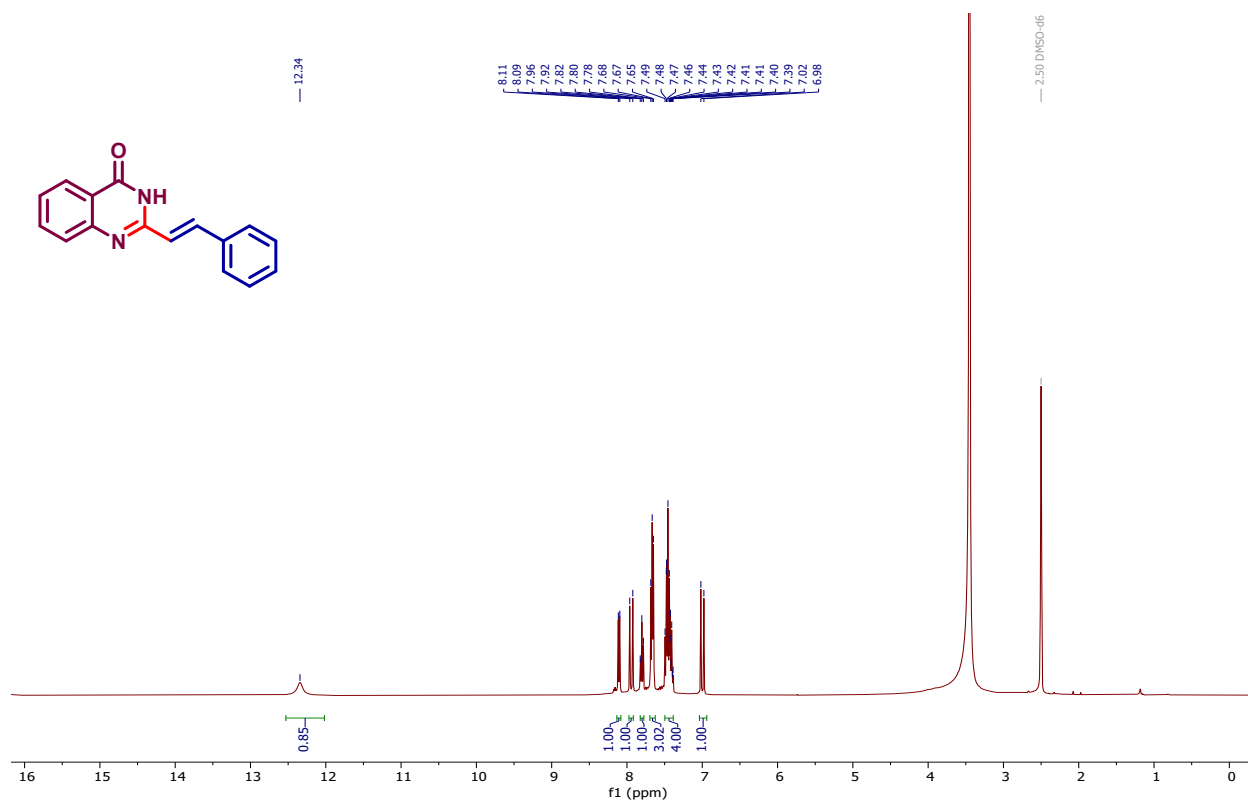


Figure S70: ¹H NMR spectrum (400 MHz) of 3za in DMSO-d₆

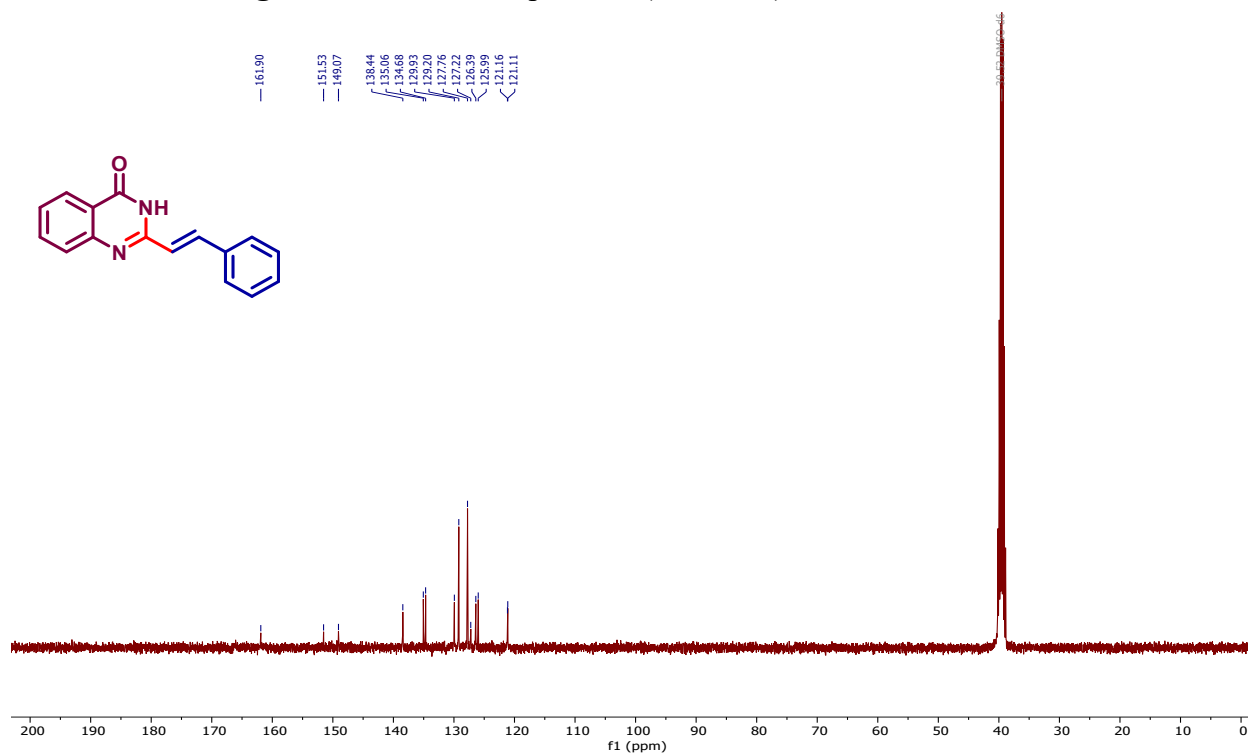


Figure S71: ¹³C NMR spectrum (100 MHz) of 3za in DMSO-d₆

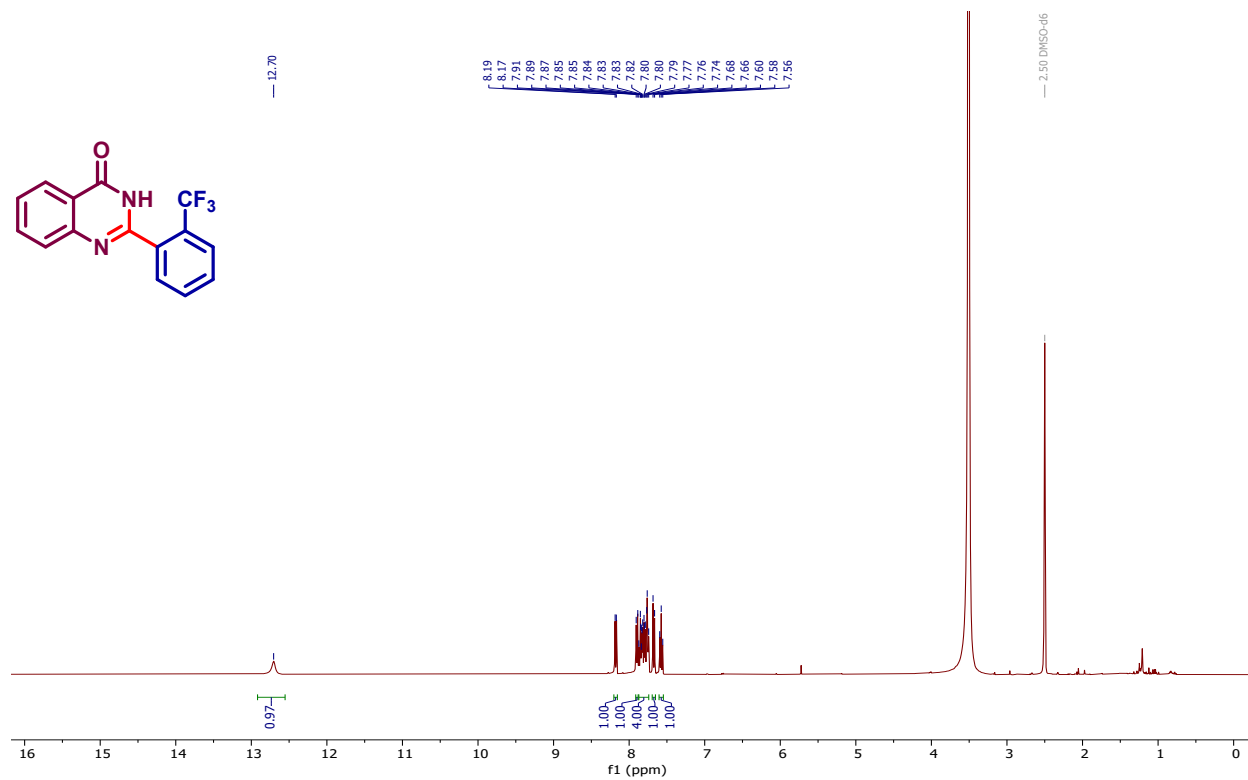


Figure S72: ¹H NMR spectrum (400 MHz) of 3zb in DMSO-d₆

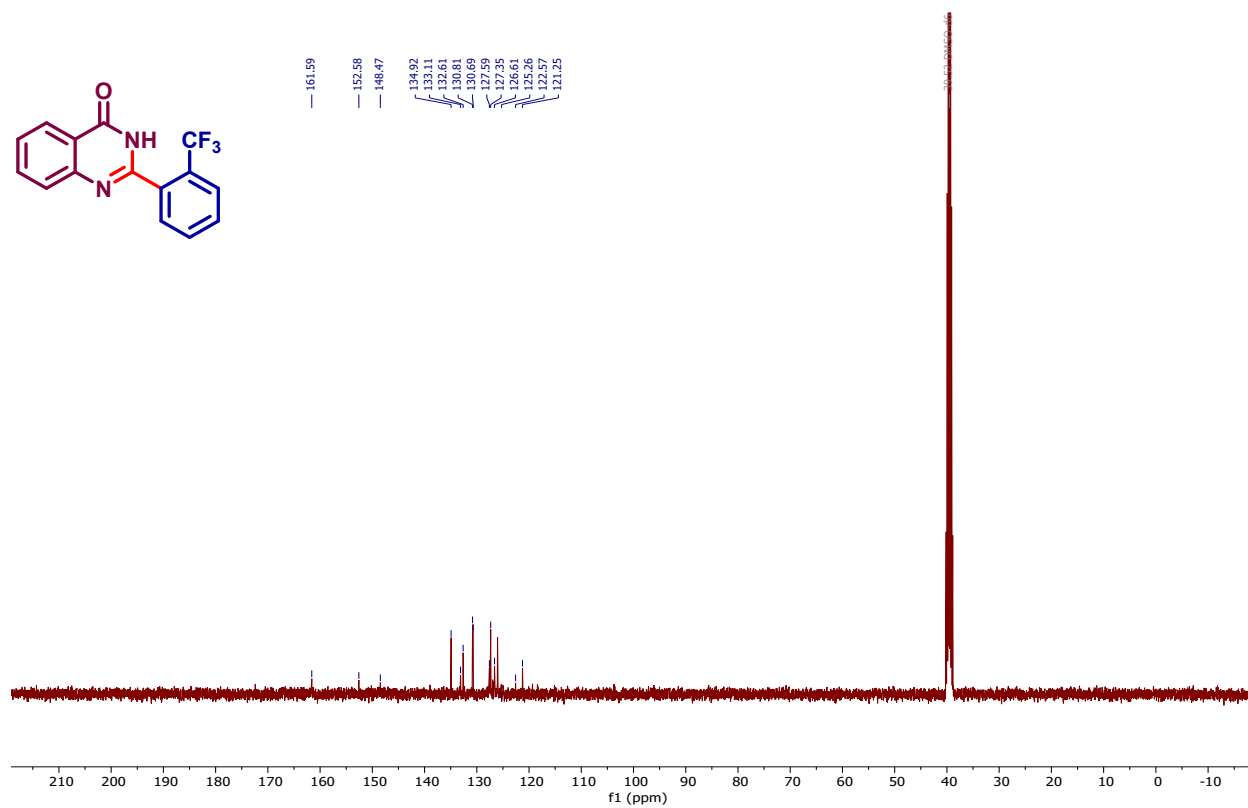


Figure S73: ¹³C NMR spectrum (100 MHz) of 3zb in DMSO-d₆

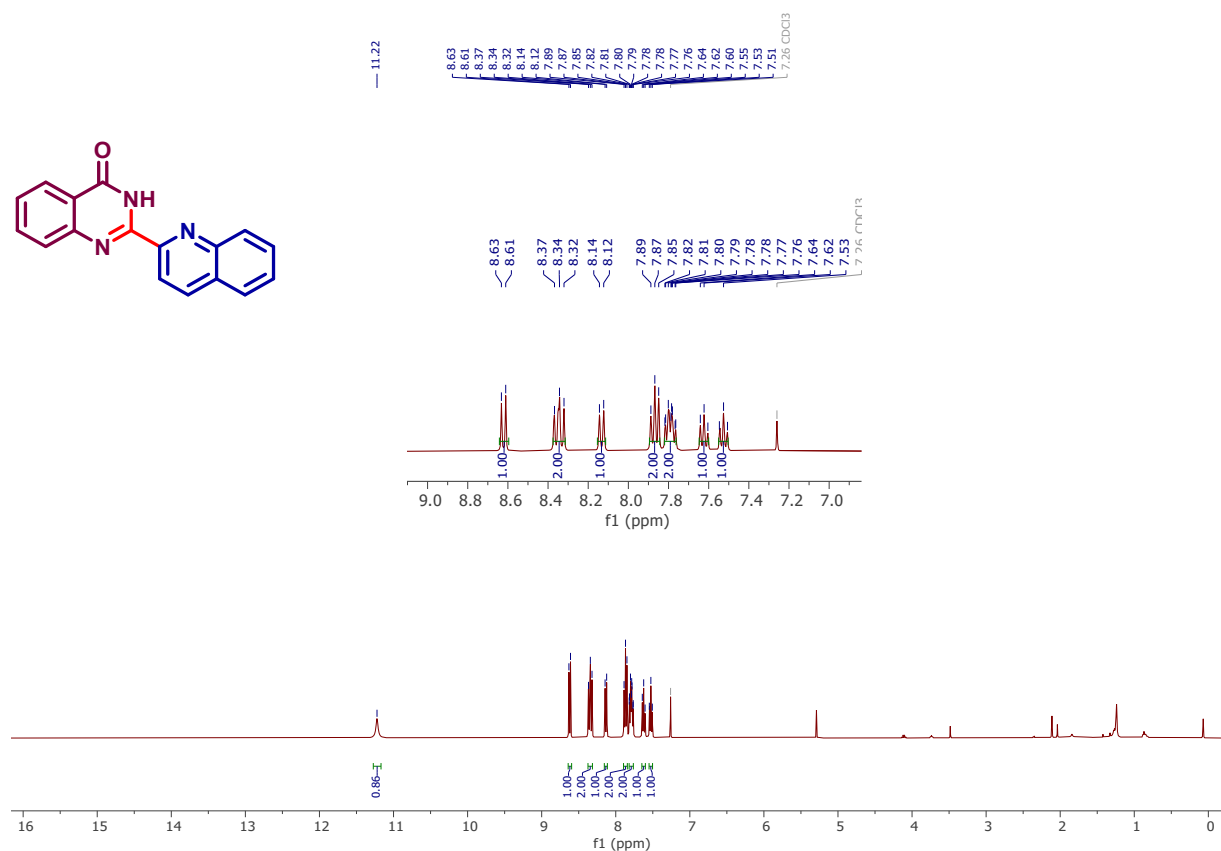


Figure S74: ¹H NMR spectrum (400 MHz) of 3zc in CDCl₃

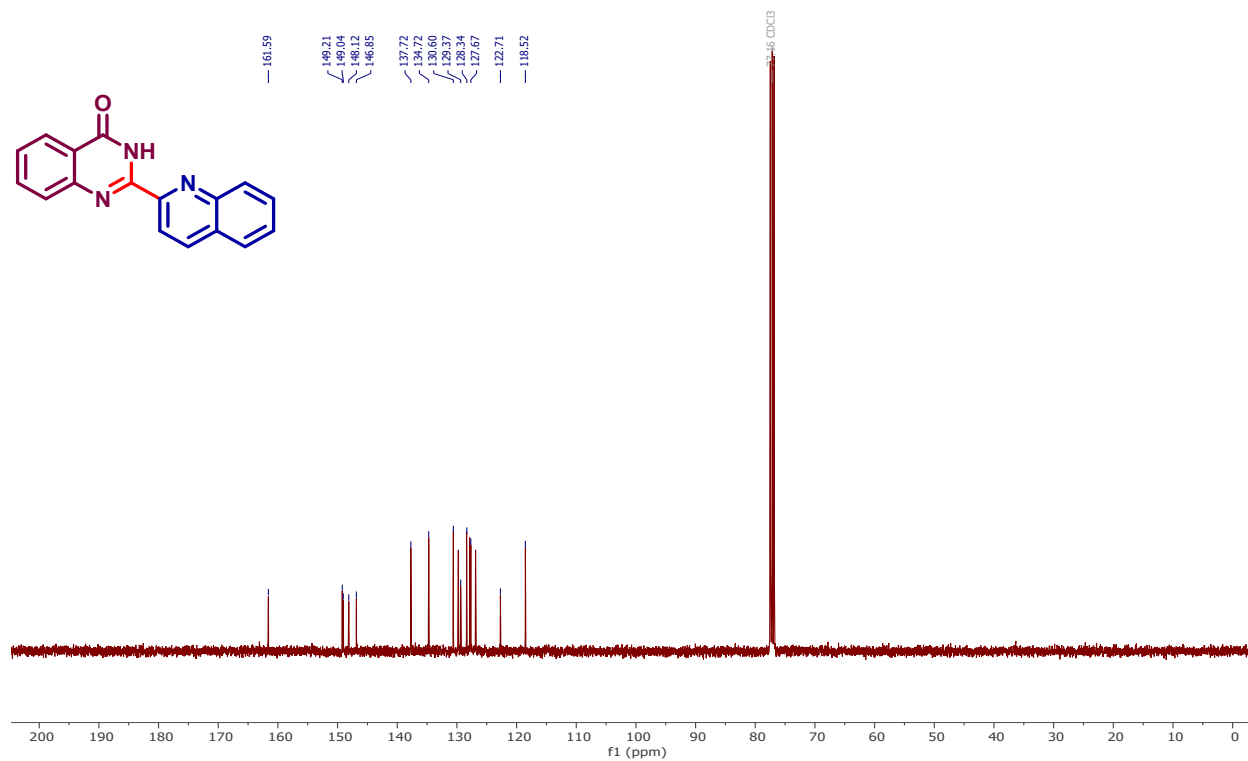


Figure S75: ¹³C NMR spectrum (100 MHz) of 3zc in CDCl₃

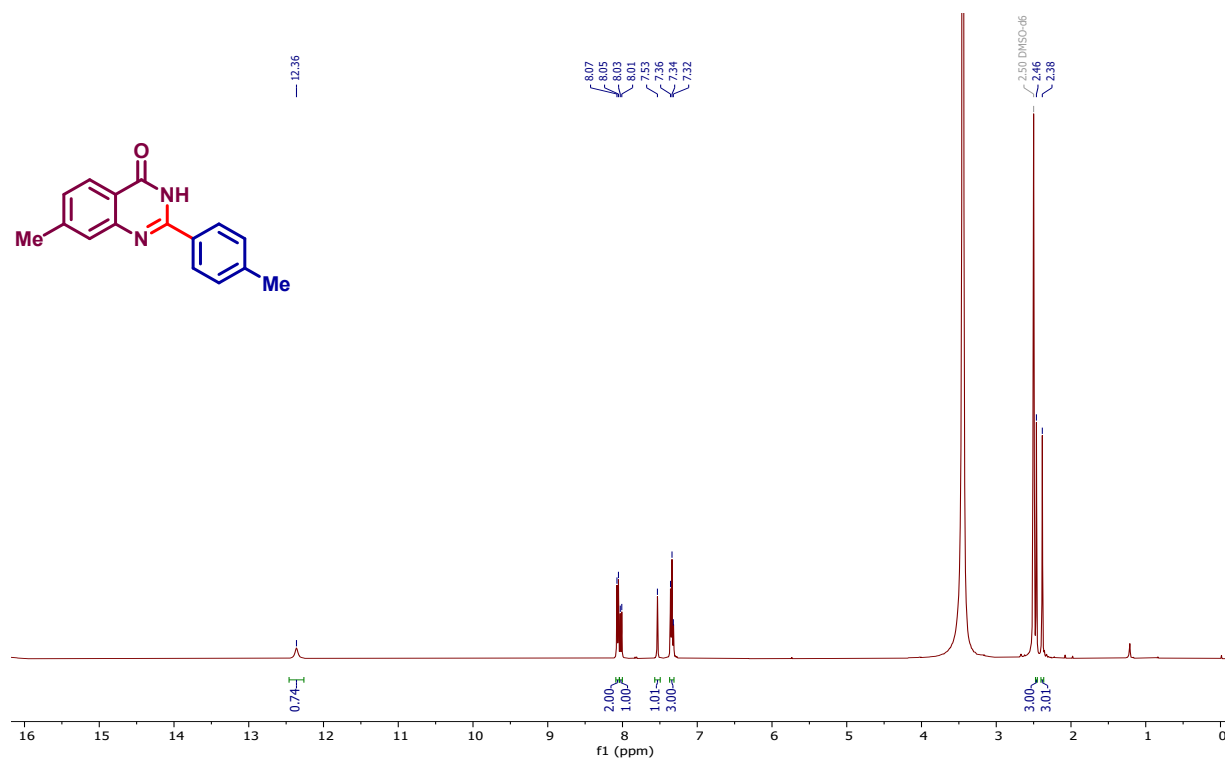


Figure S76: ¹H NMR spectrum (400 MHz) of 6a in DMSO-d₆

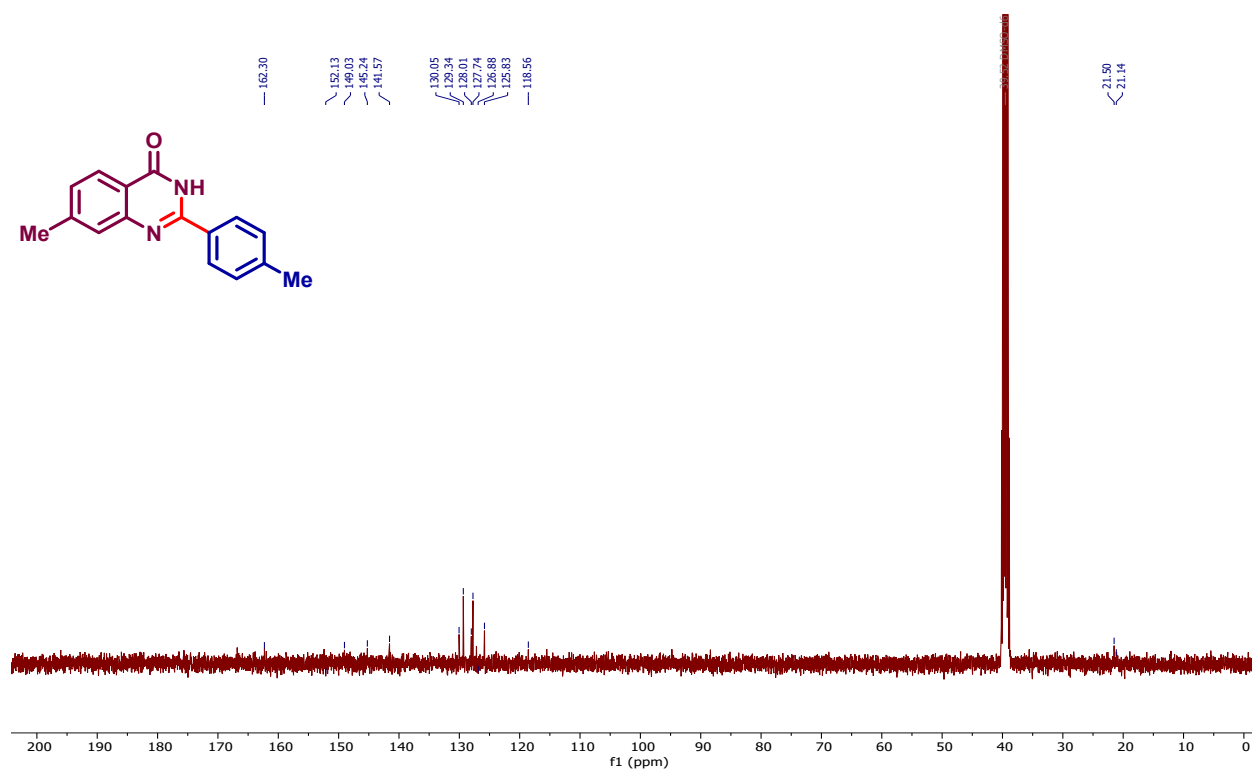


Figure S77: ¹³C NMR spectrum (100 MHz) of 6a in DMSO-d₆

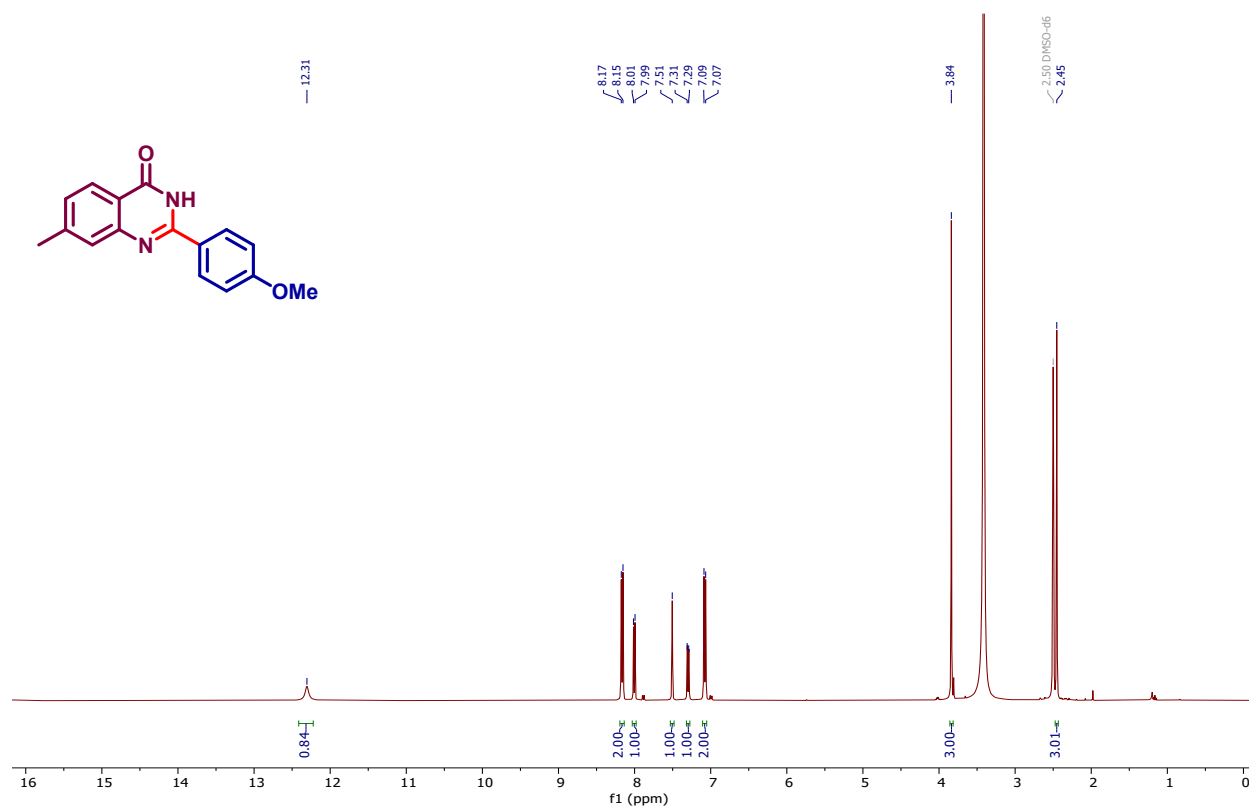


Figure S78: ¹H NMR spectrum (400 MHz) of 6b in DMSO-d₆

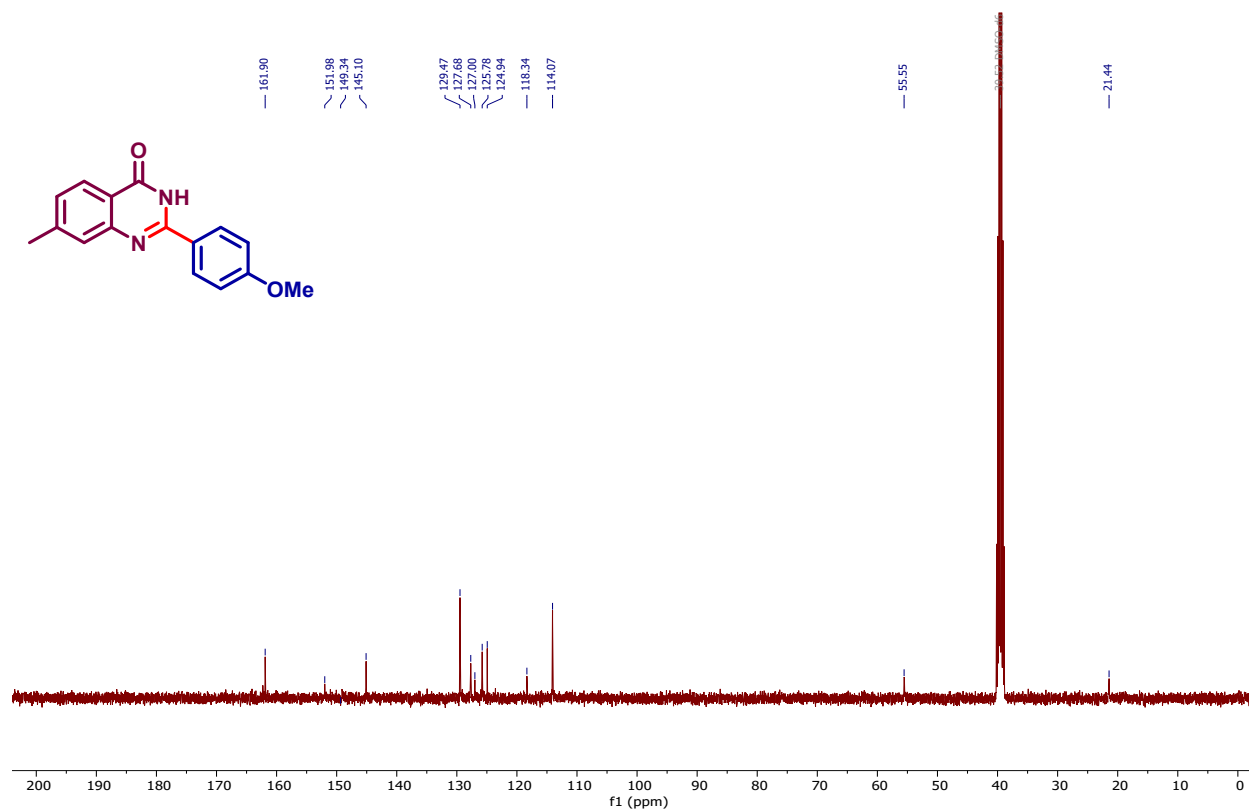


Figure S79: ¹³C NMR spectrum (100 MHz) of 6b in DMSO-d₆

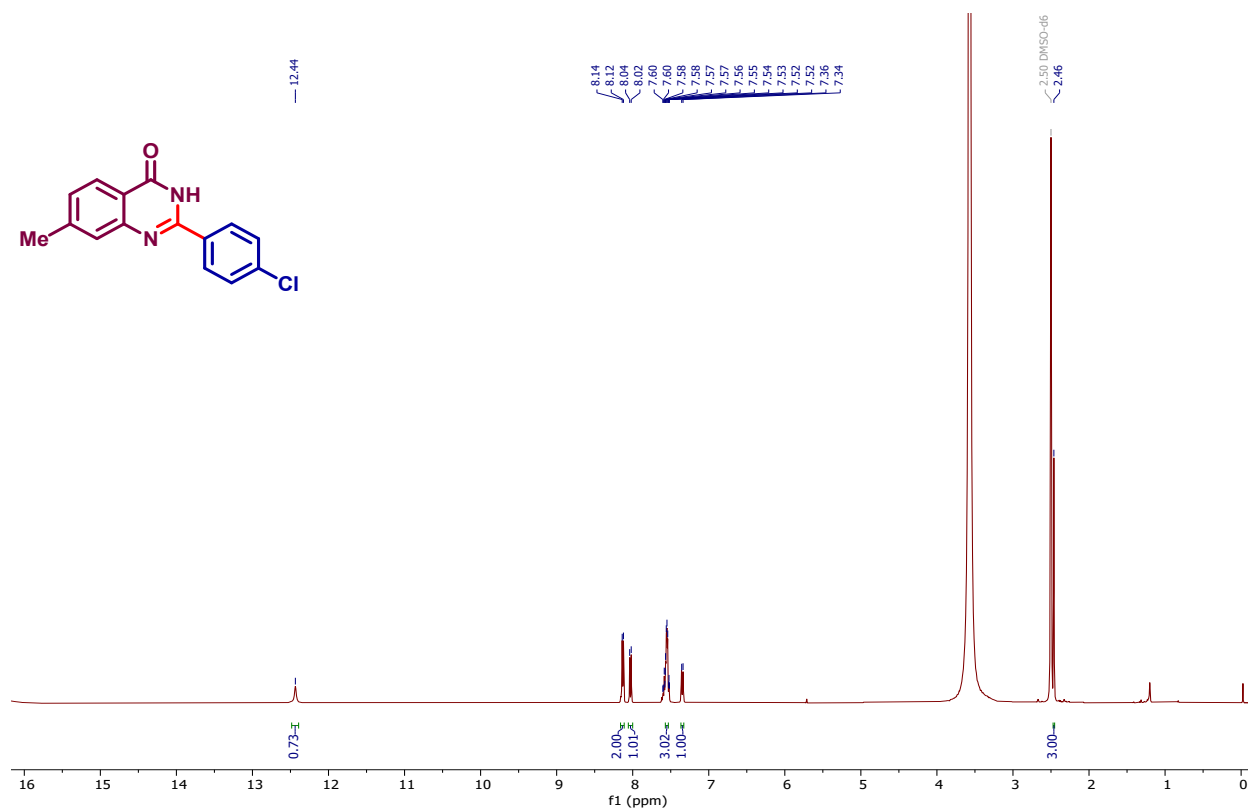


Figure S80: ¹H NMR spectrum (400 MHz) of 6c in DMSO-d₆

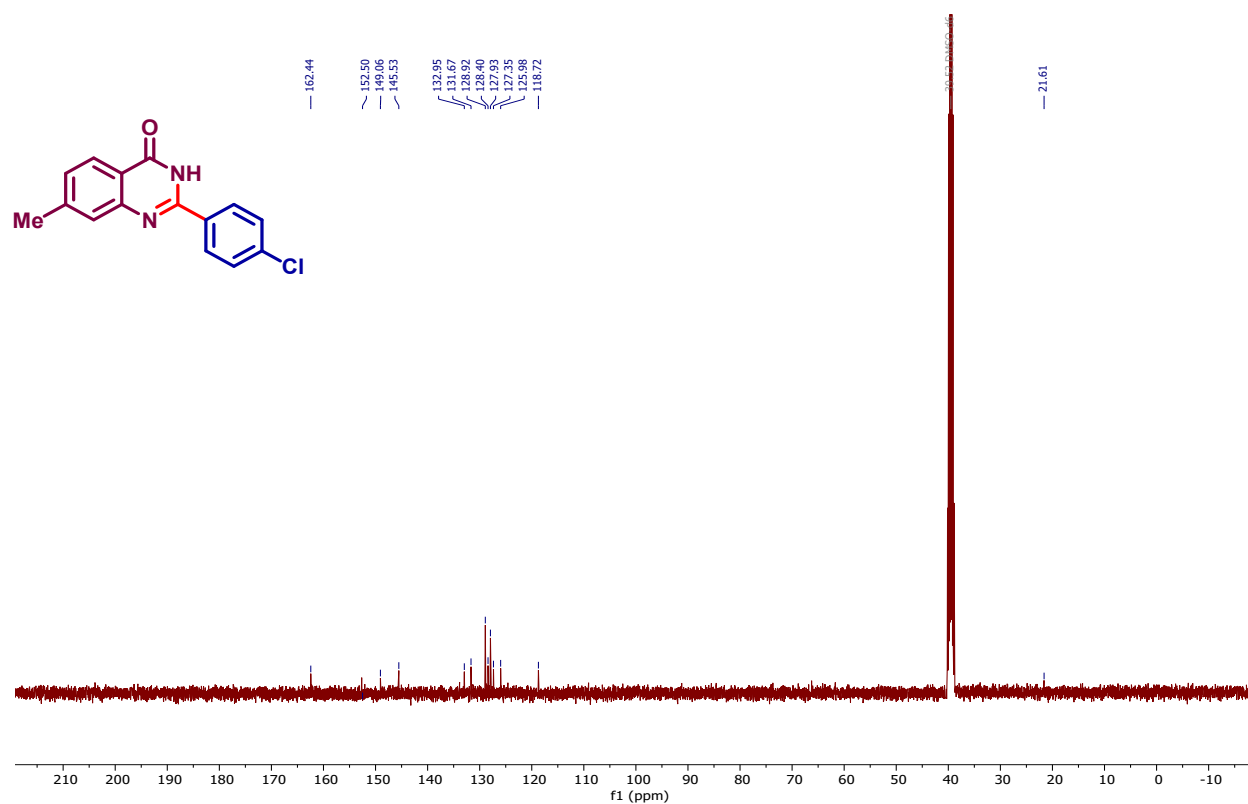


Figure S81: ¹³C NMR spectrum (100 MHz) of 6c in DMSO-d₆

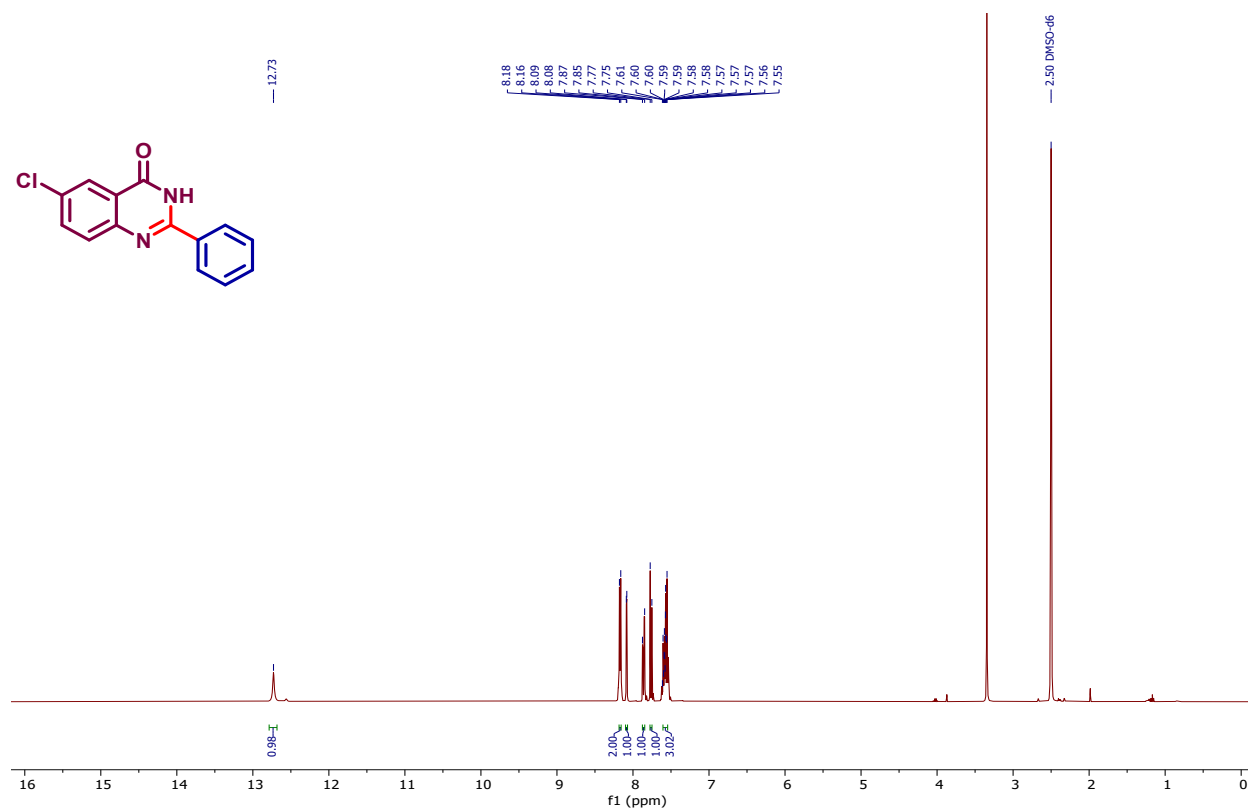


Figure S82: ¹H NMR spectrum (400 MHz) of 7a in DMSO-d₆

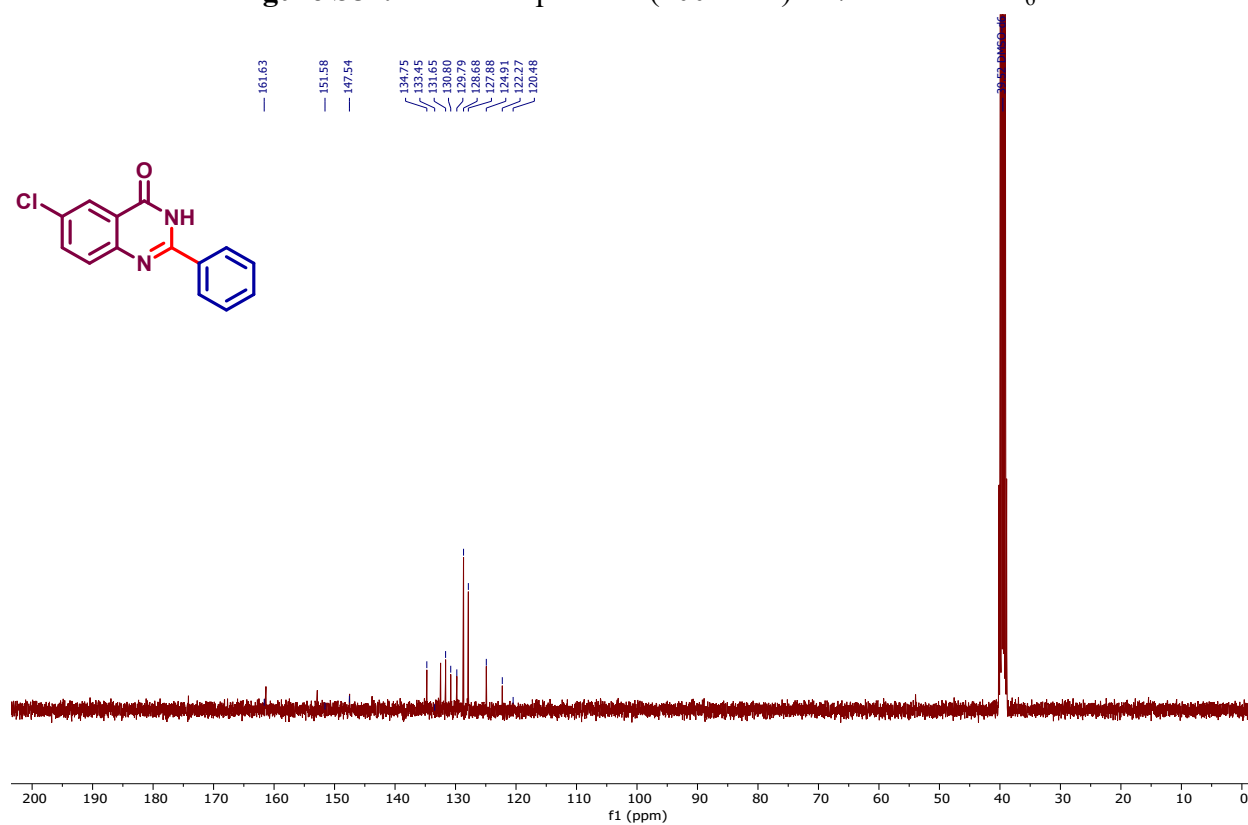


Figure S83: ¹³C NMR spectrum (100 MHz) of 7a in DMSO-d₆

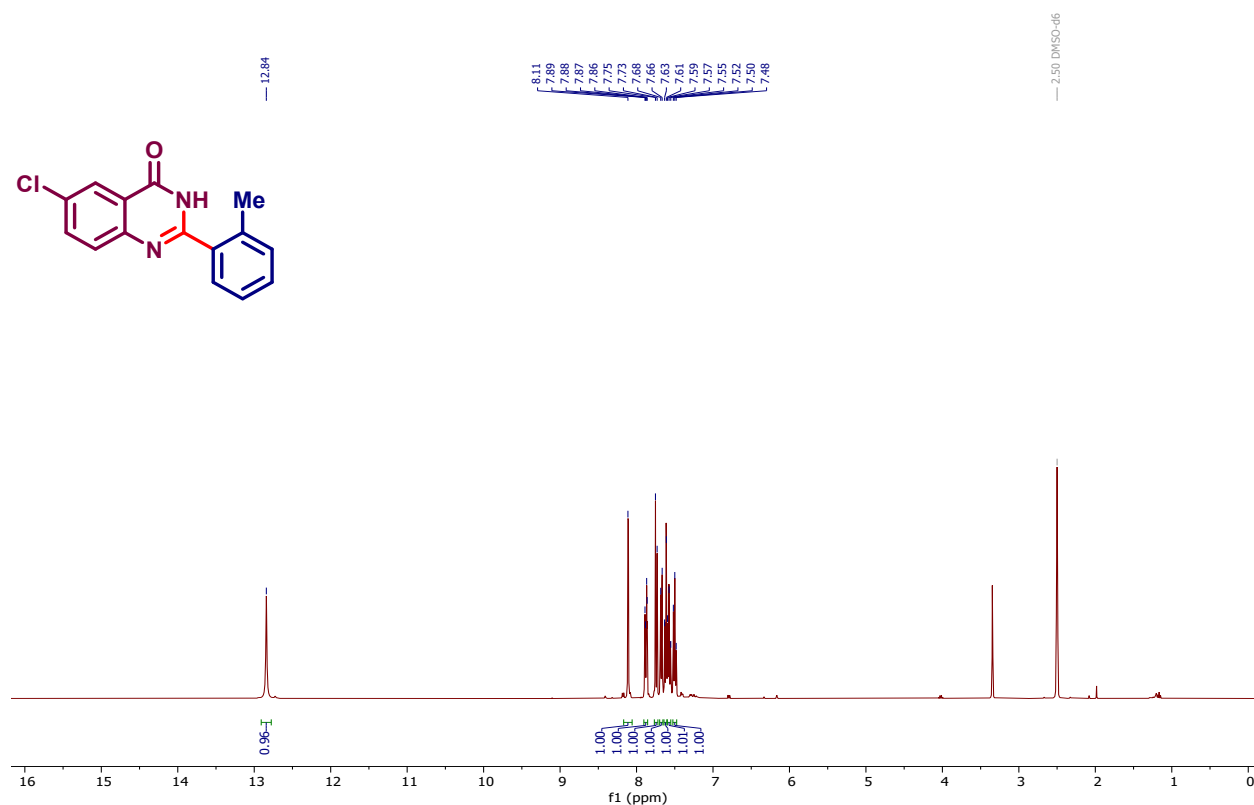


Figure S84: ¹H NMR spectrum (400 MHz) of 7b in DMSO-d₆

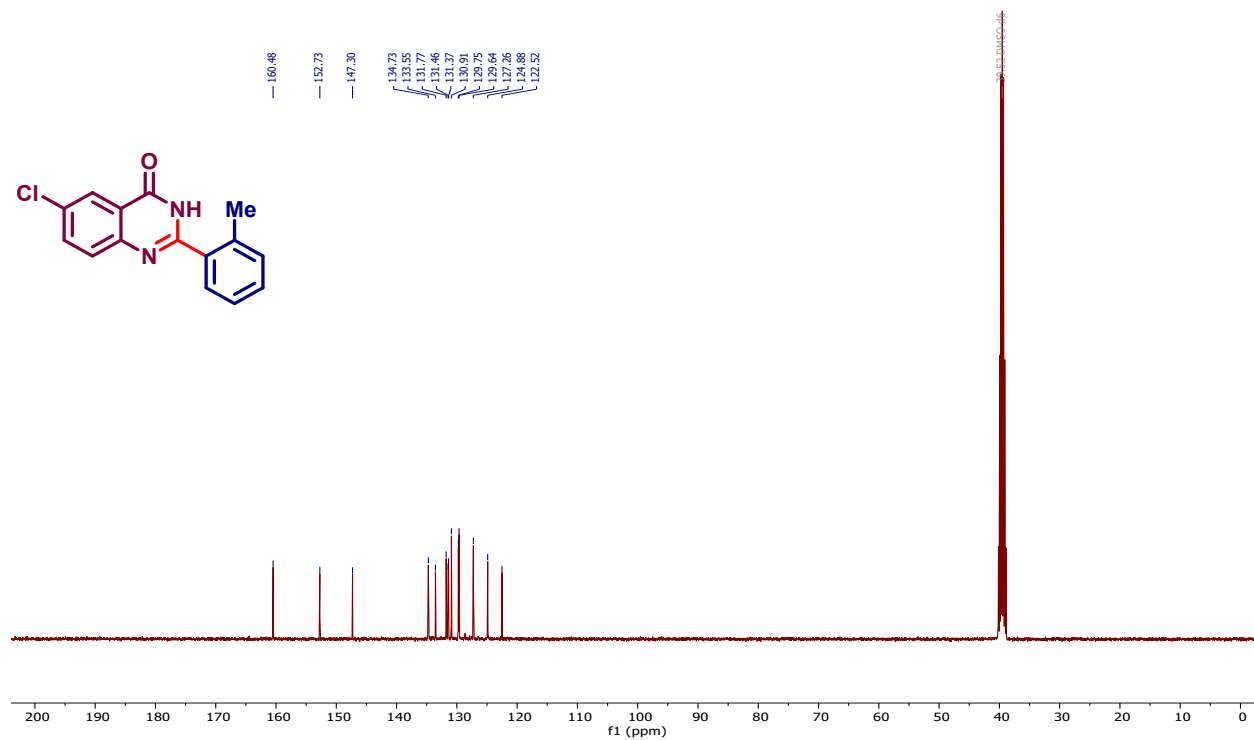


Figure S85: ¹³C NMR spectrum (100 MHz) of 7b in DMSO-d₆

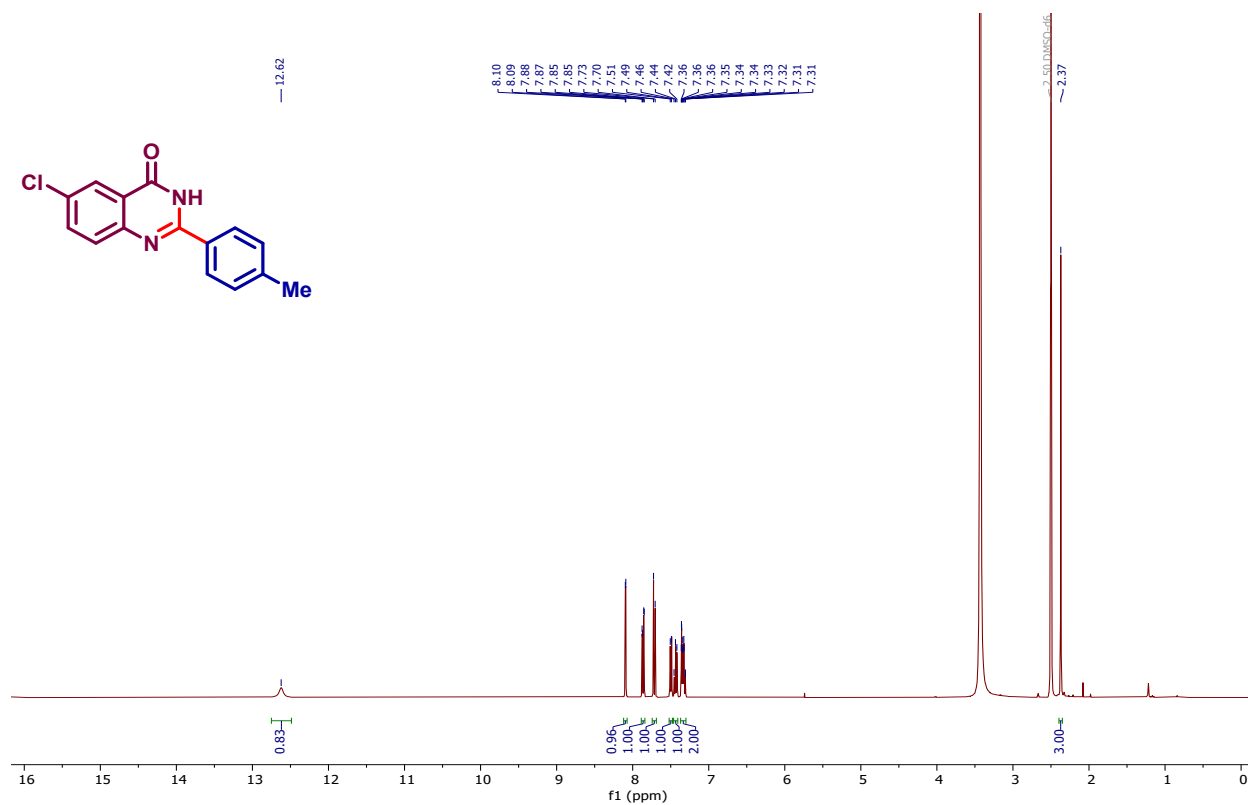


Figure S86: ¹H NMR spectrum (400 MHz) of 7c in DMSO-d₆

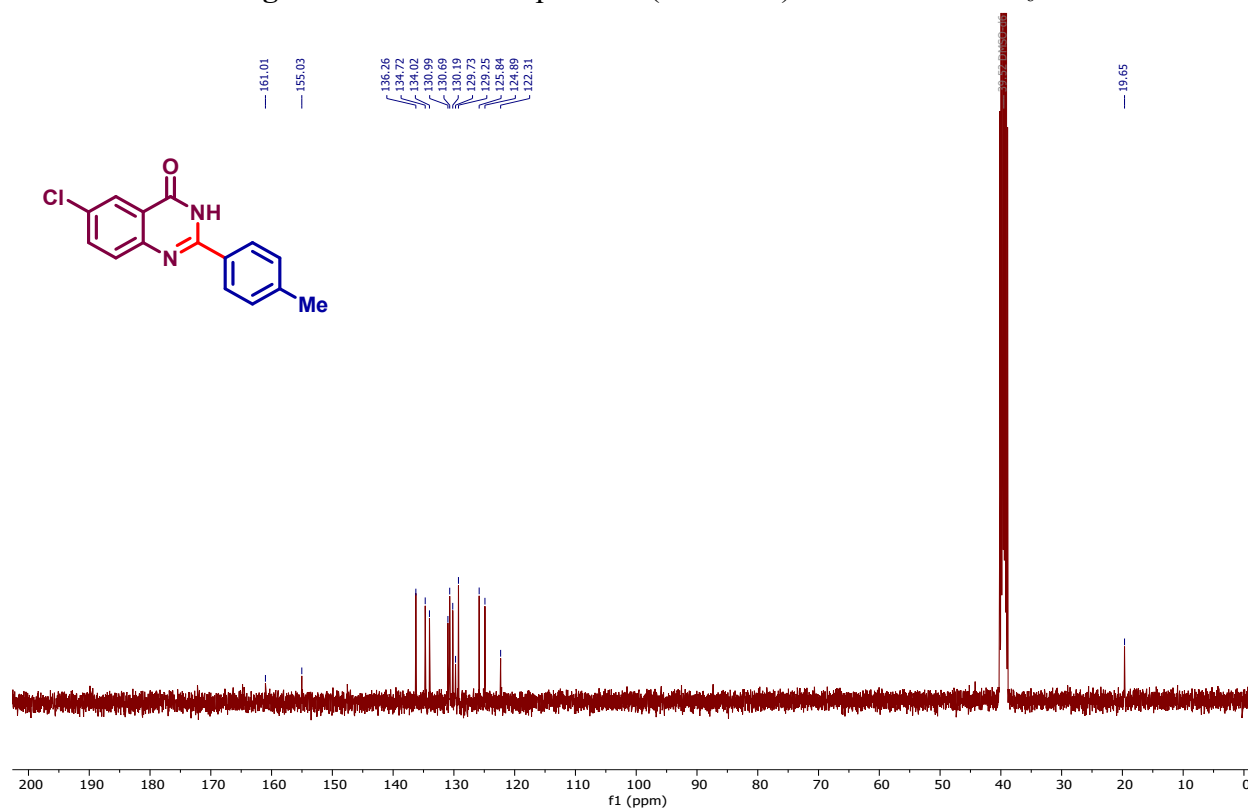


Figure S87: ¹³C NMR spectrum (100 MHz) of 7c in DMSO-d₆

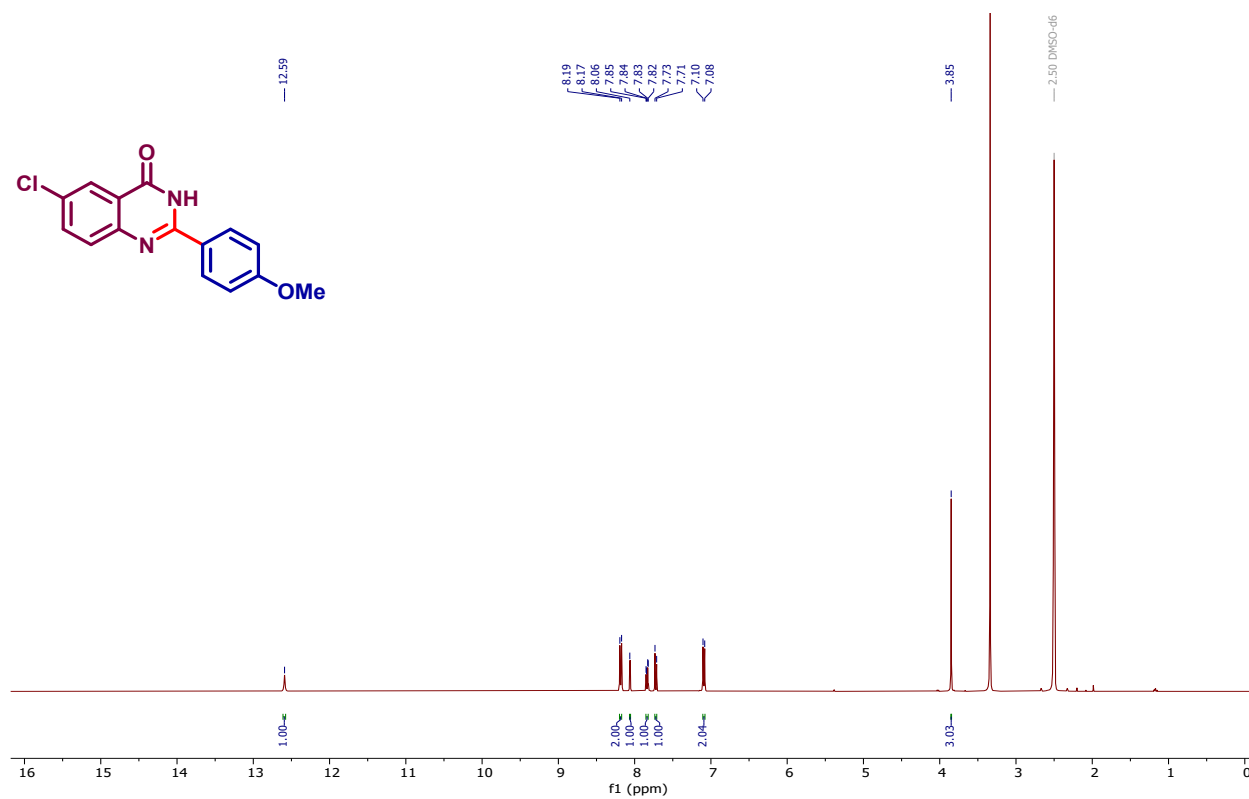


Figure S88: ¹H NMR spectrum (400 MHz) of 7d in DMSO-d₆

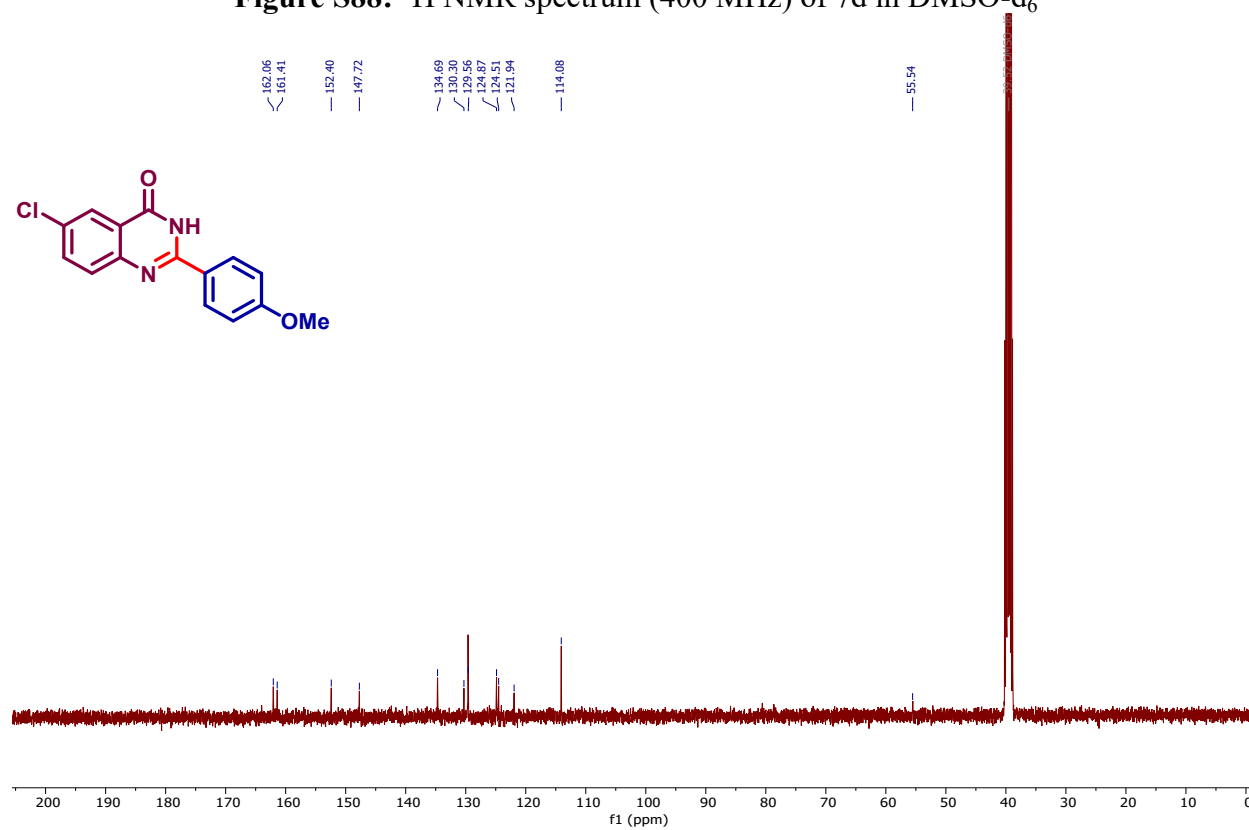


Figure S89: ¹³C NMR spectrum (100 MHz) of 7d in DMSO-d₆

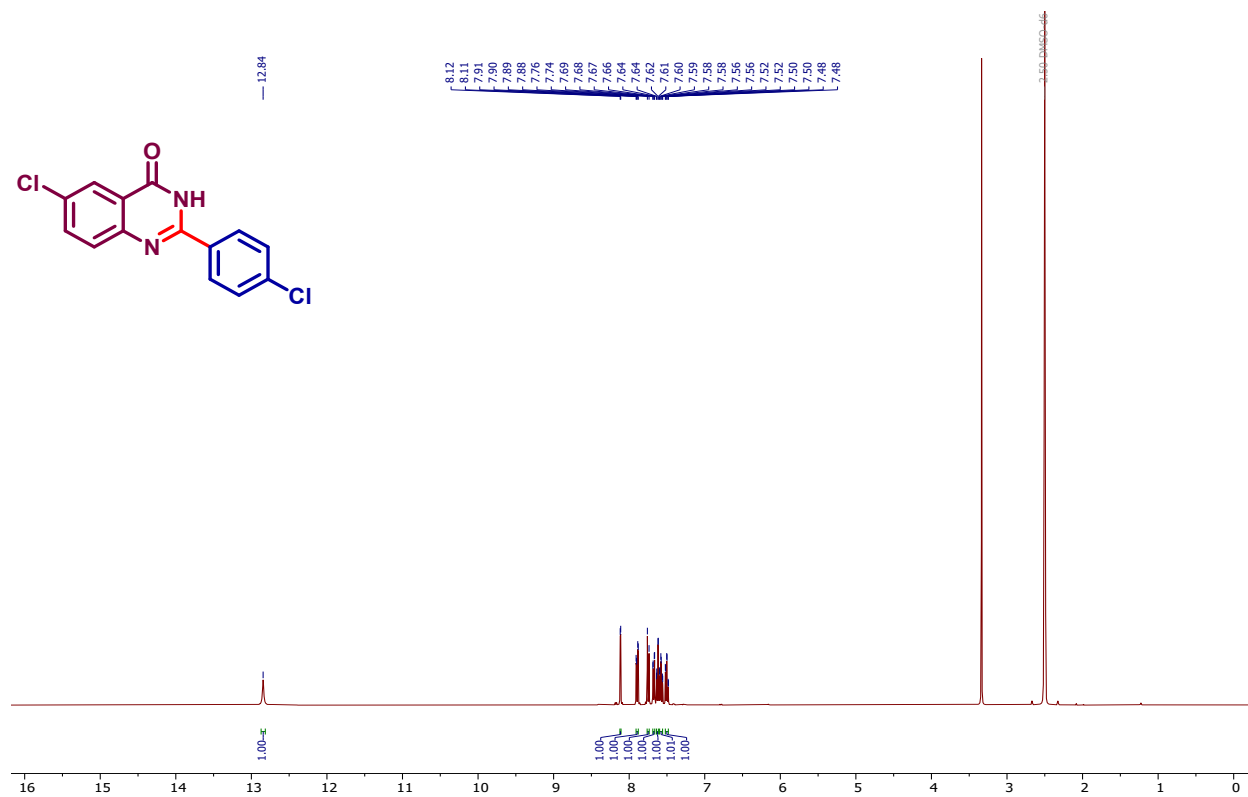


Figure S90: ¹H NMR spectrum (400 MHz) of 7e in DMSO-d₆

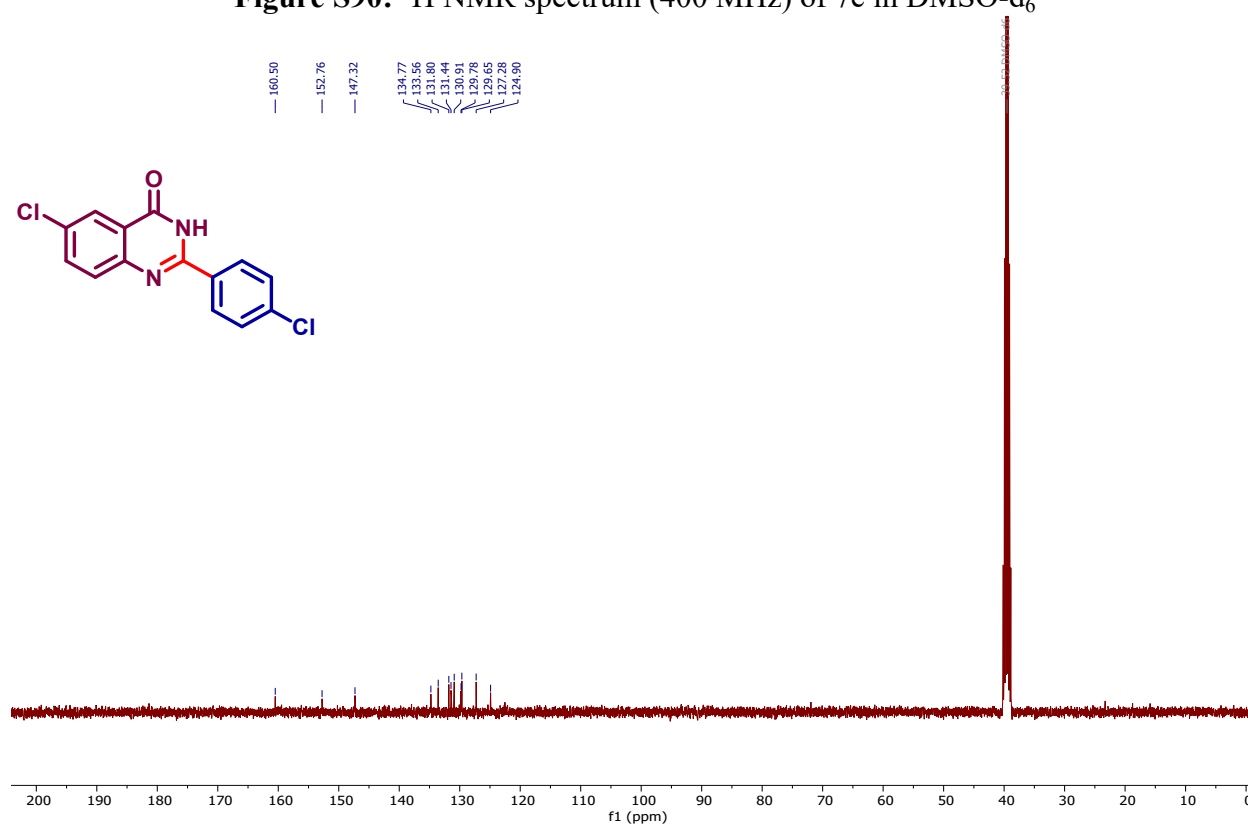


Figure S91: ¹³C NMR spectrum (100 MHz) of 7e in DMSO-d₆

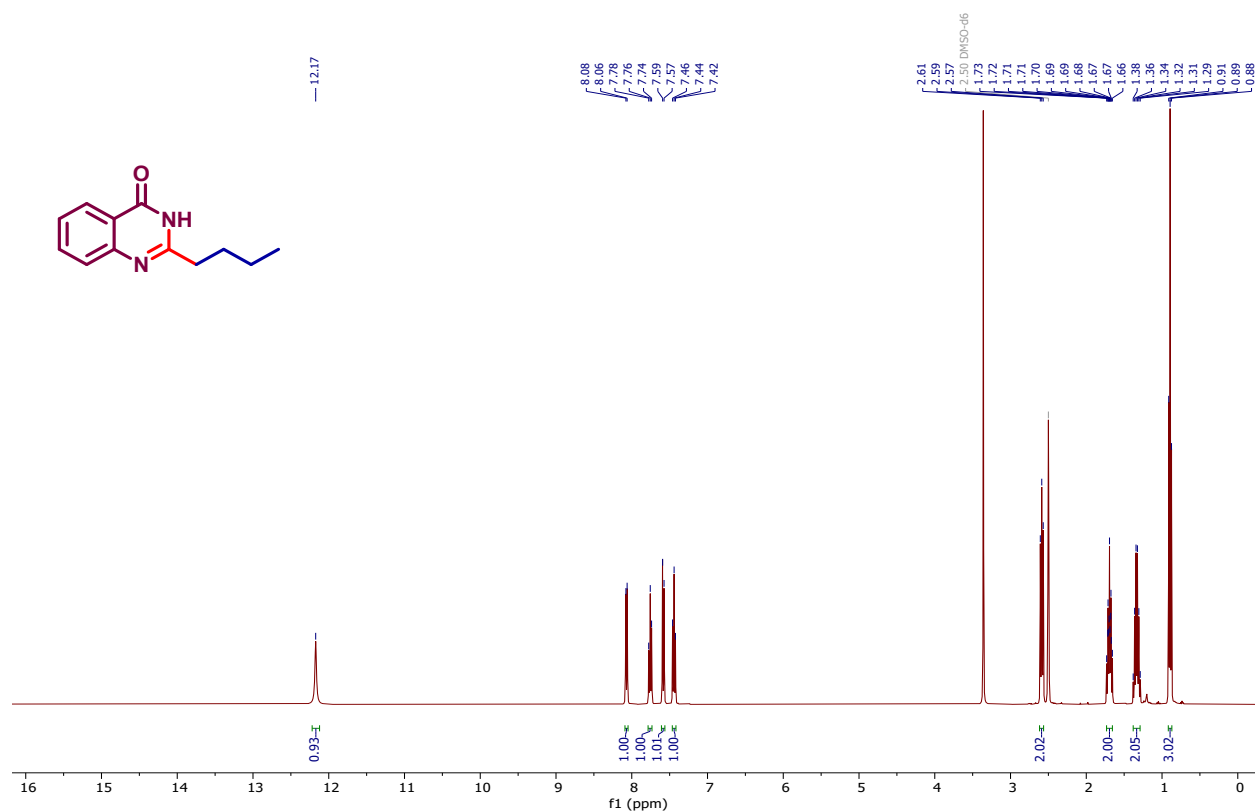


Figure S92: ¹H NMR spectrum (400 MHz) of 9a in DMSO-d₆

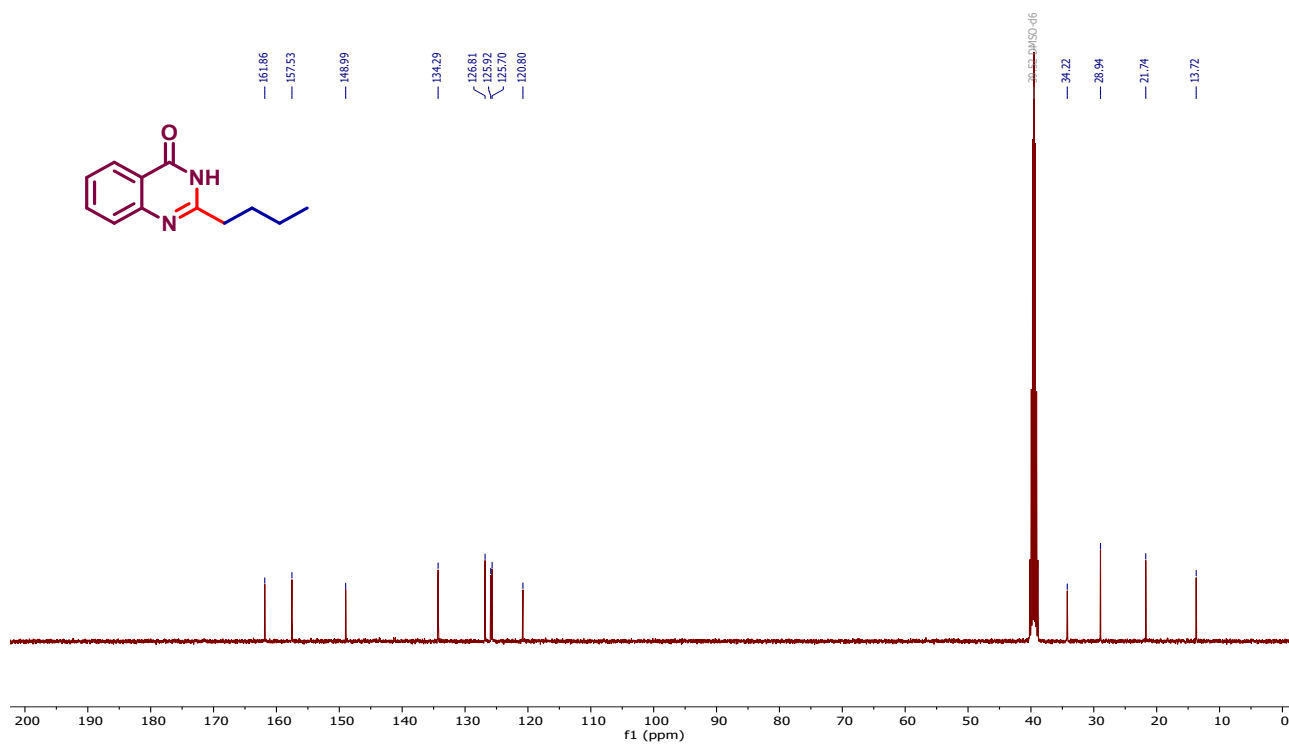


Figure S93: ¹³C NMR spectrum (100 MHz) of 9a in DMSO-d₆

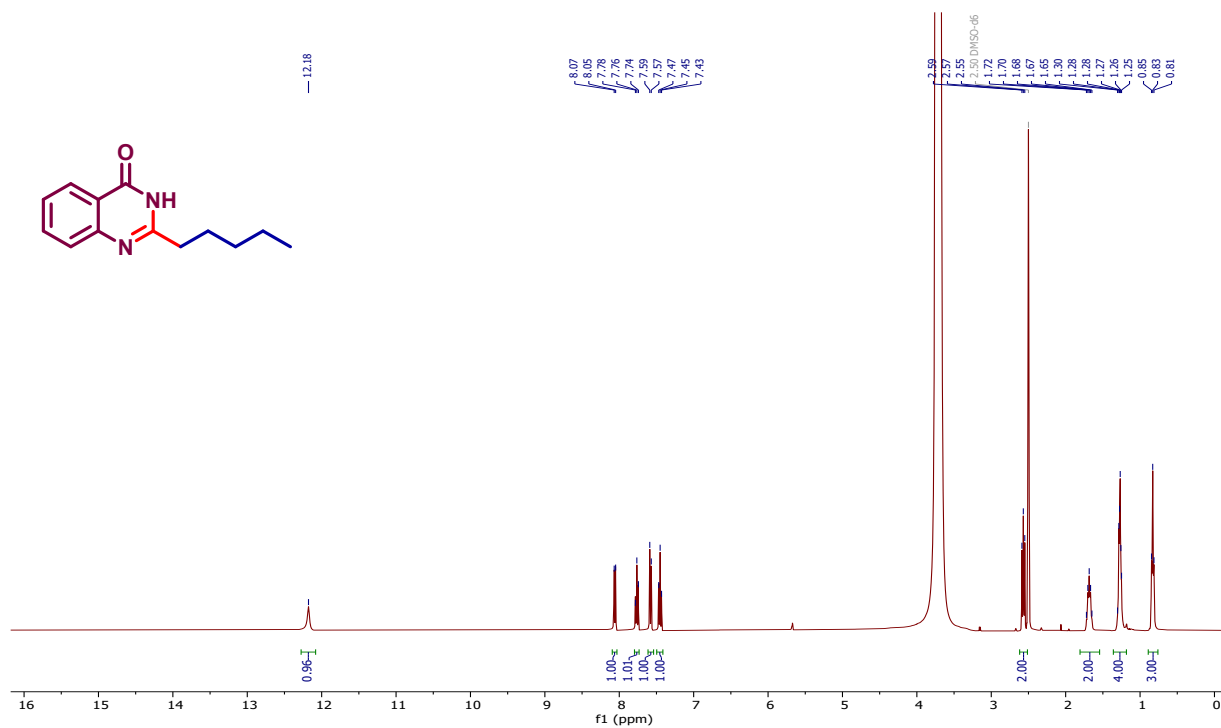


Figure S94: ¹H NMR spectrum (400 MHz) of 9b in DMSO-d₆

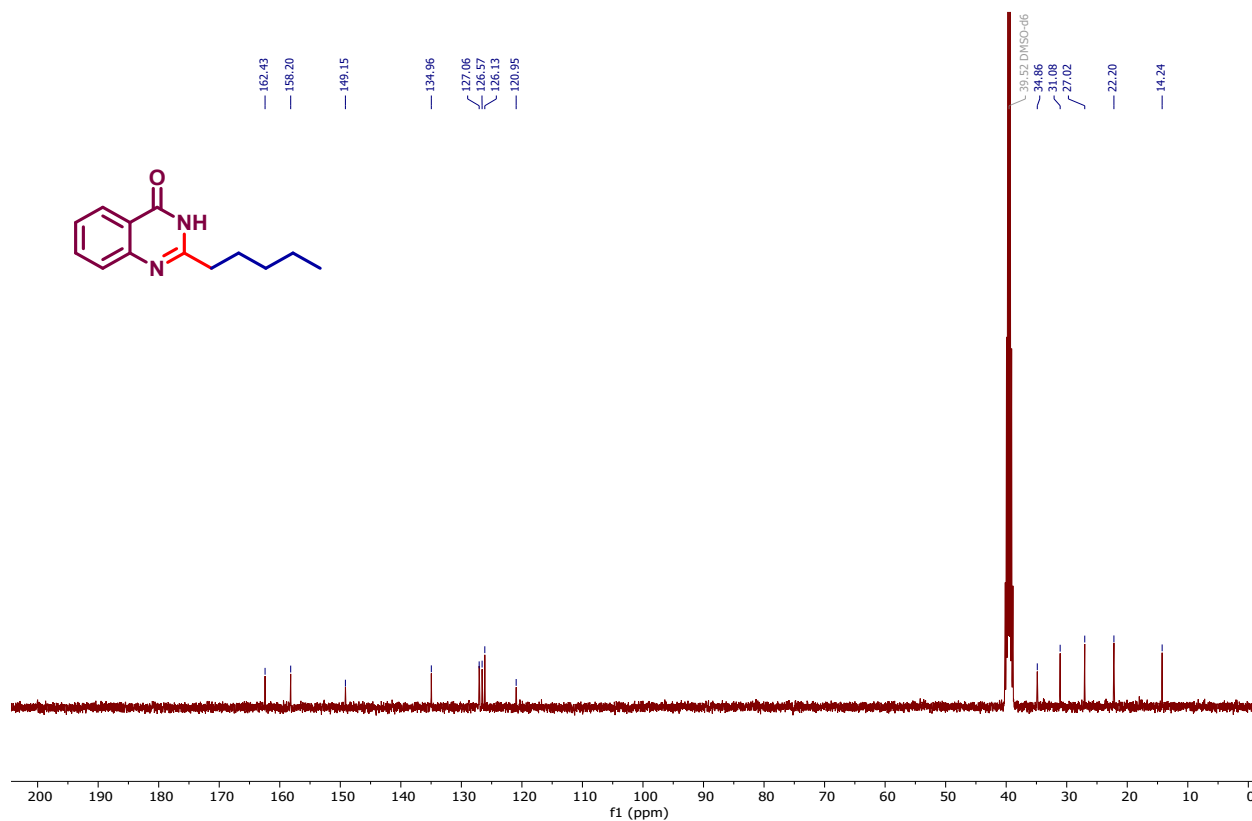


Figure S95: ¹³C NMR spectrum (100 MHz) of 9b in DMSO-d₆

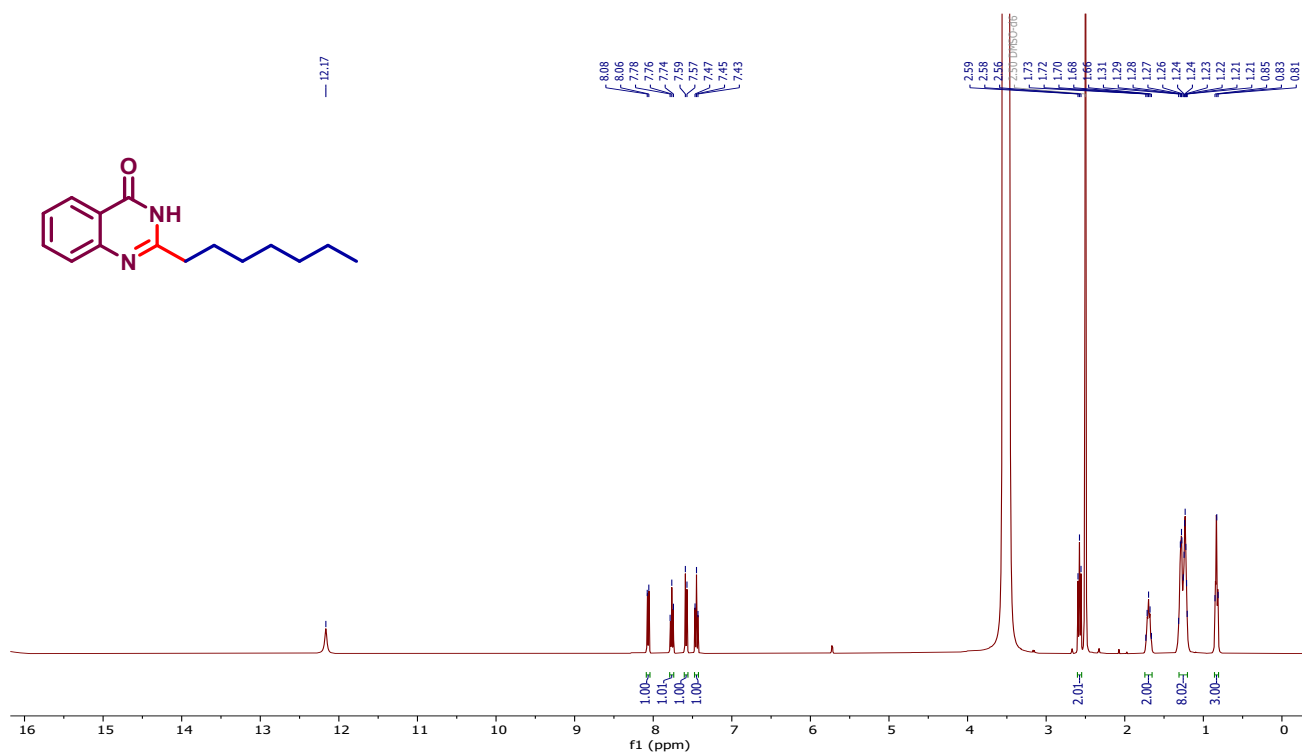


Figure S96: ¹H NMR spectrum (400 MHz) of 9c in DMSO-d₆

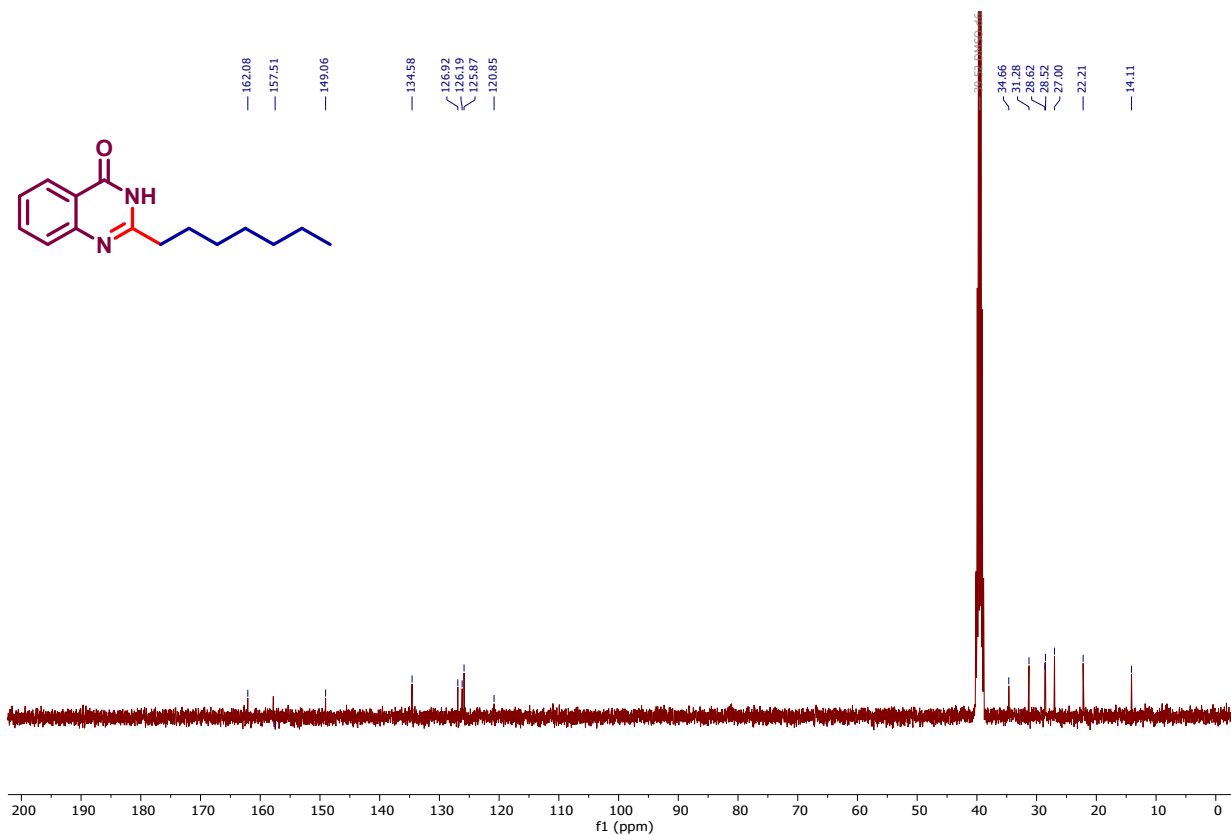


Figure S97: ¹³C NMR spectrum (100 MHz) of 9c in DMSO-d₆

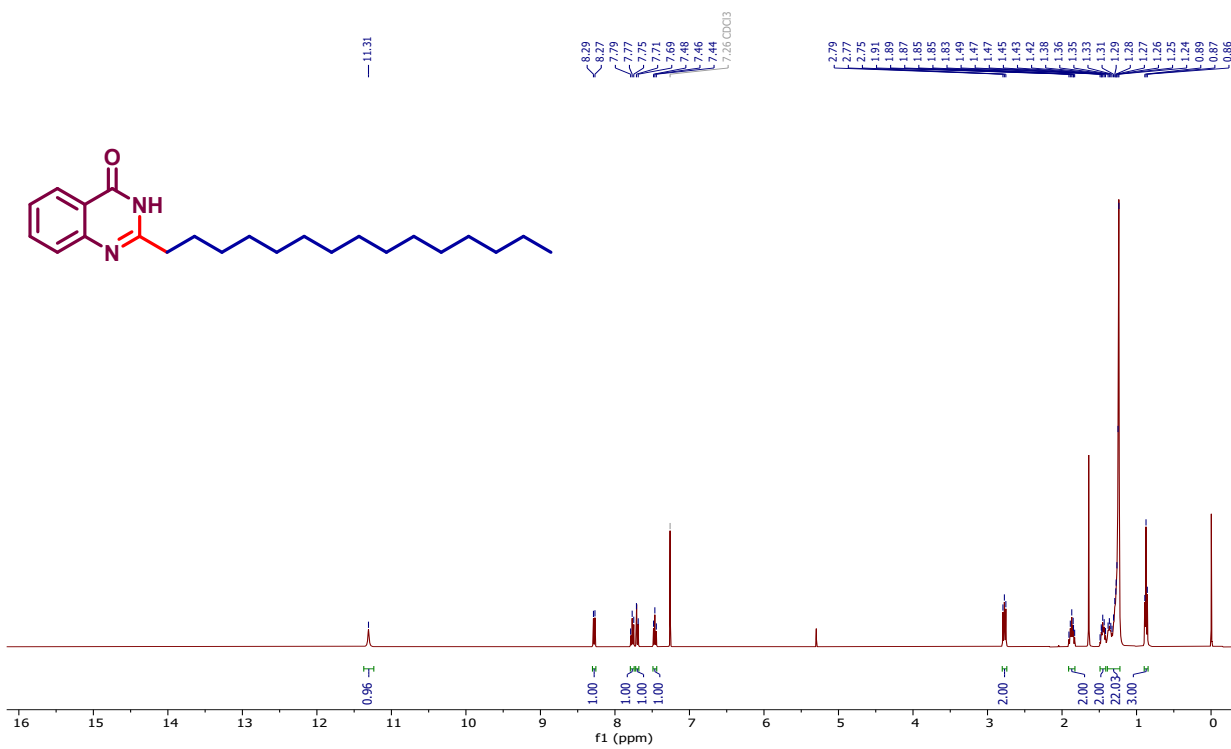


Figure S98: ¹H NMR spectrum (400 MHz) of 9d in CDCl₃

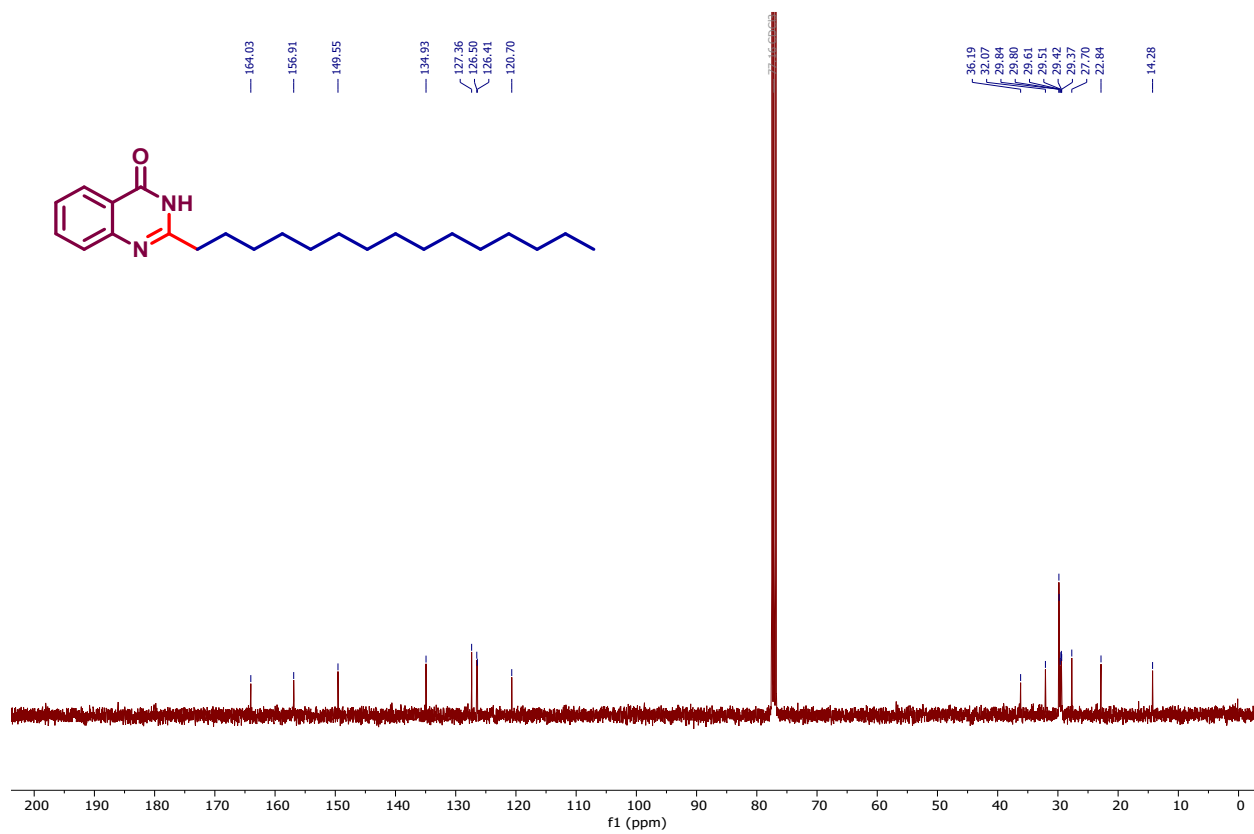


Figure S99: ¹³C NMR spectrum (100 MHz) of 9d in CDCl₃

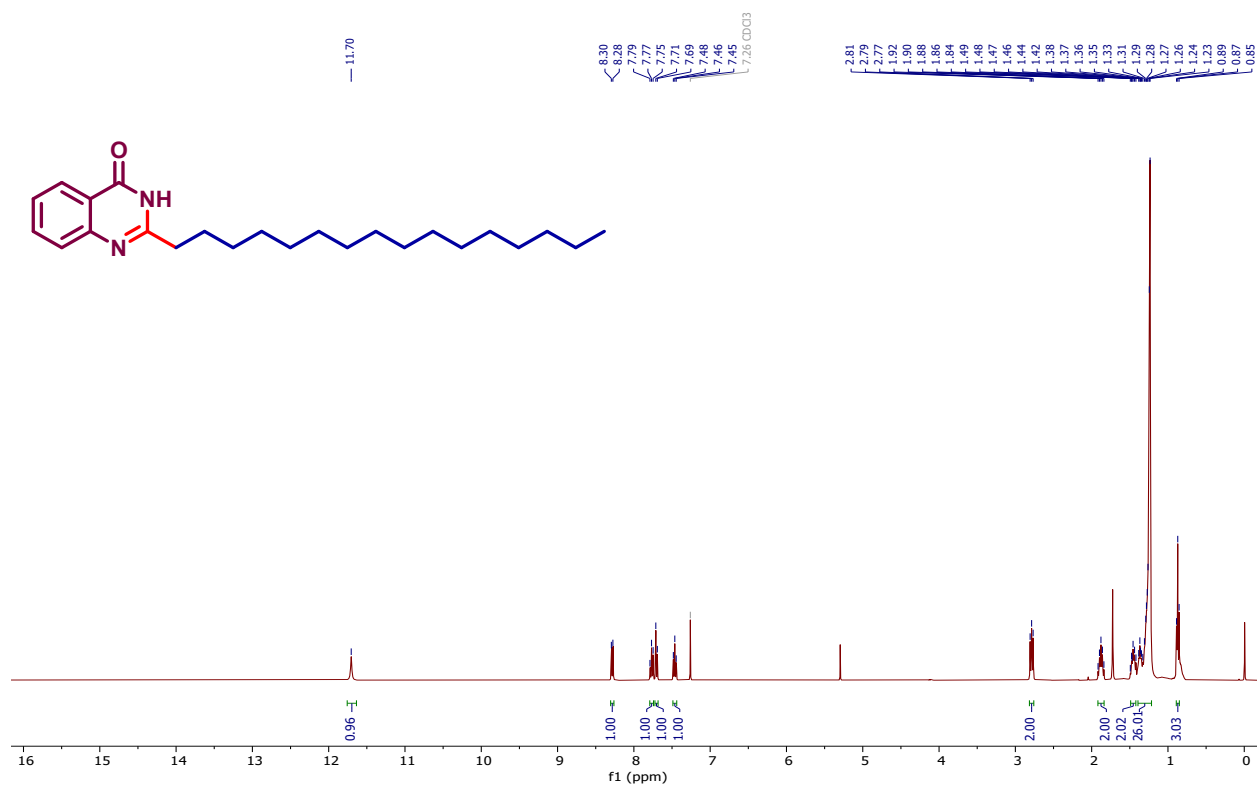


Figure S100: ¹H NMR spectrum (400 MHz) of 9e in CDCl₃

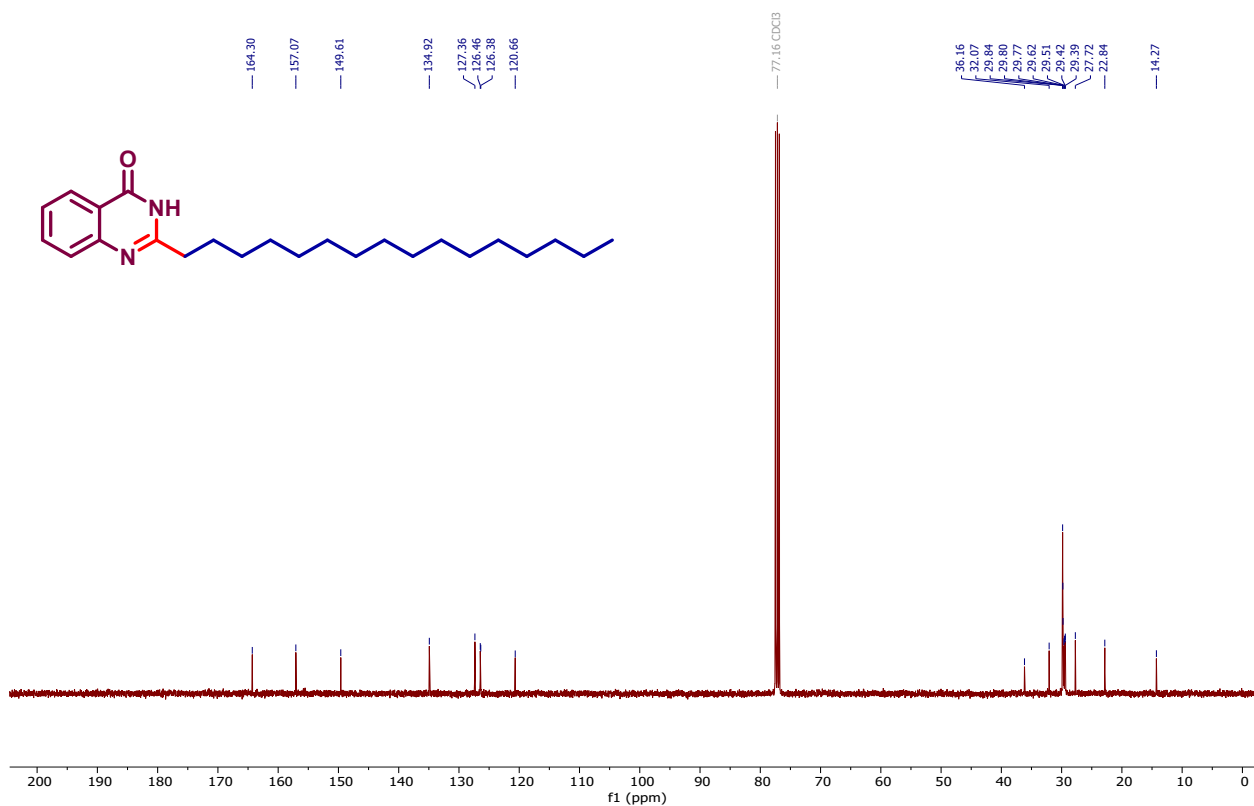
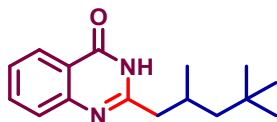
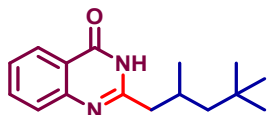


Figure S101: ¹³C NMR spectrum (100 MHz) of 9e in CDCl₃



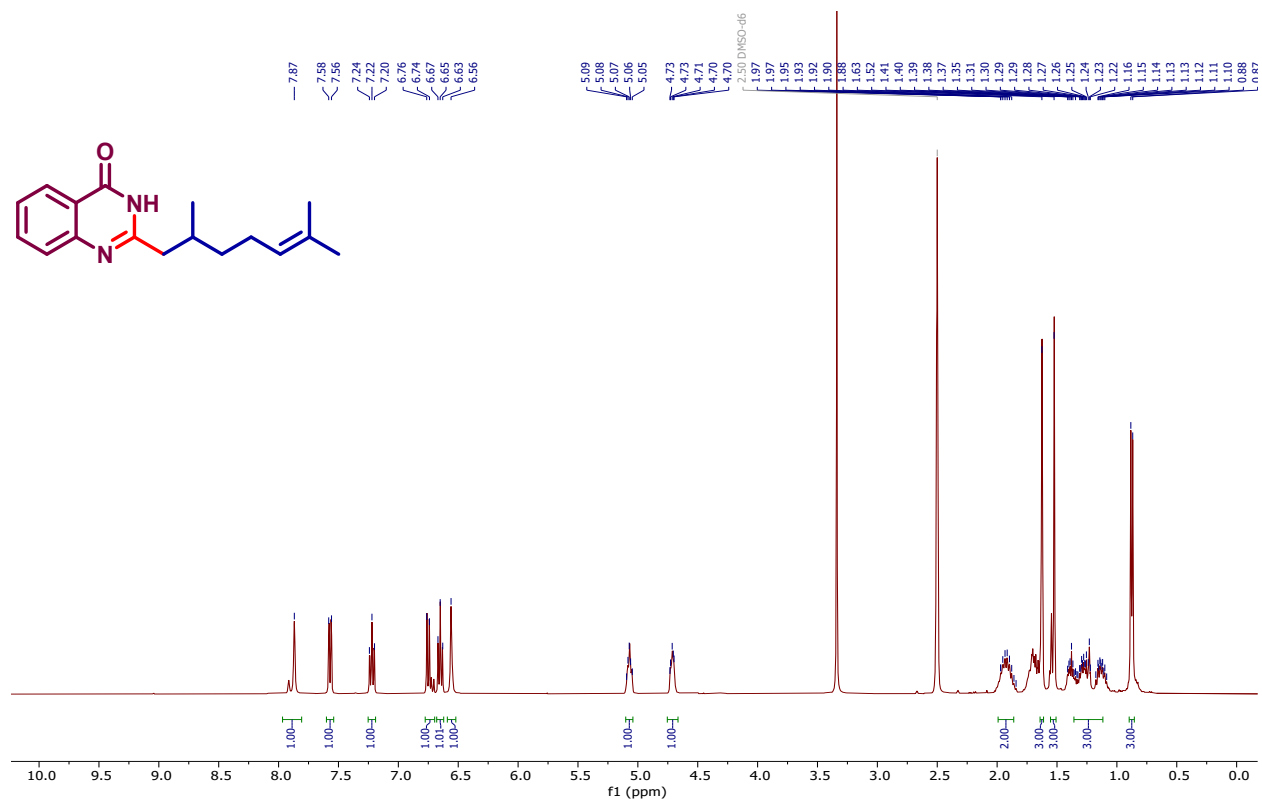


Figure S104: ¹H NMR spectrum (400 MHz) of 9g in DMSO-d₆

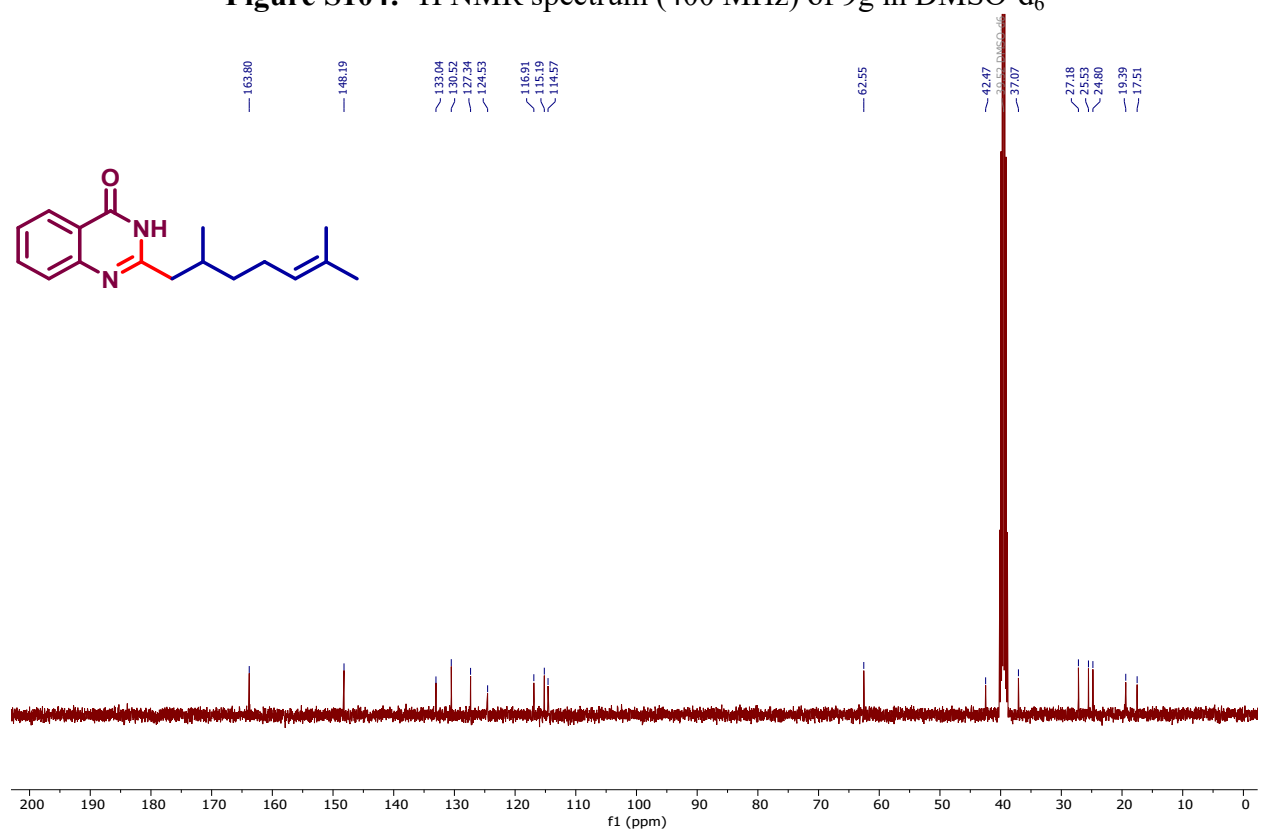


Figure S105: ¹³C NMR spectrum (100 MHz) of 9g in DMSO-d₆

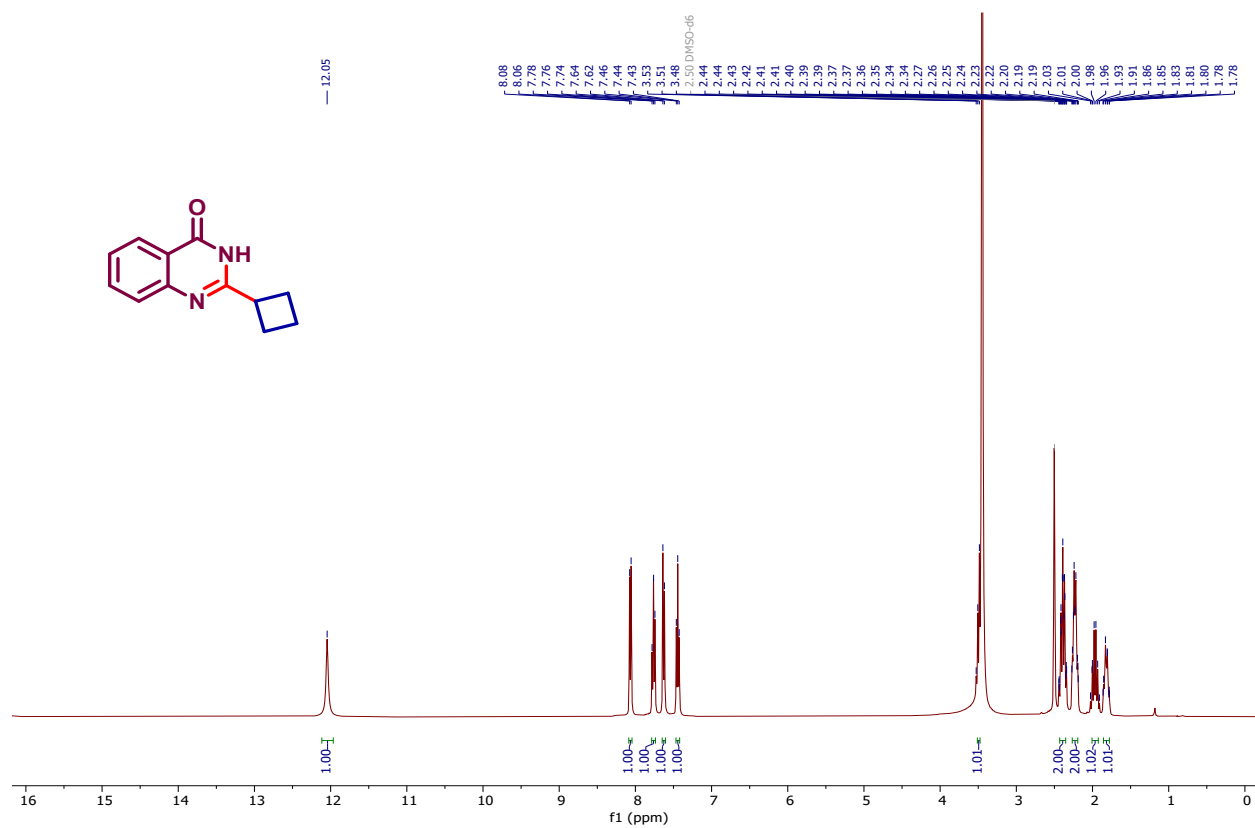


Figure S106: ¹H NMR spectrum (400 MHz) of 9h in DMSO-d₆

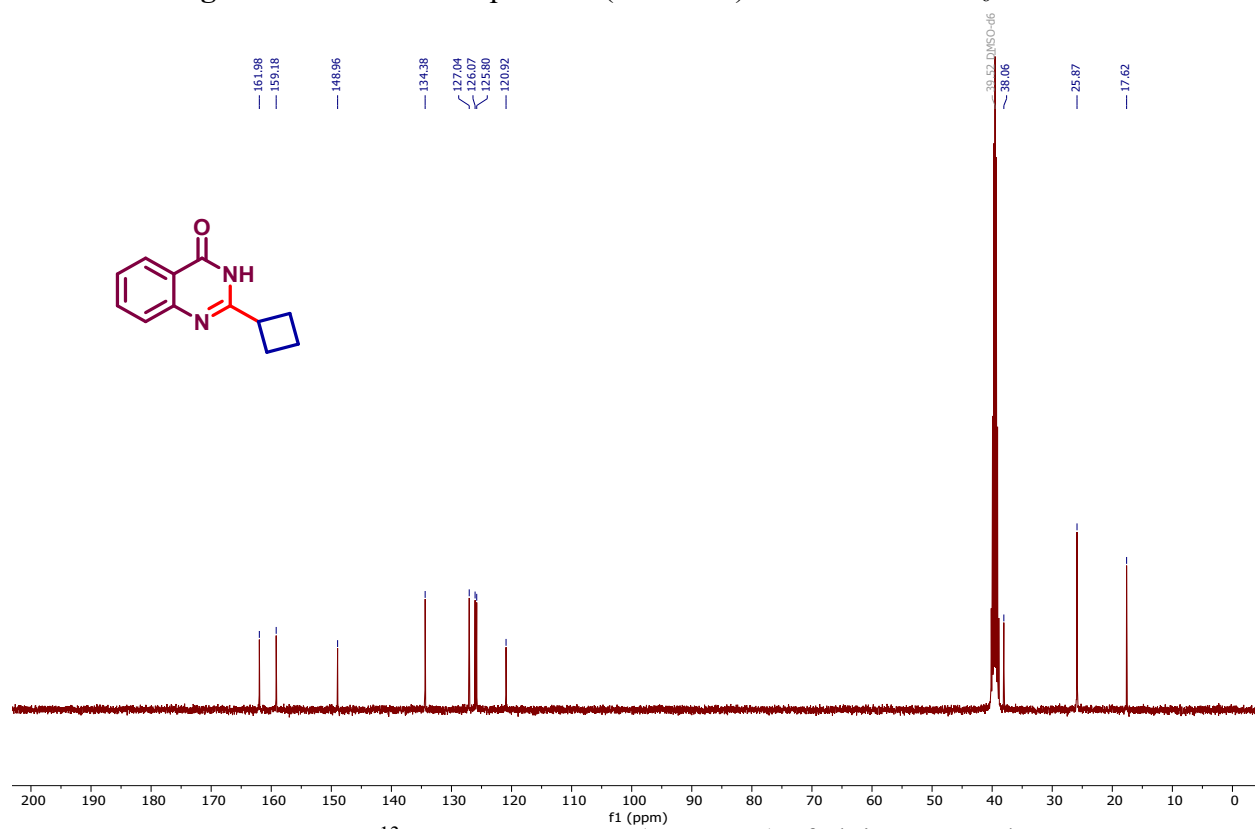


Figure S107: ¹³C NMR spectrum (100 MHz) of 9h in DMSO-d₆

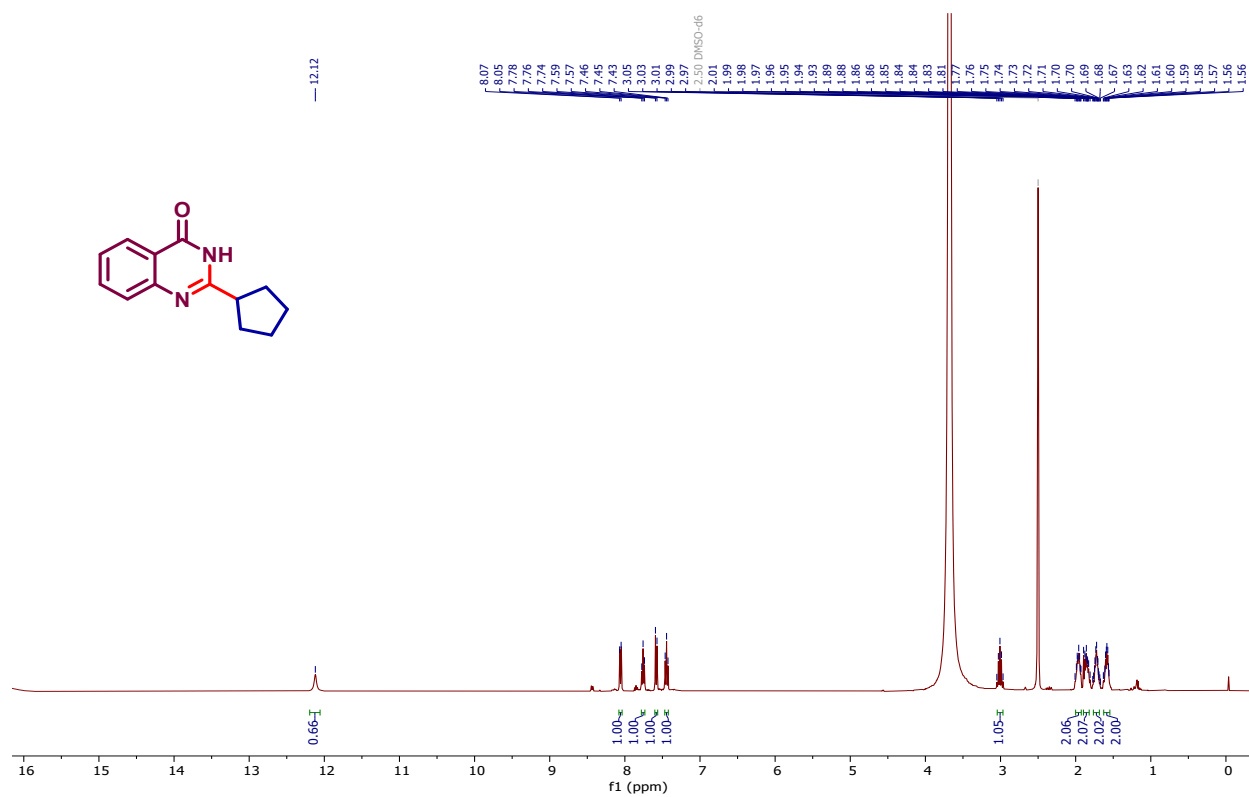


Figure S108: ¹H NMR spectrum (400 MHz) of 9i in DMSO-d₆

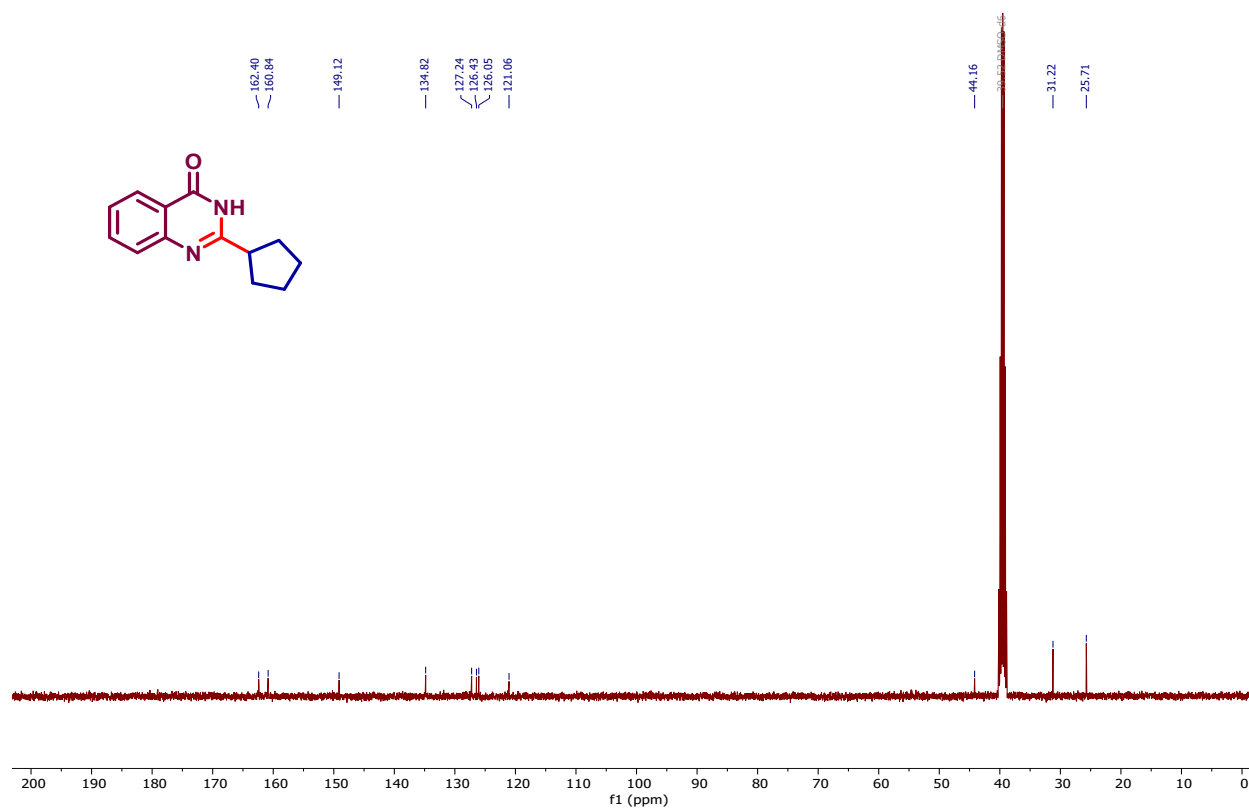


Figure S109: ¹³C NMR spectrum (100 MHz) of 9i in DMSO-d₆

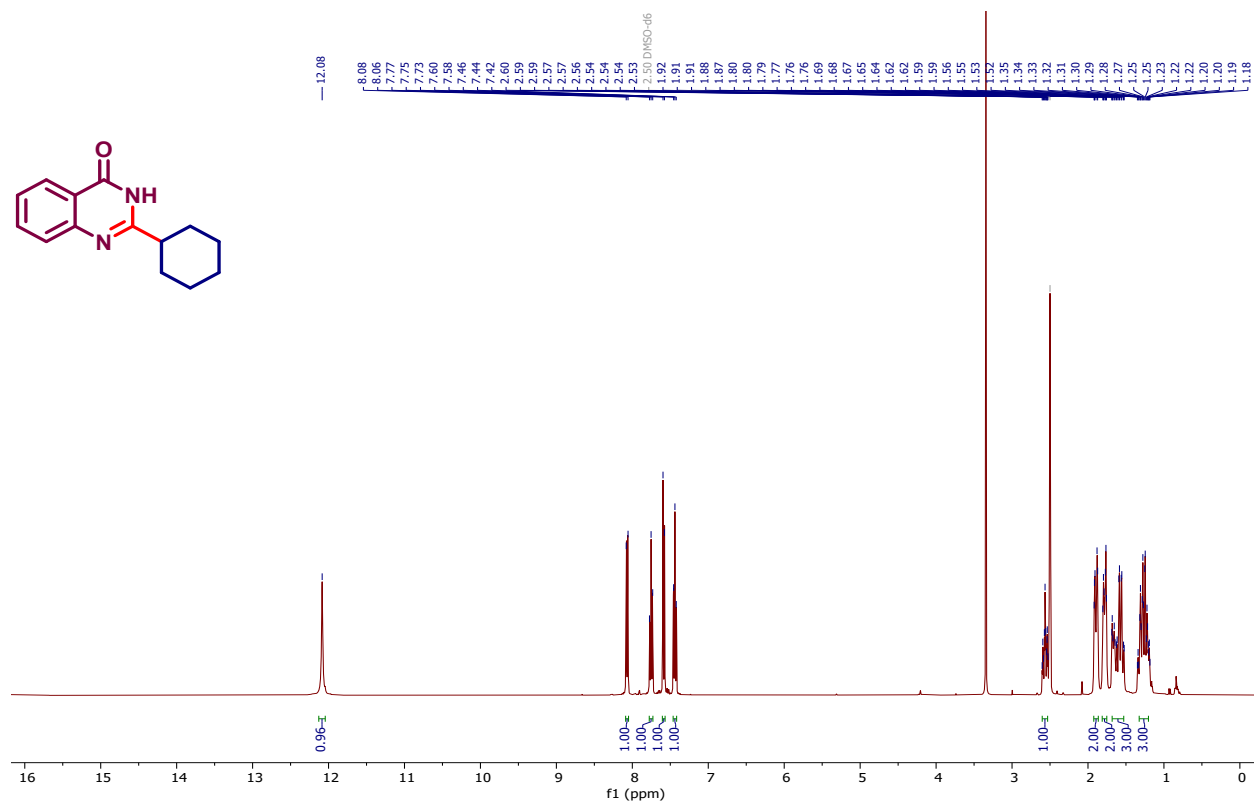


Figure S110: ¹H NMR spectrum (400 MHz) of 9j in DMSO-d₆

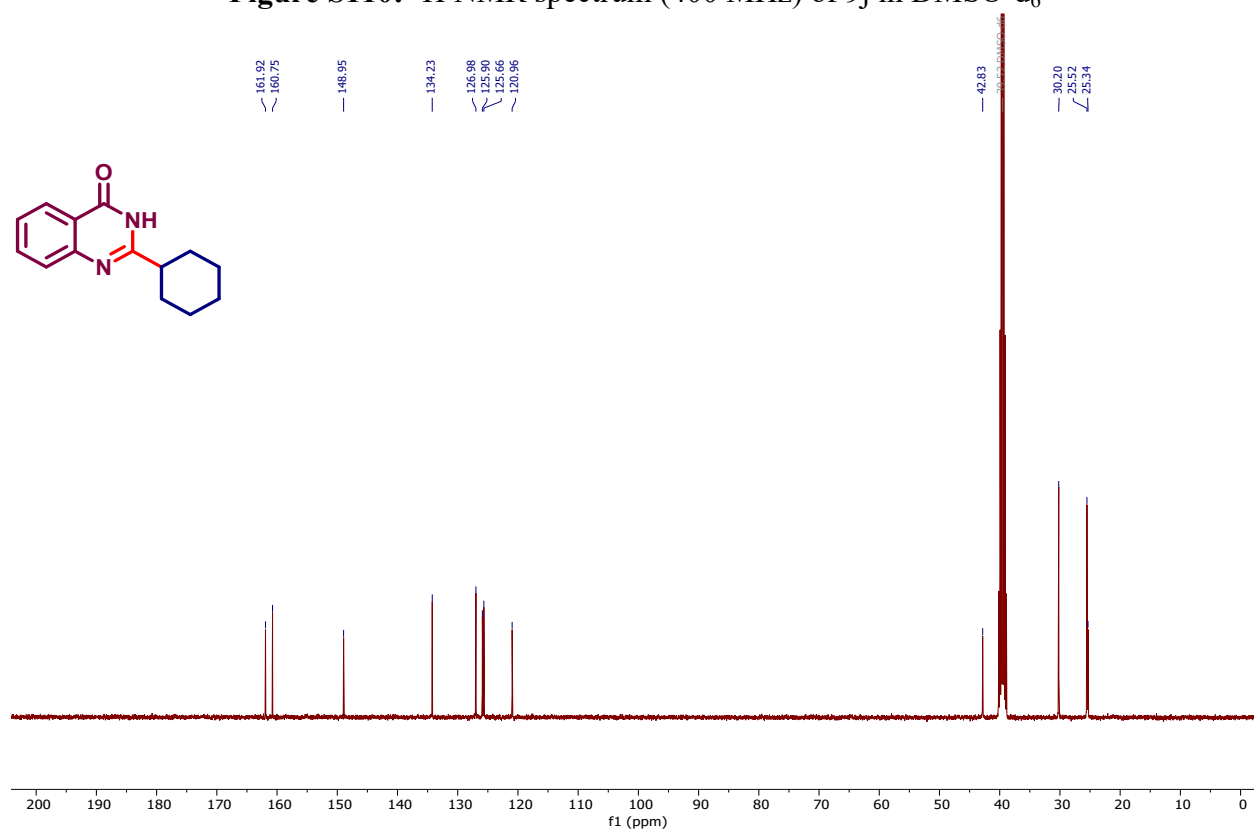


Figure S111: ¹³C NMR spectrum (100 MHz) of 9j in DMSO-d₆

References:

1. A. Mishra and M. Shahid, *J. Phys. Chem. C* **2010**, *114*, 16726–16739
2. P. R. Thorve and B. Maji, *Catal. Sci. Technol.* **2021**, *11*, 1116–1124
3. S. Halder, S. Mandal, A. Biswas and D. Adhikari, *Green Chem.* **2023**, *25*, 2840–2845
4. B. Sardar, R. Jamatia, A. Samanta and D. Srimani, *J. Org. Chem.* **2022**, *87*, 5556–5567
5. D. Pal, A. Mondal and D. Srimani, *Catal. Sci. Technol.*, **2022**, *12*, 3202–3208
6. A. K. Bains, Y. Ankit, and D. Adhikari. *ChemSusChem*. **2021**, *14*, 324
7. M. Kumar, Richa, S. Sharma, V. Bhatt and N. Kumar, *Adv. Synth. Catal.* **2015**, *357*, 2862–2868
8. J. Sun, T. Tao, D. Xu, H. Cao, Q. Kong, X. Wang, Y. Liu, J. Zhao, Y. Wang, and Y. Pan, *Tetrahedron Lett.* **2018**, *21*, 2099–2102
9. R. Regar, K.S. Mehra, Bhowal, and R. J. Sankar, *Eur. J. Org. Chem.* **2019**, *47*, 6278–6284