Supporting Information

Unlocking the photo-dehydrogenation ability of naphthalene monoimide towards the synthesis of quinazolinones

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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; 1,8-naphthalic anhydride; and 2,6-diisopropylaniline were purchased from Sigma-Aldrich. These 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 (from Merck) coated with silica and fluorescent indicator 254 nm 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 ^{1}H NMR, ^{13}C NMR spectroscopies and high-resolution mass spectrometry. ^{1}H 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 $CDCl_3$ (δ 7.26 ppm). Carbon chemical shifts are internally referenced to the deuterated solvent signals in $CDCl_3$ (δ 77.1 ppm). High-resolution mass spectra (HRMS) were recorded on a Waters QTOF mass spectrometer. Fluorescence quenching experiments of the **NMI** 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. UV-Vis was recorded using Varian Cary 60 (Agilent Technologies) spectrophotometer. The total volume in the cuvette was fixed at 1 ml and a cuvette of path length 1 cm was used. The photochemical reactions were conducted with eplite 50 W blue LED (455 nm). The reaction tube was kept 7-8 cm away from the light source.

2. General synthetic procedure for 2-(2,6-diisopropylphenyl)-1*H*- benzo[de]isoquinoline -1,3(2*H*)-dione (NMI) Catalyst[1]:

The NMI molecule was synthesized according to the previously reported literature procedure[1]. To a solution of 1,8-Naphthalic anhydride (5.05 mmol, 1.0 g) in glacial acetic acid (10 mL) taken in a sealed tube, 2,6-diisopropylaniline (6.06 mmol, 1.2 mL) was added and heated at 110 °C for 6 h with continuous stirring. After that, the reaction mixture was cooled to room temperature followed by filtration and washing with diethyl ether, and the resulting solution was dried. Further purification was done by column chromatography using ethyl acetate/hexane solvent mixture (3:7) as the eluent to afford **NMI** as a greenish-white shiny solid (1.156 g, 64%) The desired products were fully characterized by ^{1}H, ^{13}C NMR spectroscopies.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (dd, J = 7.3, 1.2 Hz, 2H), 8.31 (dd, J = 8.3, 1.1 Hz, 2H), 7.82 (dd, J = 8.2, 7.2 Hz, 2H), 7.48 (dd, J = 8.2, 7.3 Hz, 1H), 7.34 (d, J = 7.8 Hz, 2H), 2.76 (s, 2H), 1.17 (d, J = 6.9 Hz, 12H). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 164.3, 145.7, 134.3, 131.9, 131.8, 130.9, 129.5, 127.1, 124.1, 122.8, 29.1, 24.0.

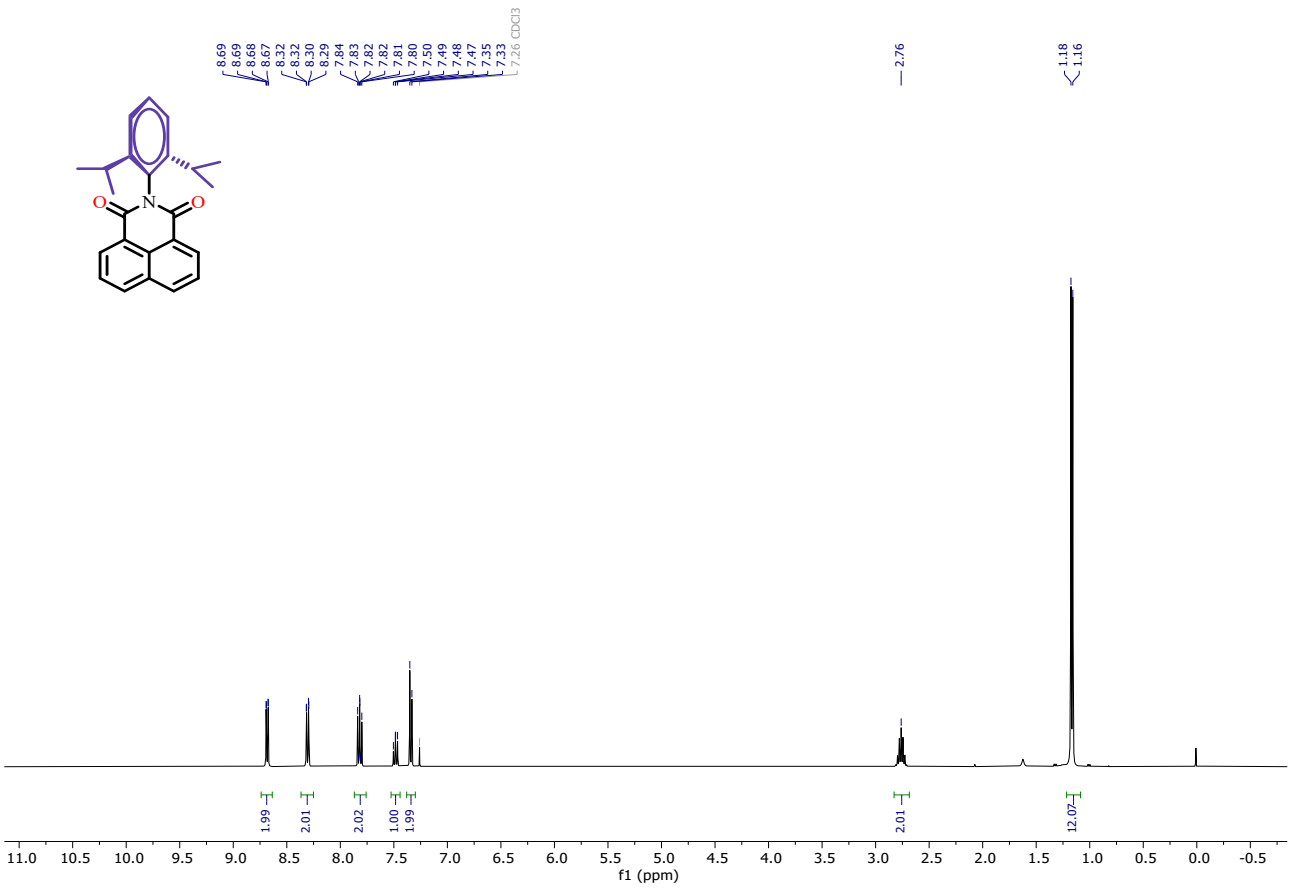


Figure S1. ^{1}H NMR spectrum (400 MHz) of **NMI** in $CDCl_3$.

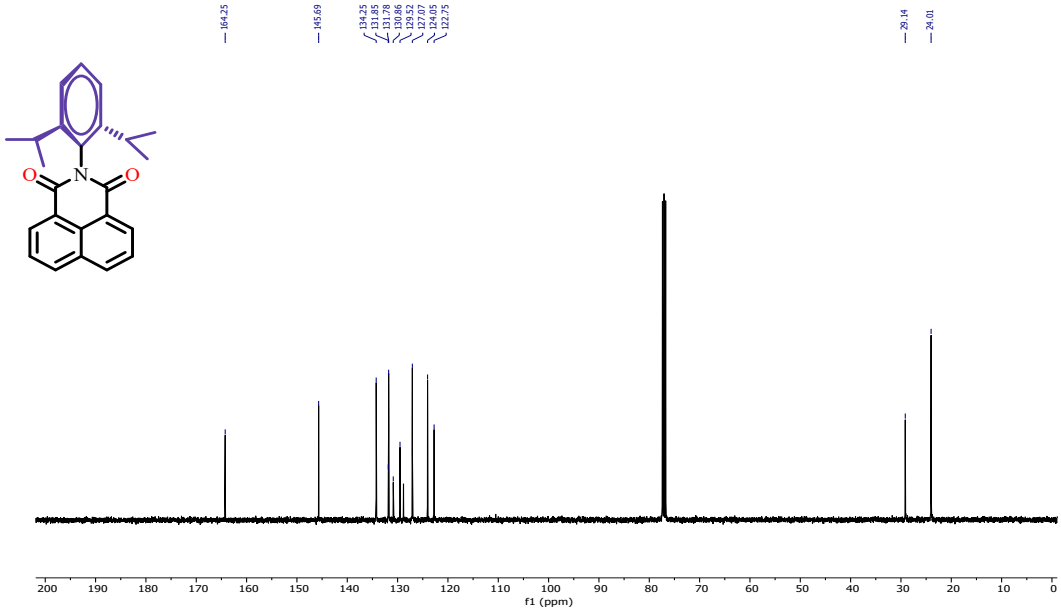
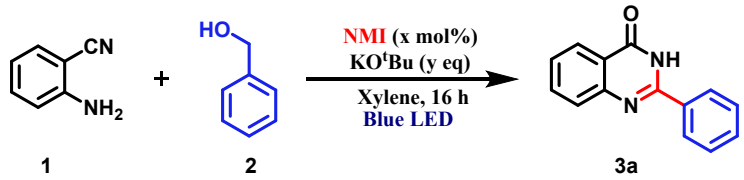


Figure S2. ^{13}C NMR spectrum (100 MHz) of **NMI** in $CDCl_3$

3. Table S1: Optimization of the reaction condition

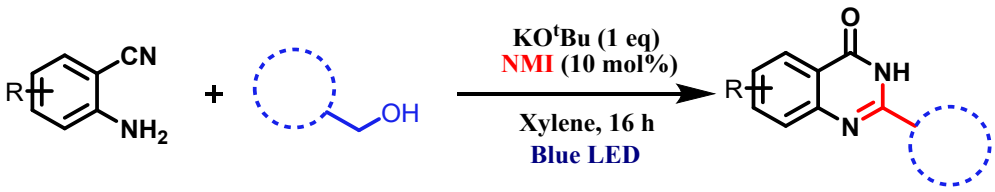


Entry	Catalyst (mol%)	Base (equiv.)	Time (h)	Solvent	Yield* (%)
1	5	KO^{t}Bu (1)	16	Toluene	18
2	10	KO^{t}Bu (1)	16	Toluene	28
3	**10**	**KO^{t}Bu (1)**	**16**	**Xylene**	**88**
4	10	KO^{t}Bu (0.5)	16	Xylene	45
5	10	KO^{t}Bu (1)	12	Xylene	58
6	15	KO^{t}Bu (1)	20	Xylene	86
7	5	KOH (1)	16	Xylene	10
8	10	NaOH (1)	16	Xylene	8
9	10	KO^{t}Bu (1)	16	MeCN	trace
10	15	KO^{t}Bu (1)	16	THF	0
11	10	KO^{t}Bu (1)	16	MeOH	trace
12	-	KO^{t}Bu (1)	16	Xylene	12
13	10	-	16	Xylene	n.r

***** *Reaction conditions*: NMI (x mol %, with respect to 2-amino benzonitrile), 2-amino benzonitrile (0.5 mmol), alcohol (0.75 mmol), KO^{t}Bu (y mmol), solvent (2 mL) in Blue LED, 16 h (isolated yield).

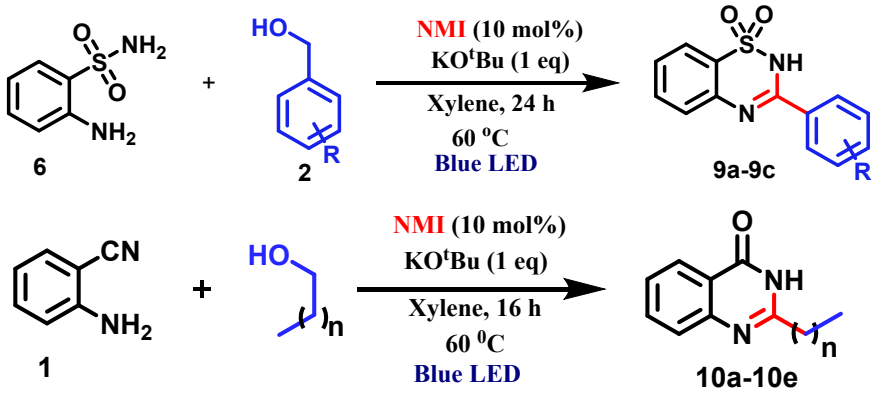
4. General procedure

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



A 15 mL vial tube was charged with 10 mol% of **NMI**, 0.5 mmol of *o*-aminobenzonitrile, KO^{t}Bu (0.5 mmol), and alcohol (0.75 mmol) in 2 mL xylene. The reaction mixture was stirred under blue light irradiation for 16 h in an open atmosphere. Upon completion, the reaction mixture was worked up in ethyl acetate and brine mixture. Then the organic layer was collected, dried over $MgSO_4$, and concentrated *in vacuo*. The residue was purified by column chromatography using hexane/ethyl acetate (4:1 to 2:1 gradually) as eluent to afford pure products. The desired products were fully characterized by ^{1}H, ^{13}C NMR spectroscopies.

b) General synthetic procedure for the synthesis of 2*H*-benzo[1,2,4]thiadiazine-1,1-dioxide derivatives or quinazolinone derivatives from aliphatic alcohols:

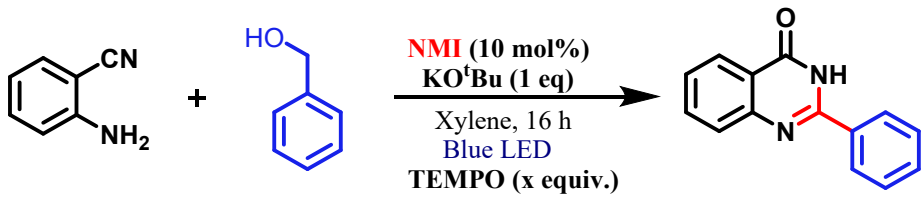


A 15 mL vial was charged with 10 mol% of **NMI**, 0.5 mmol of 2-aminobenzenesulfonamide or 2-aminobenzonitrile, KO^{t}Bu (0.5 mmol), and aromatic/aliphatic alcohol (0.75 mmol) in 2 mL xylene. The reaction mixture was stirred under blue light irradiation for 24 h in an oil bath at 60 ^{O}C. Upon completion, the reaction mixture was cooled and worked up in ethyl acetate and brine mixture. Then the organic layer was collected, dried over $MgSO_4$, and concentrated *in vacuo*. The residue was purified by column chromatography using hexane/ethyl acetate (1:1

to 1:4) as eluent to afford pure products. The desired products were fully characterized by ^{1}H, ^{13}C NMR spectroscopies.

5. Mechanistic investigation:

a) Procedure for radical quenching experiment:



In a typical reaction, a 15 mL vial was charged with **NMI** (10 mol%), benzyl alcohol (0.75 mmol), 2-aminobenzonitrile (0.5 mmol) KO^{t}Bu (0.5 mmol), and the varying equivalent of TEMPO dissolved in 2 mL xylene. The reaction mixture was stirred under blue light irradiation for 16 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 1.2 equivalent of TEMPO complete quenching of the reaction occurs.

Product formation on varying equivalent of TEMPO addition

Tempo (x Equiv.)	Product formation
0.6	14%
1.2	0%

b) Observation of color changes during the reaction:

The molecule **NMI** when dissolved in xylene gives a colorless solution. Then KO^{t}Bu was added to it and kept the solution in dark. There was no visual color change under the dark condition. On the other hand, as soon as visible light is irradiated on the reaction mixture, the solution first turns into orange, which slowly darkens and changed to wine-red. The resulting wine-red solution was analysed by both UV-vis and EPR spectroscopies**.**

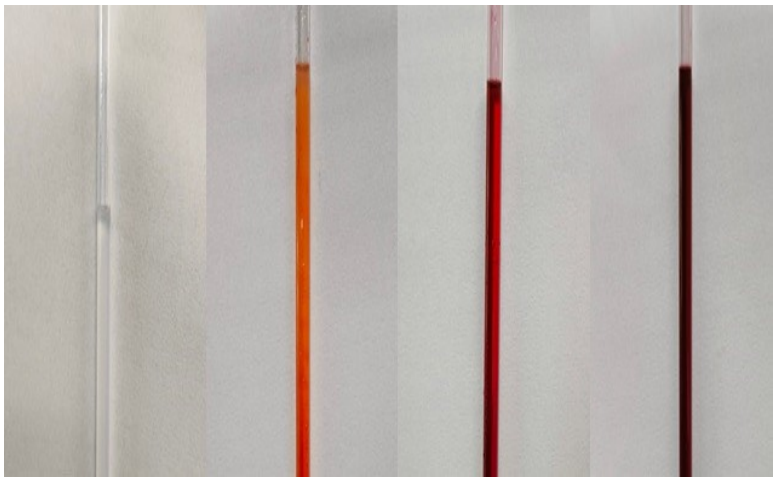


Figure S3. The progression of color during exposing the NMI and KO^{t}Bu in xylene to visible light. The molecule NMI alone in xylene is a colorless solution.

c) EPR analysis of NMI radical anion:

In a solution of **NMI** (0.028 mmol, 10 mg) in xylene, KO^{t}Bu (0.178 mmol, 20 mg) was added. Under the dark condition, this solution is completely colorless. Then the reaction mixture was irradiated with white light for 5 minutes which prompted a sharp color change to wine red. The X-band (9.4 GHz) EPR measurement of this solution was carried out at room temperature. A sharp signal at g = 2.005 was observed, which indicated the formation of a **NMI** radical anion.

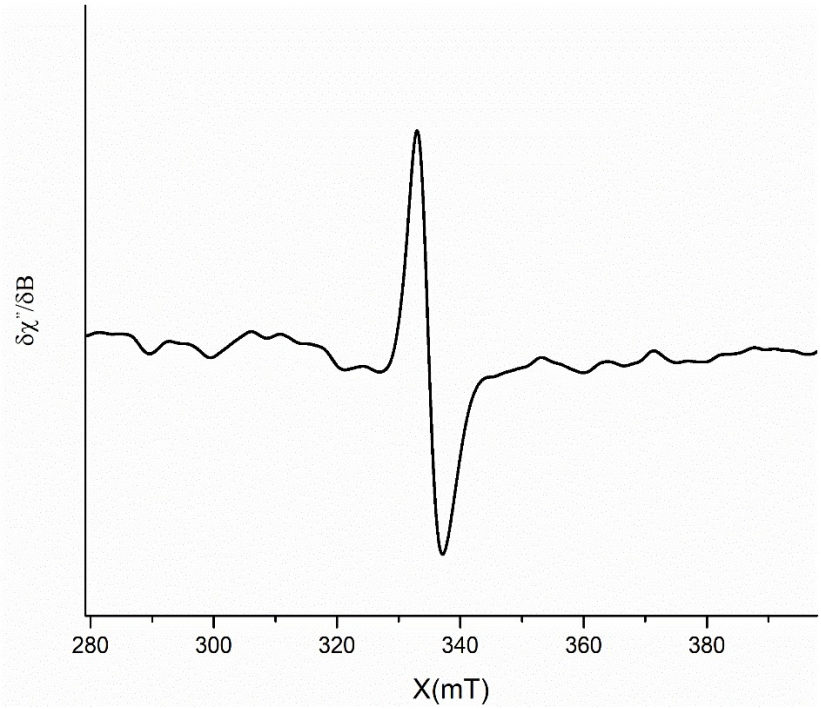


Figure S4. X-band (9.4 GHz) EPR signal of **NMI** radical anion obtained by adding KO^{t}Bu and after shining visible light. During the data acquisition the modulation frequency was 100 kHz, and the power was 5 mW.

6. UV-Visible absorption spectra:

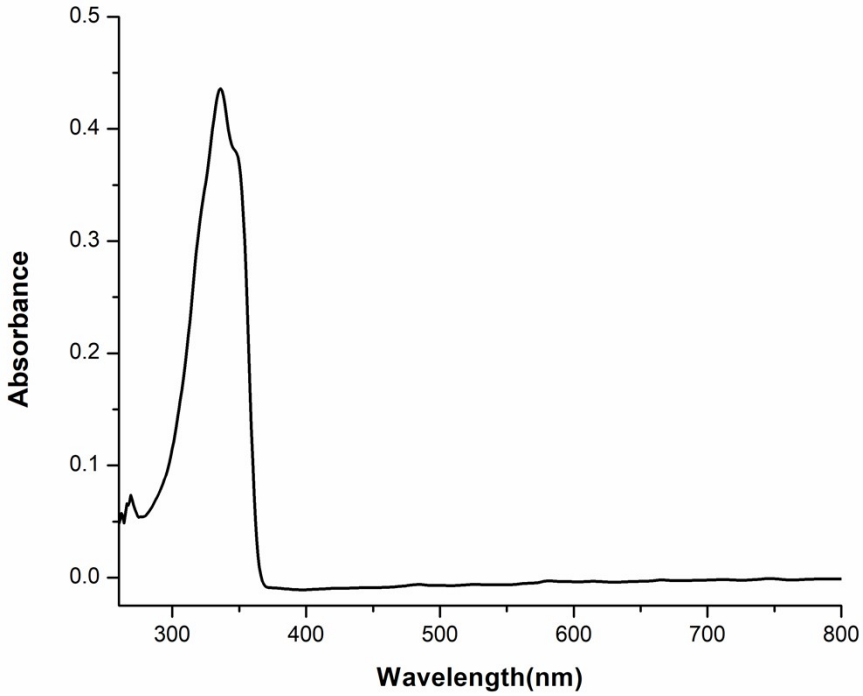


Figure S5. UV-visible spectra of **NMI** in xylene (6.7×10^{-5} M solution was taken)

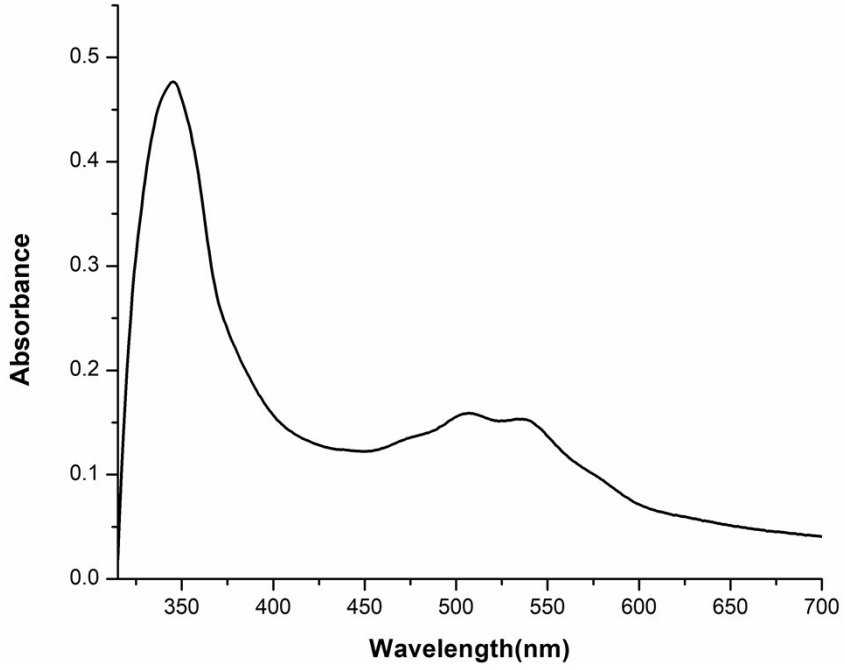


Figure S6. UV-visible spectra of **NMI** in xylene after the addition of KO^{t}Bu and light excitation.

7. Fluorescence quenching experiment and Stern-Volmer plot:

The Stern-Volmer quenching experiments were carried out to explore the intramolecular reductive quenching of the photocatalyst **NMI** by varying concentration of KO^{t}Bu. The emission spectra were collected from a Cary Eclipse Fluorescence Spectrofluorometer. The **NMI** was dissolved in deaerated xylene and the solution was excited at 345 nm. The monitoring wavelength was the corresponding maxima of the emission band; λ_{max} = 382 nm (for **NMI**). Relative fluorescence intensities were measured for solutions containing **NMI** (6.7×10^{-5} M) with varying KO^{t}Bu concentration (15 mM to 65 mM). There was no change in the shape of the fluorescence spectrum but the intensity was decreasing gradually with increasing quencher (KO^{t}Bu) concentration.

Preparation of stock sample: In a Schlenk flask, 2×10^{-3} M solution of **NMI** was prepared in 5 mL dry xylene. The stock solution was diluted to 6.7×10^{-5} M in 3 mL of dry xylene. For each quencher concentration, samples were prepared separately. The Stern-Volmer relationship (equation 1) was established by taking the ratio of the integrated fluorescence intensities (I_0/I_n) in the absence and presence of electron donors and the concentration of donors used as quenchers [Q]. In this present case, the [Q] is KO^{t}Bu.

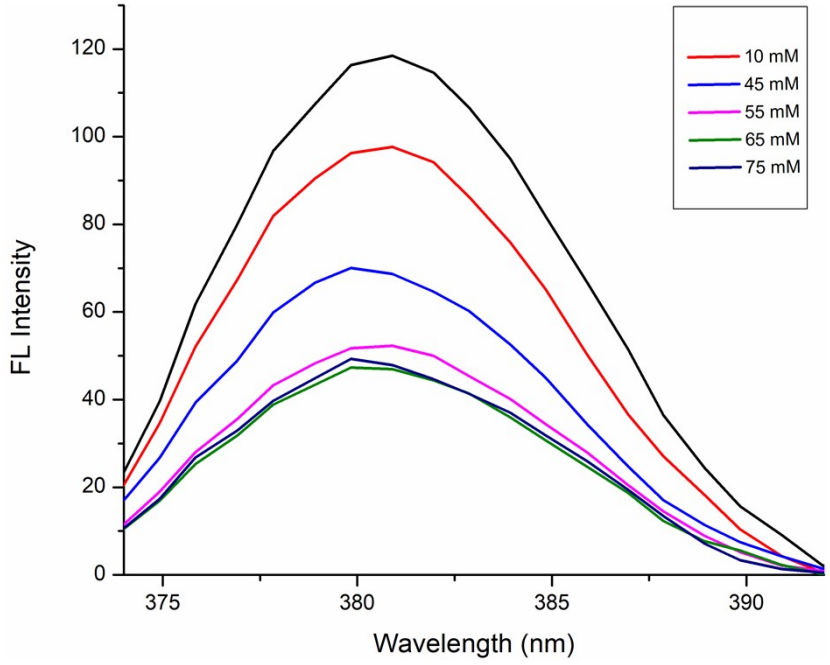


Figure S7. Fluorescence emission spectra of **NMI** (λ_{max} - 381 nm) and its intensity quenching by addition of successive aliquots of KO^{t}Bu. Experiments were carried out in oxygen-free Xylene solution at 298 K with **NMI** concentration of 10^{-5} M, excited at 345 nm.

$$I_0/I = 1 + K_{SV}[Q]\text{……(1)}$$

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.

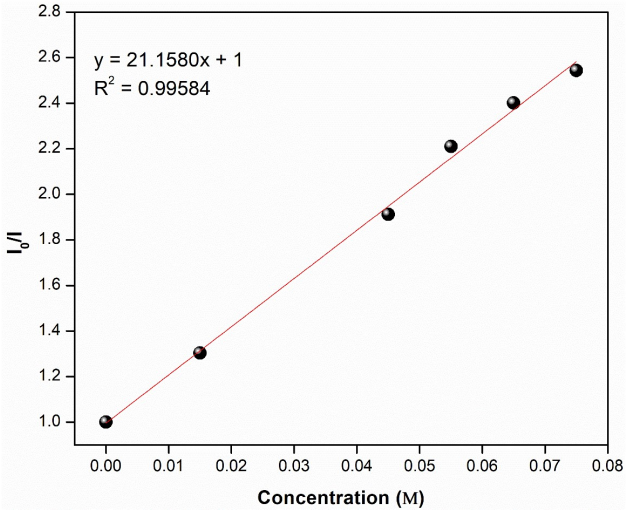


Figure S8. Stern-Volmer quenching of **NMI** showing a linear correlation with increasing quencher (KO^{t}Bu) concentration.

8. Detection of H_2O_2 during alcohol oxidation:

For oxidation of alcohols, presence of H_2O_2 in the reaction mixture was analyzed by UV−Vis spectroscopy[2] using the iodometric assay based on peak of I_3^- at λ_{max} = 345 nm; ε = 26 000 M^{-1} cm^{-1} upon reaction with KI. In a typical reaction, a 5 mL vial was charged with benzyl alcohol (1 mmol), KO^{t}Bu (1 mmol), **NMI** (10 mol%) in 5 mL dry xylene and was closed with a rubber septum. The resulting solution was spurged with O_2. The reaction mixture was stirred for 6 h under blue 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 H_2SO_4 (pH = 2) was 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 H_2O_2 oxidizes I^- to I_2, which reacts with an excess of I^- to form I_3^-. The chemical reactions are as follows[2]

(i) $H_2O_2 + 2I^- + 2H^+ \rightarrow 2H_2O + I_2$

(ii) $I_2\,(aq) + I^- \rightarrow I_3^-$

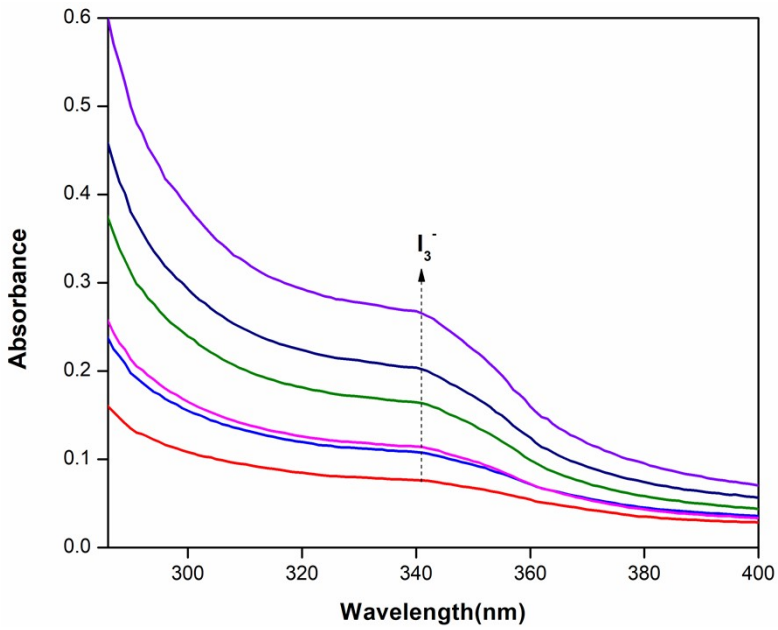
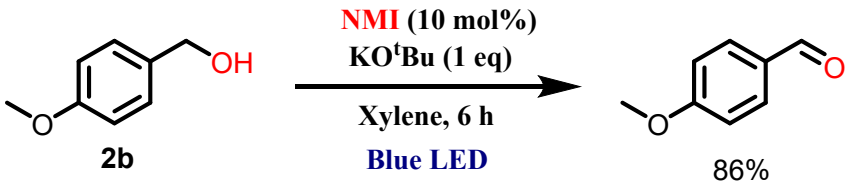


Figure S9: UV-Visible spectrum of I_3^- ion formation in the presence of H_2O_2.

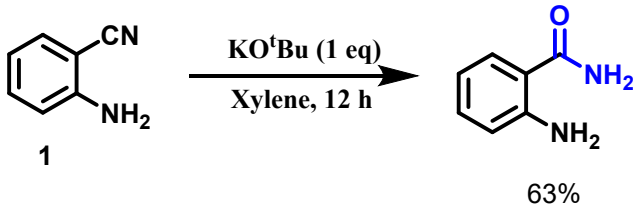
9. Mechanistic insight into the reaction:

a) Photo catalysed alcohol dehydrogenation:



A 15 mL vial tube was charged with 10 mol% of **NMI**, KO^{t}Bu (0.5 mmol), and 4-methoxy benzyl alcohol (0.5 mmol) in 2 mL xylene. The reaction mixture was stirred under blue light irradiation for 6 h in an open atmosphere. Upon completion, the reaction mixture was worked up in ethyl acetate and brine mixture. Then the organic layer was collected, dried and analyzed by ^{1}H NMR spectroscopy. It is found that 86% of 4-methoxy benzaldehyde formed after 6 h under photochemical condition.

b) KO^{t}Bu mediated hydration of *O*-aminobenzonitrile (1):

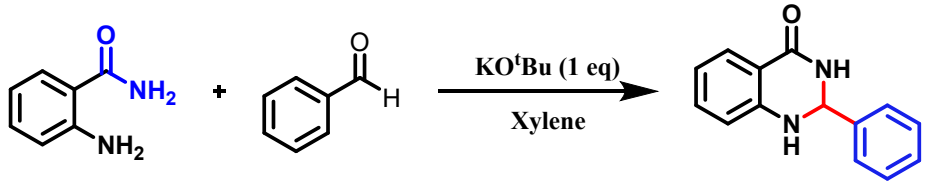


1

63%

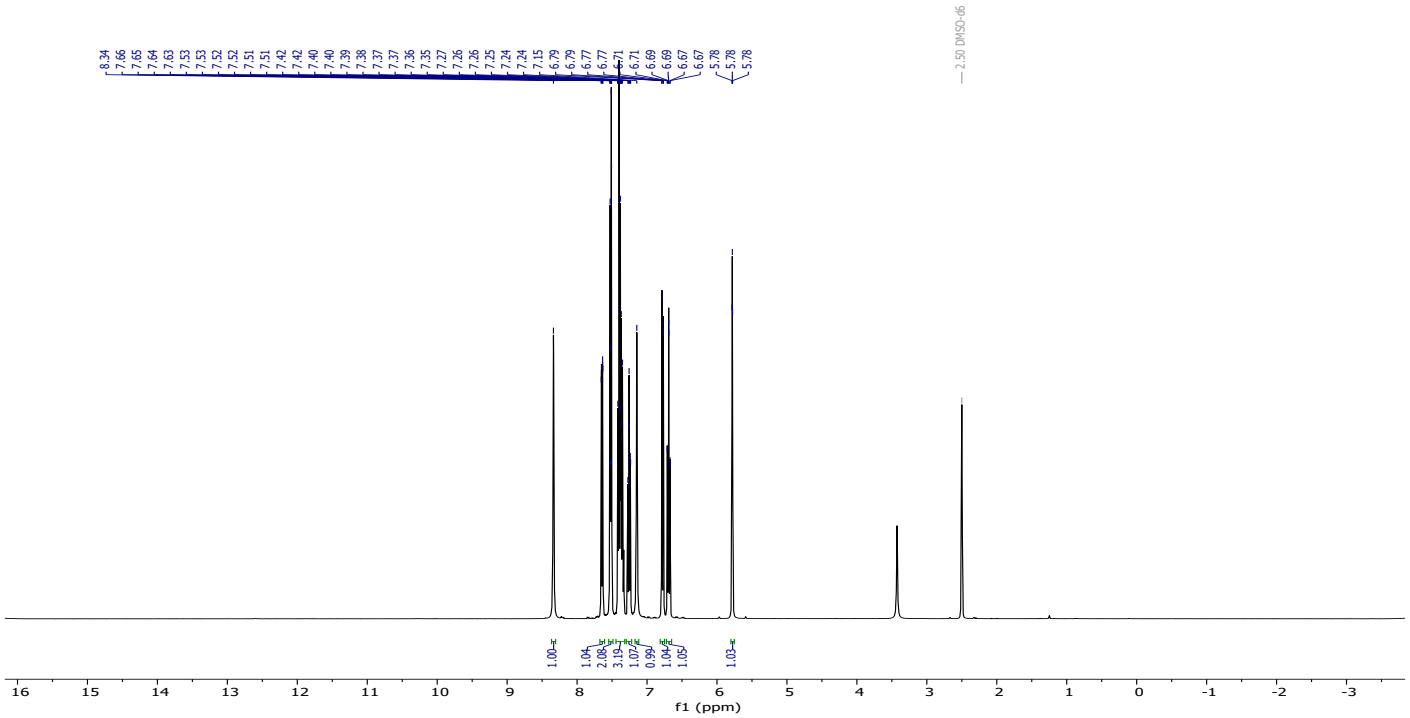
A 15 mL vial was charged with 0.5 mmol of 2-aminobenzonitrile and KO^{t}Bu (0.5 mmol) in 2 mL xylene. The reaction mixture was stirred in an open atmosphere for 12 h. Upon completion, the reaction mixture was extracted with ethyl acetate and evaporated *in vacuo*. Then the residue was purified by column chromatography on silica gel using hexane and ethyl acetate as eluent (3:2), giving 63% isolated yield of 2-aminobenzamide.

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



11
60%

A 15 mL vial tube was charged with 0.5 mmol of 2-aminobenzamide and KO^{t}Bu (0.5 mmol) in 2 mL xylene. 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 gel employing ethyl acetate in hexane (3:2) as an eluent. The intermediate product **11** was isolated in 60% yield. This control reaction proves that this condensation and cyclization event only requires a base. The molecule **11** was fully characterized by ^{1}H and ^{13}C NMR spectroscopies.



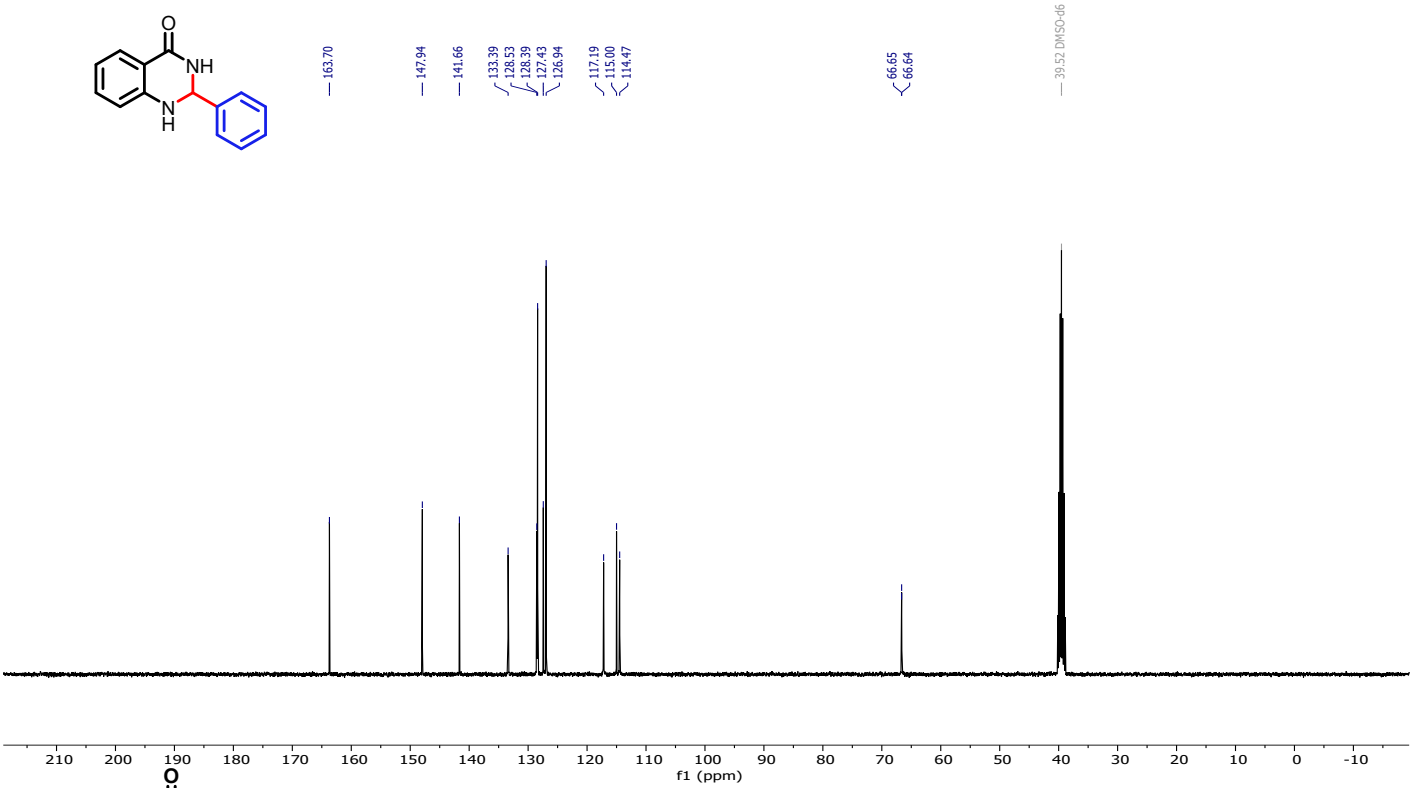
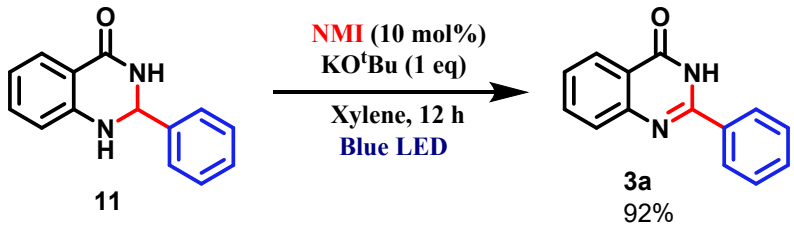


Figure S10: ^{1}H NMR spectrum (400 MHz) of **11** in DMSO-d_6.

Figure S11: ^{13}C NMR spectrum (100 MHz) of **11** in DMSO-d_6.

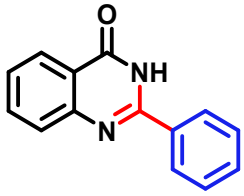
d) NMI catalysed dehydrogenation of intermediate 2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one, 11:



A 15 mL vial tube was charged with 0.5 mmol of 2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one, **11**, 10 mol% of catalyst **NMI** and KO^{t}Bu (0.5 mmol) in 2 mL xylene. The reaction mixture was stirred under blue light irradiation 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 (1:3) as an eluent. The desired product **3a** was separated in 92% isolated yield, suggesting effective dehydrogenation of the cyclic aminal intermediate by **NMI** under photoredox condition.

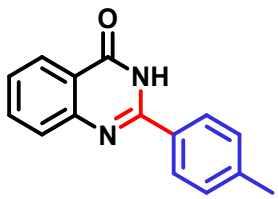
Analytical data:

(E)-1-benzylidene-1*H*-indene (3a) [3]:



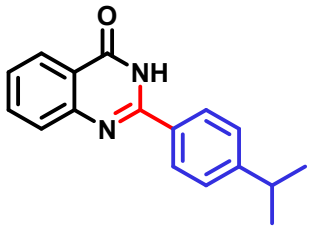
White solid, 88% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.55 (s, 1H), 8.17 (ddd, J = 9.4, 7.9, 1.5 Hz, 3H), 7.88 – 7.80 (m, 1H), 7.77 – 7.72 (m, 1H), 7.60 – 7.49 (m, 4H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 162.5, 152.5, 149.0, 134.8, 133.0, 131.6, 128.8, 128.0, 128.0, 127.7, 126.8, 126.1, 121.2.

2-(*p*-tolyl) quinazolin-4(3*H*)-one (3b) [3]:



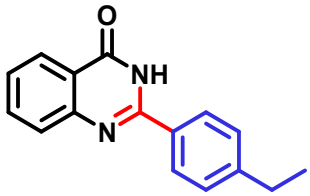
White solid, 81% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.59 (s, 1H), 8.26 (dd, J = 7.9, 1.5 Hz, 1H), 8.23 – 8.18 (m, 2H), 7.94 (ddd, J = 8.6, 7.1, 1.6 Hz, 1H), 7.84 (dd, J = 8.3, 1.2 Hz, 1H), 7.62 (ddd, J = 8.2, 7.1, 1.2 Hz, 1H), 7.46 (d, J = 8.0 Hz, 2H), 2.62 (p, J = 1.9 Hz, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 162.6, 152.6, 149.0, 141.8, 134.9, 130.2, 129.5, 128.0, 127.6, 126.7, 126.1, 121.1, 21.2

2-(4-isopropylphenyl) quinazolin-4(3*H*)-one (3c):



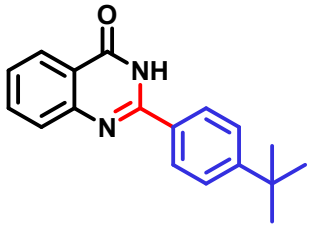
White solid, 76% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.48 (s, 1H), 8.22 – 8.06 (m, 3H), 7.82 (ddd, J = 8.5, 7.0, 1.6 Hz, 1H), 7.73 (dd, J = 8.3, 1.2 Hz, 1H), 7.50 (ddd, J = 8.1, 7.1, 1.2 Hz, 1H), 7.40 (d, J = 8.2 Hz, 2H), 2.96 (hept, J = 6.9 Hz, 1H), 1.23 (d, J = 6.9 Hz, 6H).^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 162.7, 152.7, 152.6, 149.3, 135.0, 130.8, 128.3, 127.9, 127.0, 126.9, 126.3, 121.4, 33.8, 24.0.

2-(4-ethylphenyl) quinazolin-4(3*H*)-one (3d):



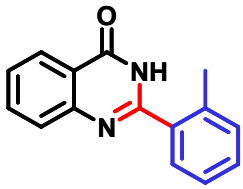
White solid, 83% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.48 (s, 1H), 8.15 (dd, J = 7.9, 1.6 Hz, 1H), 8.13 – 8.08 (m, 2H), 7.82 (ddd, J = 8.5, 7.0, 1.6 Hz, 1H), 7.72 (dd, J = 8.3, 1.2 Hz, 1H), 7.50 (ddd, J = 8.1, 7.0, 1.2 Hz, 1H), 7.40 – 7.34 (m, 2H), 2.68 (q, J = 7.6 Hz, 2H), 1.21 (t, J = 7.6 Hz, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 162.7, 152.7, 149.3, 148.4, 135.4, 130.6, 128.5, 128.2, 127.9, 126.3, 121.4, 28.5, 15.8

2-(4-(tert-butyl)phenyl)quinazolin-4(3*H*)-one (3e)[4]:



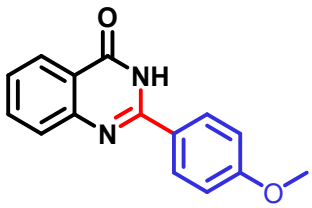
White solid, 87% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.50 (s, 1H), 8.14 (td, J = 7.0, 1.7 Hz, 3H), 7.83 (s, 1H), 7.73 (dd, J = 8.3, 1.2 Hz, 1H), 7.60 – 7.46 (m, 3H), 1.32 (s, 9H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 162.3, 154.3, 152.,2 148.9, 134.6, 129.9, 127.6, 127.5, 126.4, 125.9, 125.5, 120.9, 34.7, 30.9.

2-phenylquinazolin-4(3*H*)-one (3f)[3]:



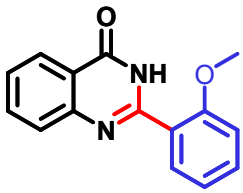
White solid, 78% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.45 (s, 1H), 8.17 (dd, J = 7.9, 1.6 Hz, 1H), 7.86 – 7.81 (m, 1H), 7.69 (d, J = 8.1 Hz, 1H), 7.56 – 7.50 (m, 2H), 7.42 (dd, J = 7.4, 1.5 Hz, 1H), 7.37 – 7.32 (m, 2H), 2.38 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 162.0, 154.6, 148.9, 136.3, 134.7, 134.5, 130.8, 130.1, 129.4, 127.6, 126.9, 126.0, 125.9, 121.2, 19.8.

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



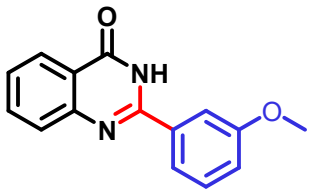
White solid, 73% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.42 (s, 1H), 8.21 – 8.17 (m, 2H), 8.13 (d, J = 6.5 Hz, 1H), 7.81 (s, 1H), 7.73 – 7.68 (m, 1H), 7.48 (s, 1H), 7.09 (d, J = 8.9 Hz, 2H), 3.85 (s, 3H) ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 162.9, 161.9, 152.6, 149.2, 135.3, 129.5, 127.3, 126.2, 124.0, 120.7, 114.8, 56.3.

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



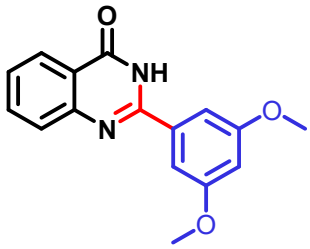
White solid, 70% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.11 (s, 1H), 8.15 (dd, J = 8.0, 1.5 Hz, 1H), 7.83 (s, 1H), 7.70 (dt, J = 7.9, 1.5 Hz, 2H), 7.53 (dt, J = 2.9, 0.9 Hz, 2H), 7.19 (dd, J = 8.5, 1.0 Hz, 1H), 7.09 (d, J = 1.0 Hz, 1H), 3.86 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 160.8, 156.7, 152.0, 148.6, 134.0, 131.8, 130.1, 127.0, 126.2, 125.4, 122.3, 120.6, 120.0, 111.5, 55.3.

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



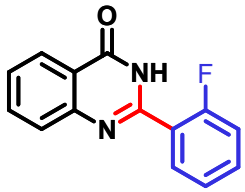
White solid, 66% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.54 (s, 1H), 8.17 – 8.14 (m, 1H), 7.86 – 7.74 (m, 4H), 7.53 (t, J = 6.9 Hz, 1H), 7.46 (t, J = 8.0 Hz, 1H), 7.15 (dd, J = 7.8, 3.1 Hz, 1H), 3.86 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 162.1, 159.2, 152.9, 134.5, 133.9, 129.6, 127.3, 126.5, 125.7, 120.8, 120.0, 117.5, 112.3, 55.2.

2-(3,5-dimethoxyphenyl) quinazolin-4(3*H*)-one (3j)[4]:



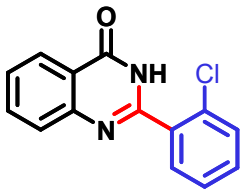
White solid, 72% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.52 (s, 1H), 8.15 (dd, J = 7.9, 1.6 Hz, 1H), 7.88 – 7.81 (m, 1H), 7.78 – 7.73 (m, 1H), 7.53 (ddd, J = 8.1, 7.0, 1.2 Hz, 1H), 7.38 (d, J = 2.3 Hz, 2H), 6.70 (t, J = 2.3 Hz, 1H), 3.84 (s, 6H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 163.1, 152.5, 152.1, 149.1, 135.3, 127.8, 126.9, 126.4, 125.2, 121.7, 121.1, 111.9, 111.1, 56.2.

2-(2-fluorophenyl) quinazolin-4(3*H*)-one (3k)[3]:



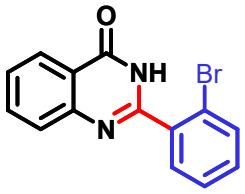
White solid, 60% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.59 (s, 1H), 8.18 (d, J = 7.7 Hz, 1H), 7.91 – 7.68 (m, 3H), 7.58 (dt, J = 21.2, 7.1 Hz, 2H), 7.38 (q, J = 8.9 Hz, 2H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 161.36, 160.67, 158.18 (d, $^{1}J_{C\text{-}F}$ = 249 Hz), 149.78, 148.52, 134.43, 132.73, 132.64, 130.9, 130.9, 127.3, 126.9, 125.7, 124.5, 124.4, 122.2, 122.1, 121.0, 116.1, 115.9.

2-(2-chlorophenyl) quinazolin-4(3*H*)-one (3l)[3]:



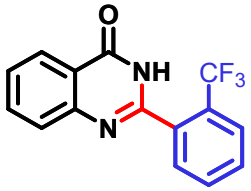
White solid, 71% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.64 (s, 1H), 8.18 (dd, J = 7.9, 1.6 Hz, 1H), 7.89 – 7.82 (m, 1H), 7.69 (ddd, J = 15.8, 7.8, 1.4 Hz, 2H), 7.64 – 7.55 (m, 3H), 7.51 (dd, J = 7.4, 1.5 Hz, 1H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 161.4, 152.3, 148.6, 134.6, 133.8, 131.6, 131.5, 130.9, 129.6, 127.5, 127.3, 127.1, 125.9, 121.3.

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



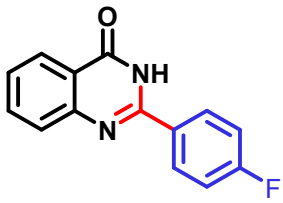
White solid, 66% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.65 (s, 1H), 8.18 (dd, J = 8.0, 1.6 Hz, 1H), 7.86 (ddd, J = 8.5, 7.2, 1.6 Hz, 1H), 7.70 (ddd, J = 15.3, 7.9, 1.5 Hz, 2H), 7.65 – 7.53 (m, 3H), 7.50 (td, J = 7.4, 1.4 Hz, 1H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 161.4, 152.3, 148.6, 134.6, 133.8, 131.7, 130.9, 129.6, 127.5, 127.1, 125.9, 121.3.

2-(2-(trifluoromethyl) phenyl) quinazolin-4(3*H*)-one (3n)[5]:



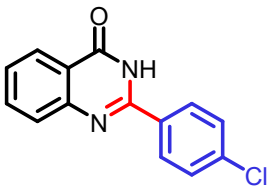
White solid, 73% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.67 (s, 1H), 8.15 (dd, J = 8.1, 1.5 Hz, 1H), 7.89 – 7.86 (m, 1H), 7.84 – 7.81 (m, 1H), 7.80 – 7.77 (m, 1H), 7.76 – 7.72 (m, 2H), 7.65 (dd, J = 8.3, 1.2 Hz, 1H), 7.57 – 7.52 (m, 1H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 161.6, 152.6, 148.6, 134.9, 132.7, 130.9, 130.7, 127.7, 127.4 (q, $^{2}J_{C-F}$ = 31 Hz), 126.7, 126.6 (q, $^{3}J_{C-F}$ = 4 Hz), 126.1,125.4 122.7 (q, $^{1}J_{C-F}$ = 272.1 Hz), 121.4. ^{19}F NMR (376 MHz, DMSO-d_6) δ -57.08.

2-(4-fluorophenyl) quinazolin-4(3*H*)-one (3o) [3]:



White solid, 71% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.57 (s, 1H), 8.31 – 8.19 (m, 2H), 8.15 (dd, J = 7.9, 1.5 Hz, 1H), 7.89 – 7.79 (m, 1H), 7.73 (d, J = 8.1 Hz, 1H), 7.52 (t, J = 7.5 Hz, 1H), 7.39 (t, J = 8.8 Hz, 2H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 164.7, 162.2 (d, $^{1}J_{C-F}$ = 248 Hz), 161.7, 150.8, 148.0, 134.0, 129.8, 129.7, 128.6, 128.6, 126.9, 126.0, 125.3, 120.3, 115.1, 114.9.

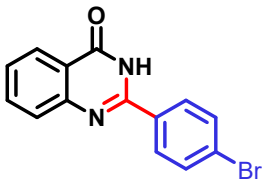
2-(4-chlorophenyl) quinazolin-4(3*H*)-one(3p) [3]:



White solid, 72% yield. ^{1}H NMR (400 MHz, DMSO-d6) δ 12.63 (s, 1H), 8.22 – 8.19 (m, 2H), 8.16 (dd, J = 7.9, 1.6 Hz, 1H), 7.85 (d, J = 1.6 Hz, 1H), 7.75 (d, J = 8.1 Hz, 1H), 7.65 – 7.61

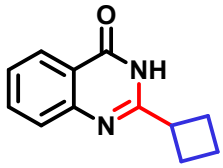
(m, 2H), 7.54 (s, 1H). $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ 162.2, 151.4, 148.6, 136.3, 134.7, 131.6, 129.7, 128.7, 127.6, 126.8, 125.9, 121.0.

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



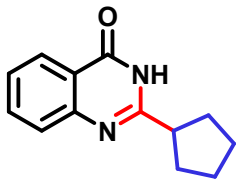
White solid, 65% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.62 (s, 1H), 8.24 – 8.13 (m, 3H), 7.84 (dd, J = 6.9, 1.5 Hz, 1H), 7.77 – 7.70 (m, 1H), 7.67 – 7.59 (m, 2H), 7.57 – 7.51 (m, 1H). $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ 162.2, 151.3, 148.5, 136.3, 134.7, 131.5, 129.6, 128.7, 127.5, 126.8, 125.8, 120.9.

2-cyclobutylquinazolin-4(3*H*)-one (3r)[7]:



White solid, 81% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.06 (s, 1H), 8.07 (dd, J = 7.9, 1.6 Hz, 1H), 7.84 – 7.70 (m, 1H), 7.70 – 7.57 (m, 1H), 7.51 – 7.37 (m, 1H), 3.49 (t, J = 8.6 Hz, 1H), 2.40 (td, J = 9.2, 2.6 Hz, 2H), 2.28 – 2.19 (m, 2H), 2.04 – 1.91 (m, 1H), 1.87 – 1.77 (m, 1H). $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ 162.7, 159.1, 148.9, 135.1, 127.0, 126.0, 125.3, 123.1, 37.5, 26.2, 19.3.

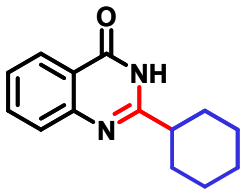
2-cyclopentylquinazolin-4(3*H*)-one (3s)[7]:



White solid, 88% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.13 (s, 1H), 8.07 (d, J = 7.9 Hz, 1H), 7.74 (d, J = 7.6 Hz, 1H), 7.58 (d, J = 8.1 Hz, 1H), 7.44 (d, J = 7.5 Hz, 1H), 3.08 – 2.92

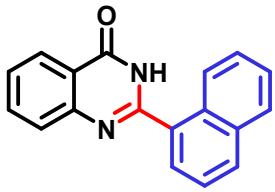
(m, 1H), 2.02 – 1.83 (m, 4H), 1.80 – 1.54 (m, 4H). $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ 161.7, 160.2, 148.7, 134.0, 126.8, 125.7, 125.5, 120.7, 43.6, 30.6, 25.2.

2-cyclohexylquinazolin-4(3*H*)-one (3t)[6]:



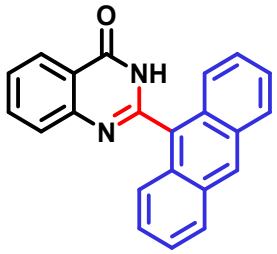
White solid, 78% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.10 (s, 1H), 8.07 (dd, J = 7.9, 1.5 Hz, 1H), 7.76 (ddd, J = 8.5, 7.1, 1.6 Hz, 1H), 7.59 (dd, J = 8.3, 1.2 Hz, 1H), 7.48 – 7.39 (m, 1H), 2.57 (s, 1H), 1.96 – 1.74 (m, 4H), 1.58 (dd, J = 12.3, 3.3 Hz, 3H), 1.38 – 1.15 (m, 3H). $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ 162.0, 160.8, 149.0, 134.3, 127.0, 126.0, 125.7, 121.0, 42.9, 30.2, 25.5, 25.4.

2-(naphthalen-1-yl) quinazolin-4(3*H*)-one (3u)[3]:



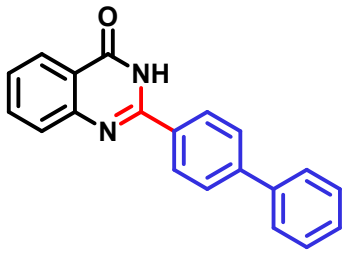
White solid, 68% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.68 (s, 1H), 8.22 (dd, J = 8.0, 1.5 Hz, 1H), 8.19 – 8.09 (m, 2H), 8.08 – 8.00 (m, 1H), 7.87 (ddd, J = 8.5, 7.1, 1.6 Hz, 1H), 7.80 (dd, J = 7.2, 1.3 Hz, 1H), 7.74 (dd, J = 8.2, 1.2 Hz, 1H), 7.67 – 7.56 (m, 4H). $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) 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.

2-(anthracen-9-yl) quinazolin-4(3*H*)-one (3v)[3]:



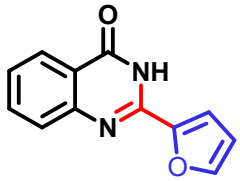
White solid, 74% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.86 (s, 1H), 8.84 (s, 1H), 8.32 (dd, J = 8.0, 1.5 Hz, 1H), 8.25 – 8.19 (m, 2H), 7.94 – 7.88 (m, 1H), 7.79 (ddd, J = 17.8, 8.5, 1.2 Hz, 3H), 7.66 (ddd, J = 8.1, 7.2, 1.2 Hz, 1H), 7.61 – 7.53 (m, 4H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 161.8, 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.

2-([1,1'-biphenyl]-4-yl)quinazolin-4(3*H*)-one (3w) [3]:



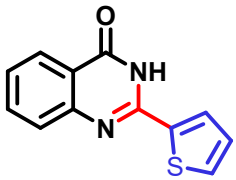
White solid, 68% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.60 (s, 1H), 8.32 – 8.28 (m, 2H), 8.17 (dd, J = 7.9, 1.5 Hz, 1H), 7.88 – 7.84 (m, 3H), 7.80 – 7.76 (m, 3H), 7.55 – 7.50 (m, 3H), 7.44 (d, J = 7.3 Hz, 1H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 162.4, 142.9, 139.0, 134.8, 131.6, 129.2, 128.5, 128.3, 126.9, 126.9, 126.7, 126.0.

2-(furan-2-yl)quinazolin-4(3*H*)-one (3x) [3]:



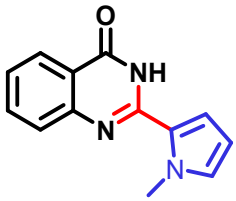
White solid, 71% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.49 (s, 1H), 8.11 (dd, J = 7.9, 1.5 Hz, 1H), 7.98 (d, J = 1.7 Hz, 1H), 7.83 – 7.74 (m, 1H), 7.67 (d, J = 8.1 Hz, 1H), 7.62 (d, J = 3.6 Hz, 1H), 7.47 (t, J = 7.5 Hz, 1H), 6.73 (dd, J = 3.6, 1.7 Hz, 1H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 161.6, 148.7, 146.6, 146.1, 144.0, 134.6, 127.3, 126.5, 126.0, 121.2, 114.5, 112.5.

2-(thiophen-2-yl)quinazolin-4(3*H*)-one (3y) [3]:



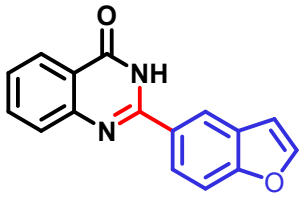
White solid, 73% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.48 (s, 1H), 8.60 (dd, J = 2.9, 1.3 Hz, 1H), 8.13 (dd, J = 8.0, 1.5 Hz, 1H), 7.87 (s, 1H), 7.82 (ddd, J = 8.5, 7.1, 1.6 Hz, 1H), 7.75 – 7.68 (m, 2H), 7.50 (ddd, J = 8.1, 7.1, 1.2 Hz, 1H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 161.7, 148.5, 147.9, 135.0, 134.2, 128.3, 127.0, 126.9, 126.6, 126.0, 125.5, 120.6.

2-(1-methyl-1H-pyrrol-2-yl) quinazolin-4(3*H*)-one (3z)[6]:



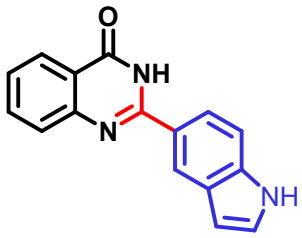
White solid, 60% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.07 (s, 1H), 8.09 (dd, J = 7.9, 1.6 Hz, 1H), 7.77 (ddd, J = 8.4, 7.1, 1.6 Hz, 1H), 7.62 (dd, J = 8.2, 1.1 Hz, 1H), 7.42 (ddd, J = 8.0, 7.1, 1.2 Hz, 1H), 7.22 (dd, J = 4.0, 1.8 Hz, 1H), 7.10 (t, J = 2.1 Hz, 1H), 6.15 (dd, J = 4.0, 2.5 Hz, 1H), 4.07 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 161.4, 148.2, 146.2, 133.8, 129.5, 125.2, 125.1, 123.3, 119.8, 114.2, 107.1, 37.0.

2-(benzofuran-5-yl) quinazolin-4(3H)-one (3za):



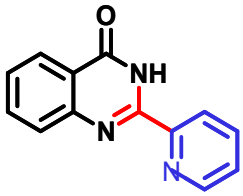
White solid, 64% yield.^{1}H NMR (400 MHz, DMSO-d_6) δ 12.70 (s, 1H), 10.11 (s, 1H), 8.39 – 8.35 (m, 2H), 8.17 (dd, J = 7.9, 1.5 Hz, 1H), 8.08 – 8.05 (m, 2H), 7.87 (ddd, J = 8.4, 7.0, 1.6 Hz, 1H), 7.78 (dd, J = 8.2, 1.2 Hz, 1H), 7.56 (ddd, J = 8.1, 7.0, 1.2 Hz, 1H).^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 192.9, 162.2, 151.5, 148.5, 137.9, 137.8, 134.8, 129.6, 128.6, 128.4, 127.8, 127.2, 126.0, 121.2. **HRMS** (ESI, m/z) calcd. for $C_{16}H_{10}N_2O_2$ [M+H]+ : 263.0815; found: 263.1261

2-(1H-indol-5-yl) quinazolin-4(3*H*)-one (3zb):



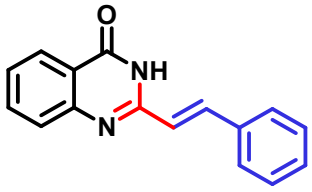
White solid, 67% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.64 (s, 1H), 8.41 (s, 1H), 8.19 (dd, J = 8.1, 1.5 Hz, 1H), 7.95 – 7.91 (m, 1H), 7.88 – 7.80 (m, 2H), 7.70 – 7.58 (m, 3H), 7.57 (q, J = 3.2 Hz, 1H), 6.68 (d, J = 2.5 Hz, 1H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 161.5, 160.2, 157.1, 138.9, 136.0, 128.7, 128.4, 127.8, 127.2, 126.9, 123.3, 122.8, 122.0, 120.1, 112.4, 103.2. **HRMS** (ESI, m/z) calcd. for $C_{16}H_{11}N_3O$ [M + H]$^{+}$: 262.0975; found: 262.0985

2-(pyridin-2-yl) quinazolin-4(3*H*)-one (3zc) [3]:



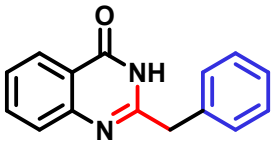
White solid, 59% yield.^{1}H NMR (400 MHz, DMSO-d_6) δ 11.87 (s, 1H), 8.79 – 8.75 (m, 1H), 8.48 – 8.45 (m, 1H), 8.20 (dd, J = 8.0, 1.5 Hz, 1H), 8.09 (d, J = 1.7 Hz, 1H), 7.91 – 7.80 (m, 2H), 7.70 – 7.65 (m, 1H), 7.58 (s, 1H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 161.1, 150.2, 149.3, 149.0, 148.7, 138.3, 135.0, 128.0, 127.6, 126.8, 126.4, 122.4, 122.3.

(E)-2-(4-styrylphenyl) quinazolin-4(3H)-one (3zd) [4]:



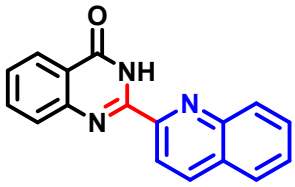
White solid, 63% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.35 (s, 1H), 8.11 (dd, J = 8.0, 1.6 Hz, 1H), 7.95 (d, J = 16.2 Hz, 1H), 7.80 (d, J = 7.0 Hz, 1H), 7.67 (dd, J = 8.0, 6.0 Hz, 3H), 7.50 – 7.42 (m, 4H), 7.01 (d, J = 16.2 Hz, 1H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 161.8, 151.4, 149.0, 138.3, 135.0, 134.6, 129.8, 129.1, 127.7, 127.2, 126.3, 125.9, 121.1, 121.1.

2-benzylquinazolin-4(3*H*)-one (3ze):



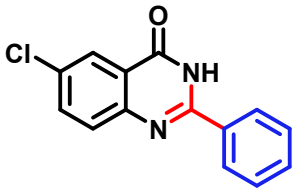
White solid, 75% yield, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.44 (s, 1H), 8.08 (dd, J = 8.0, 1.5 Hz, 1H), 7.77 (s, 1H), 7.61 (dd, J = 8.3, 1.1 Hz, 1H), 7.47 (d, J = 1.0 Hz, 1H), 7.41 – 7.36 (m, 2H), 7.32 (t, J = 7.6 Hz, 2H), 7.25 (d, J = 7.2 Hz, 1H), 3.94 (s, 2H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 161.91, 156.01, 148.94, 136.60, 134.44, 128.91, 128.54, 126.96, 126.84, 126.26, 125.74, 120.77, 40.80.

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



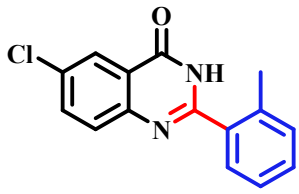
Yellow solid, 78% yield. ^{1}H NMR (400 MHz, Chloroform-d) δ 11.22 (s, 1H), 8.62 (d, J = 8.6 Hz, 1H), 8.44 – 8.26 (m, 2H), 8.13 (d, J = 8.5 Hz, 1H), 7.92 – 7.84 (m, 2H), 7.84 – 7.72 (m, 2H), 7.62 (dd, J = 8.3, 6.8 Hz, 1H), 7.58 – 7.47 (m, 1H). ^{13}C NMR{^{1}H} (100 MHz, Chloroform-d) δ 161.6, 149.2, 149.1, 148.1, 146.9, 137.7, 134.7, 130.6, 129.8, 129.4, 128.4, 128.3, 127.9, 127.7, 126.9, 122.7, 118.5.

6-chloro-2-phenylquinazolin-4(3*H*)-one (7a) [4]:



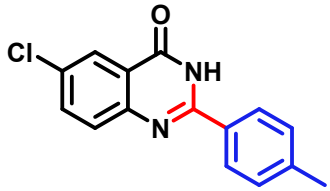
White solid, 87% yield.^{1}H NMR (400 MHz, DMSO-d_6) δ 12.73 (s, 1H), 8.20 – 8.15 (m, 2H), 8.08 (d, *J* = 2.5 Hz, 1H), 7.85 (d, *J* = 2.6 Hz, 1H), 7.76 (d, *J* = 8.7 Hz, 1H), 7.61 – 7.53 (m, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 161.8, 151.4, 149.0, 138.3, 135.0, 134.5, 129.82, 129.1, 127.7, 127., 126.3, 125.9, 121.1, 121.1.

6-chloro-2-(o-tolyl) quinazolin -4(3*H*)-one (7b):



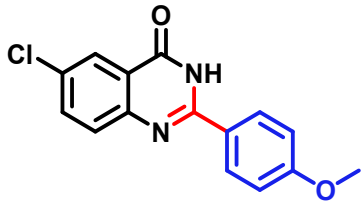
White solid, 71% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.62 (s, 1H), 8.09 (d, J = 2.5 Hz, 1H), 7.85 (dd, J = 8.7, 2.5 Hz, 1H), 7.70 (d, J = 8.7 Hz, 1H), 7.49 (dd, J = 7.6, 1.4 Hz, 1H), 7.42 (dd, J = 7.4, 1.5 Hz, 1H), 7.36 – 7.29 (m, 2H), 2.37 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 160.5, 152.8, 147.3, 134.8, 133.6, 131.8, 131.4, 131.4, 130.9, 129.8, 129.6, 127.3, 124.9, 23.3.

6-chloro-2-(p-tolyl) quinazolin-4(3*H*)-one (7c) [7]:



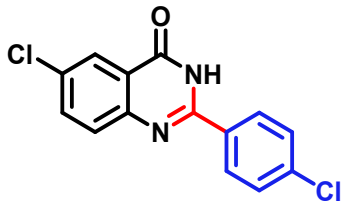
White solid, 77% yield.^{1}H NMR (400 MHz, DMSO-d_6) δ 12.63 (s, 1H), 8.10 (d, J = 2.5 Hz, 1H), 7.87 (dd, J = 8.7, 2.5 Hz, 1H), 7.72 (d, J = 8.7 Hz, 1H), 7.51 (dd, J = 7.6, 1.4 Hz, 1H), 7.43 (dd, J = 7.4, 1.5 Hz, 1H), 7.37 – 7.30 (m, 2H), 2.38 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 161.0, 155.1, 136.4, 134.8, 134.2, 131.1, 130.8, 130.3, 129.4, 125.9, 125.0, 19.8.

6-chloro-2-(4- methoxyphenyl) quinazolin-4(3*H*)-one (7d)[8]:



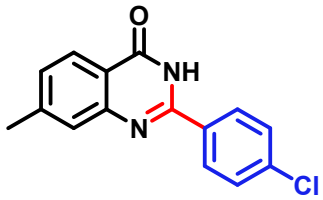
White solid, 64% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.59 (s, 1H), 8.20 – 8.17 (m, 2H), 8.06 (d, J = 2.5 Hz, 1H), 7.84 (dd, J = 8.7, 2.6 Hz, 1H), 7.72 (d, J = 8.7 Hz, 1H), 7.11 – 7.08 (m, 2H), 3.85 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 162.1, 161.4, 152.4, 147.8, 134.7, 130.3, 129.5, 124.8, 124.5, 121.9, 114.1, 55.5.

6-chloro-2-(4-chlorophenyl) quinazolin-4(3*H*)-one (7e)[8]:



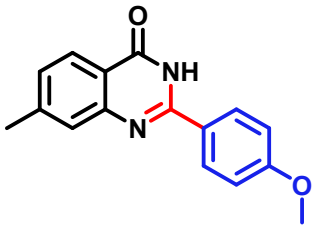
White solid,68% yield.^{1}H NMR (400 MHz, DMSO-d_6) δ 12.84 (s, 1H), 8.11 (d, J = 2.5 Hz, 1H), 7.89 (dd, J = 8.7, 2.6 Hz, 1H), 7.74 (d, J = 8.8 Hz, 1H), 7.67 (dd, J = 7.5, 1.7 Hz, 1H), 7.62 (dd, J = 8.0, 1.4 Hz, 1H), 7.57 (td, J = 7.6, 1.7 Hz, 1H), 7.50 (td, J = 7.4, 1.4 Hz, 1H). ^{13}C NMR{^{1}H} (100 MHz, DMSO-d_6) δ 160.5, 152.8, 147.3, 134.8, 133.6, 131.8, 131.4, 130.9, 129.8, 129.6, 127.3, 124.9.

2-(4-chlorophenyl)-7-methylquinazolin-4(3*H*)-one (8a)[9]:



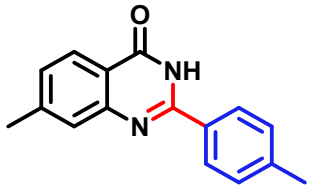
White solid,78% yield.^{1}H NMR (400 MHz, DMSO-d_6) δ 12.46 (s, 1H), 8.17 (dt, J = 6.6, 1.7 Hz, 2H), 8.03 (d, J = 8.1 Hz, 1H), 7.65 – 7.49 (m, 4H), 7.33 (dd, J = 8.1, 1.7 Hz, 1H), 2.46 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 162.6, 152.8, 149.3, 145.5, 133.2, 131.8, 129.1, 128.5, 128.2, 127.6, 126.2, 119.0, 21.5.

2-(4-methoxyphenyl)-7-methylquinazolin-4(3*H*)-one (8b)[10]:



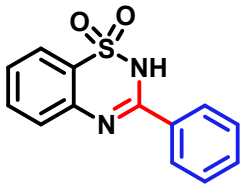
White solid, 84% yield.^{1}H NMR (400 MHz, DMSO-d_6) δ 12.33 (s, 1H), 8.20 – 8.16 (m, 2H), 8.01 (d, J = 8.0 Hz, 1H), 7.51 (d, J = 1.5 Hz, 1H), 7.30 (dd, J = 8.1, 1.7 Hz, 1H), 7.10 – 7.06 (m, 2H), 3.85 (s, 3H), 2.46 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 161.9, 151.9, 149.1, 145.0, 129.4, 127.6, 126.9, 125.7, 124.9, 118.3, 114.0, 55.4, 21.4.

7-methyl-2-(p-tolyl) quinazolin-4(3*H*)-one (8c) [7]:



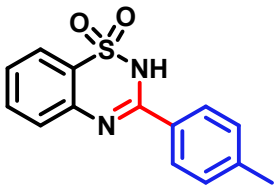
White solid,82% yield.^{1}H NMR (400 MHz, DMSO-d_6) δ 12.38 (s, 1H), 8.08 (d, J = 7.9 Hz, 2H), 8.02 (d, J = 8.0 Hz, 1H), 7.53 (s, 1H), 7.33 (t, J = 8.3 Hz, 3H), 2.46 (s, 3H), 2.38 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 162.2, 152.3, 149.0, 145.1, 141.5, 130.0, 129.3, 127.3, 127.7, 127.1, 125.8, 118.5, 21.4, 21.1.

3-phenyl-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide (9a)[3]:



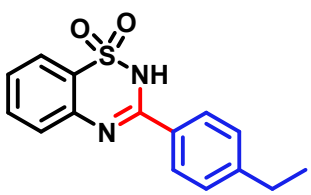
White solid,62% yield.^{1}H NMR (400 MHz, DMSO-d_6) δ 12.22 (s, 1H), 8.08 – 8.03 (m, 2H), 7.89 – 7.85 (m, 1H), 7.76 – 7.69 (m, 2H), 7.64 (dt, J = 7.3, 2.2 Hz, 3H), 7.50 (s, 1H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 155.1, 135.8, 133.37, 133.1, 132.2, 129.1, 128.5, 126.5, 123.6, 121.7, 118.8.

3-(p-tolyl)-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide (9b)[3]:



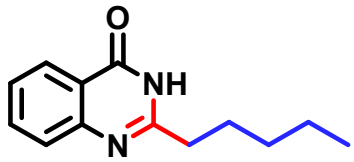
White solid,59% yield.^{1}H NMR (400 MHz, DMSO-d_6) δ 12.10 (s, 1H), 7.99 – 7.95 (m, 2H), 7.85 (dd, J = 7.9, 1.4 Hz, 1H), 7.77 – 7.71 (m, 1H), 7.64 (dd, J = 8.4, 1.1 Hz, 1H), 7.52 – 7.47 (m, 1H), 7.44 (d, J = 8.0 Hz, 2H), 2.42 (s, 3H).^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 154.7, 143.3, 135.5, 133.1, 129.5, 128.9, 128.3, 126.7, 123.34, 121.5, 118.4, 21.1.

3-(4-ethylphenyl)-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide (9c):



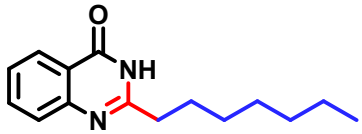
White solid,56% yield.^{1}H NMR (400 MHz, DMSO-d_6) δ 12.11 (s, 1H), 8.06 – 7.89 (m, 2H), 7.86 (dd, J = 8.0, 1.4 Hz, 1H), 7.73 (ddd, J = 8.6, 7.2, 1.5 Hz, 1H), 7.63 (dd, J = 8.5, 1.2 Hz, 1H), 7.54 – 7.37 (m, 3H), 2.72 (q, J = 7.6 Hz, 2H), 1.22 (d, J = 1.7 Hz, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 154.7, 149.4, 135.6, 133.1, 129.2, 128.4, 128.3, 126.7, 123.4, 121.5, 118.5, 28.2, 15.3.

2-pentylquinazolin-4(3*H*)-one (10a):



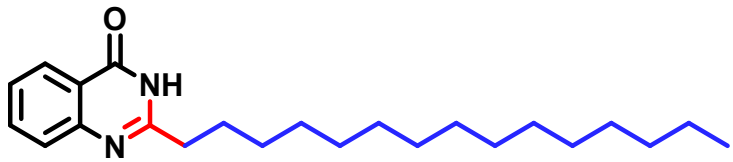
White solid, 66% yield ^{1}H NMR (400 MHz, DMSO-d_6 δ 12.18 (s, 1H), 8.07 (dd, J = 7.9, 1.6 Hz, 1H), 7.76 (ddd, J = 8.5, 7.1, 1.6 Hz, 1H), 7.59 (dd, J = 8.2, 1.1 Hz, 1H), 7.45 (ddd, J = 8.1, 7.1, 1.2 Hz, 1H), 2.62 – 2.56 (m, 2H), 1.76 – 1.67 (m, 2H), 1.31 (dt, J = 7.5, 3.0 Hz, 4H), 0.90 – 0.84 (m, 3H).^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 161.85, 157.55, 148.99, 134.30, 126.82, 125.93, 125.70, 120.79, 34.49, 30.79, 26.53, 21.87, 13.89.

2-heptylquinazolin-4(3*H*)-one (10b):



White solid, 71% yield, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.17 (s, 1H), 8.07 (dd, J = 7.9, 1.5 Hz, 1H), 7.76 (ddd, J = 8.5, 7.1, 1.6 Hz, 1H), 7.58 (dd, J = 8.3, 1.1 Hz, 1H), 7.47 – 7.43 (m, 1H), 2.61 – 2.55 (m, 2H), 1.71 (p, J = 7.3 Hz, 2H), 1.35 – 1.22 (m, 8H), 0.88 – 0.82 (m, 3H).). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 164.91, 157.54, 150.51, 133.75, 126.81, 125.93, 125.69, 122.53, 34.19, 30.75, 28.51, 26.81, 22.08, 16.84.

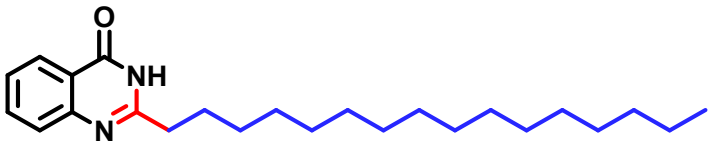
2-pentadecylquinazolin-4(3*H*)-one (10c):



White solid, 80% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.66 (s, 1H), 8.28 (dd, J = 7.9, 1.5 Hz, 1H), 7.77 (ddd, J = 8.5, 7.0, 1.6 Hz, 1H), 7.70 (dd, J = 8.2, 1.2 Hz, 1H), 7.47 (ddd, J =

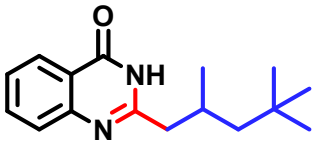
8.1, 6.9, 1.3 Hz, 1H), 2.86 – 2.72 (m, 2H), 1.94 – 1.82 (m, 2H), 1.49 – 1.41 (m, 2H), 1.38 – 1.20 (m, 22H), 0.87 (t, J = 6.8 Hz, 3H). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 164.26, 157.06, 149.59, 134.93, 127.35, 126.48, 126.38, 120.65, 36.17, 32.06, 29.83, 29.79, 29.77, 29.61, 29.51, 29.42, 29.38, 27.73, 22.84, 14.28.

2-hexadecylquinazolin-4(3H)-one (10d):



White solid, 85% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.06 (s, 1H), 8.29 (dd, J = 8.0, 1.5 Hz, 1H), 7.81 – 7.73 (m, 1H), 7.70 (dd, J = 8.3, 1.3 Hz, 1H), 7.46 (ddd, J = 8.1, 6.9, 1.3 Hz, 1H), 2.84 – 2.73 (m, 2H), 1.91 – 1.86 (m, 2H), 1.41 (dt, J = 37.2, 7.8 Hz, 4H), 1.32 – 1.21 (m, 22H), 0.87 (t, J = 6.8 Hz, 3H). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 164.43, 157.10, 149.53, 134.79, 127.22, 126.31, 126.23, 120.49, 36.02, 31.94, 29.71, 29.68, 29.65, 29.50, 29.39, 29.30, 29.28, 27.64, 22.71, 14.15.

2-(2,4,4-trimethylpentyl)quinazolin-4(3*H*)-one (10e):



White solid, 72% yield, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.22 (s, 1H), 8.07 (dd, J = 8.0, 1.5 Hz, 1H), 7.76 (ddd, J = 8.5, 7.1, 1.6 Hz, 1H), 7.60 (dd, J = 8.3, 1.2 Hz, 1H), 7.44 (ddd, J = 8.2, 7.1, 1.2 Hz, 1H), 2.57 – 2.51 (m, 1H), 2.42 (dd, J = 13.5, 7.6 Hz, 1H), 2.15 (ddq, J = 10.8, 7.0, 3.5 Hz, 1H), 1.32 (dd, J = 14.0, 3.2 Hz, 1H), 1.09 (dd, J = 13.9, 6.8 Hz, 1H), 0.93 (d, J = 6.6 Hz, 3H), 0.82 (s, 9H). $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ 161.90, 156.70, 148.92, 134.31, 126.85, 125.95, 125.68, 120.74, 49.78, 43.89, 30.80, 29.78, 28.31, 22.53.

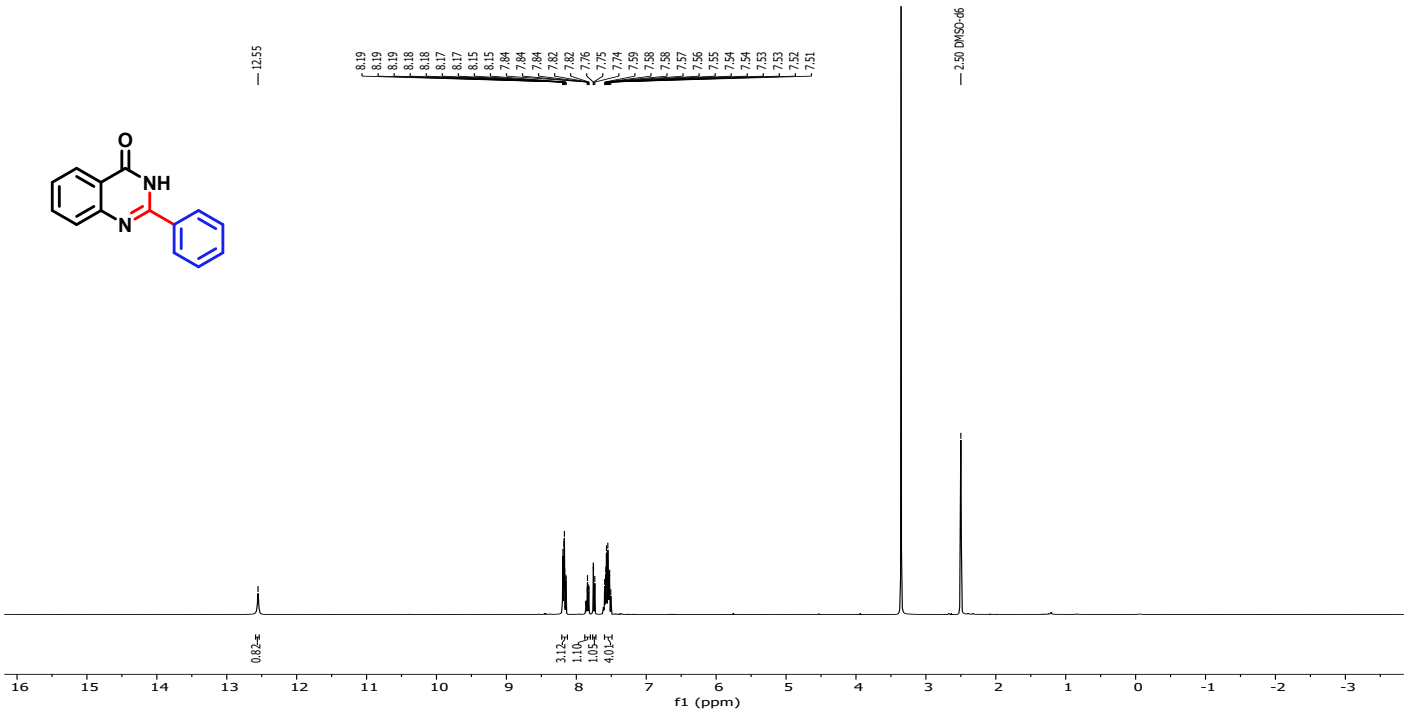


Figure S12. ^{1}H NMR spectrum (400 MHz) of **3a** in DMSO-d_6

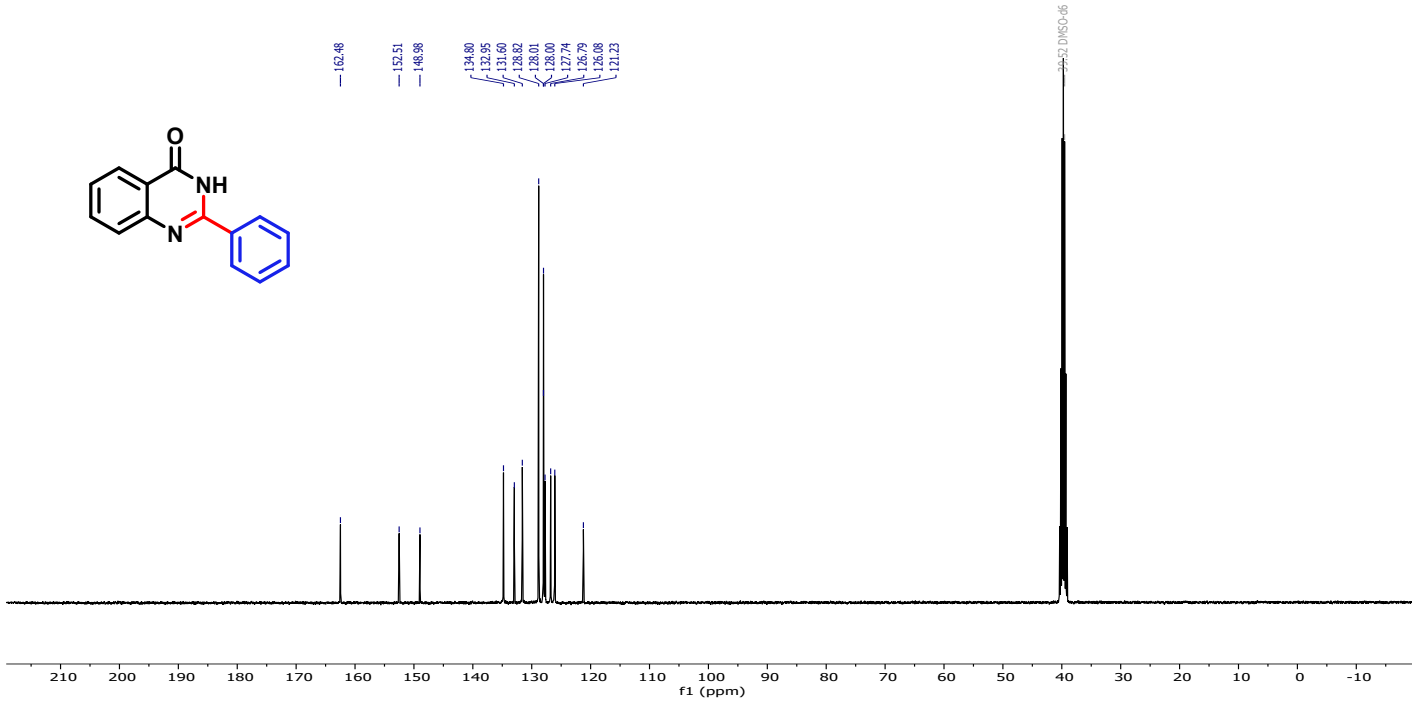


Figure S13. ^{13}C NMR spectrum (100 MHz) of **3a** in DMSO-d_6

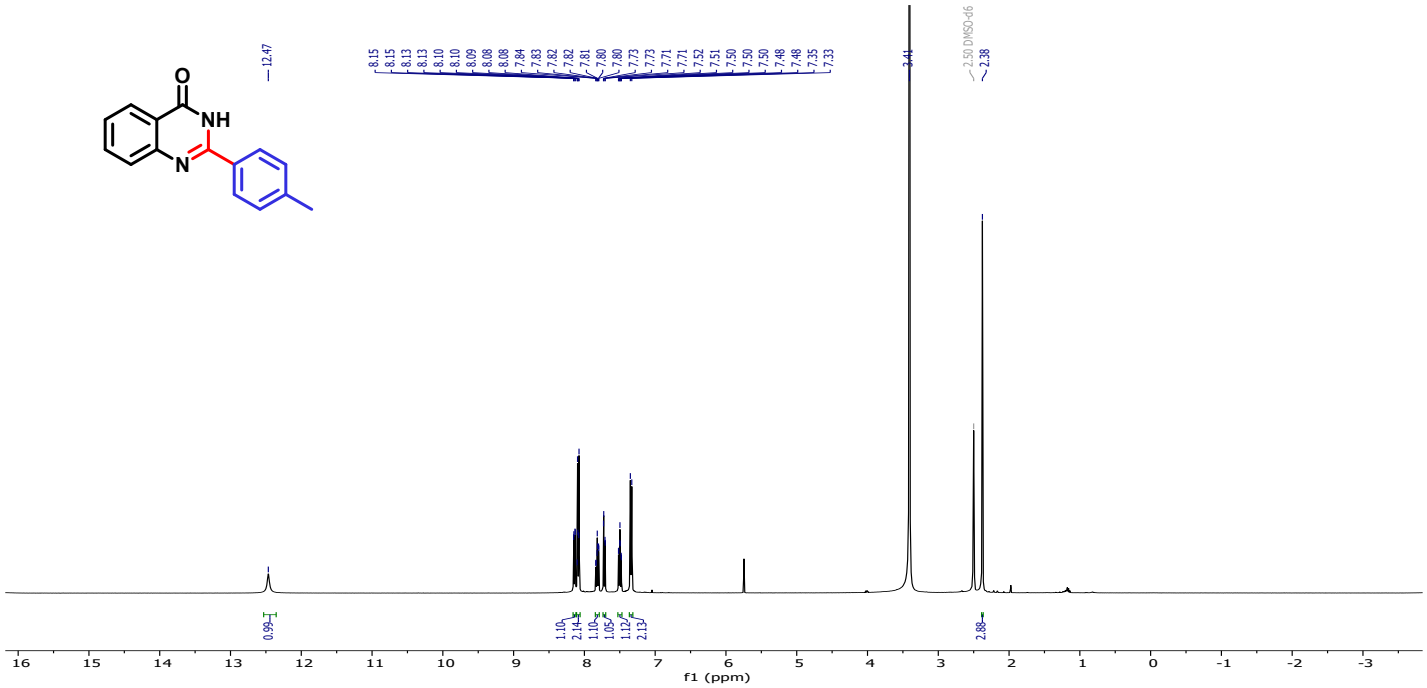


Figure S14. ^{1}H NMR spectrum (400 MHz) of **3b** in DMSO-d$_6$.

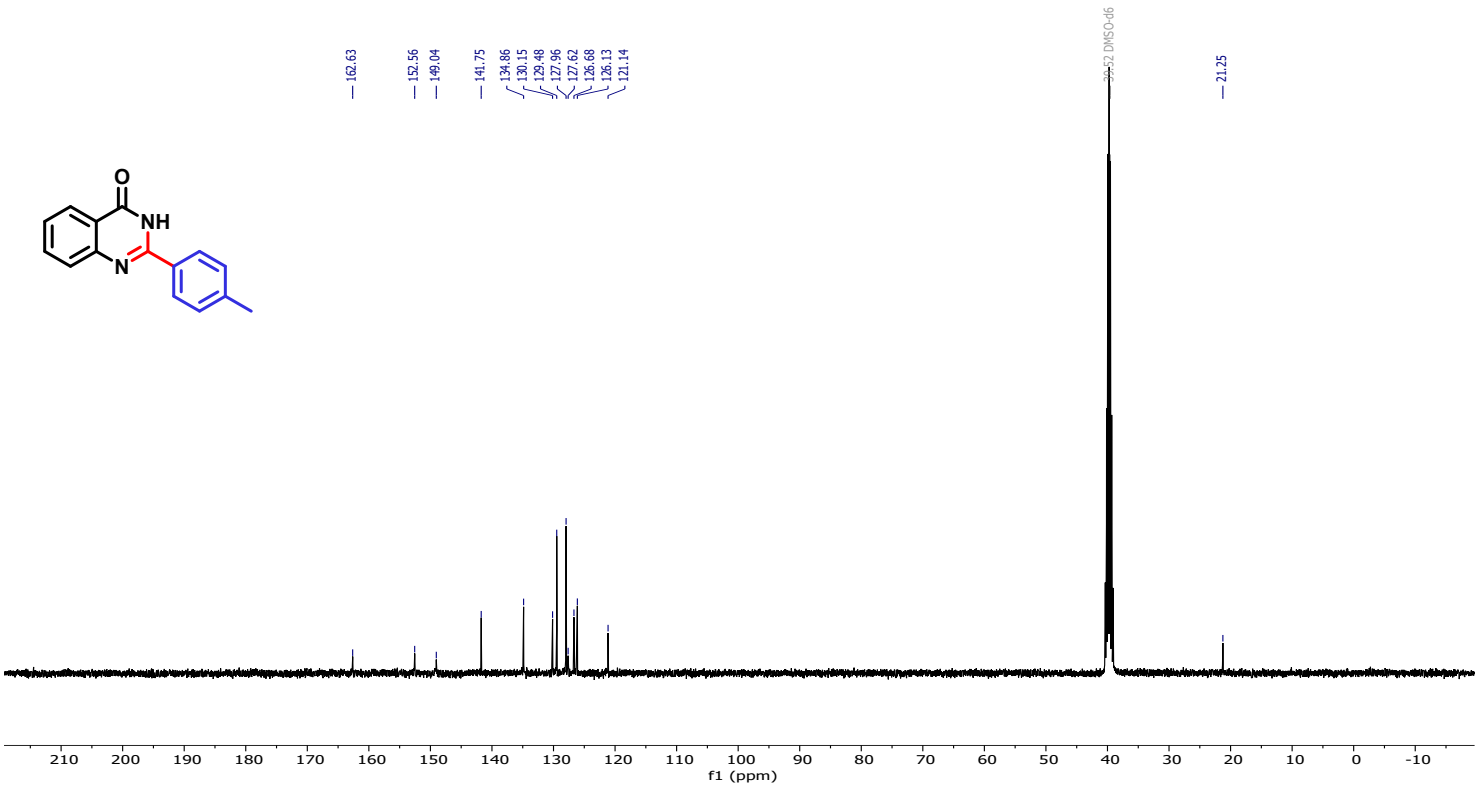


Figure S15. ^{13}C NMR spectrum (100 MHz) of **3b** in DMSO-d$_6$

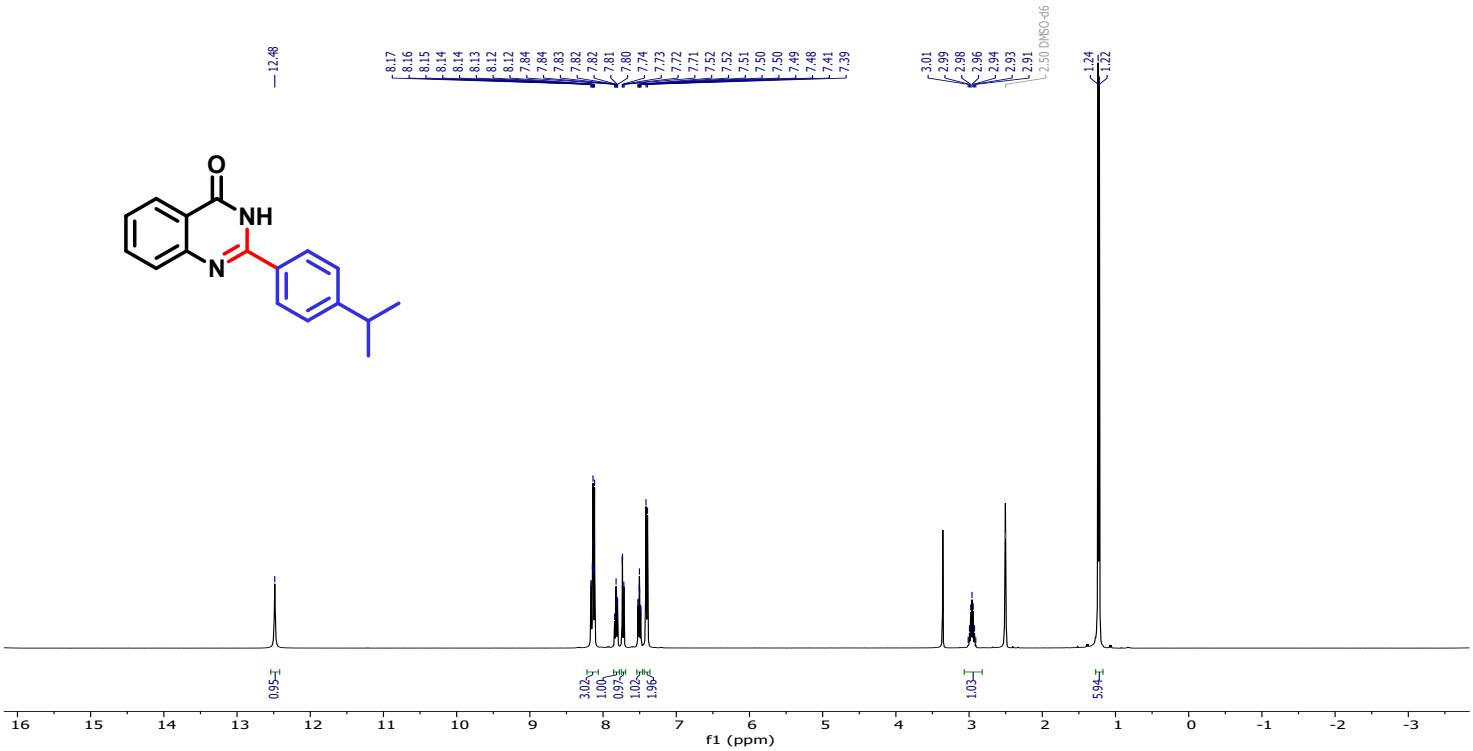


Figure S16. ^{1}H NMR spectrum (400 MHz) of 3**c** in DMSO-d_6

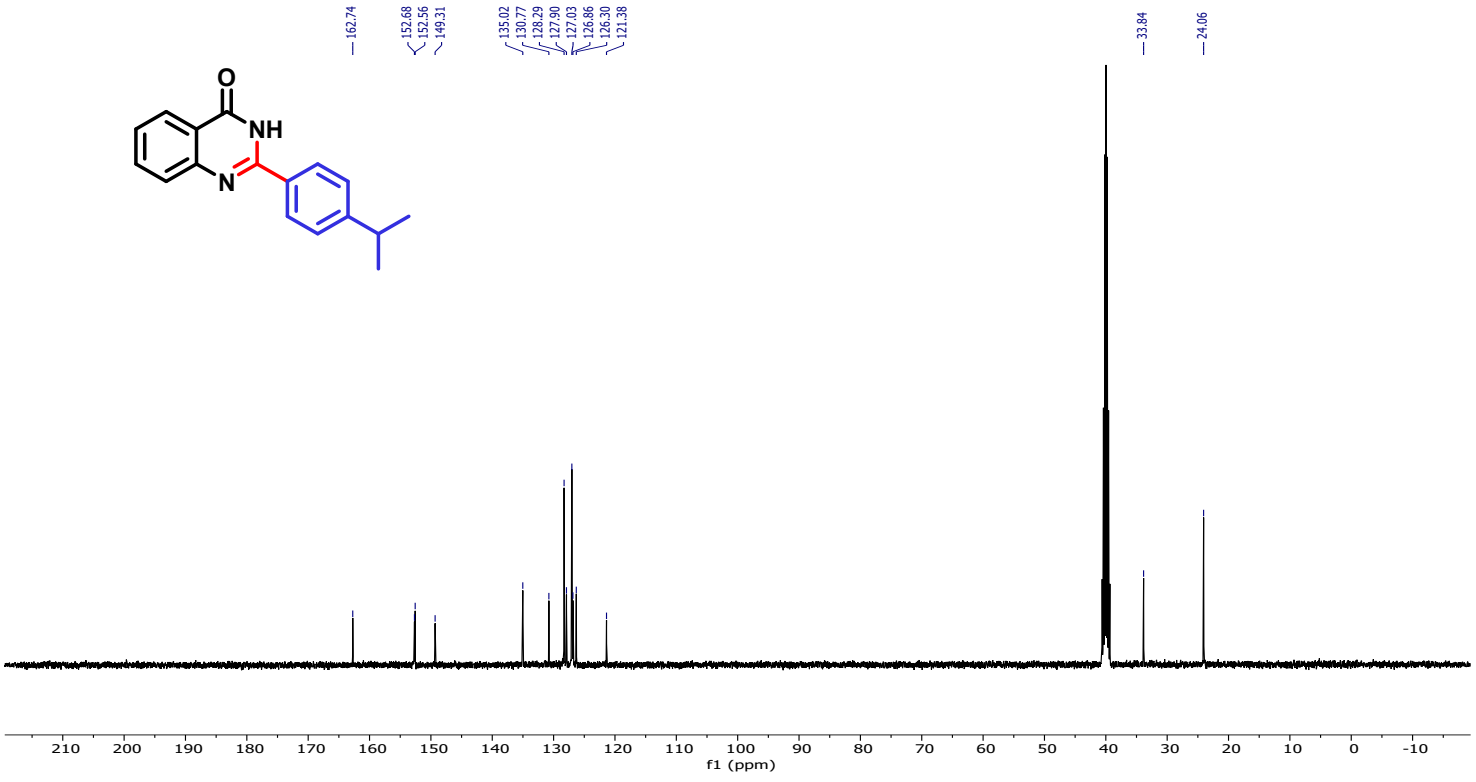


Figure S17. ^{13}C NMR spectrum (100 MHz) of **3c** in DMSO-d_6

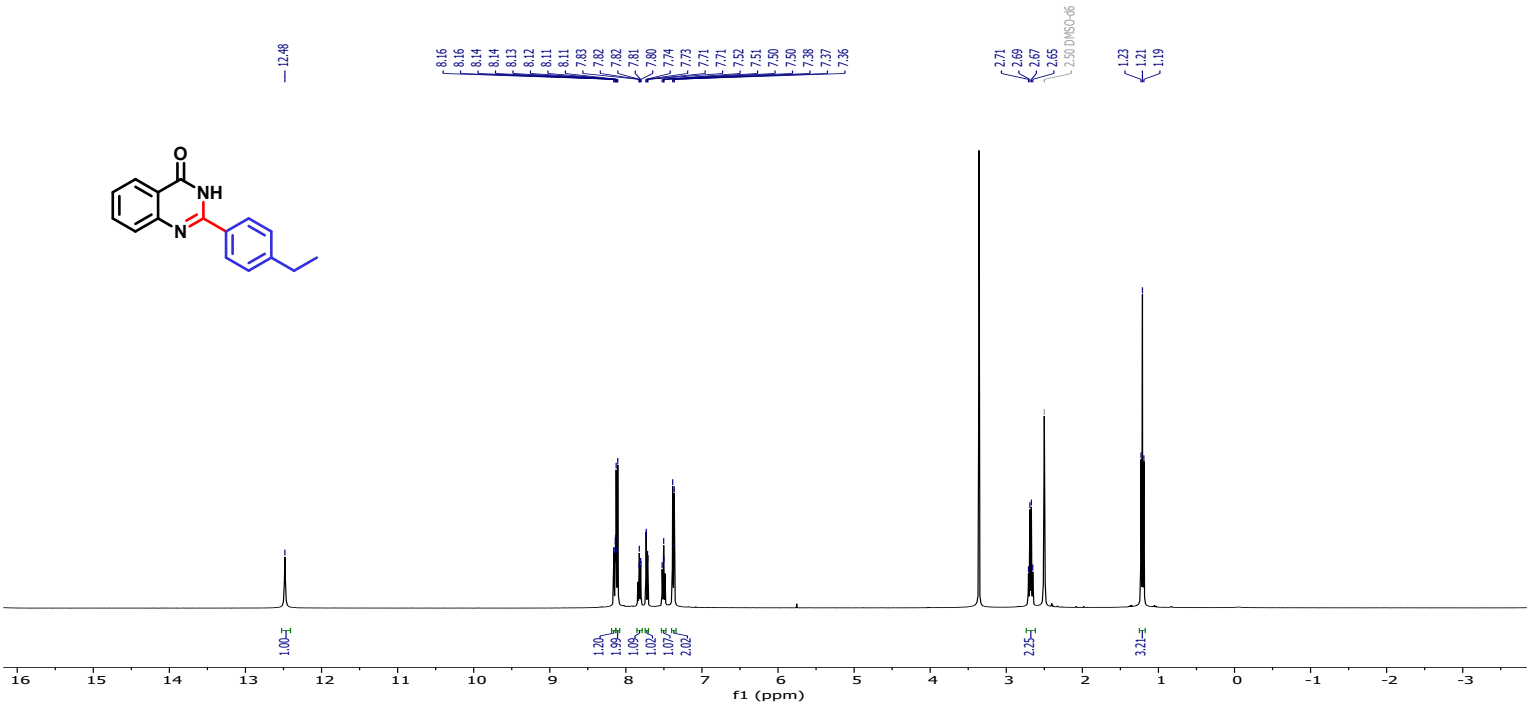


Figure S18. ^{1}H NMR spectrum (400 MHz) of **3d** in DMSO-d_6

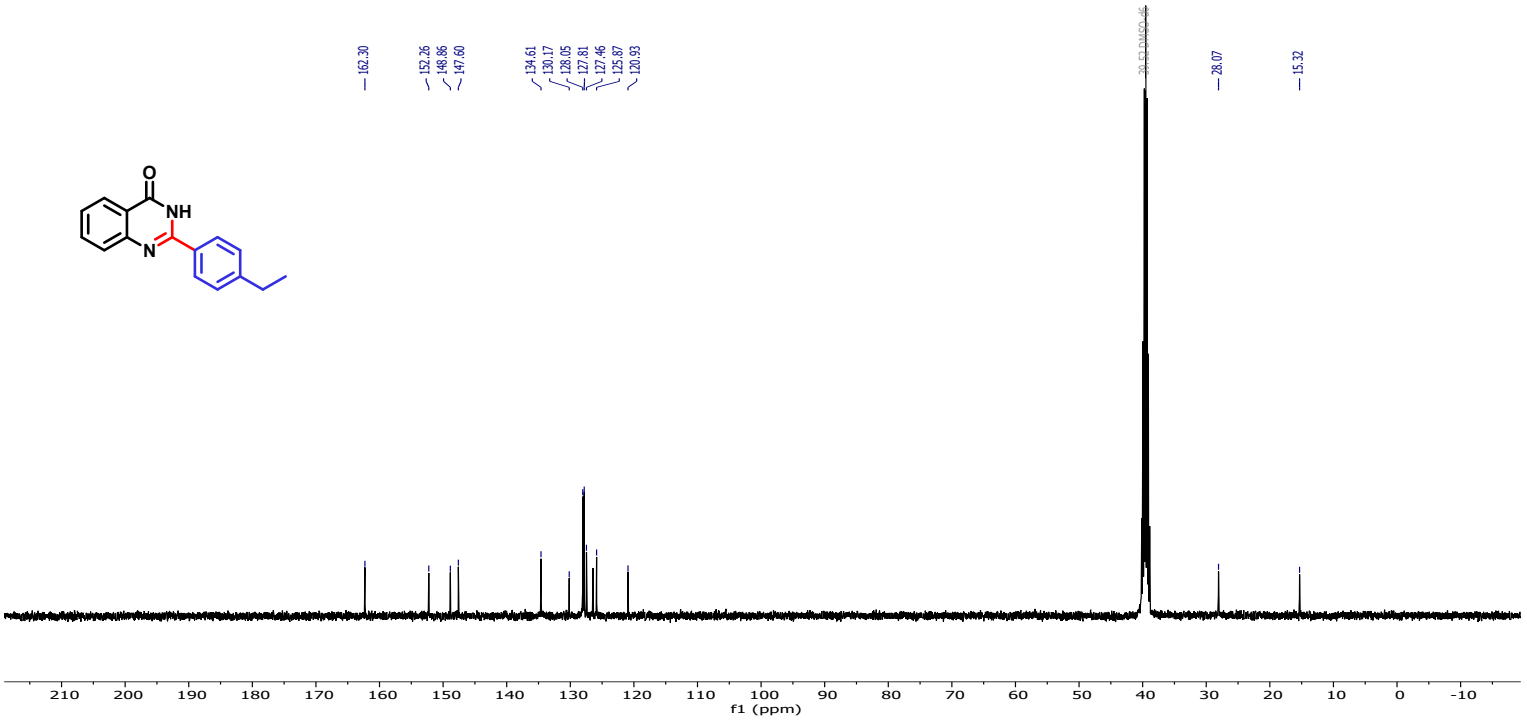


Figure S19. ^{13}C NMR spectrum (100 MHz) of **3d** in DMSO-d_6

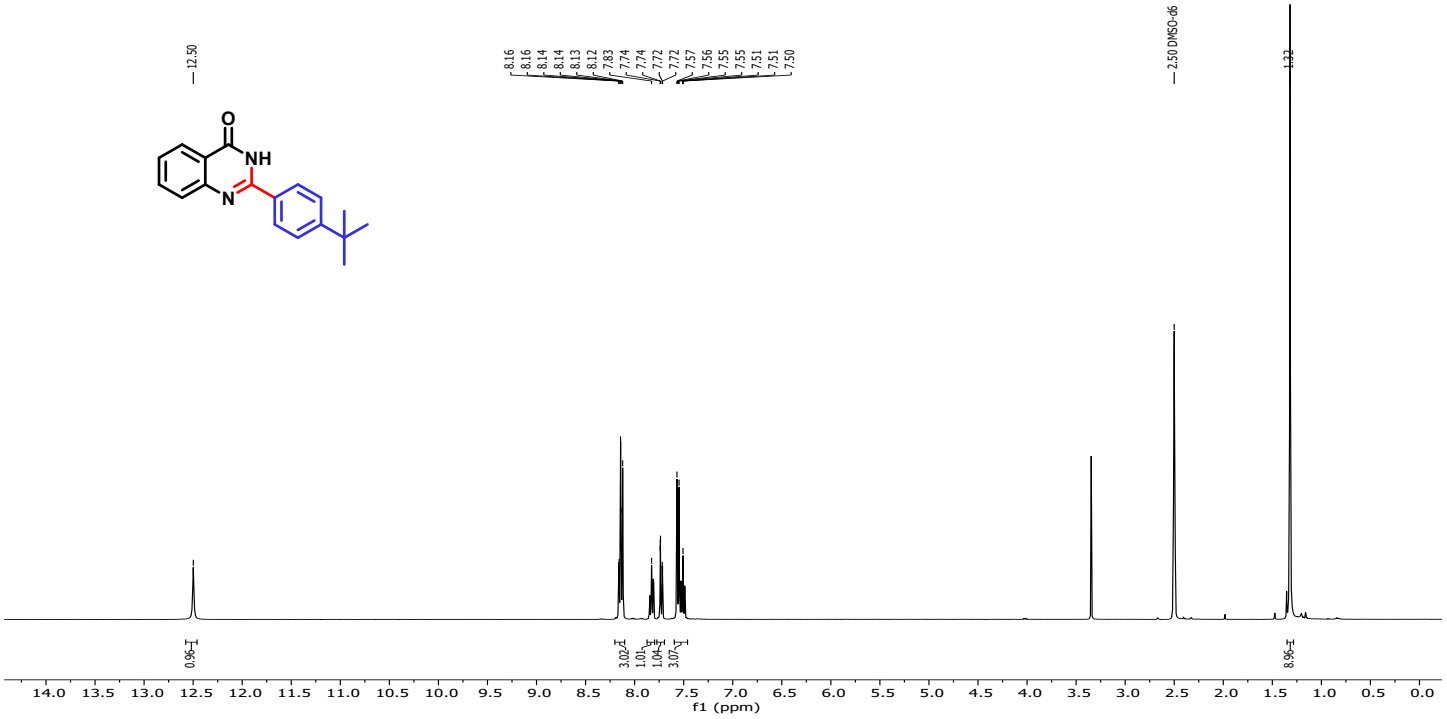


Figure S20. ^{1}H NMR spectrum (400 MHz) of **3e** in DMSO-d_6

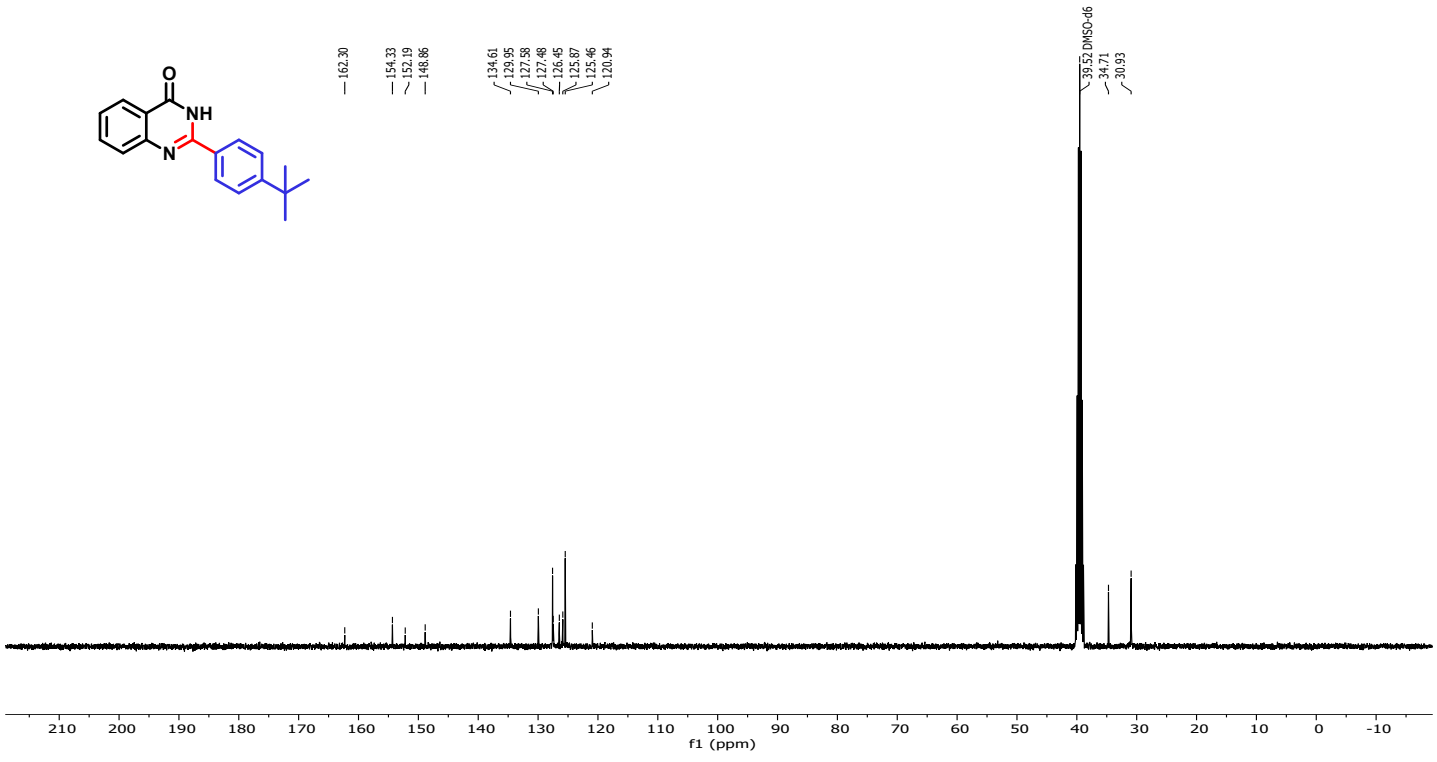


Figure S21. ^{13}C NMR spectrum (100 MHz) of **3e** in DMSO-d_6

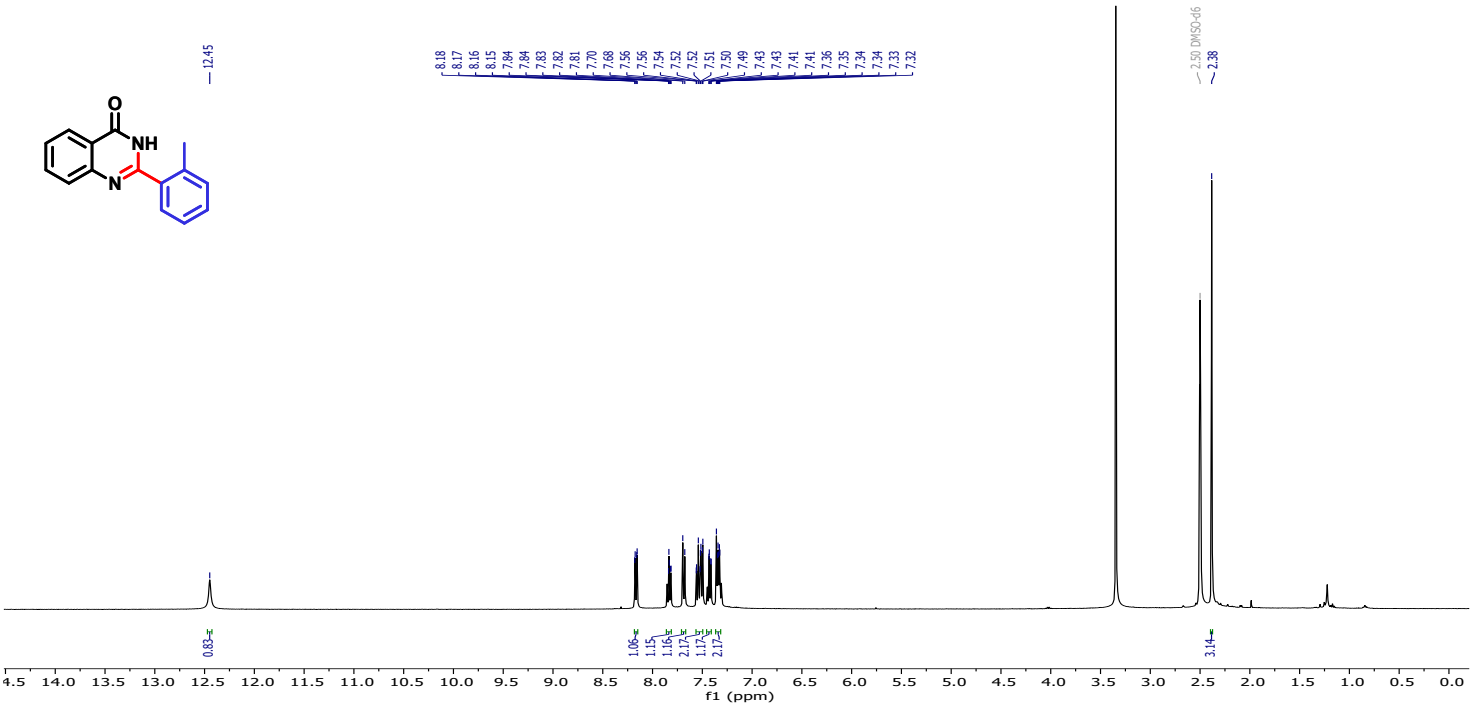


Figure S22. ^{1}H NMR spectrum (400 MHz) of **3f** in DMSO-d_6

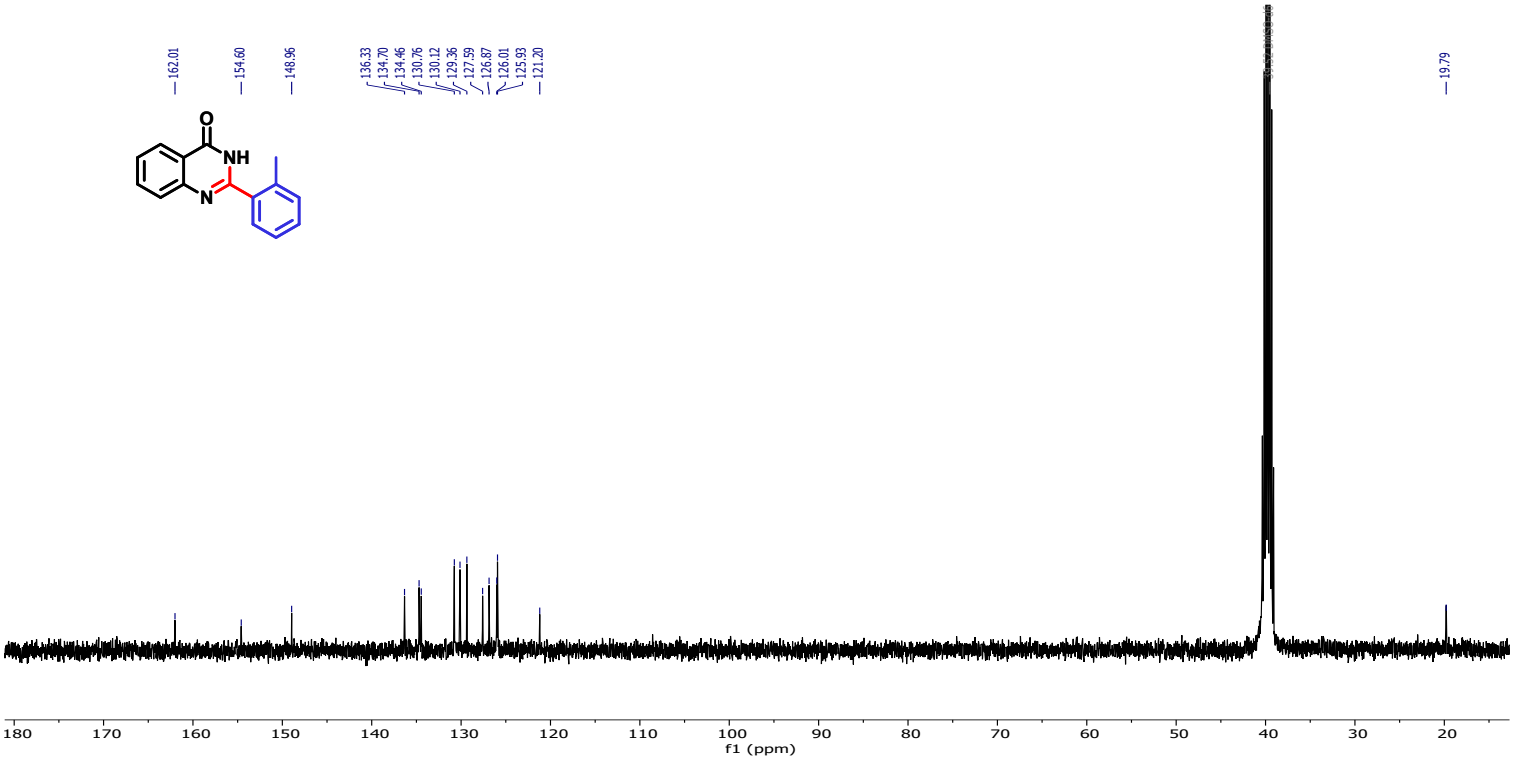


Figure S23. ^{13}C NMR spectrum (100 MHz) of **3f** in DMSO-d_6

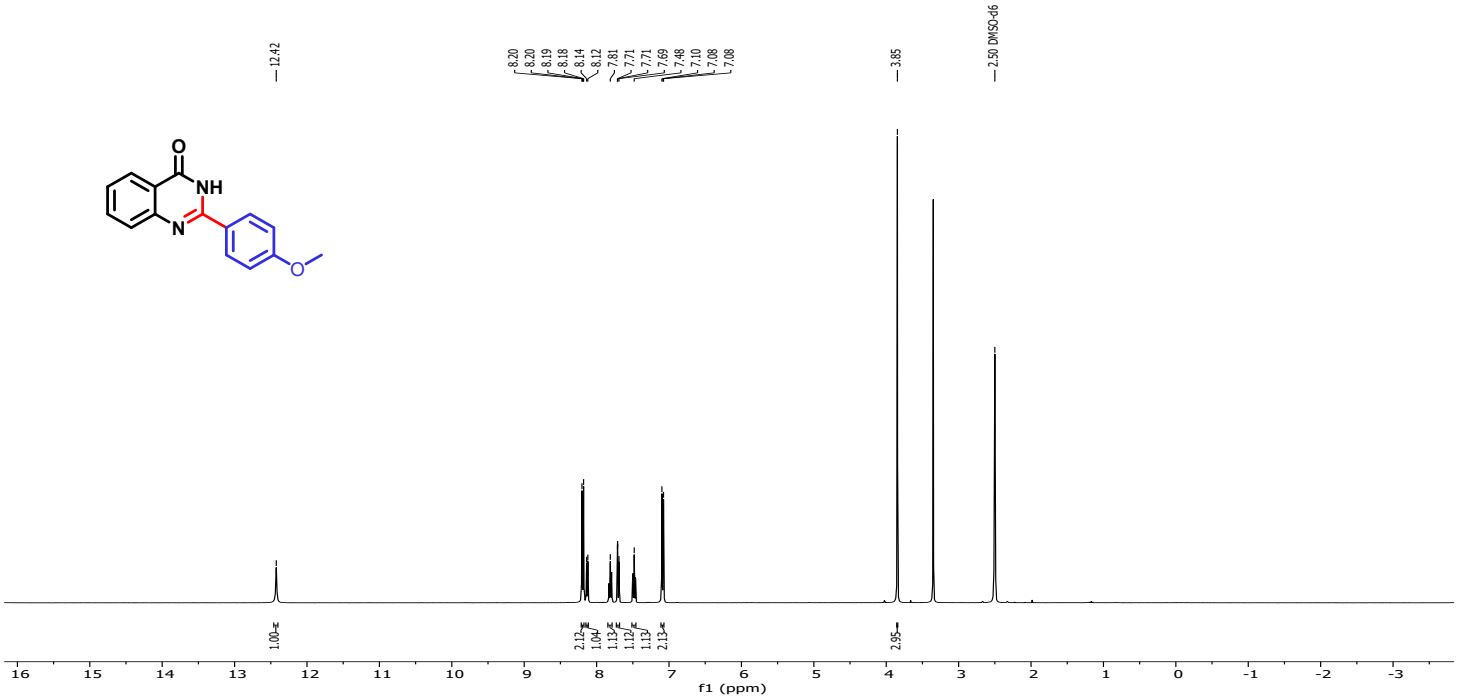


Figure S24. ^{1}H NMR spectrum (400 MHz) of **3g** in DMSO-d_6

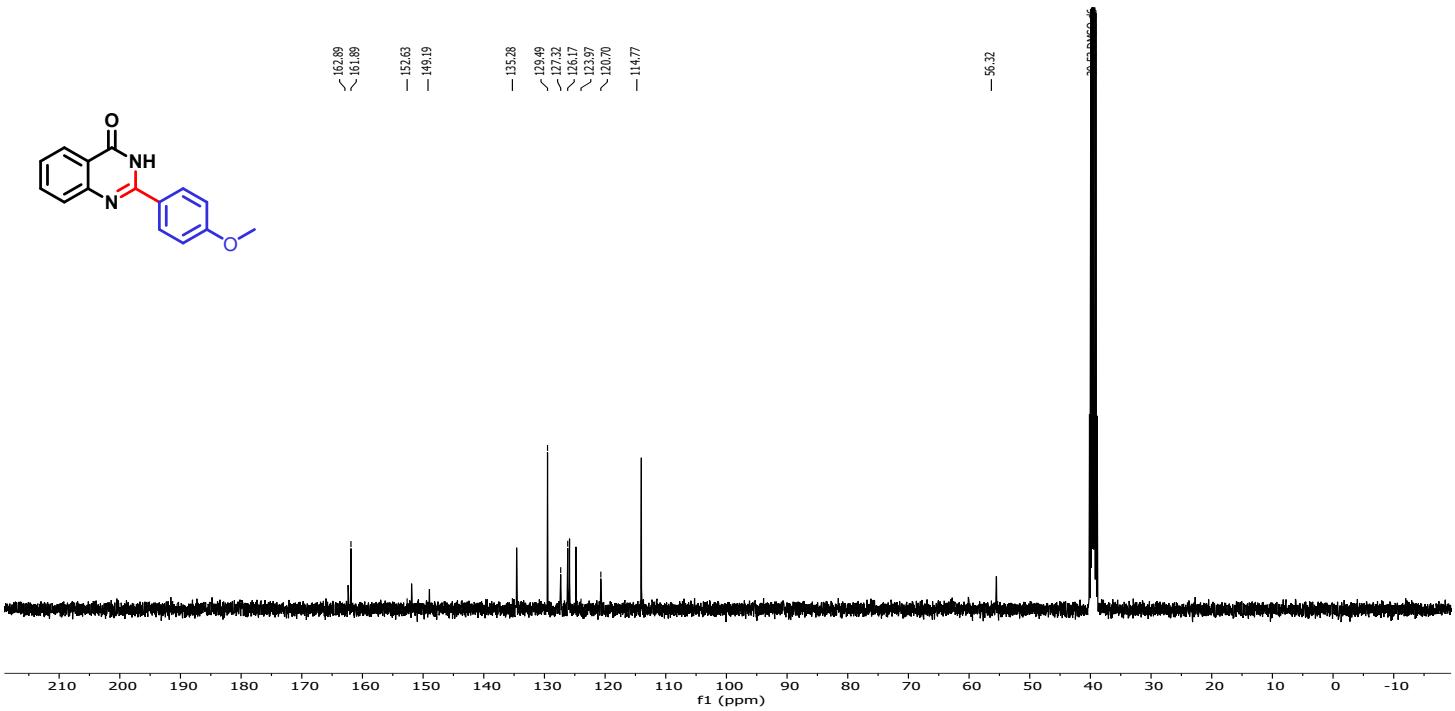


Figure S25. ^{13}C NMR spectrum (100 MHz) of **3g** in DMSO-d_6

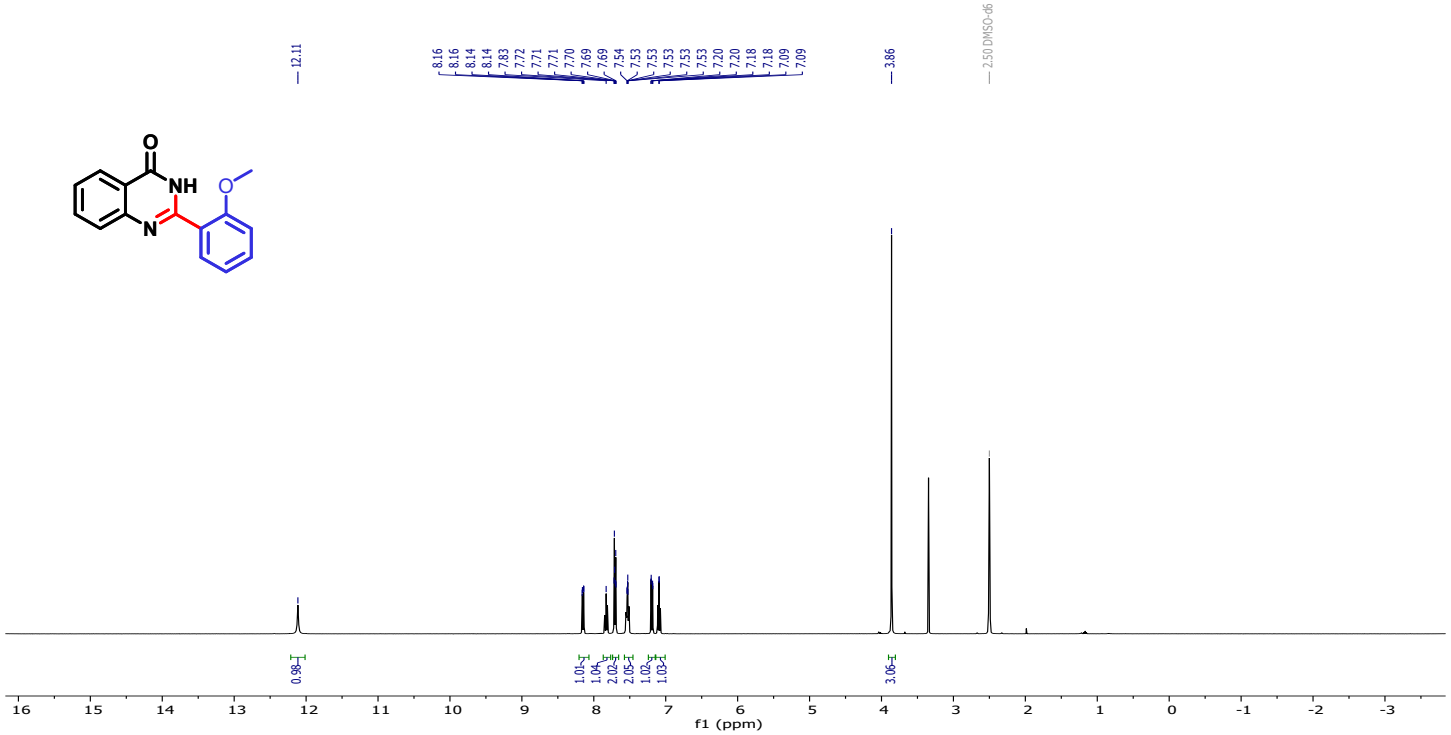


Figure S26. ^{1}H NMR spectrum (400 MHz) of **3h** in DMSO-d_6

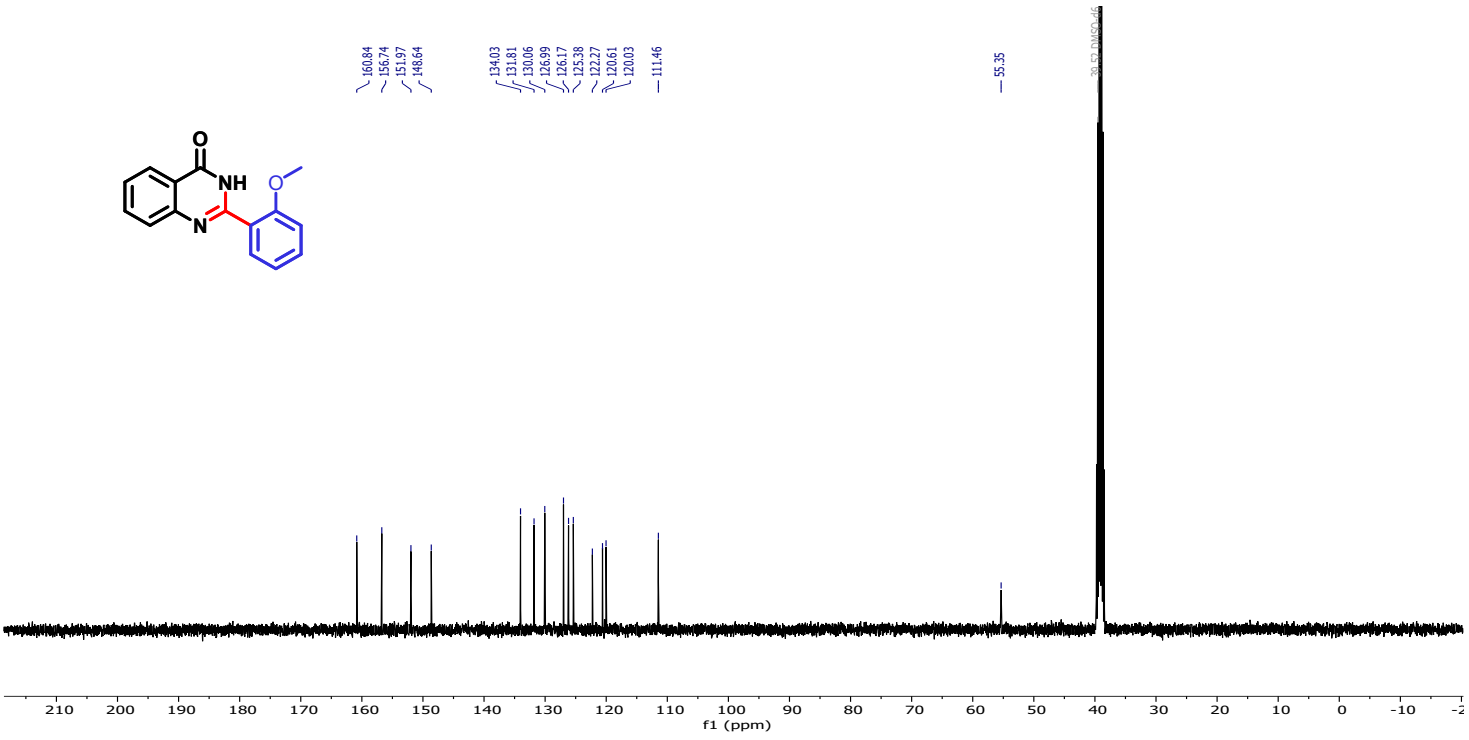


Figure S27. ^{13}C NMR spectrum (100 MHz) of **3h** in DMSO-d_6

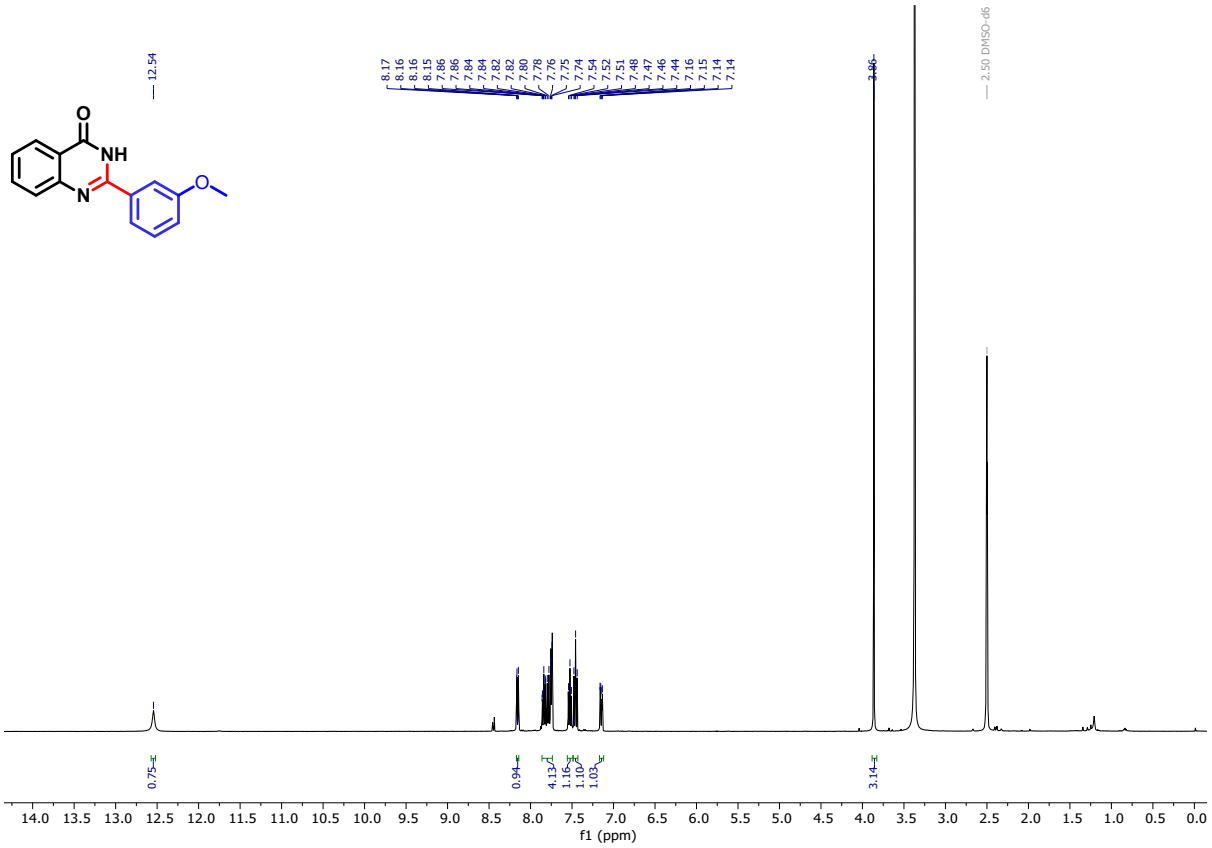


Figure S28. ^{1}H NMR spectrum (400 MHz) of **3i** in DMSO-d_6

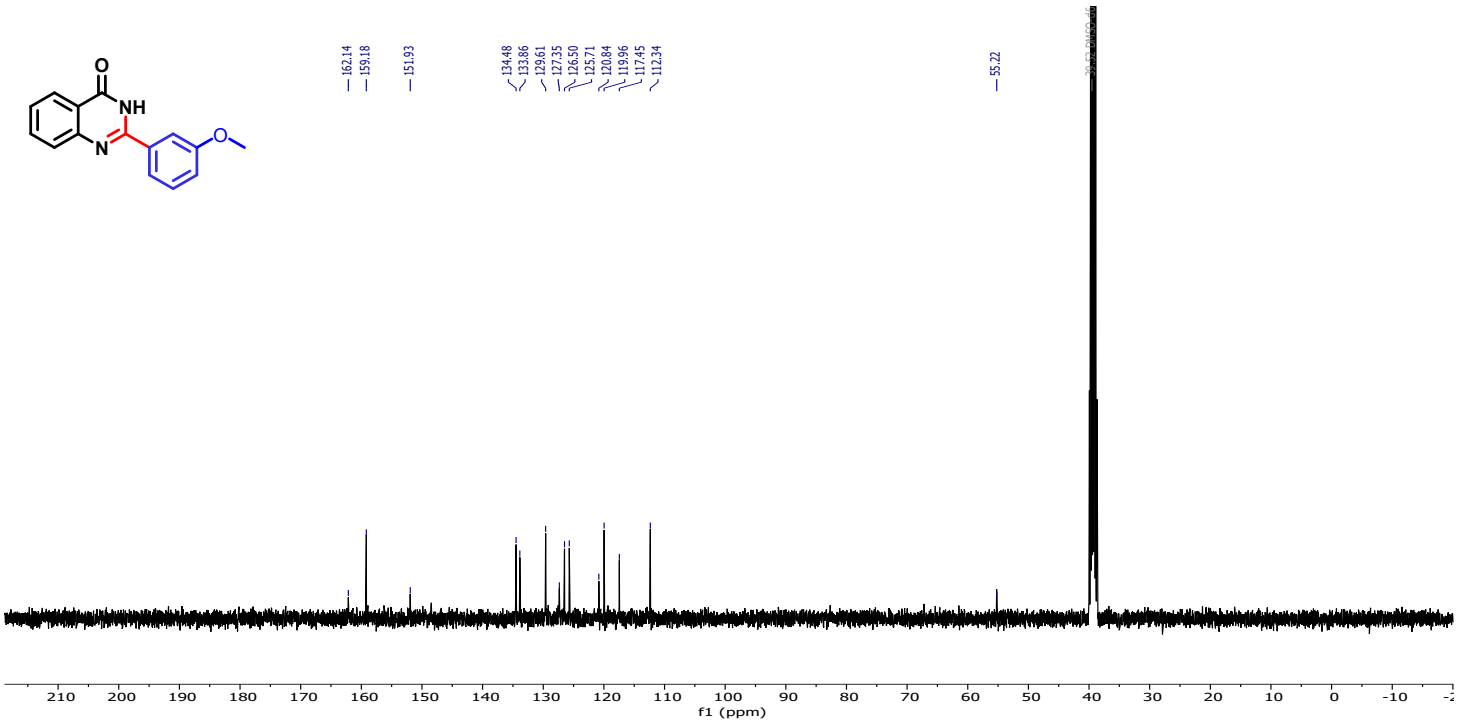


Figure S29. ^{13}C NMR spectrum (100 MHz) of **3i** in DMSO-d_6

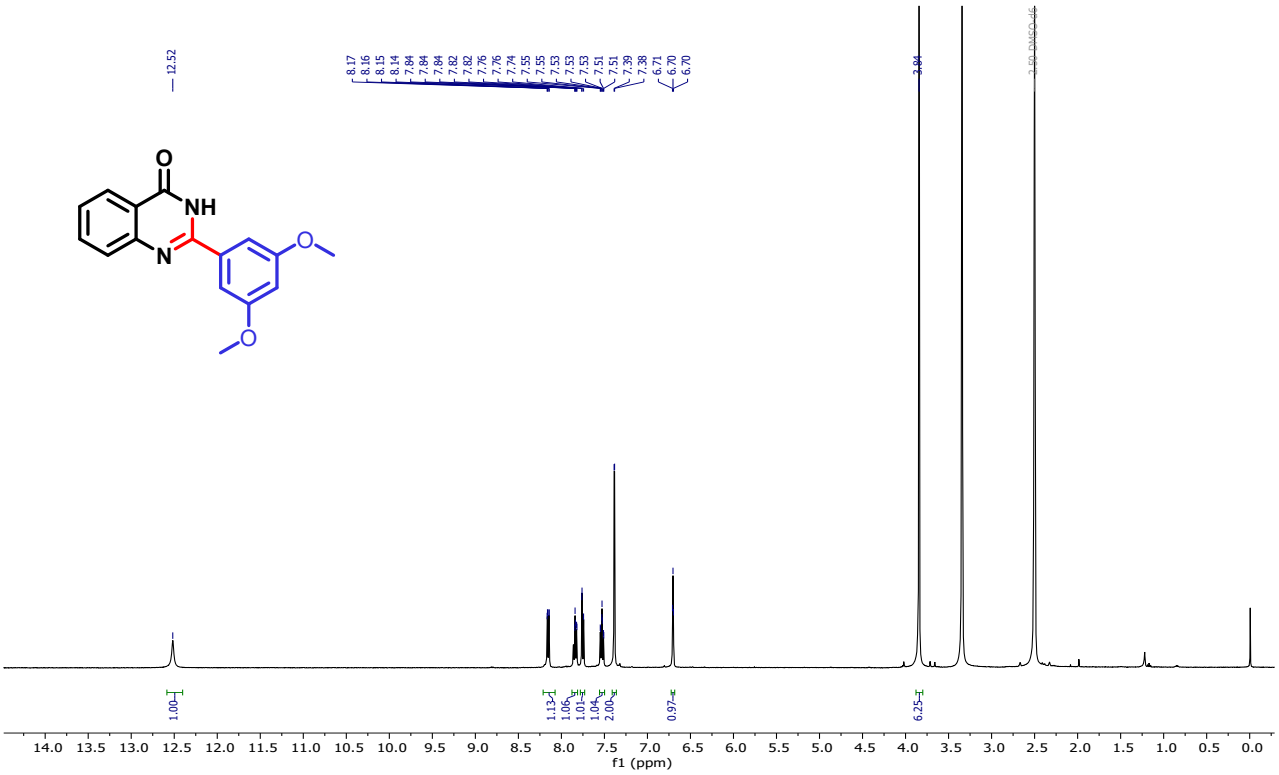


Figure S30. ^{1}H NMR spectrum (400 MHz) of **3j** in DMSO-d_6

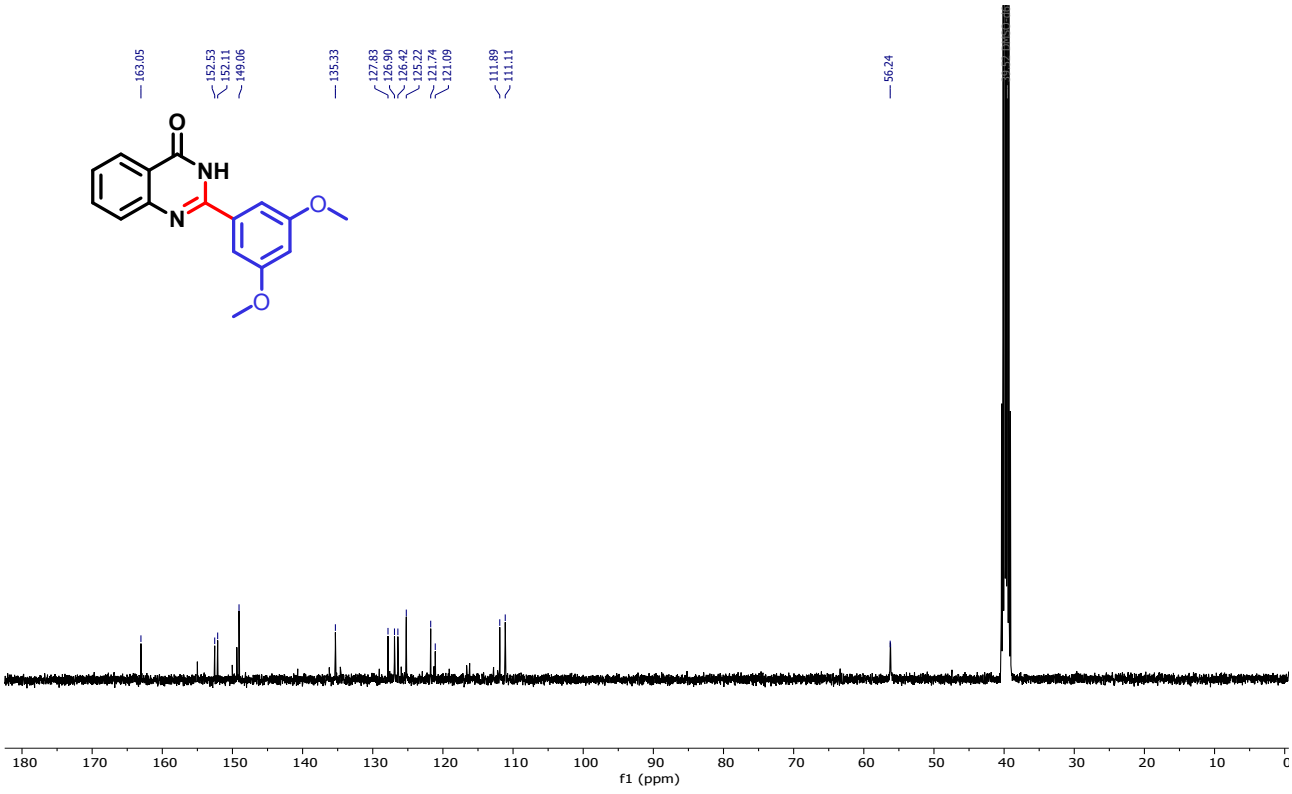


Figure S31. ^{13}C NMR spectrum (100 MHz) of **3j** in DMSO-d_6

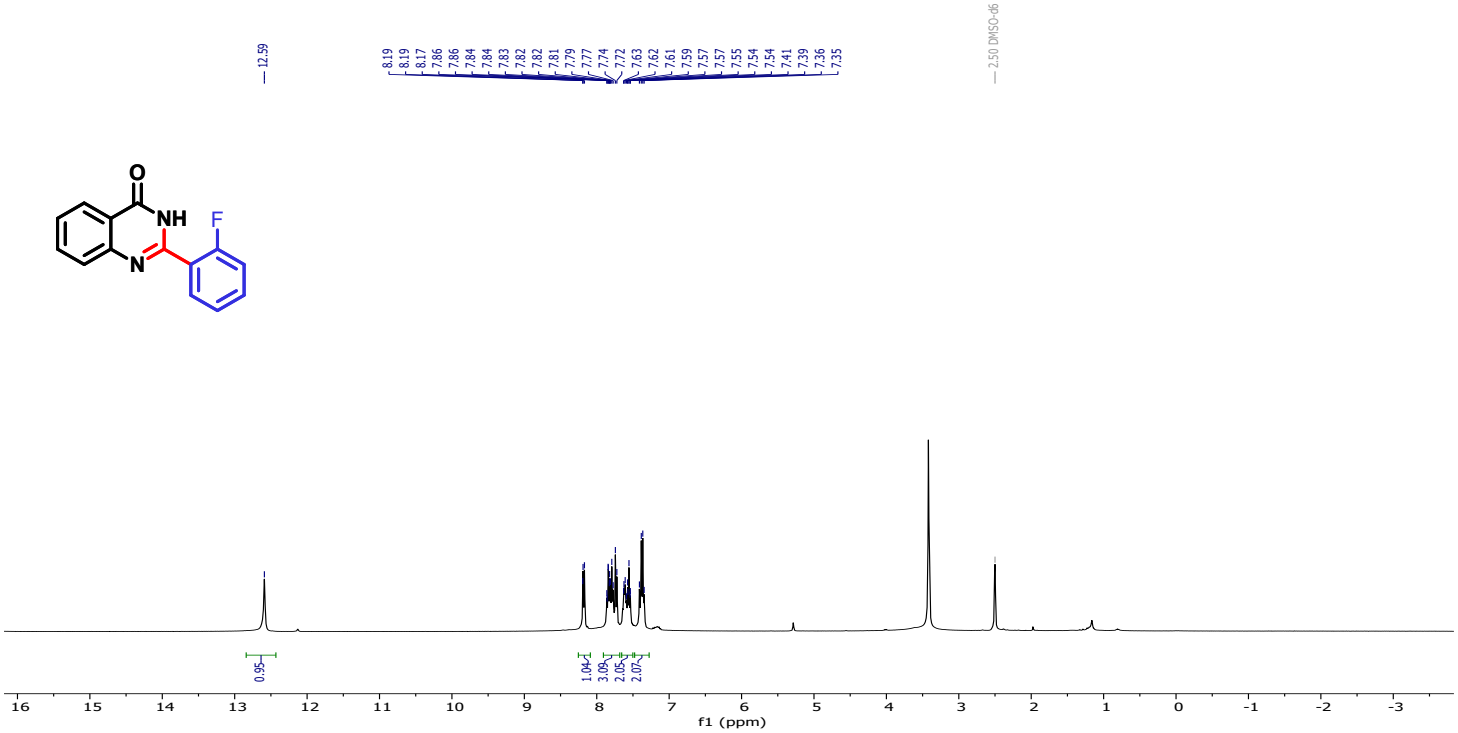


Figure S32. ^{1}H NMR spectrum (400 MHz) of **3k** in DMSO-d_6

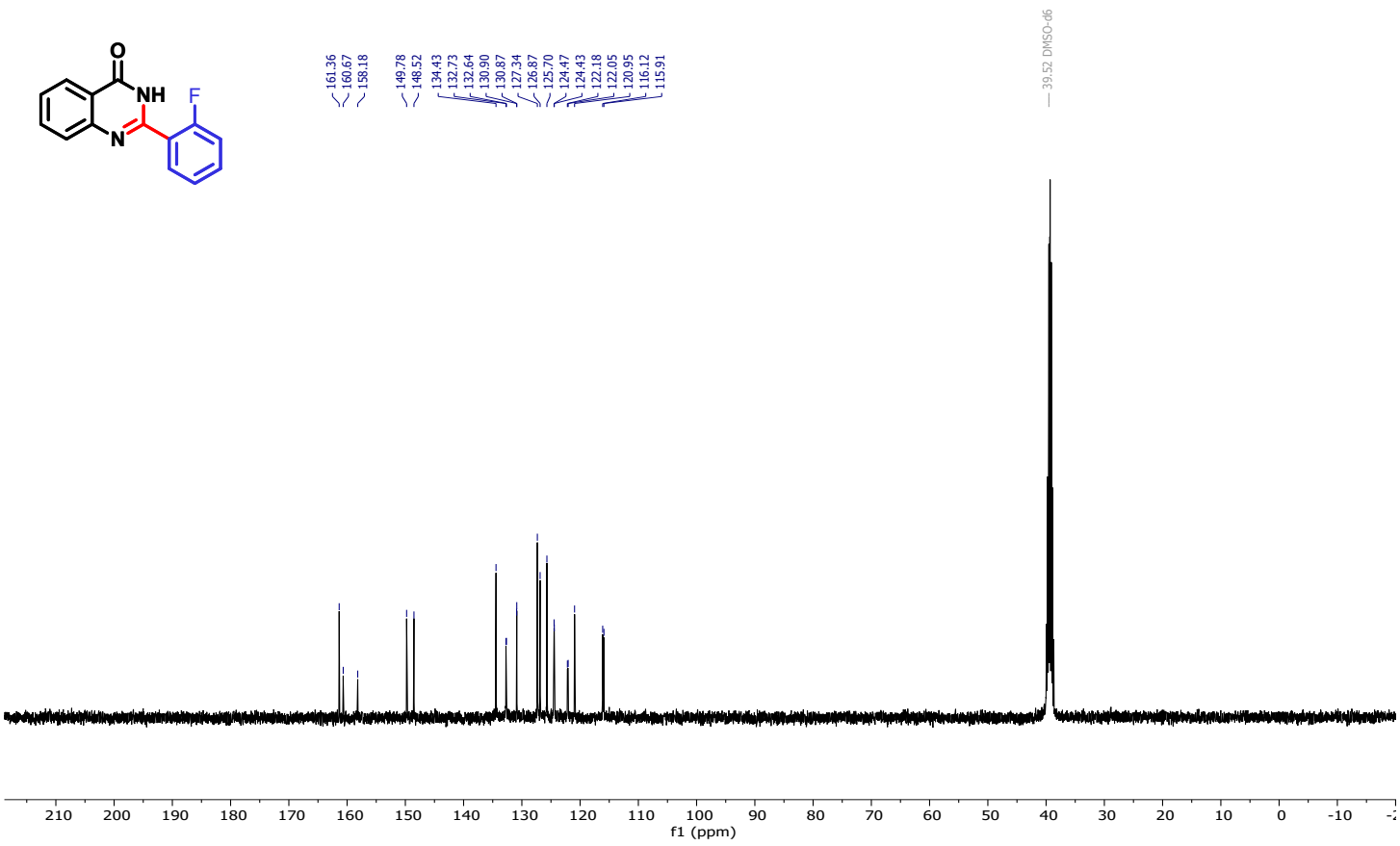


Figure S33. ^{13}C NMR spectrum (100 MHz) of **3k** in DMSO-d_6

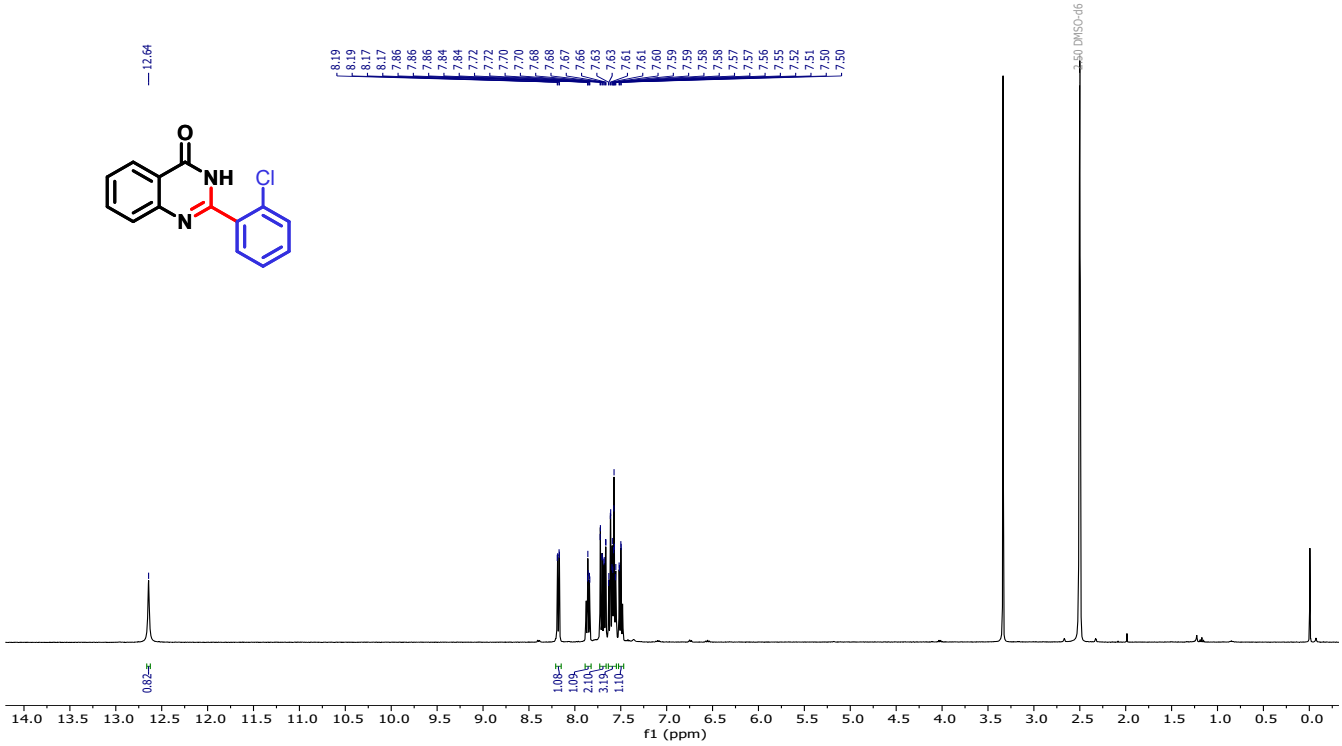


Figure S34. ^{1}H NMR spectrum (400 MHz) of **3l** in DMSO-d_6

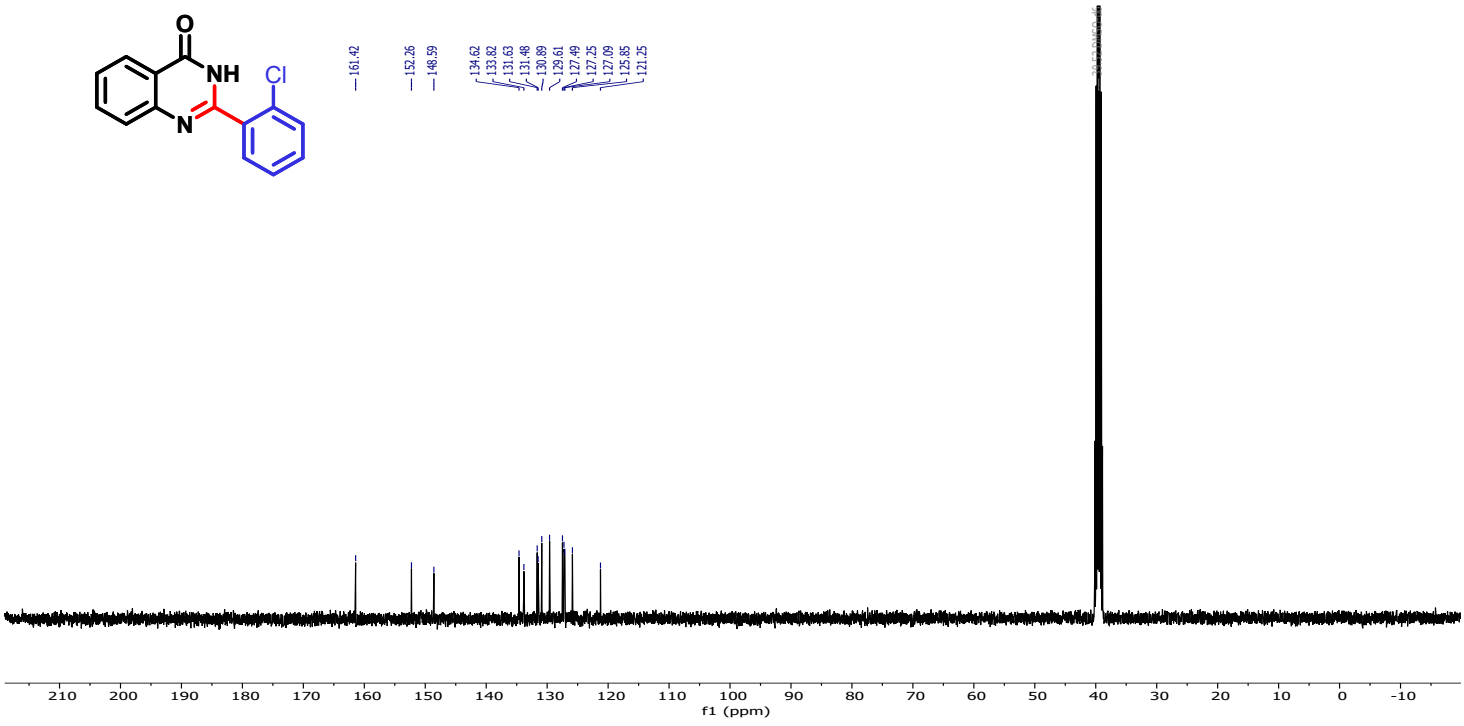


Figure S35. ^{13}C NMR spectrum (100 MHz) of **3l** in DMSO-d_6

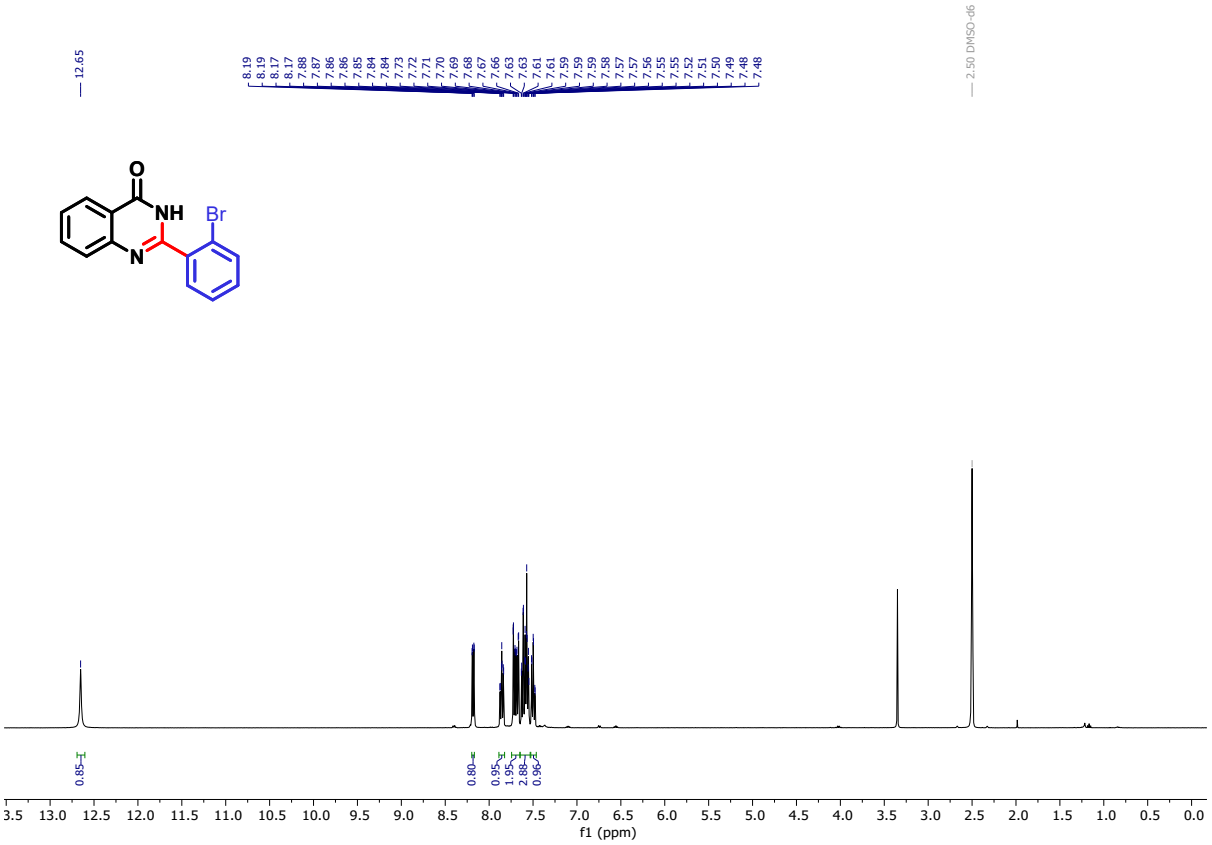


Figure S36. ^{1}H NMR spectrum (400 MHz) of **3m** in DMSO-d_6

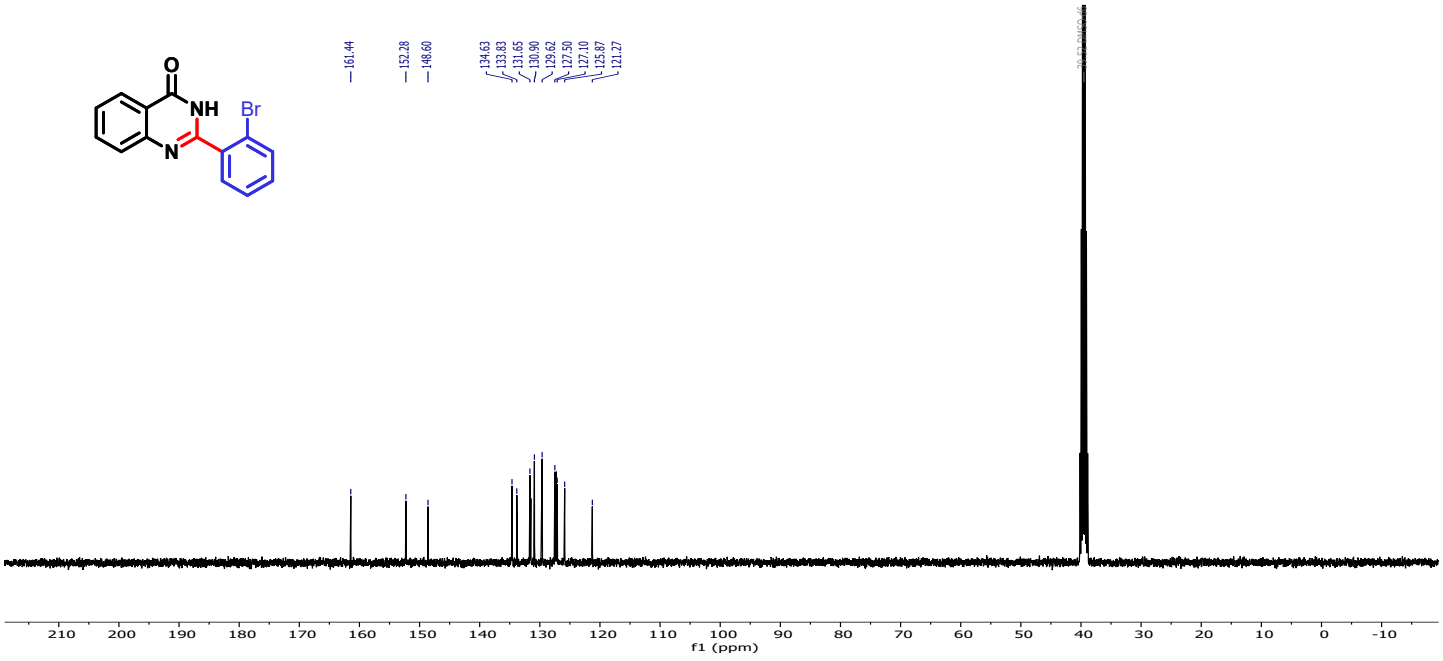


Figure S37. ^{13}C NMR spectrum (100 MHz) of **3m** in DMSO-d_6

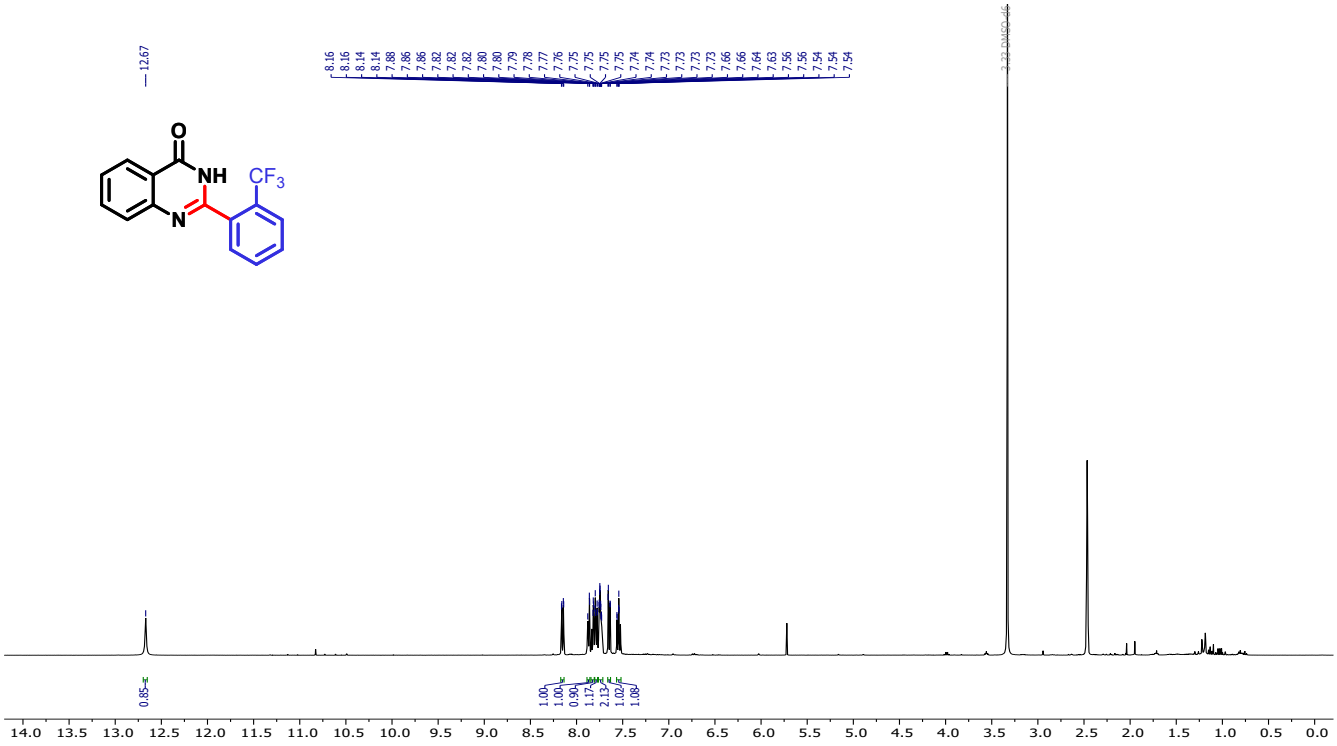


Figure S38. [1]H NMR spectrum (400 MHz) of **3n** in DMSO-d_6

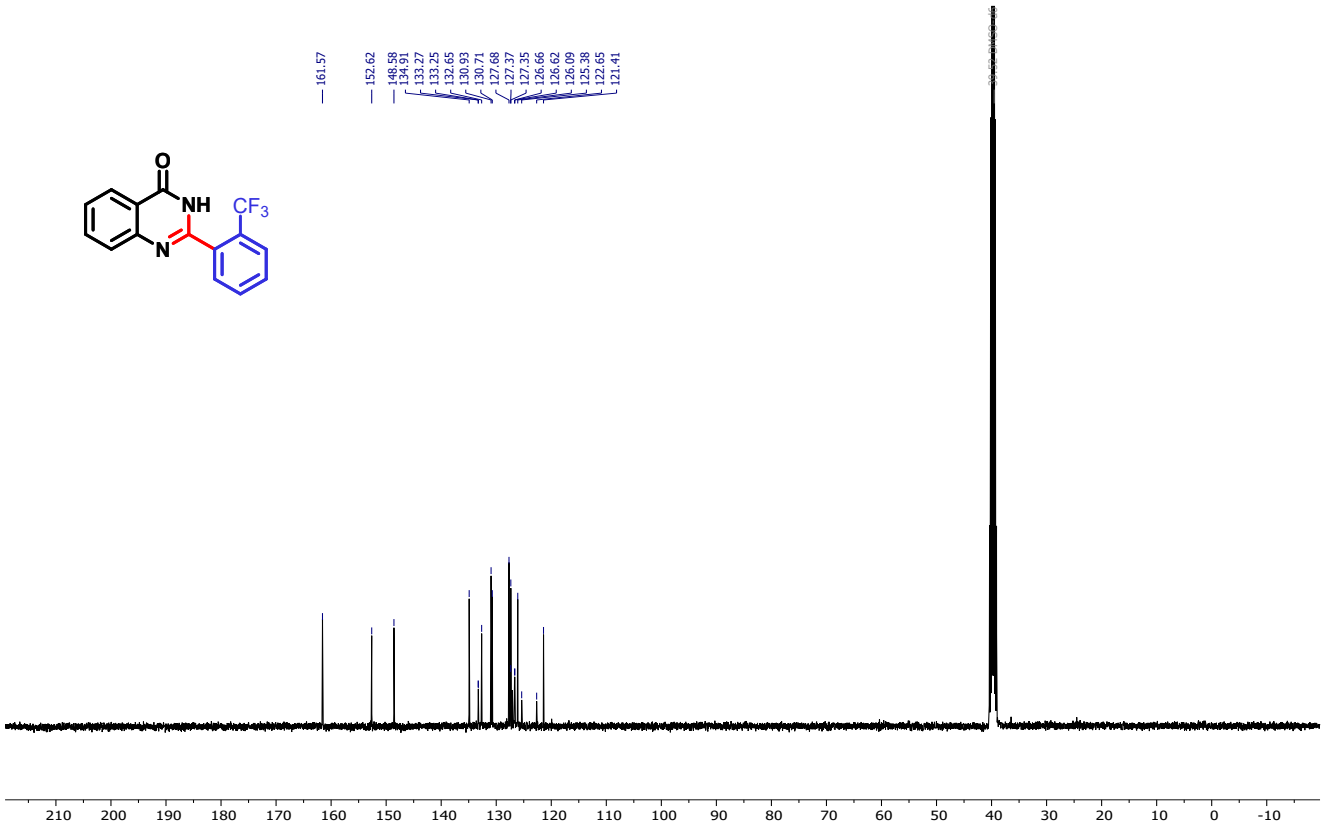


Figure S39. [13]C NMR spectrum (100 MHz) of **3n** in DMSO-d_6

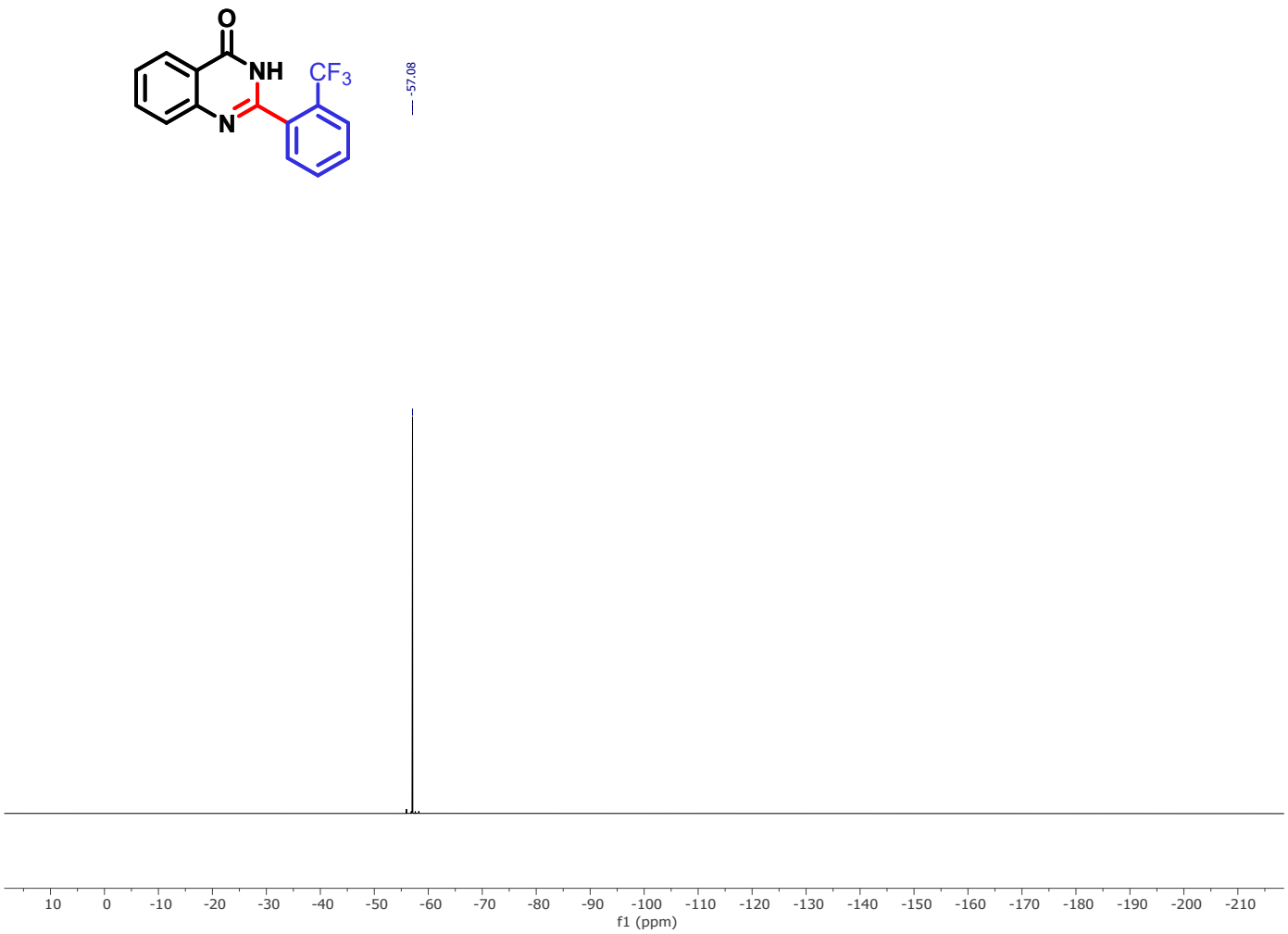


Figure S40. ^{19}F NMR spectrum (376 MHz) of **3n** in DMSO-d_6

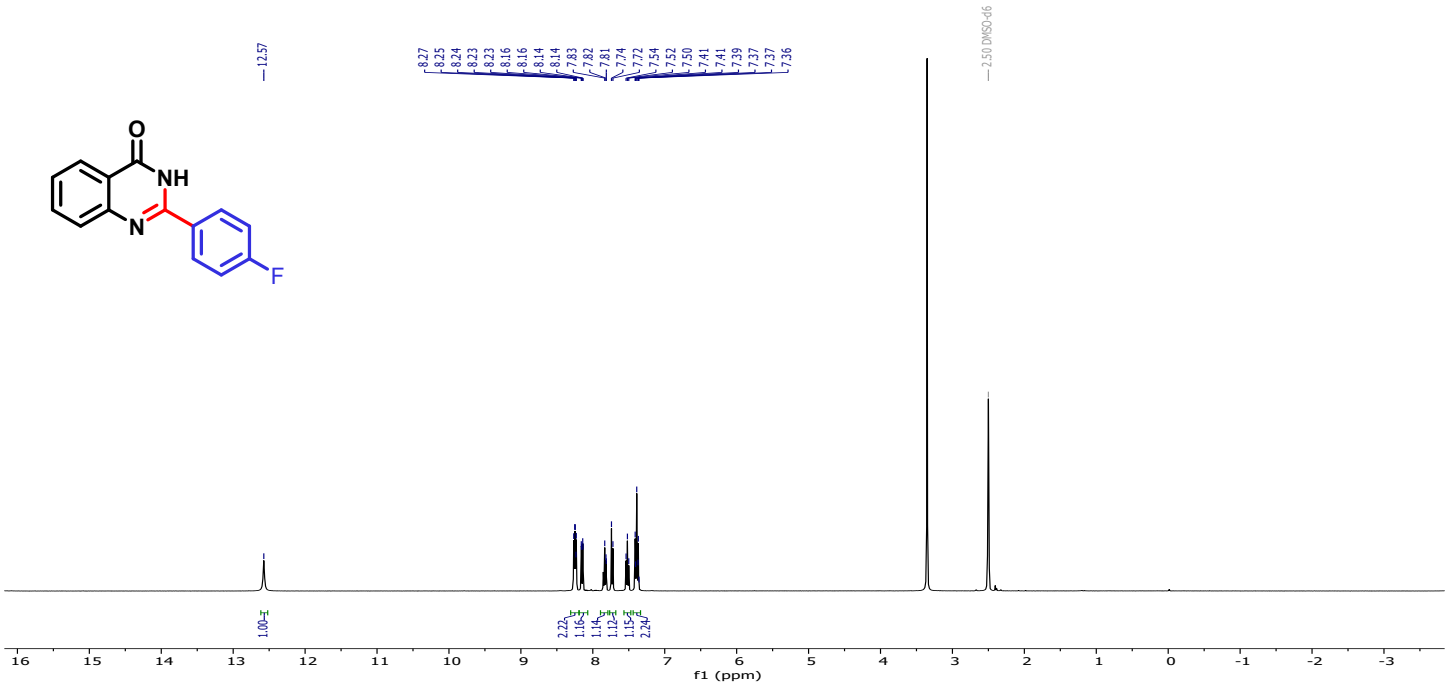


Figure S41. ^{1}H NMR spectrum (400 MHz) of **3o** in DMSO-d_6

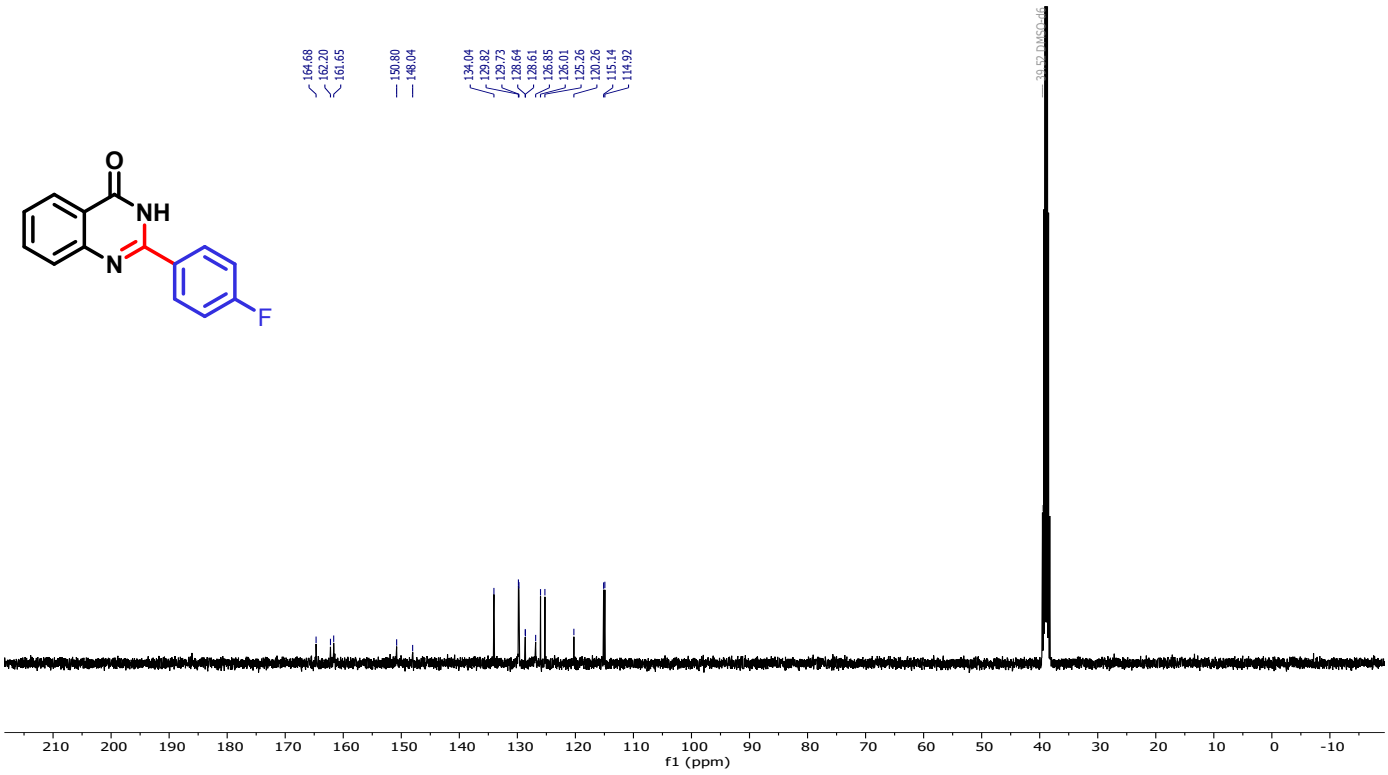


Figure S42. ^{13}C NMR spectrum (100 MHz) of **3o** in DMSO-d_6

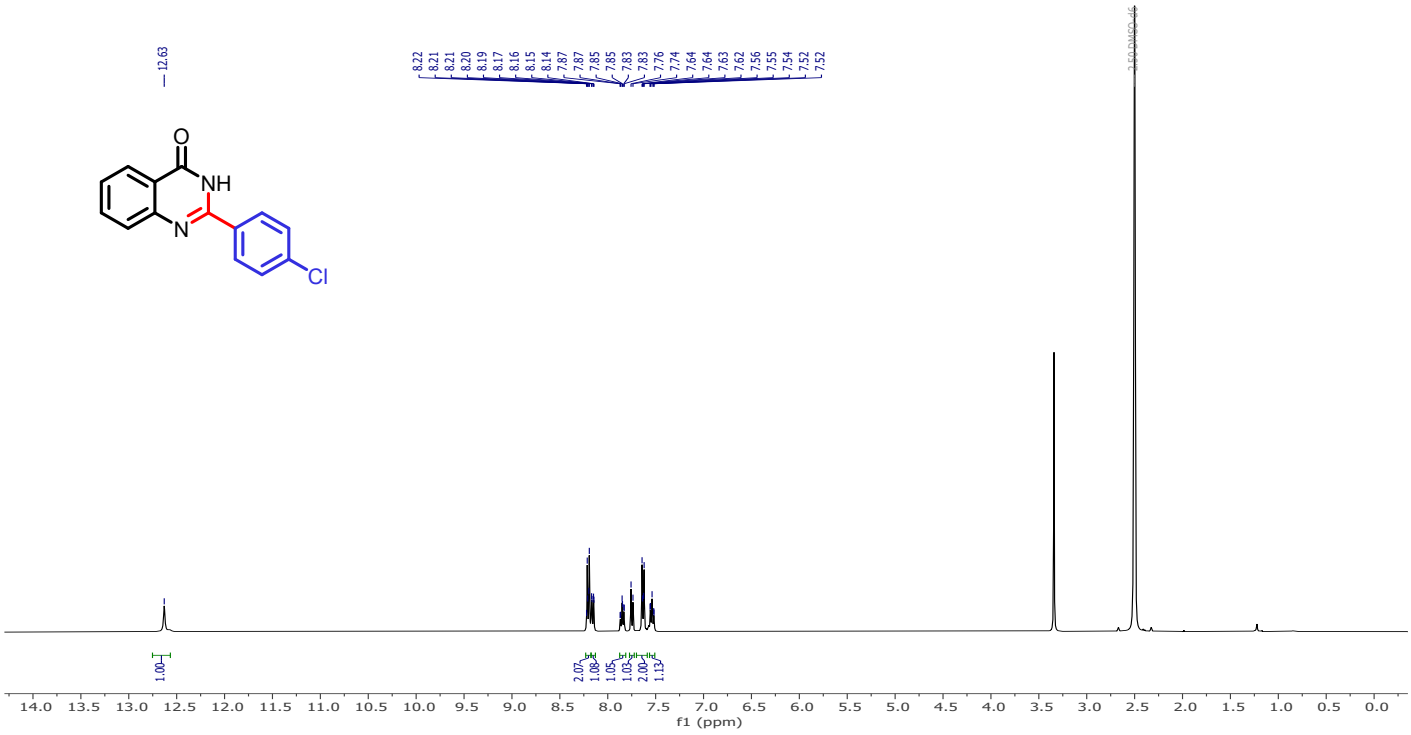


Figure S43. ^{1}H NMR spectrum (400 MHz) of **3p** in DMSO-d_6

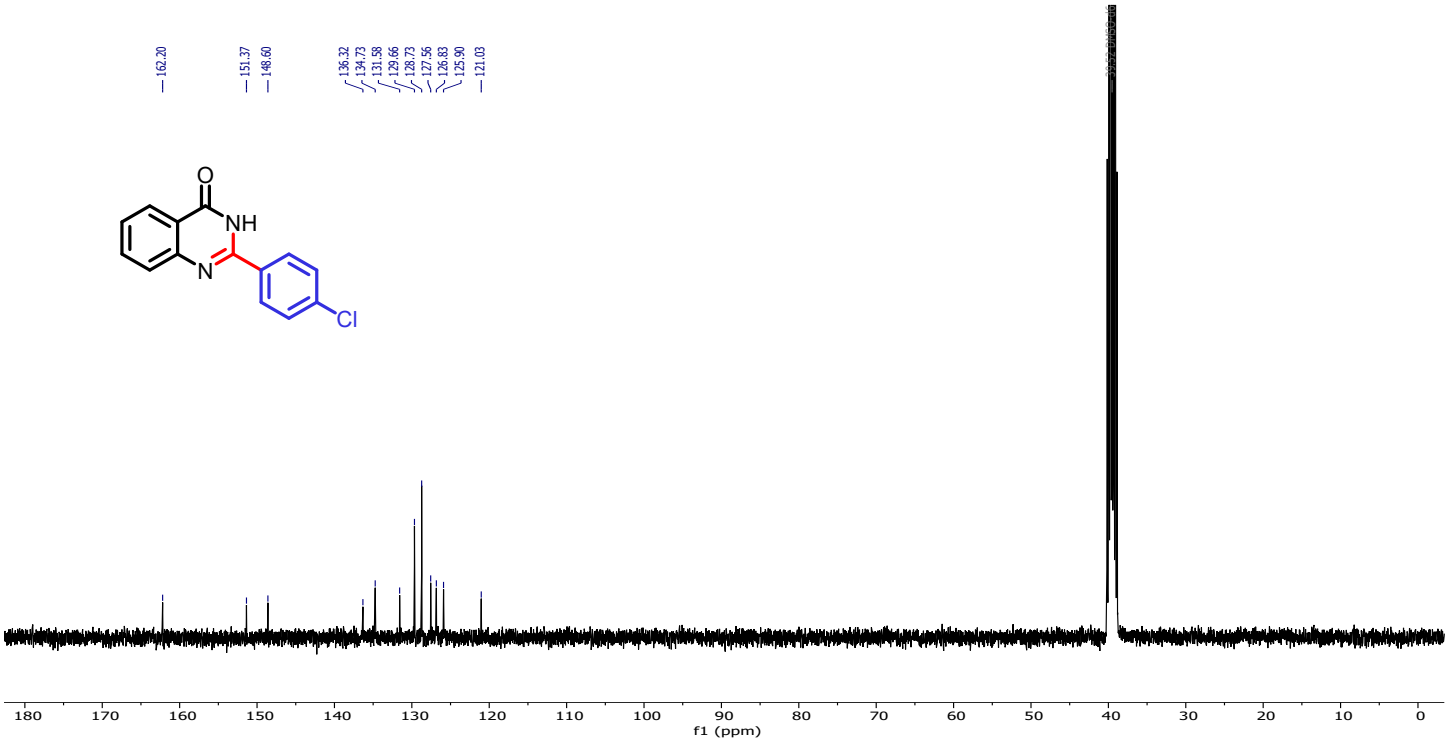


Figure S44. ^{13}C NMR spectrum (100 MHz) of **3p** in DMSO-d_6

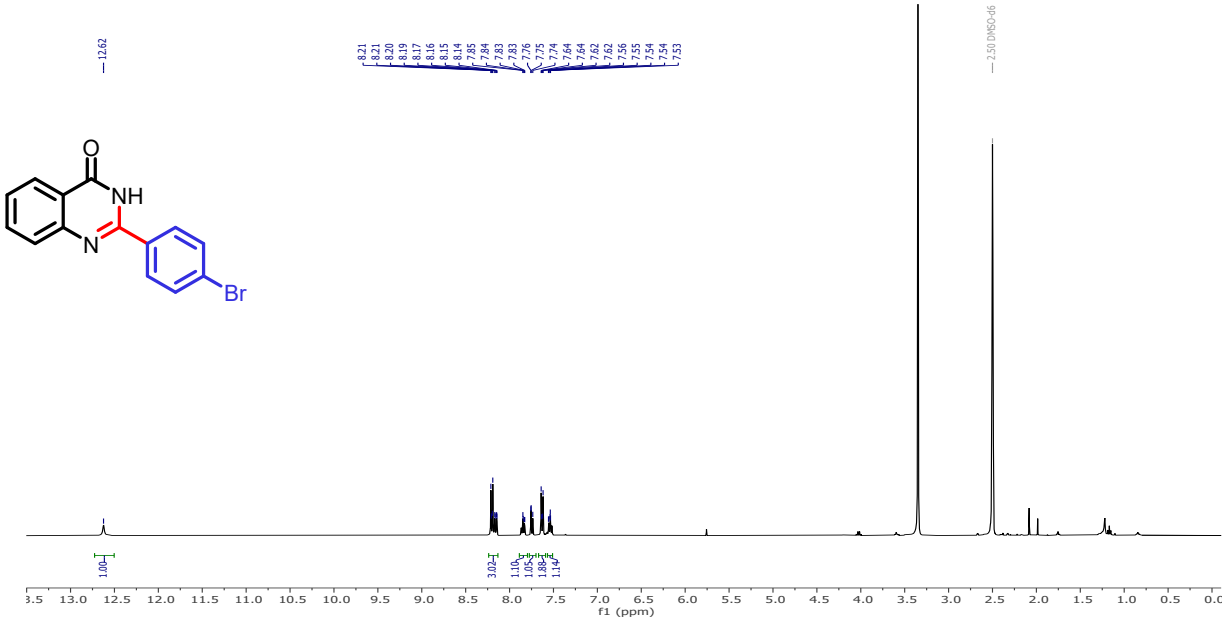


Figure S45. ^{1}H NMR spectrum (400 MHz) of **3q** in DMSO-d_6

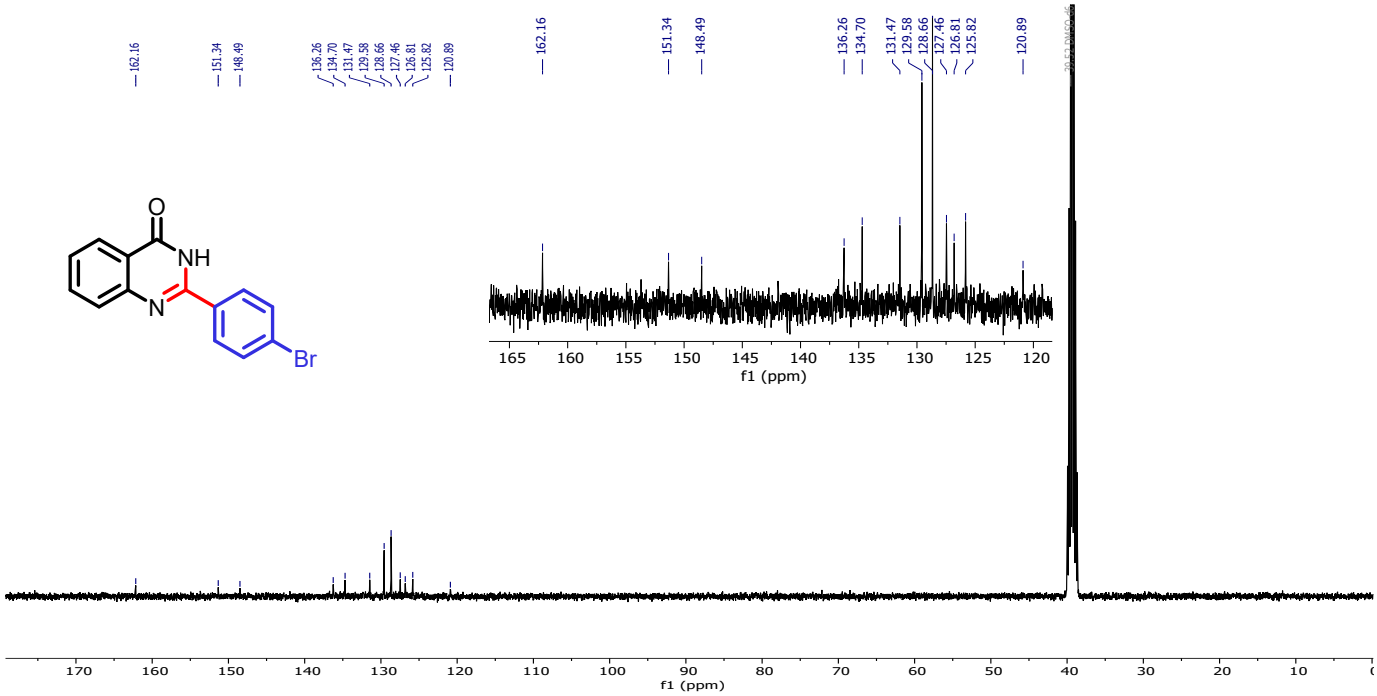


Figure S46. ^{13}C NMR spectrum (100 MHz) of **3q** in DMSO-d_6

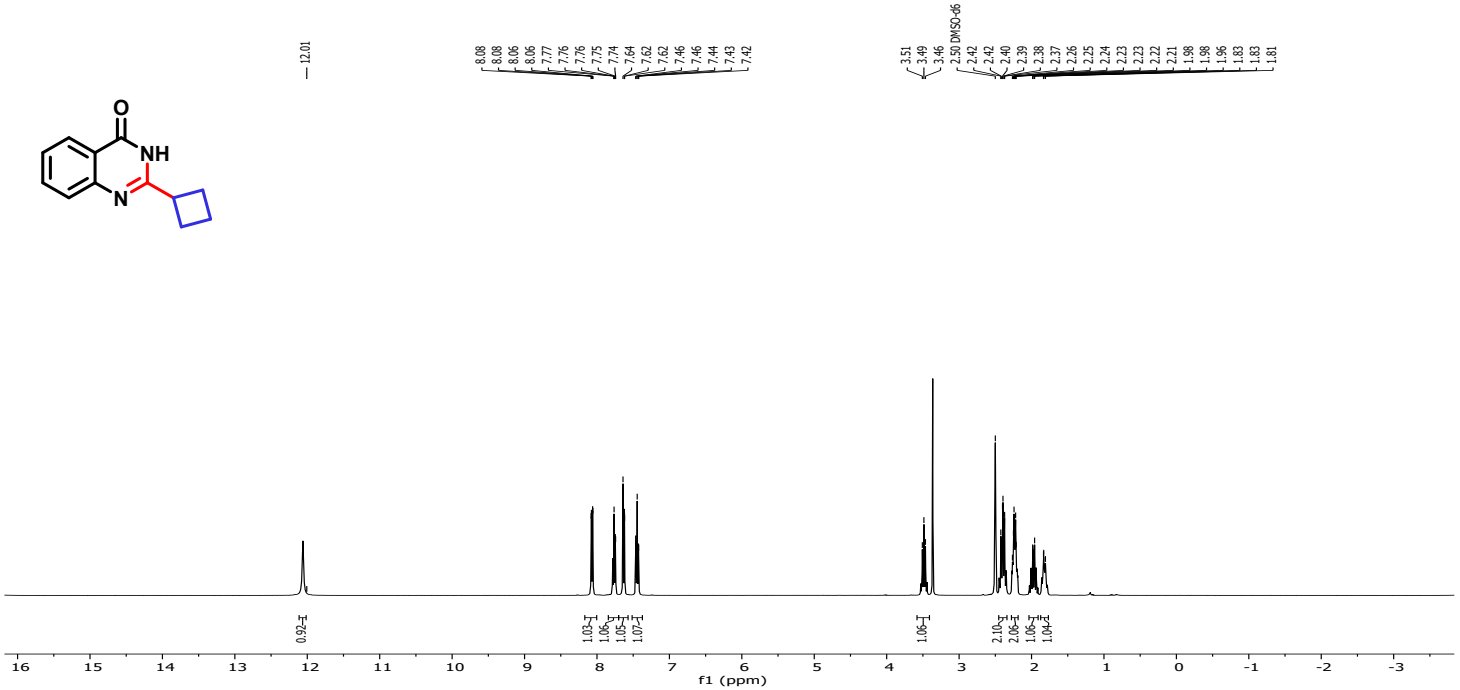


Figure S47. ^{1}H NMR spectrum (400 MHz) of **3r** in DMSO-d_6

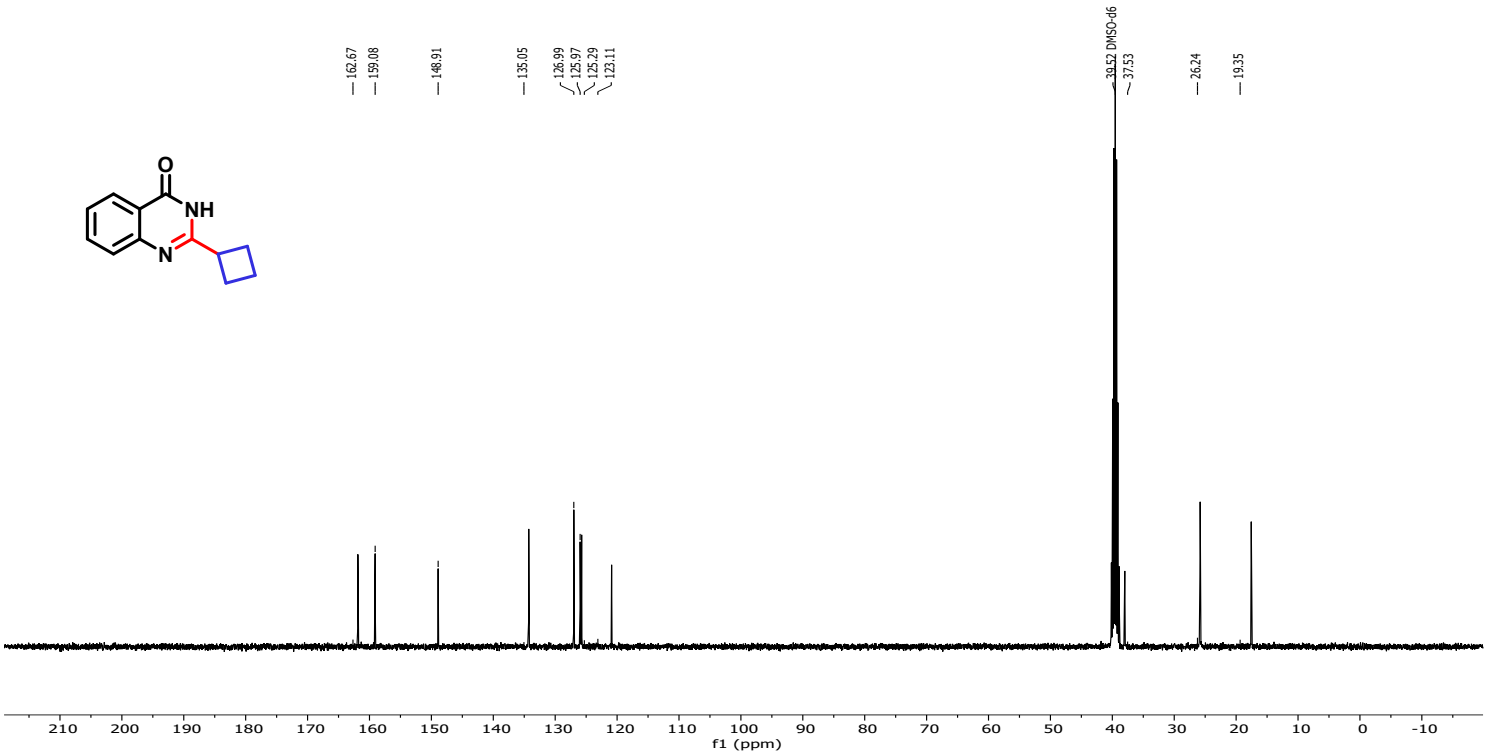


Figure S48. ^{13}C NMR spectrum (100 MHz) of **3r** in DMSO-d_6

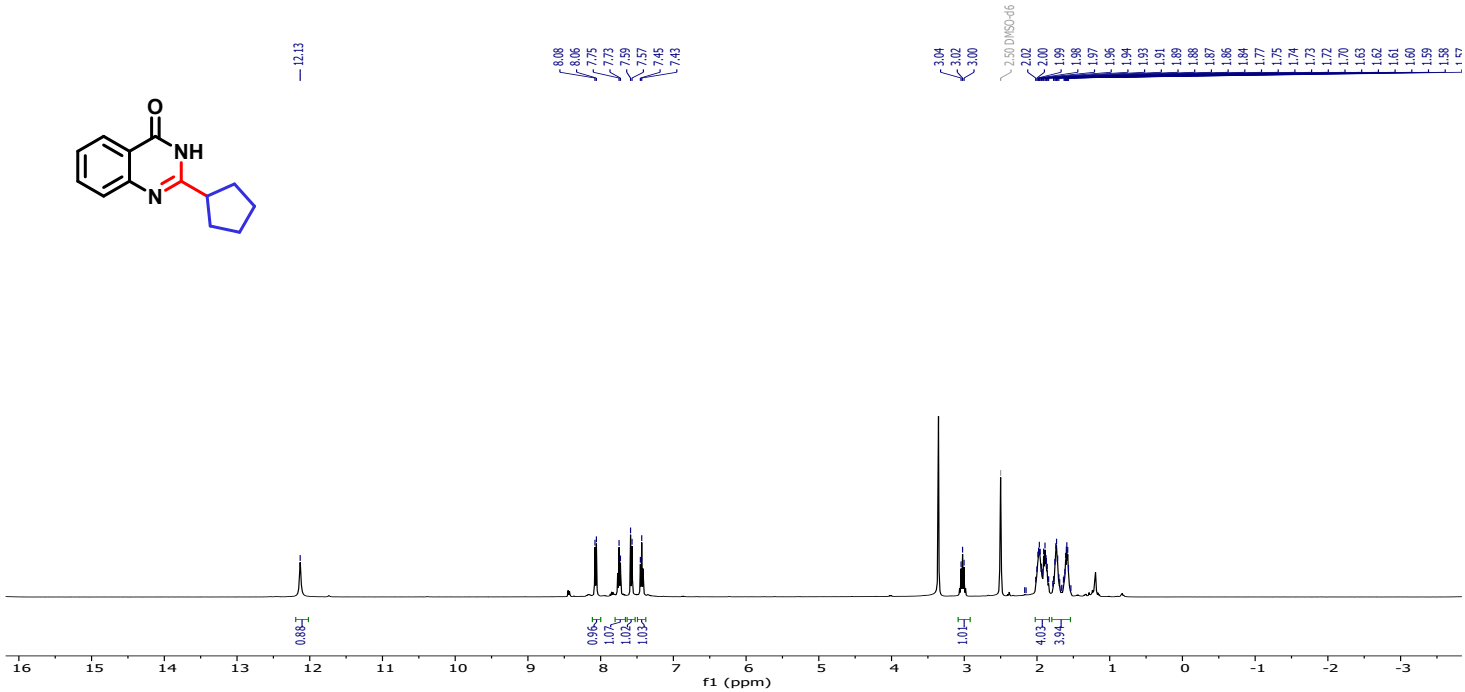


Figure S49. ^{1}H NMR spectrum (400 MHz) of **3s** in DMSO-d_6

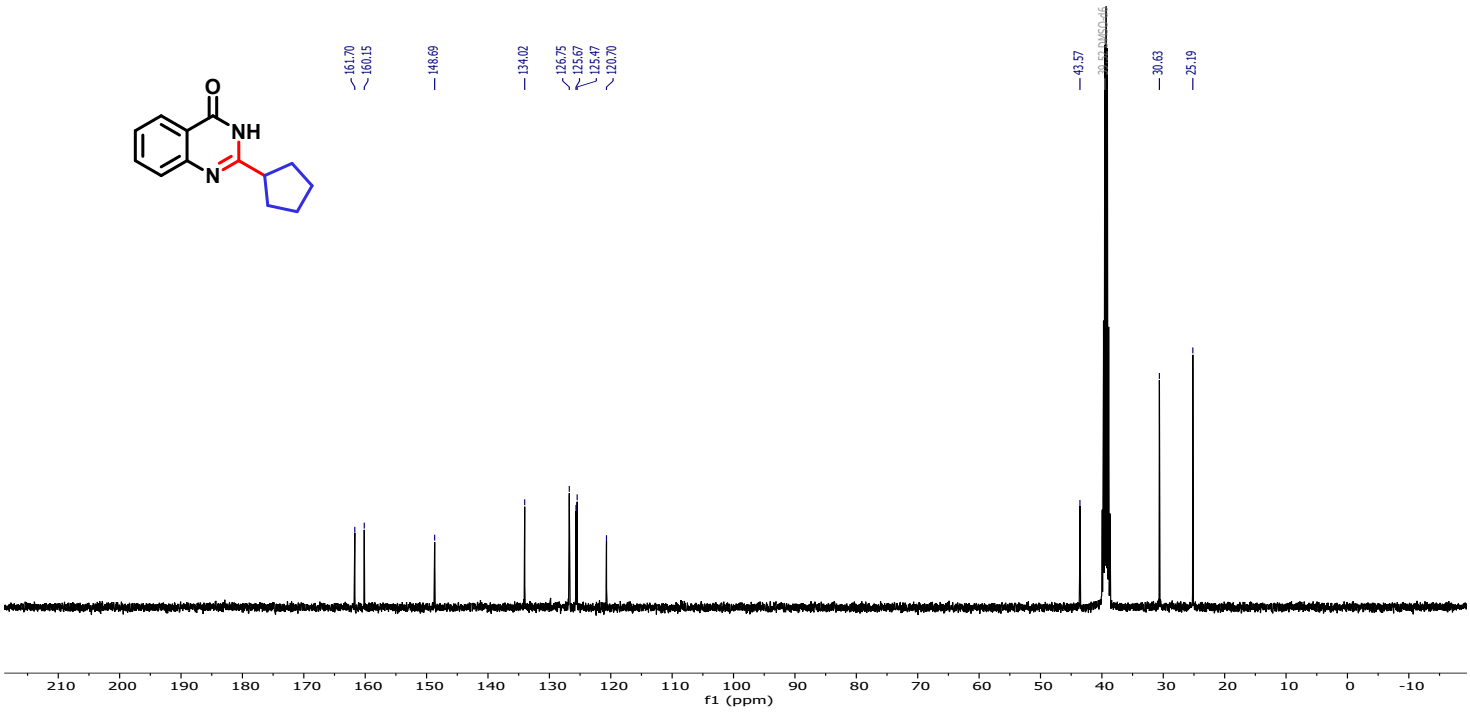


Figure S50. ^{13}C NMR spectrum (100 MHz) of **3s** in DMSO-d_6

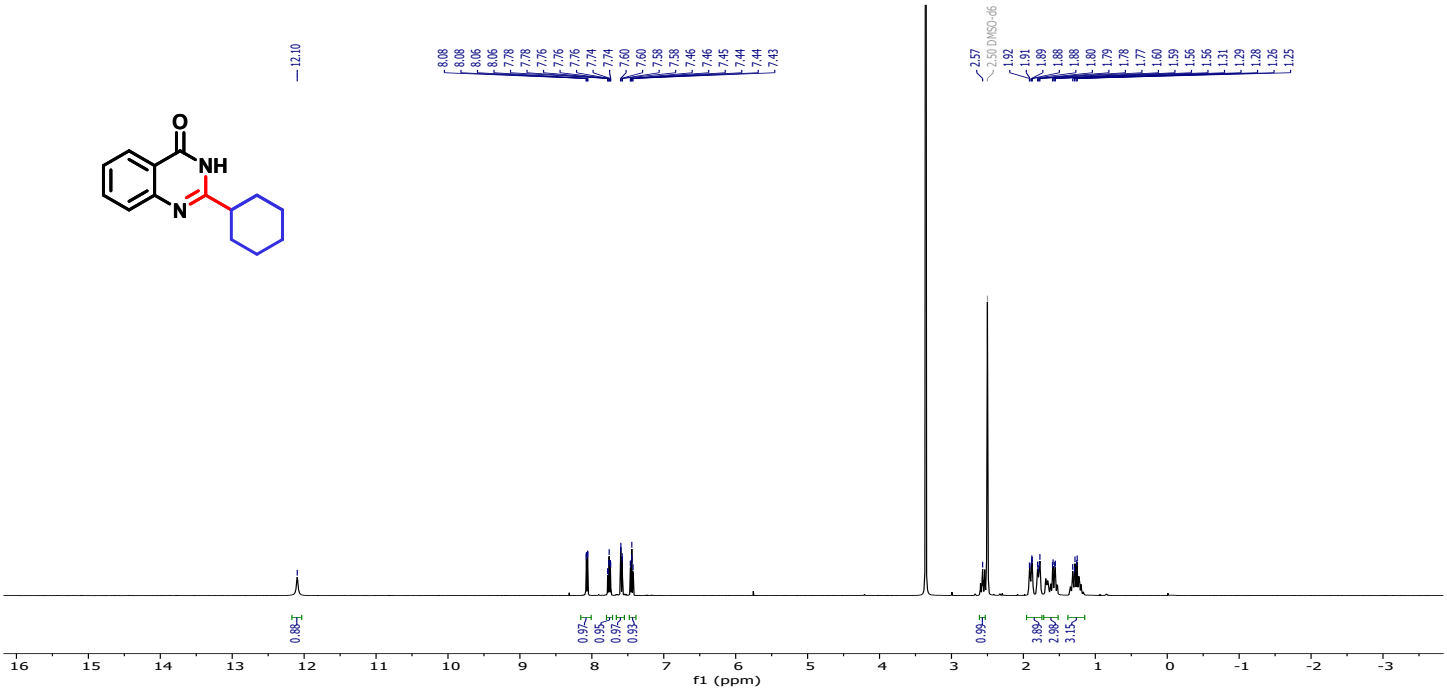


Figure S51. ^{1}H NMR spectrum (400 MHz) of **3t** in DMSO-d_6

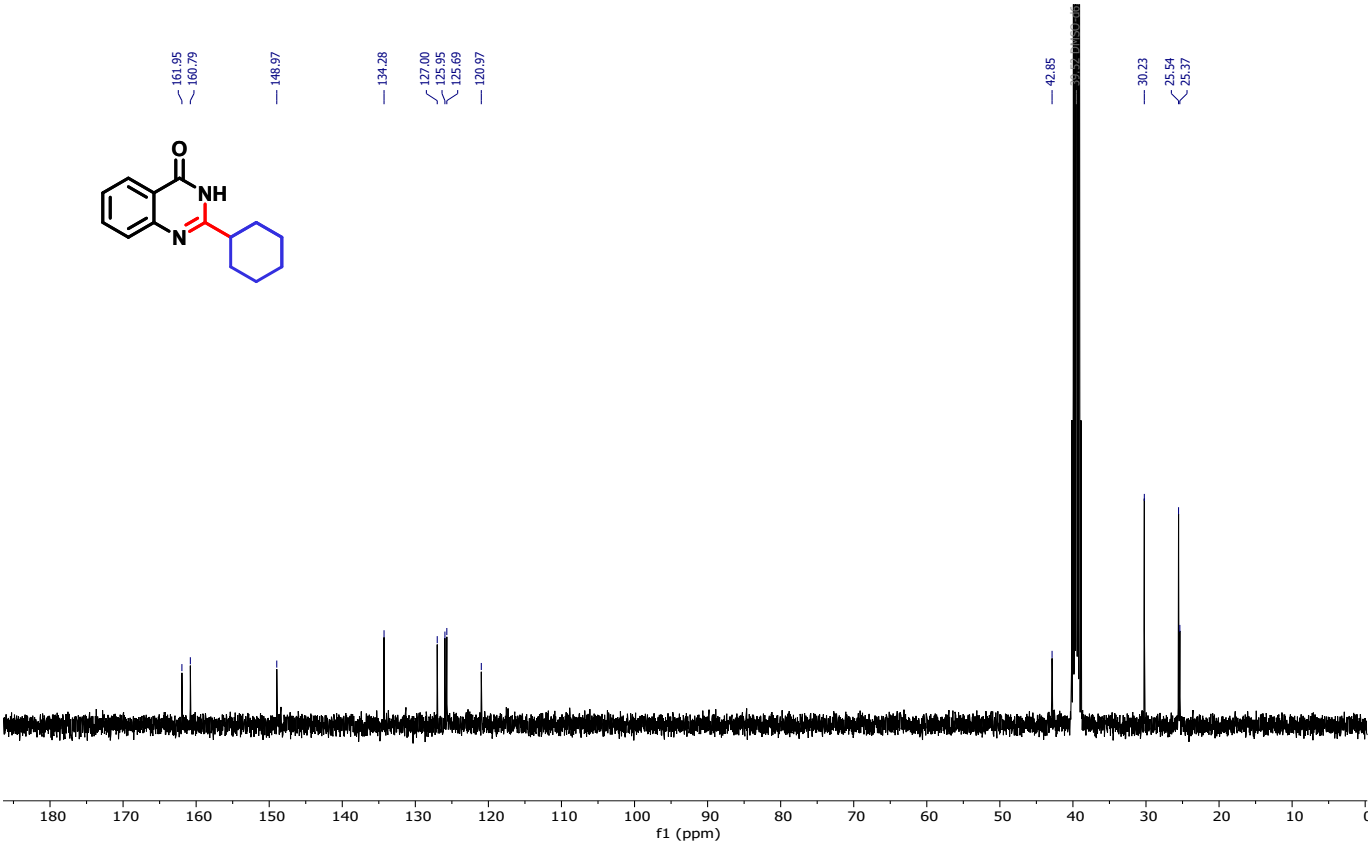


Figure S52. ^{13}C NMR spectrum (100 MHz) of **3t** in DMSO-d_6

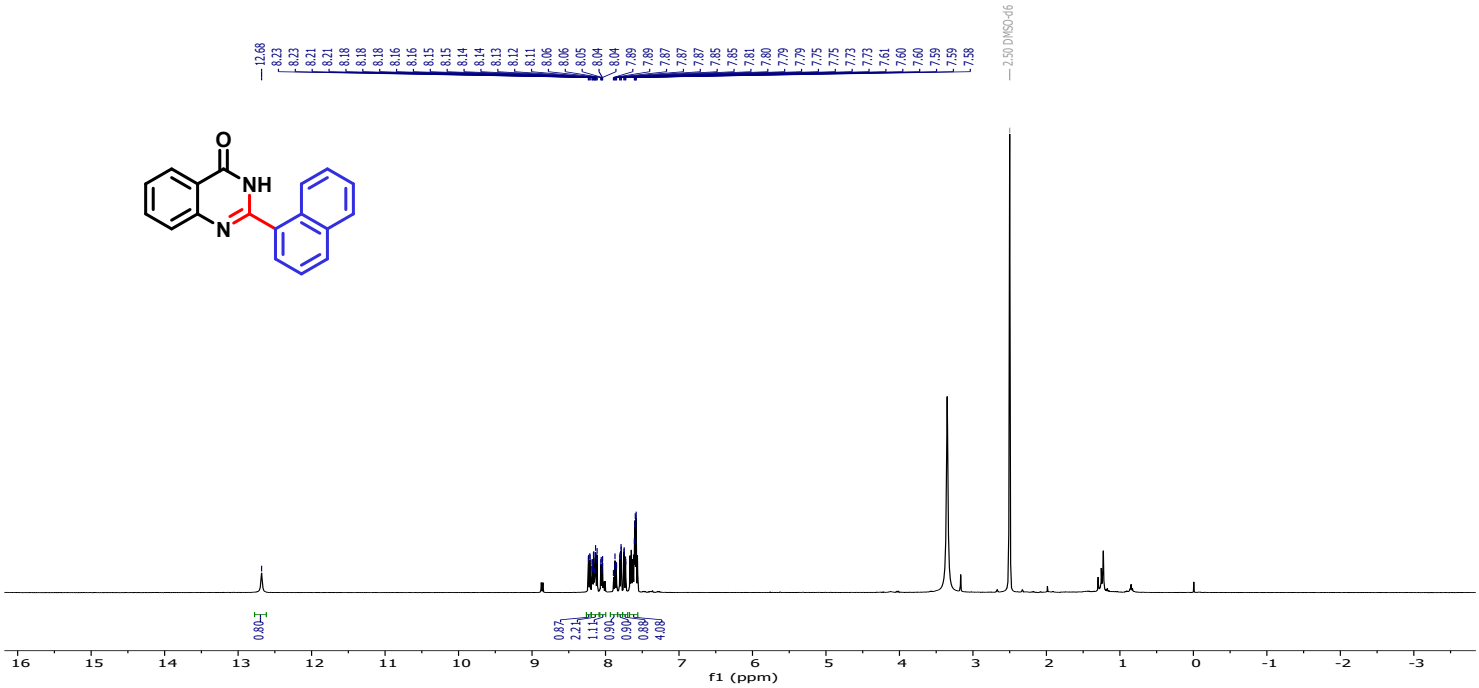


Figure S53. ^{1}H NMR spectrum (400 MHz) of **3u** in DMSO-d_6

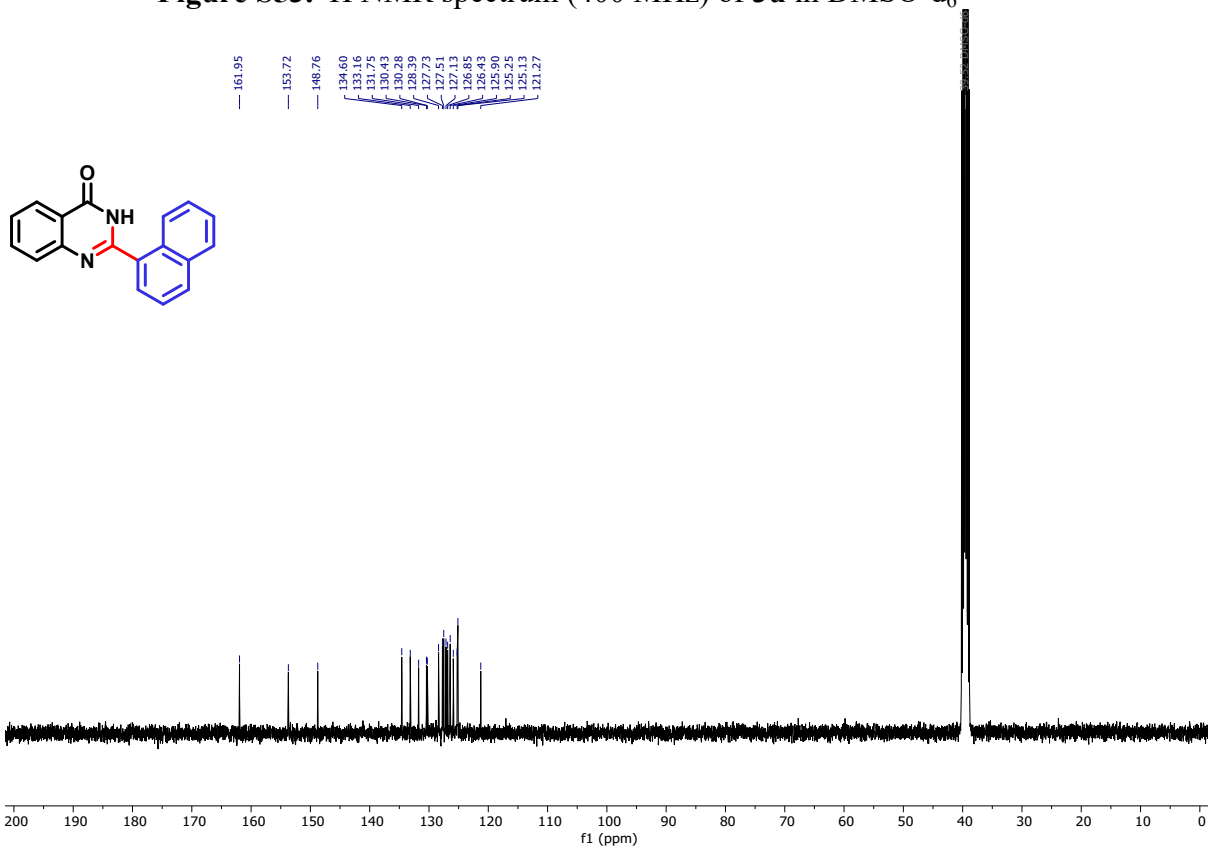


Figure S54. ^{13}C NMR spectrum (100 MHz) of **3u** in DMSO-d_6

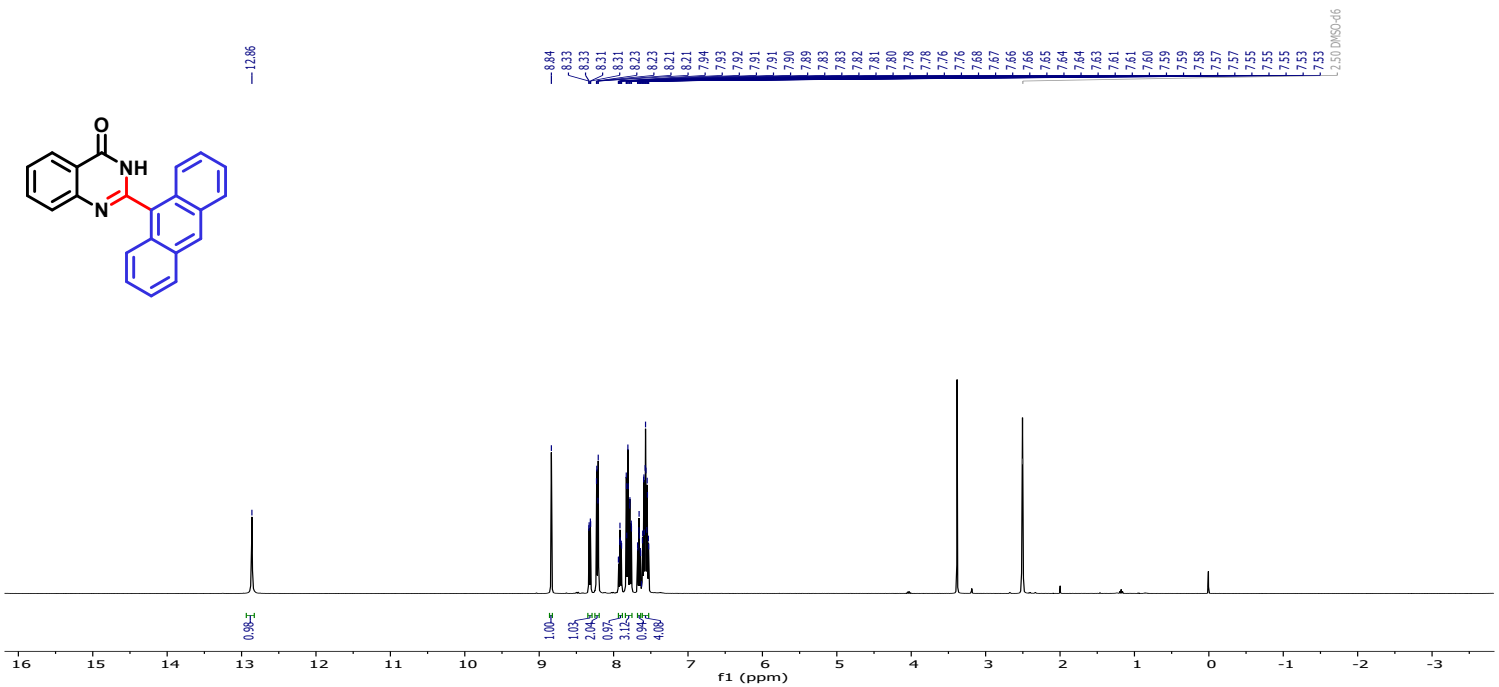


Figure S55. ^{1}H NMR spectrum (400 MHz) of **3v** in DMSO-d_6

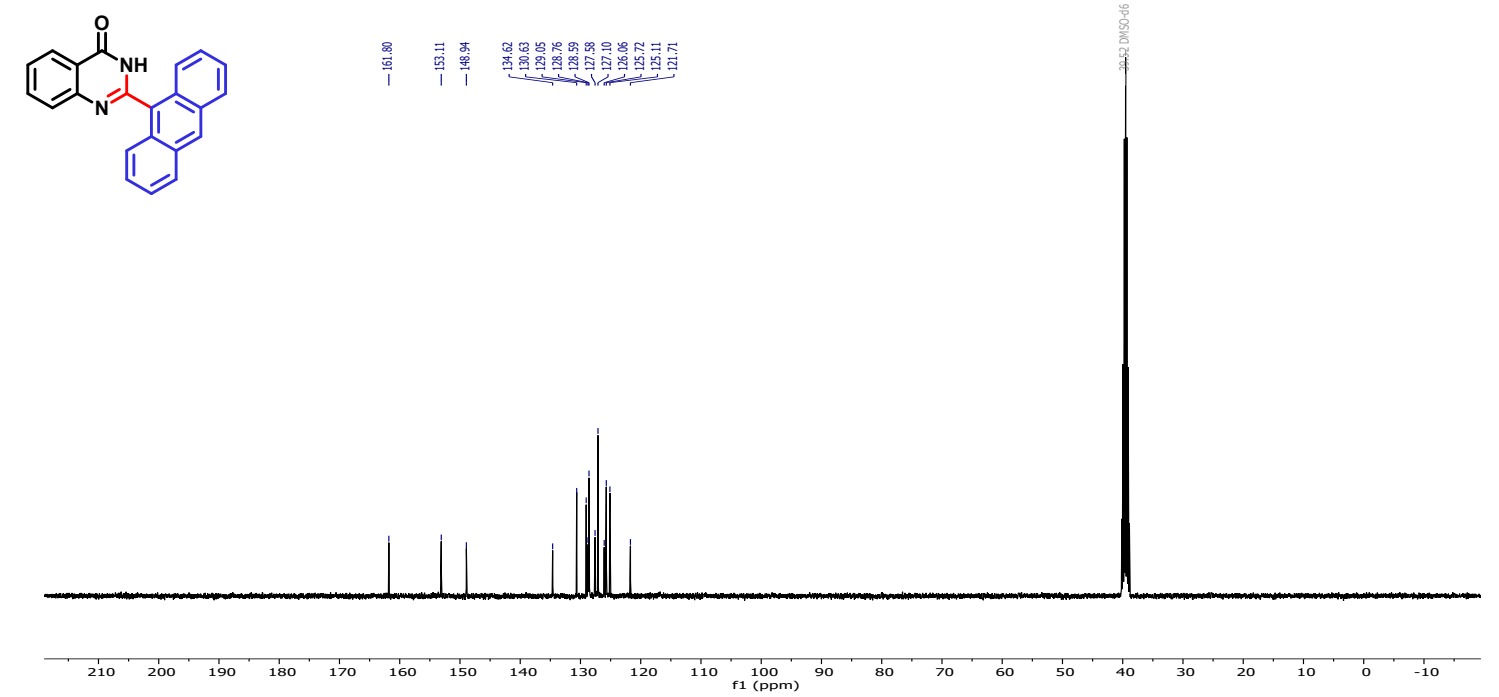


Figure S56. ^{13}C NMR spectrum (100 MHz) of **3v** in DMSO-d_6

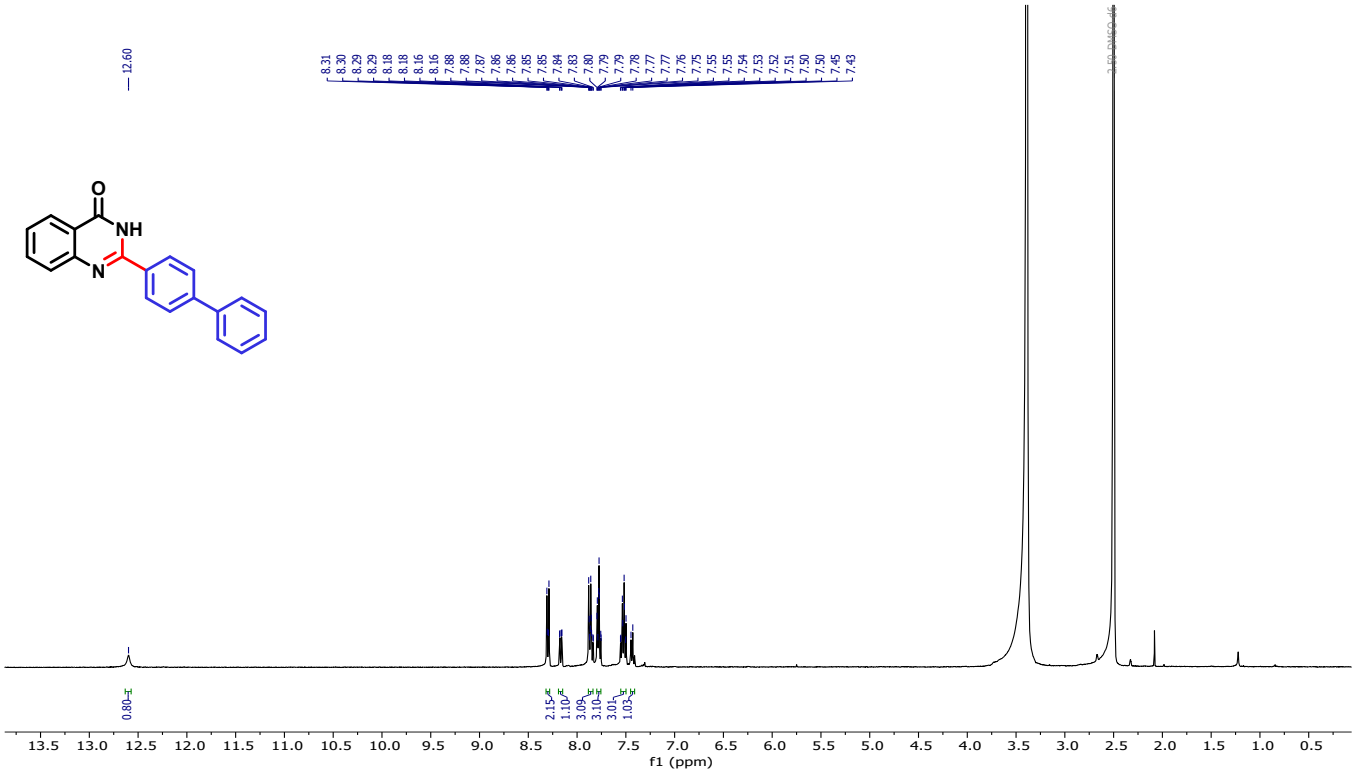


Figure S57. ^{1}H NMR spectrum (400 MHz) of **3w** in DMSO-d_6

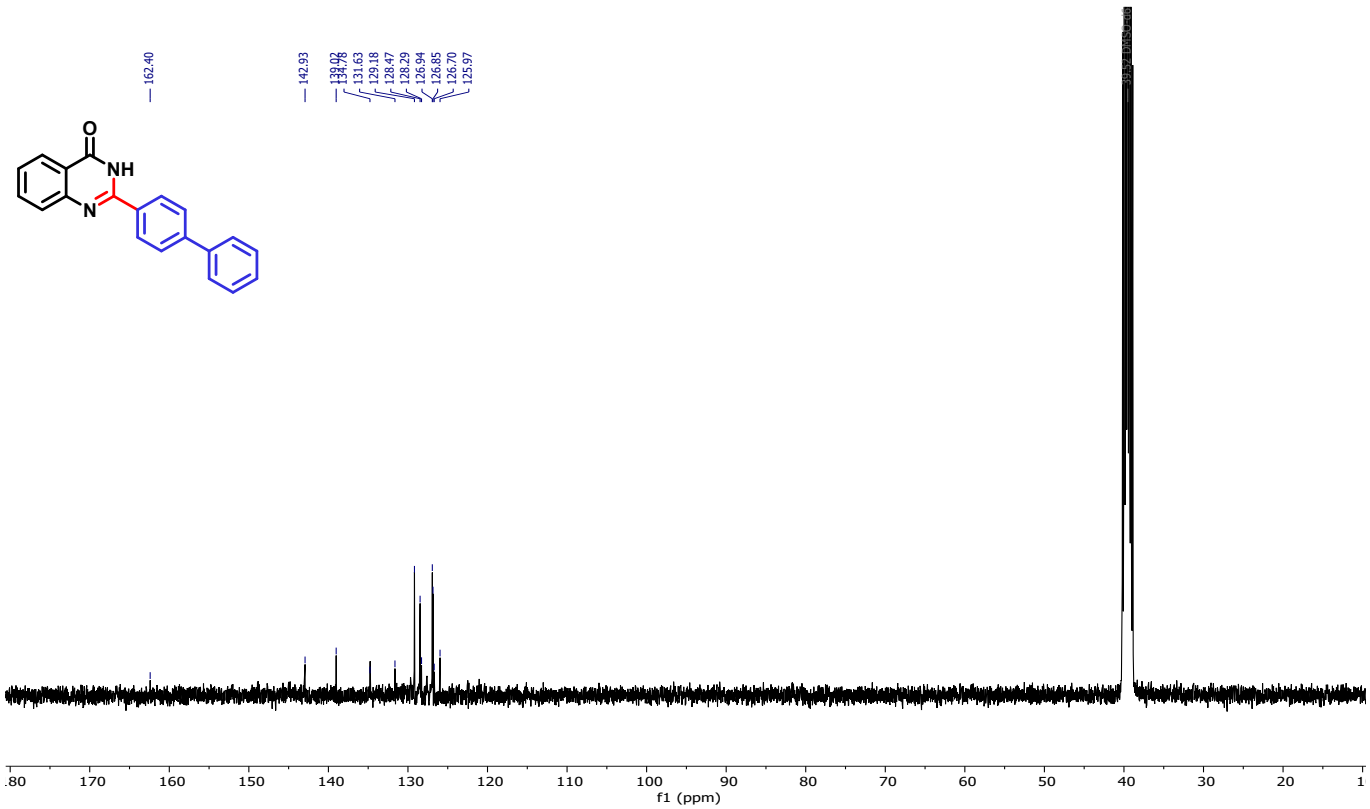


Figure S58. ^{13}C NMR spectrum (100 MHz) of **3w** in DMSO-d_6

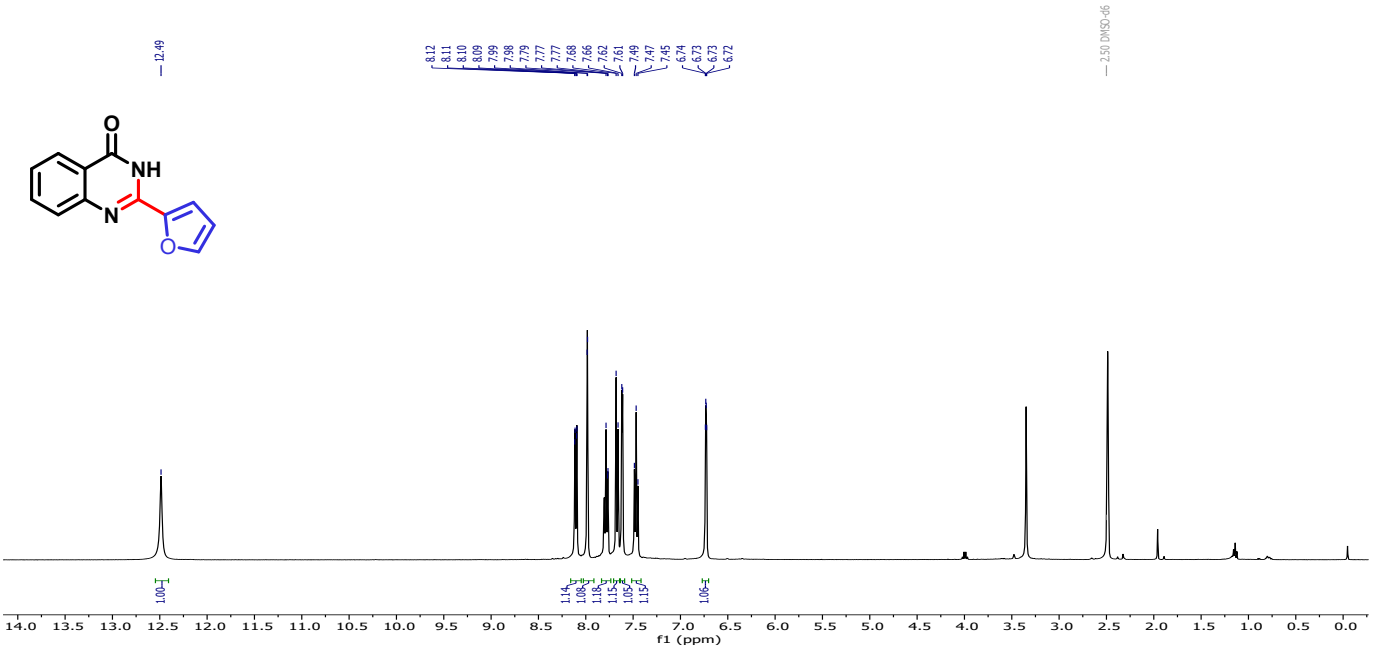


Figure S59. ^{1}H NMR spectrum (400 MHz) of **3x** in DMSO-d_6

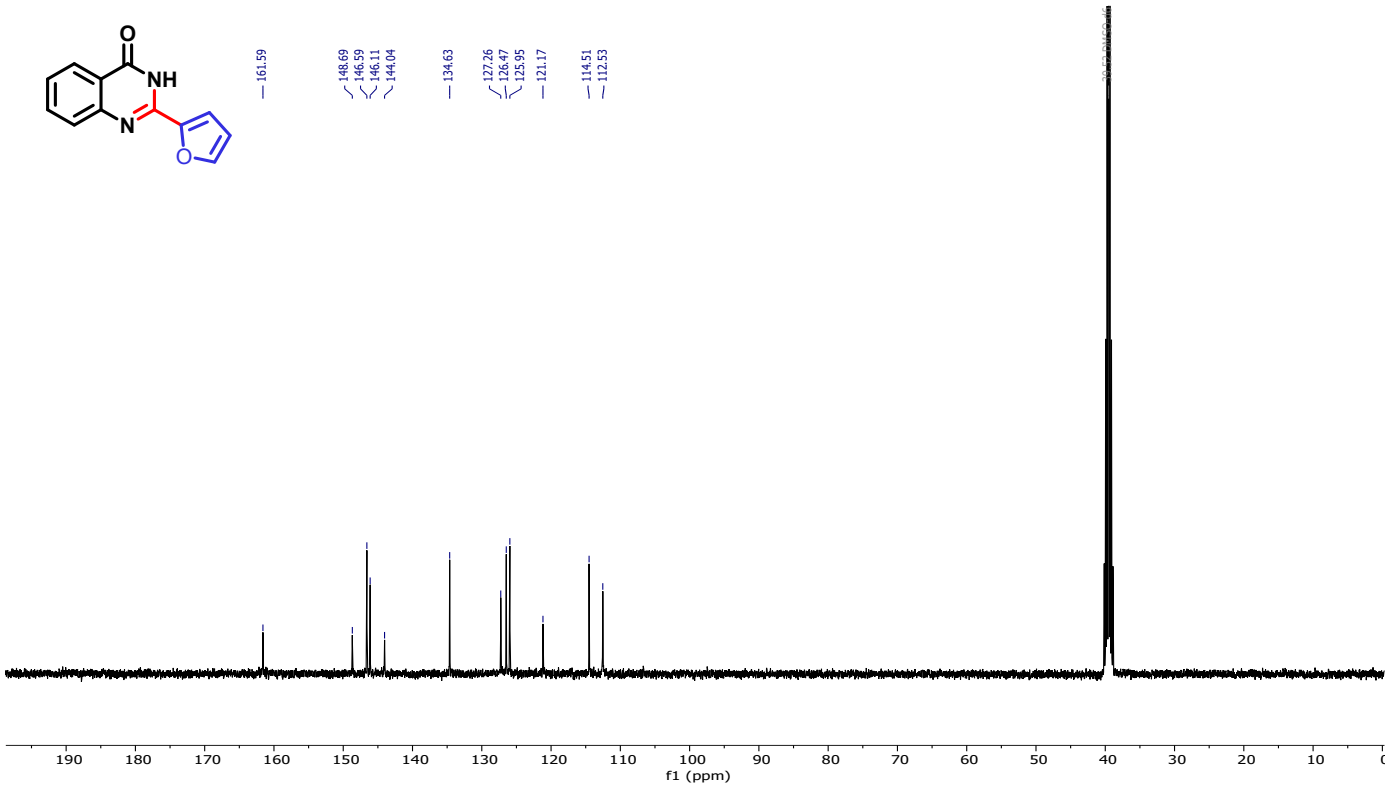


Figure S60. ^{13}C NMR spectrum (100 MHz) of **3x** in DMSO-d_6

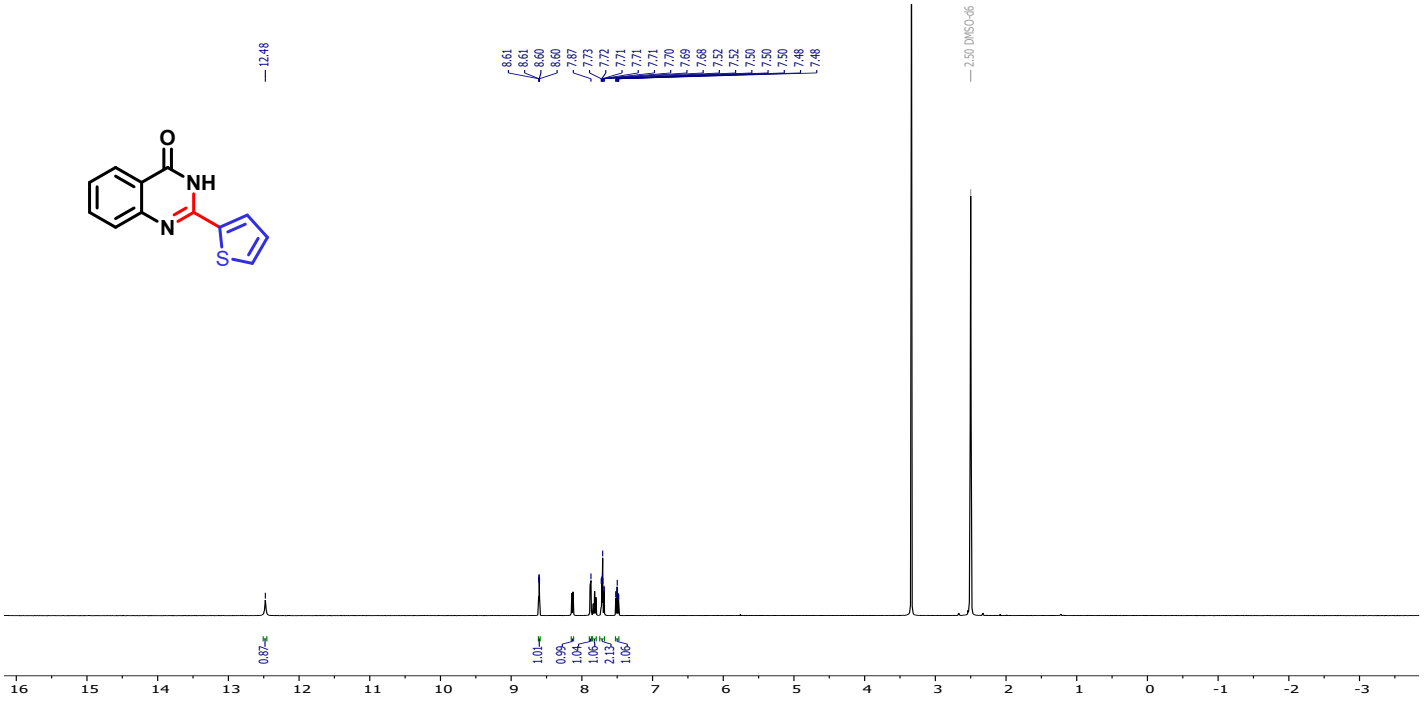


Figure S61. ^{1}H NMR spectrum (400 MHz) of **3y** in DMSO-d_6

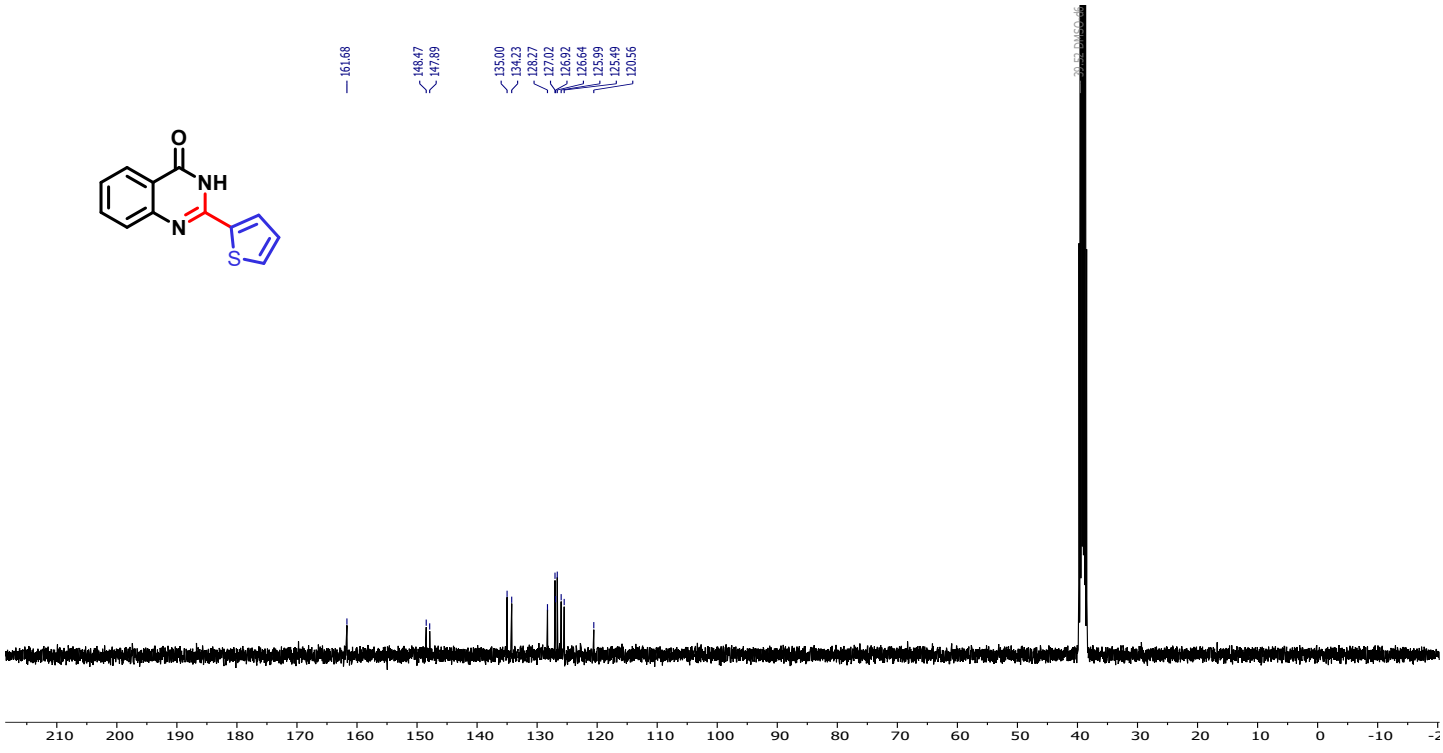


Figure S62. ^{13}C NMR spectrum (100 MHz) of **3y** in DMSO-d_6

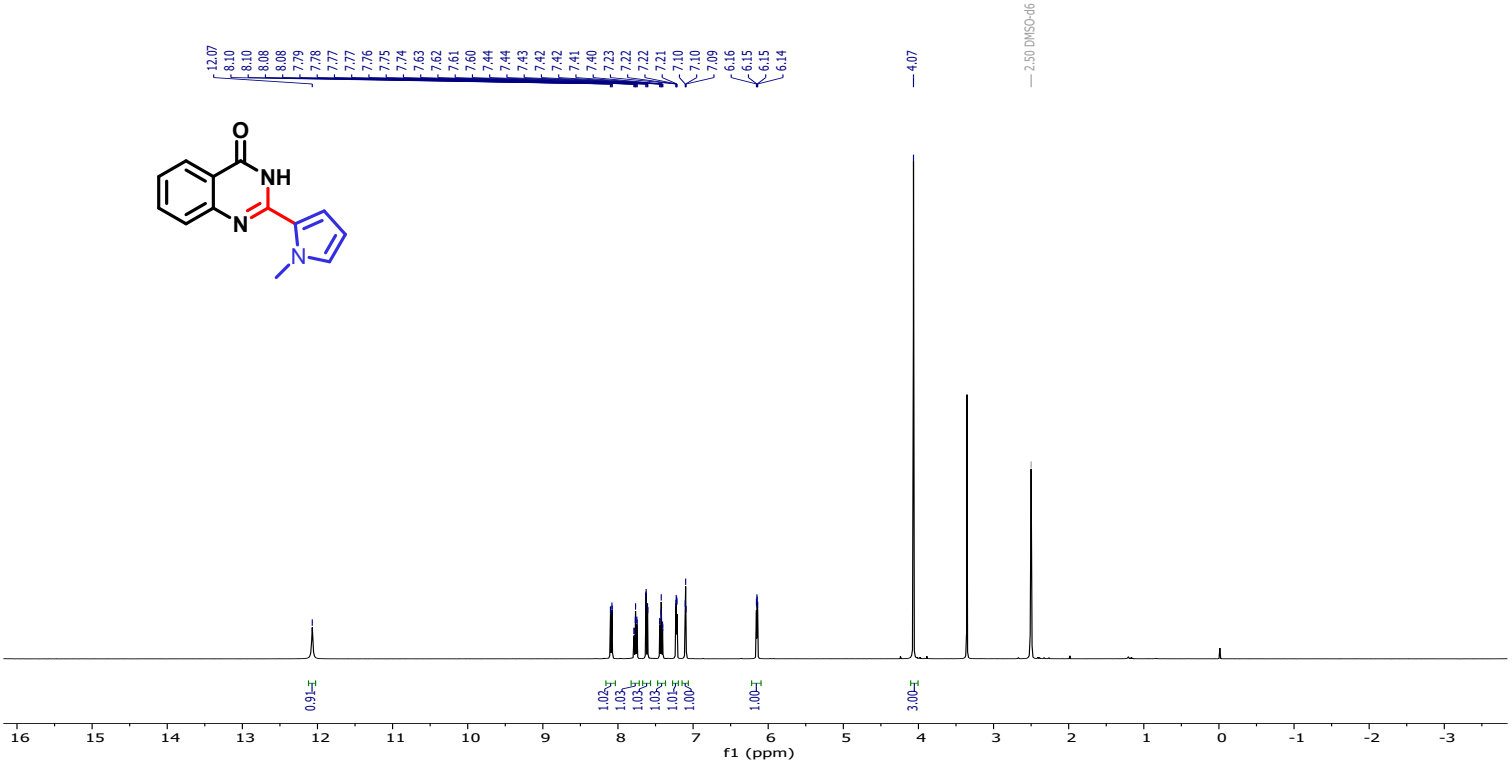


Figure S63. ^{1}H NMR spectrum (400 MHz) of **3z** in DMSO-d_6

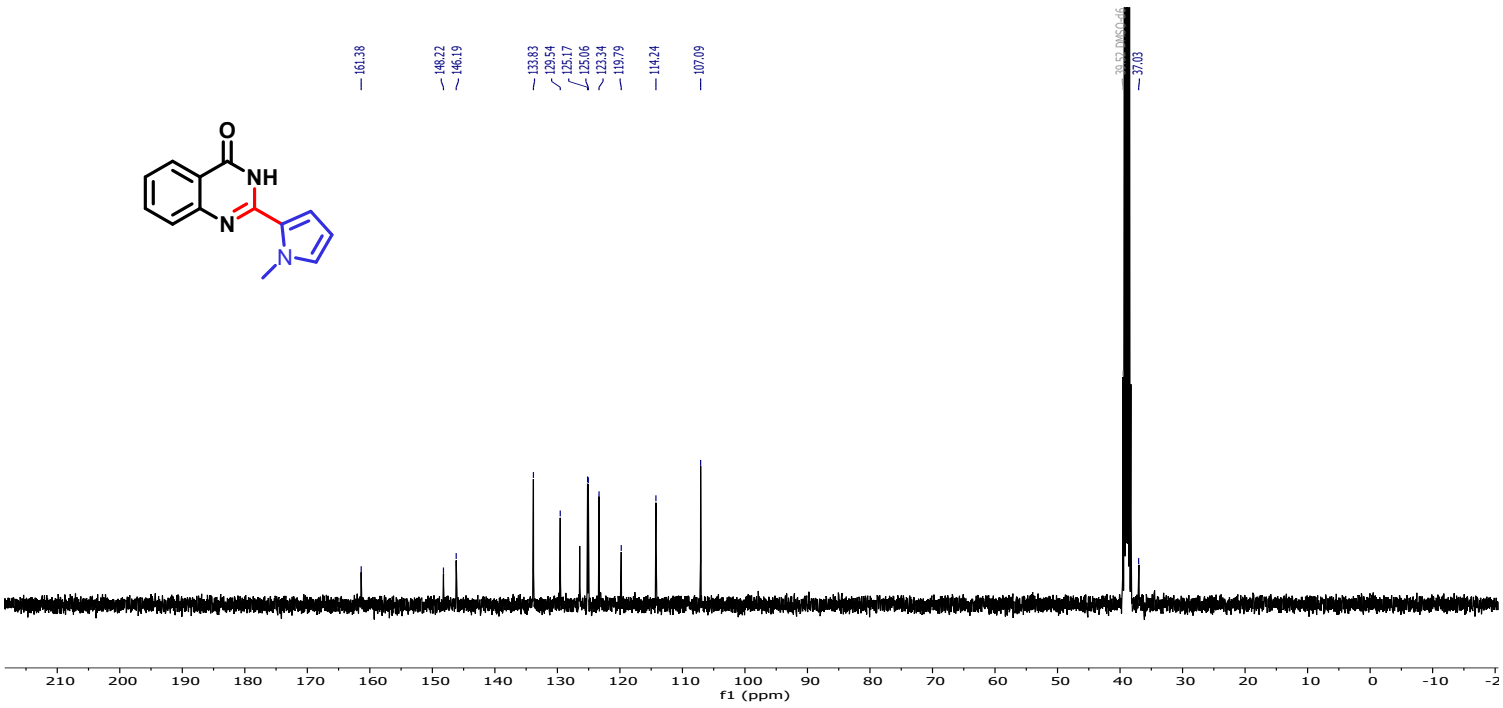


Figure S64. ^{13}C NMR spectrum (100 MHz) of **3z** in DMSO-d_6

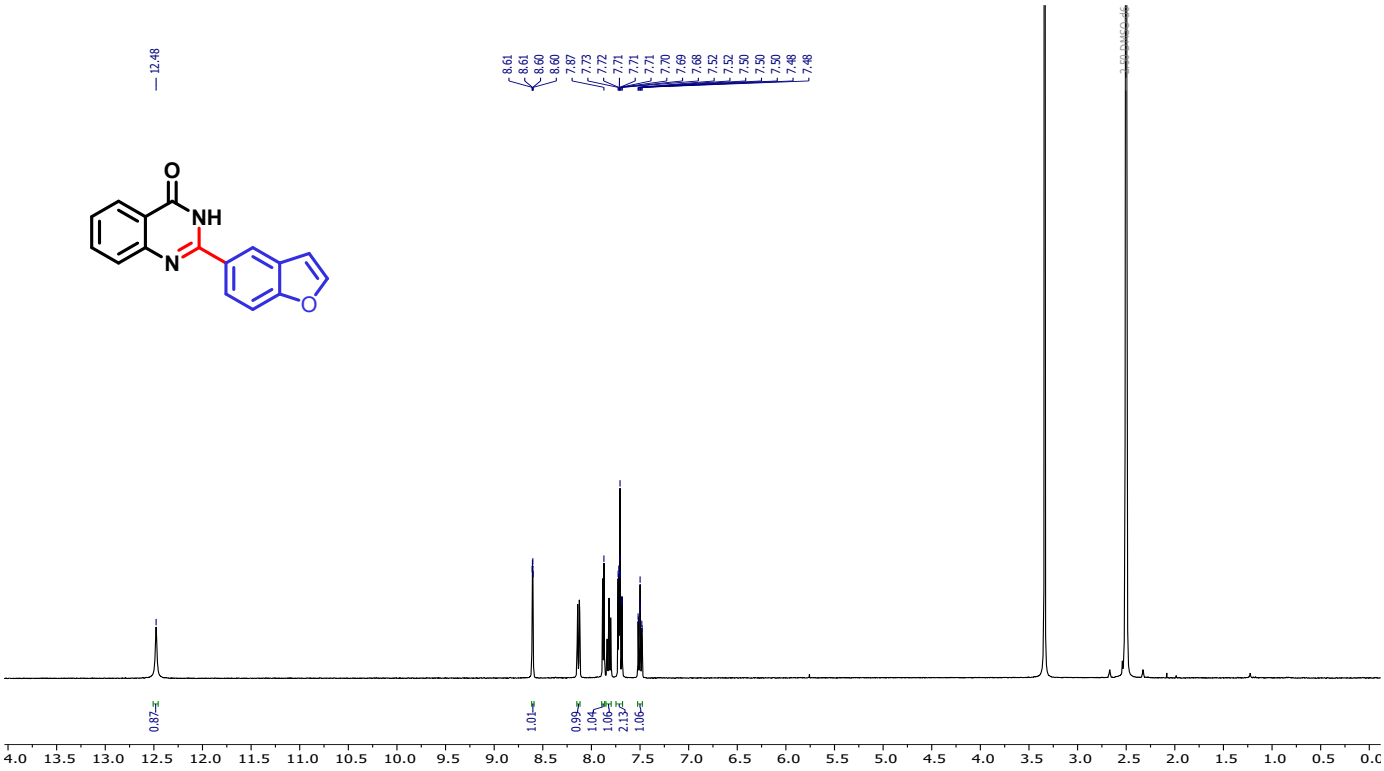


Figure S65. ^{1}H NMR spectrum (400 MHz) of **3za** in DMSO-d_6

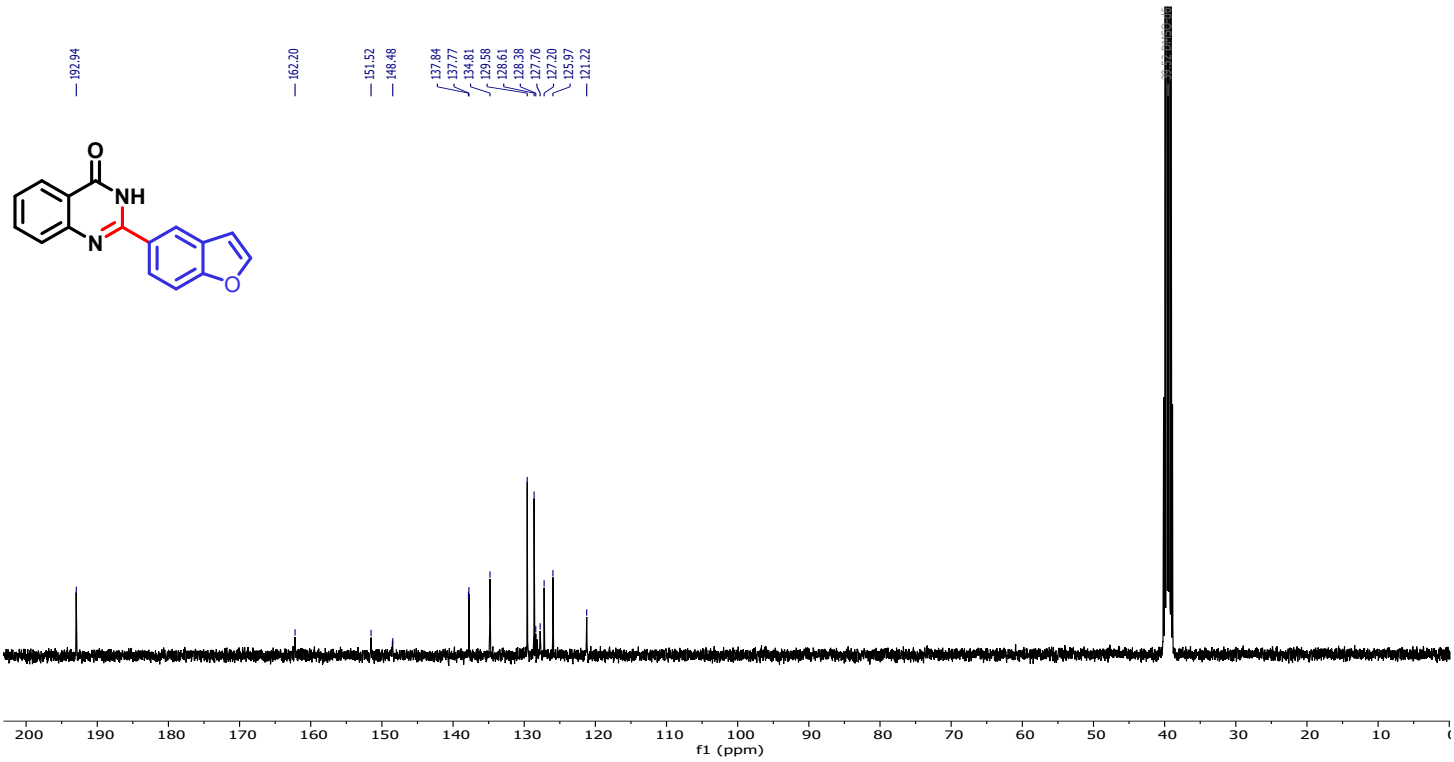


Figure S66. ^{13}C NMR spectrum (100 MHz) of **3za** in DMSO-d_6

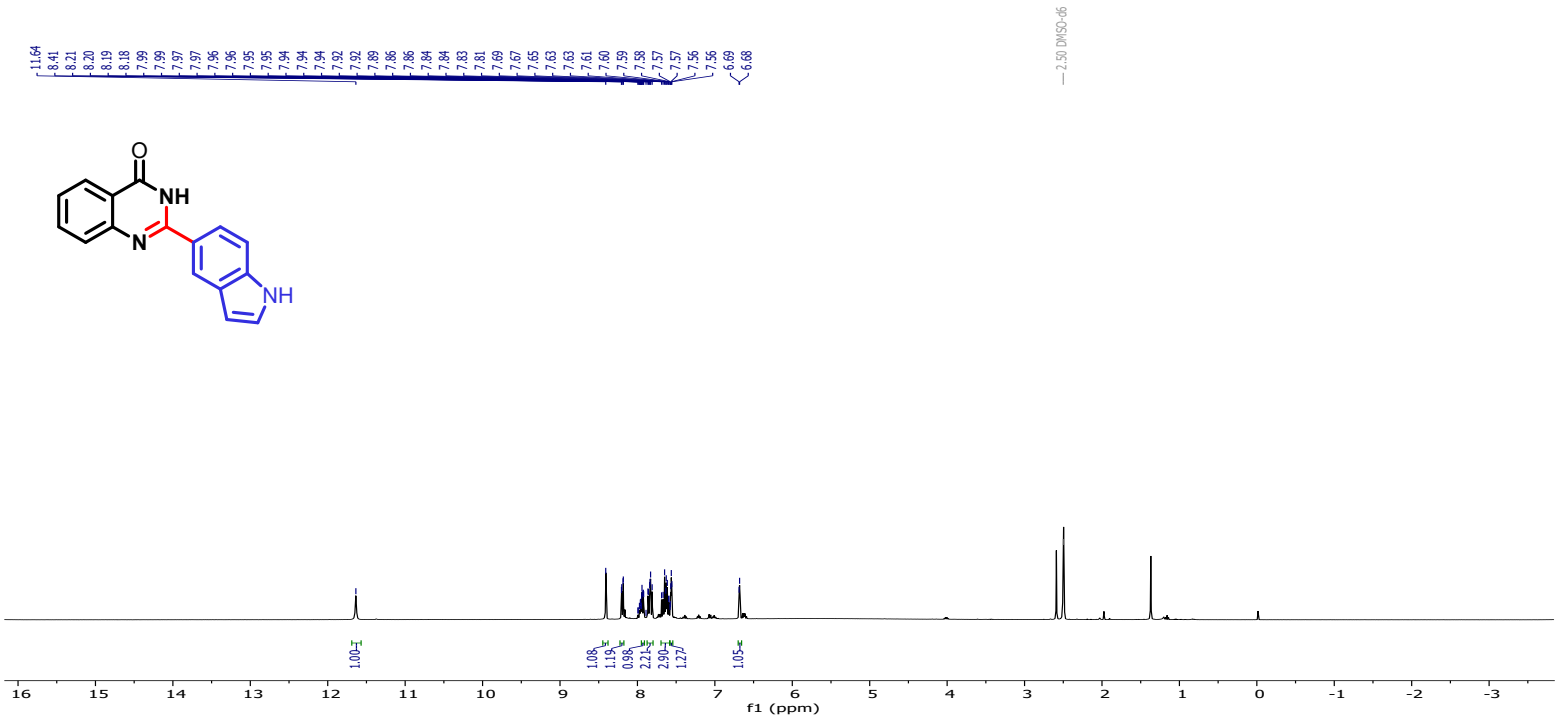


Figure S67. ^{1}H NMR spectrum (400 MHz) of **3zb** in DMSO-d_6

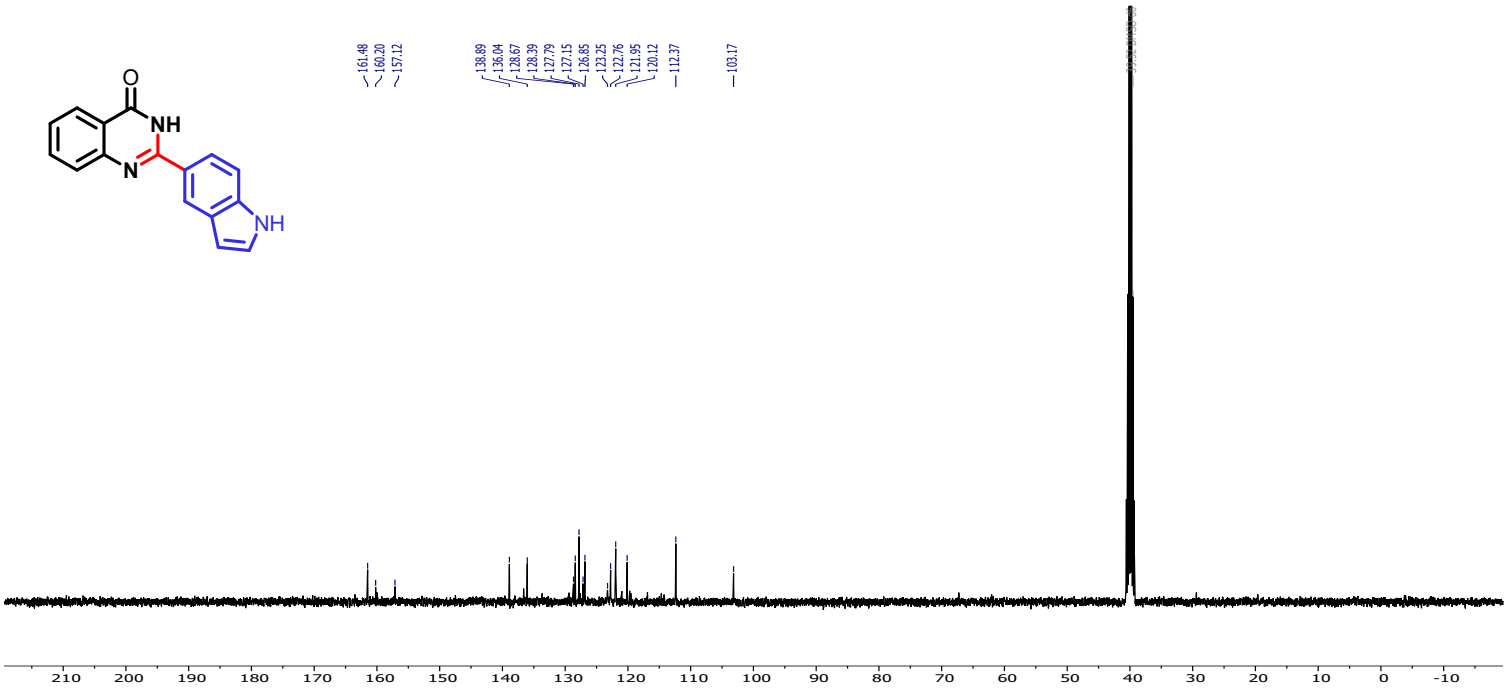


Figure S68. ^{13}C NMR spectrum (100 MHz) of **3zb** in DMSO-d_6

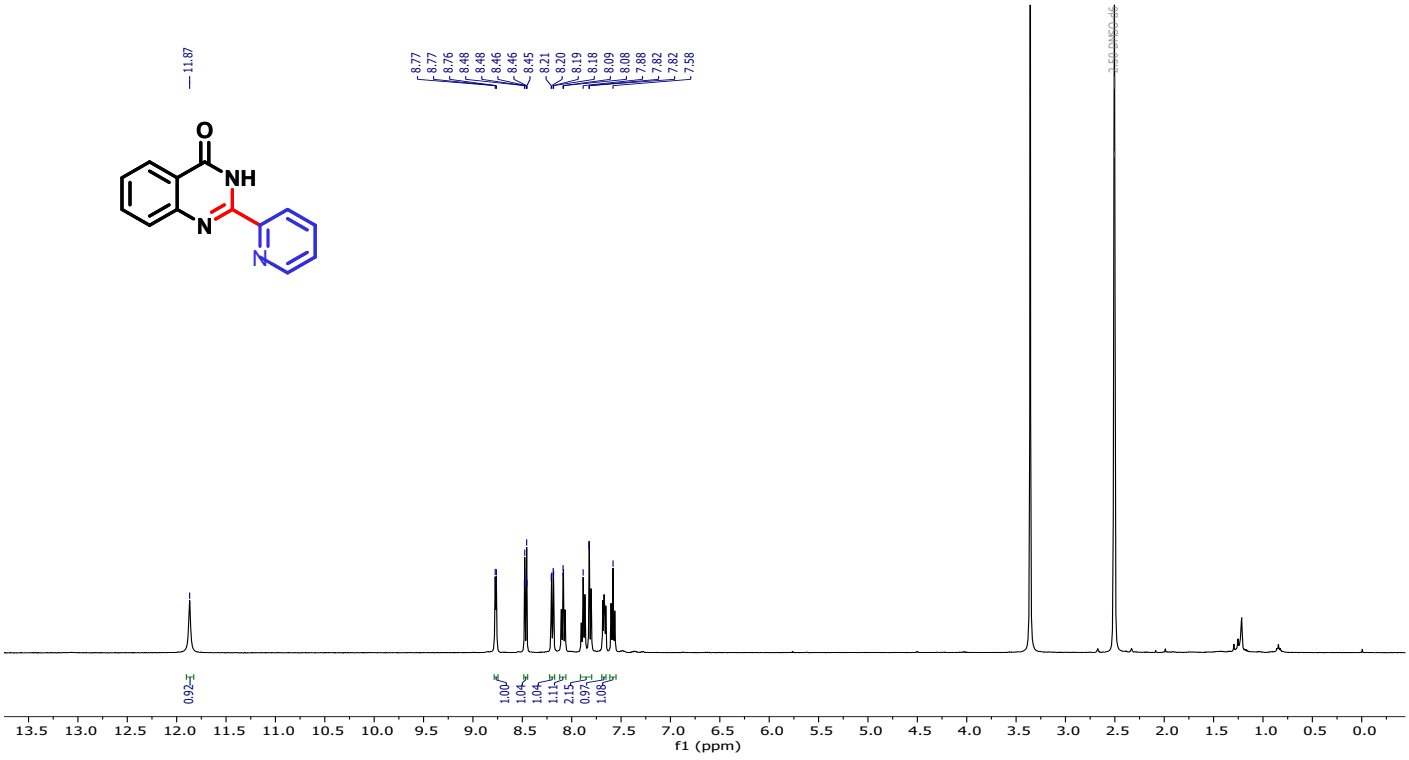


Figure S69. ^{1}H NMR spectrum (400 MHz) of **3zc** in DMSO-d_6

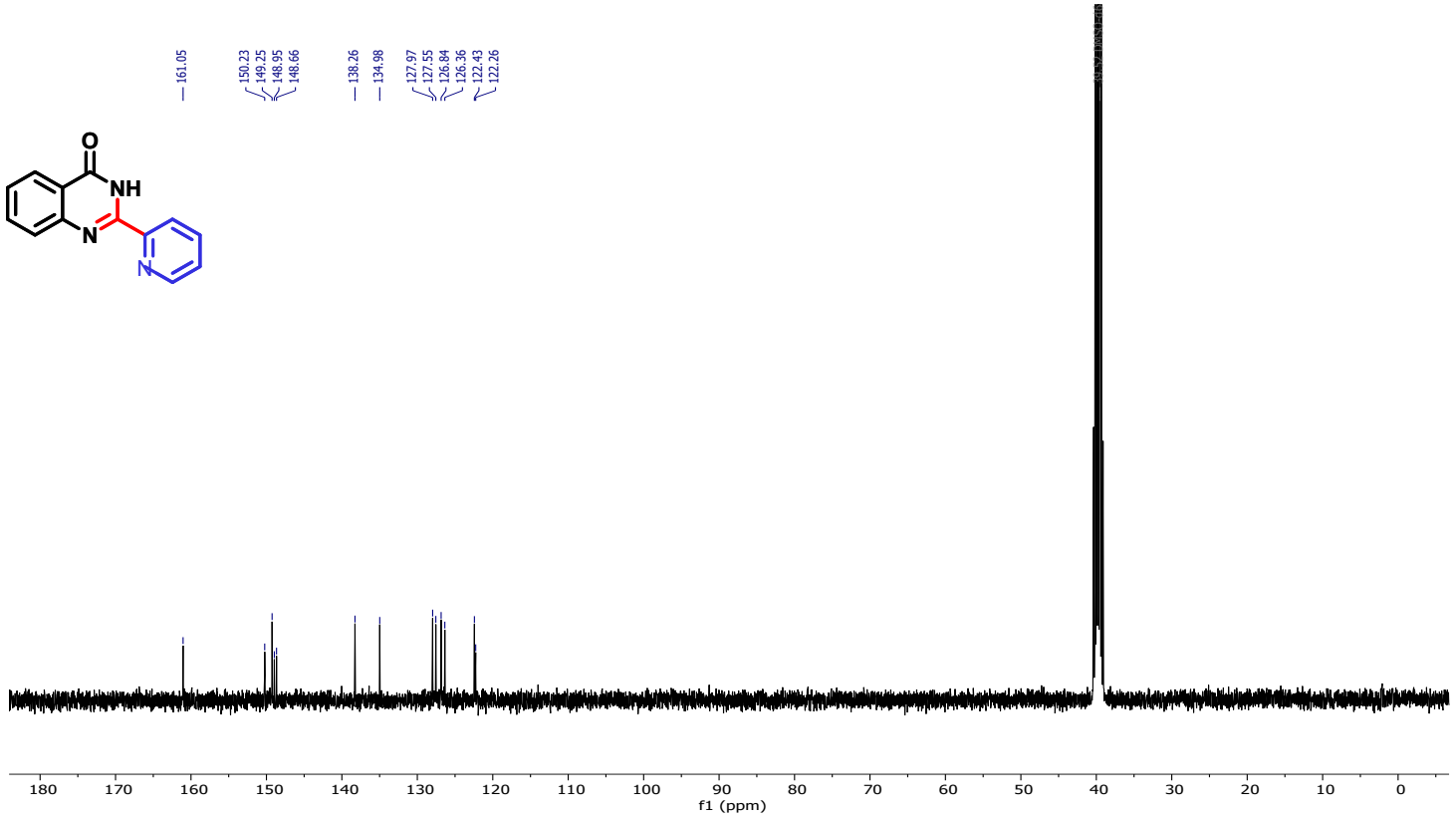


Figure S70. ^{13}C NMR spectrum (100 MHz) of **3zc** in DMSO-d_6

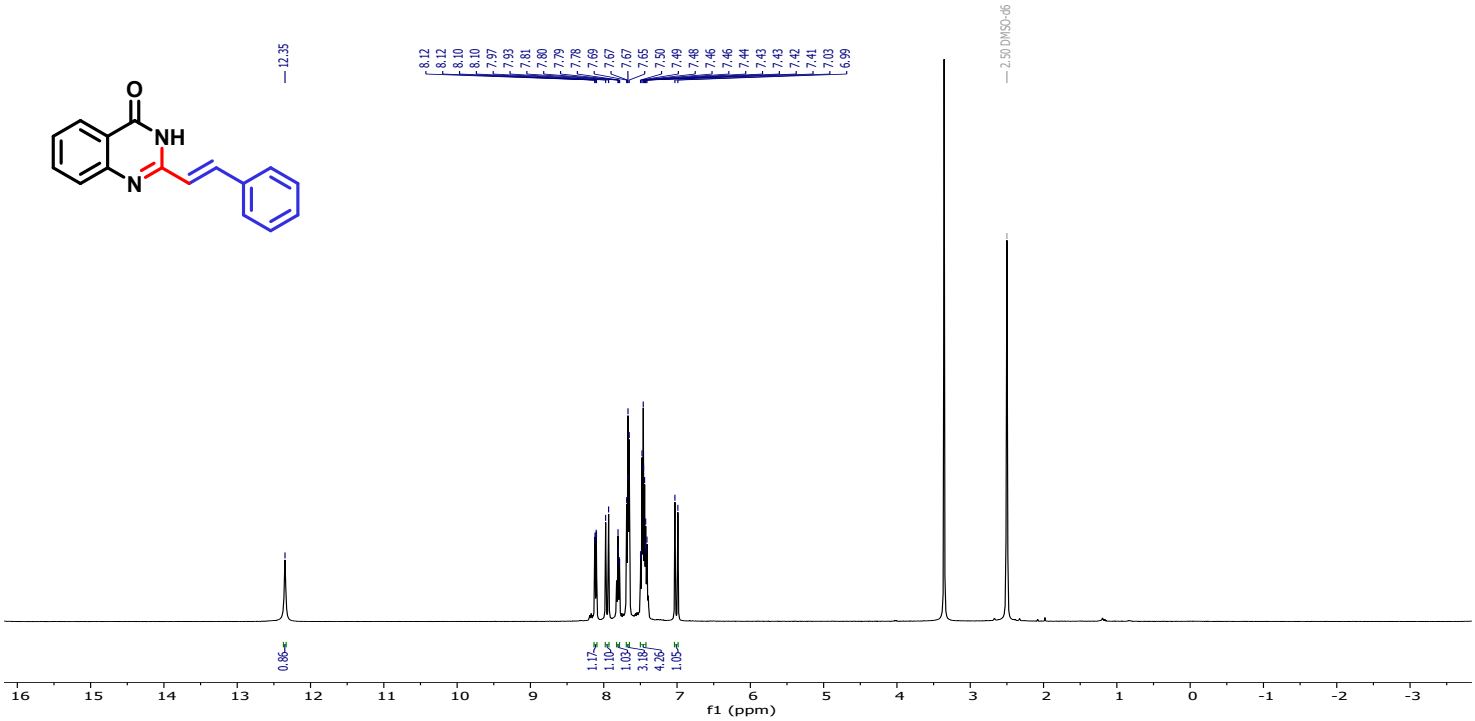


Figure S71. [1]H NMR spectrum (400 MHz) of **3zd** in DMSO-d_6

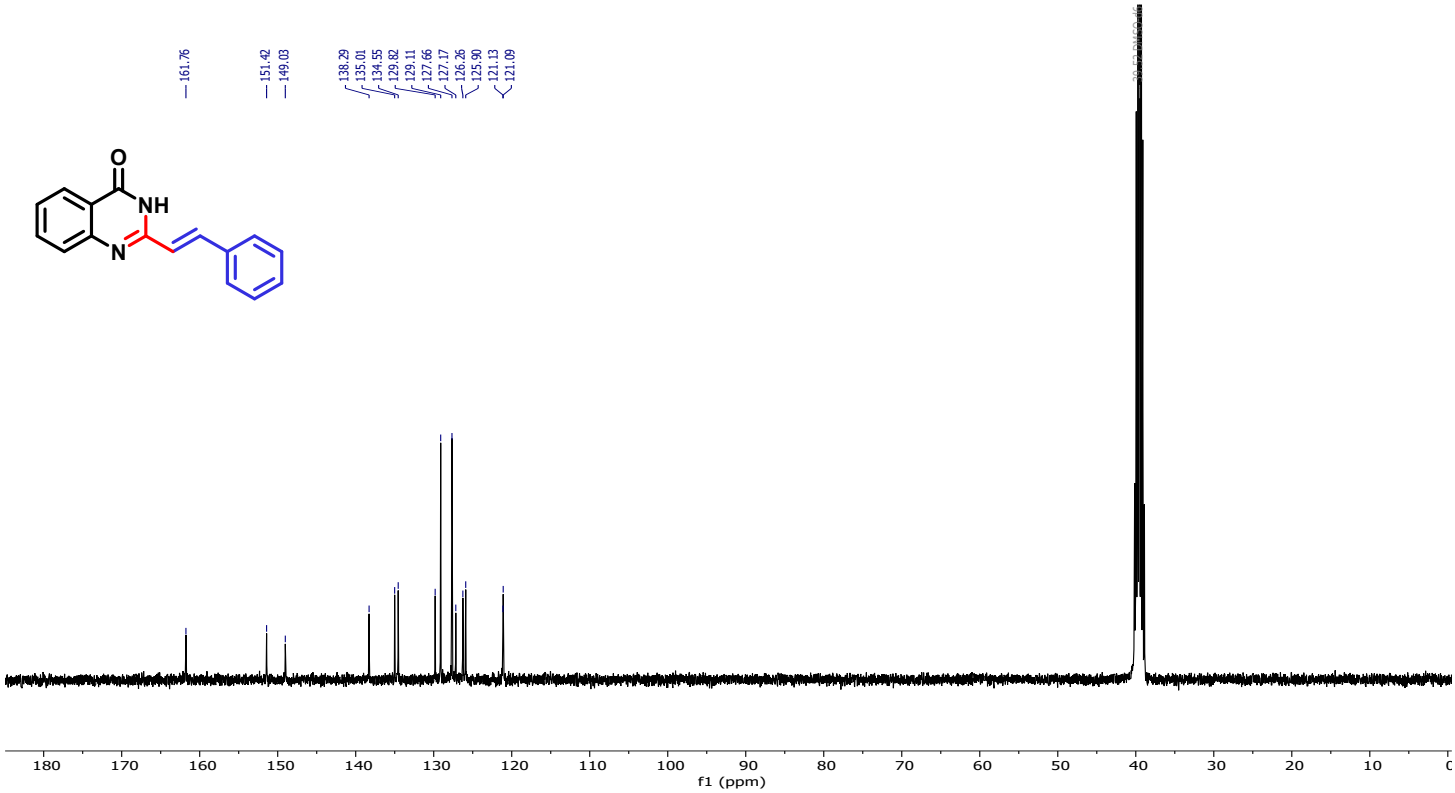


Figure S72. [13]C NMR spectrum (100 MHz) of **3zd** in DMSO-d_6

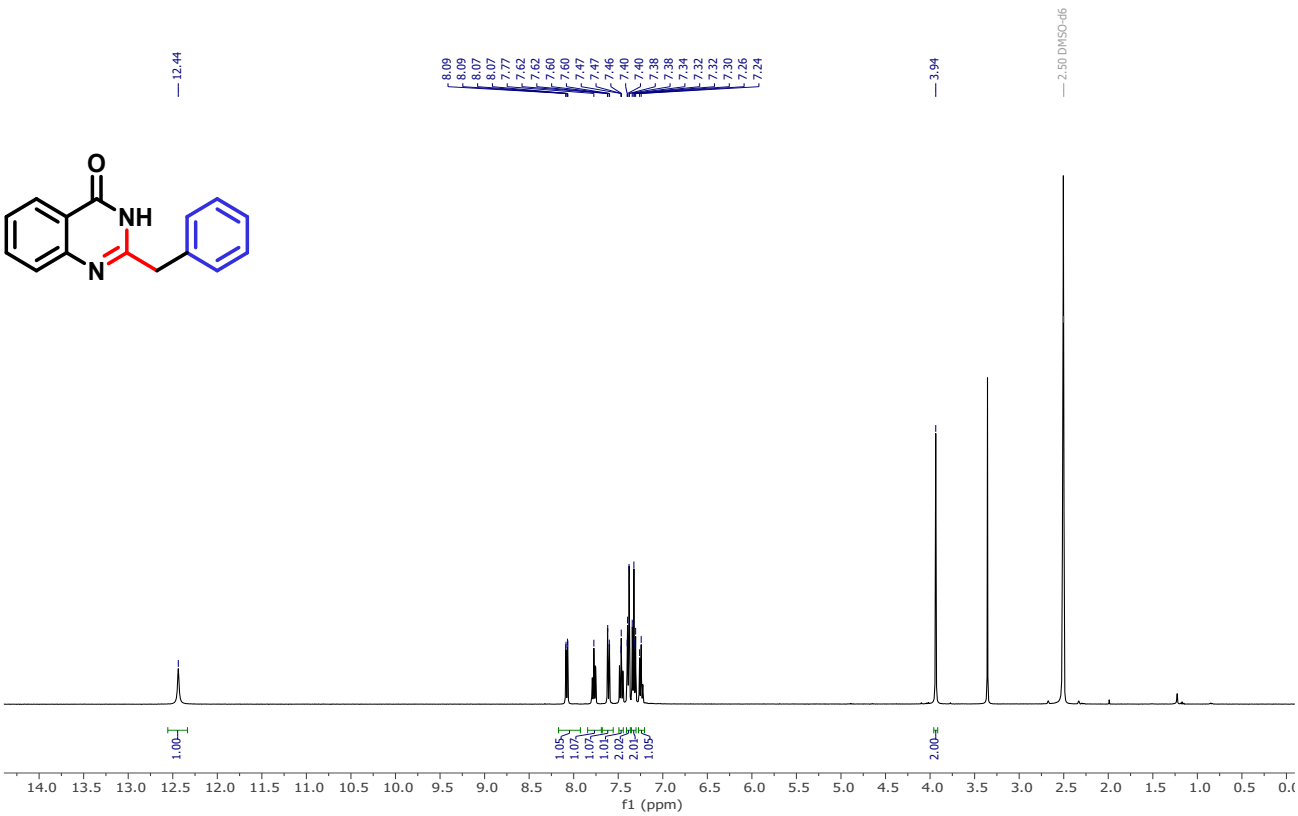


Figure S73. ^{13}C NMR spectrum (100 MHz) of **3ze** in DMSO-d_6

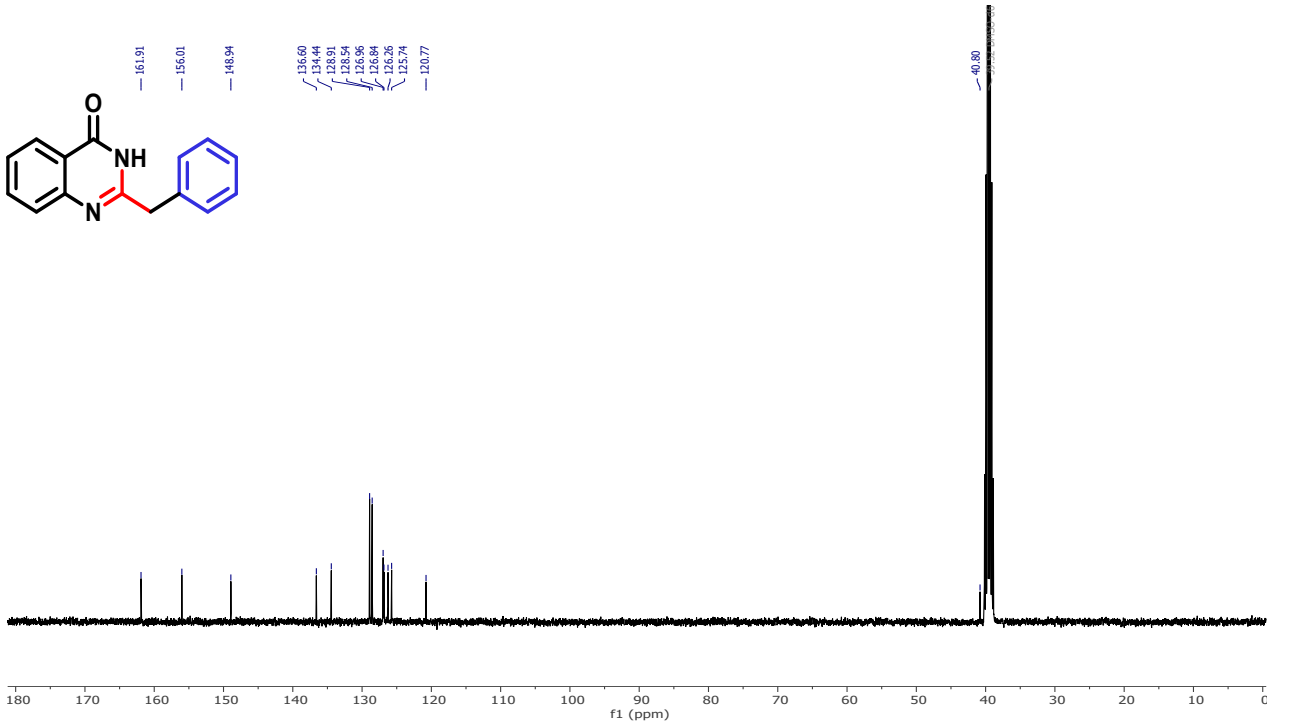


Figure S74. ^{13}C NMR spectrum (100 MHz) of **3ze** in DMSO-d_6

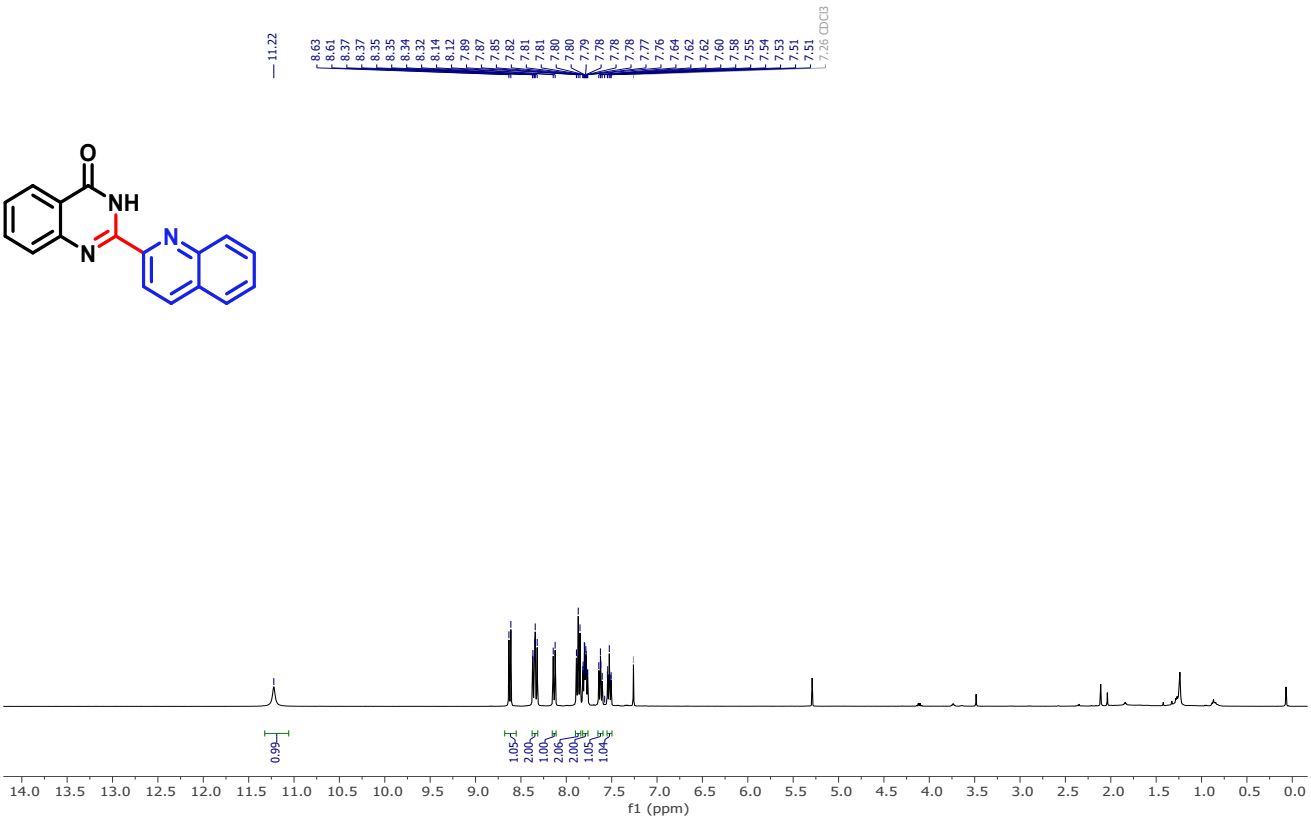


Figure S75. 1H NMR spectrum (400 MHz) of **3zf** in DMSO-d6

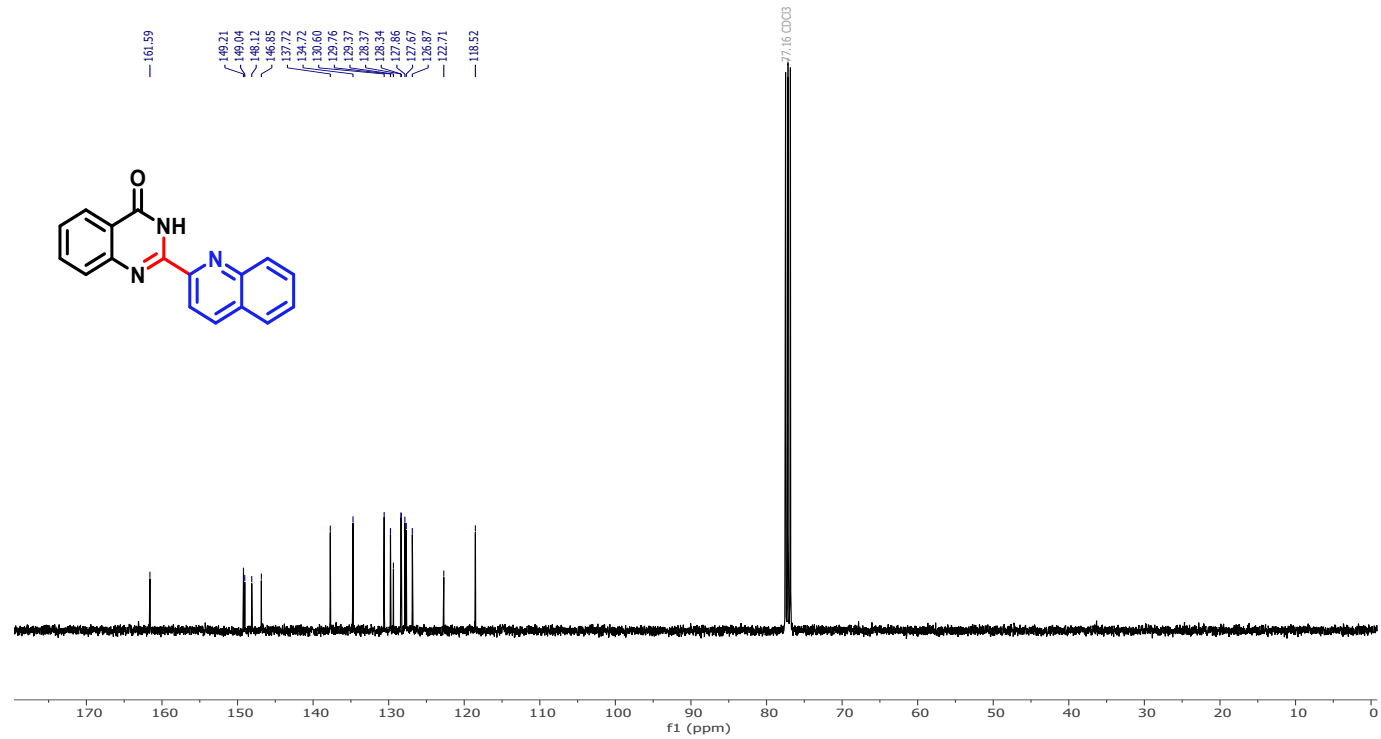


Figure S76. ^{13}C NMR spectrum (100 MHz) of **3zf** in DMSO-d6

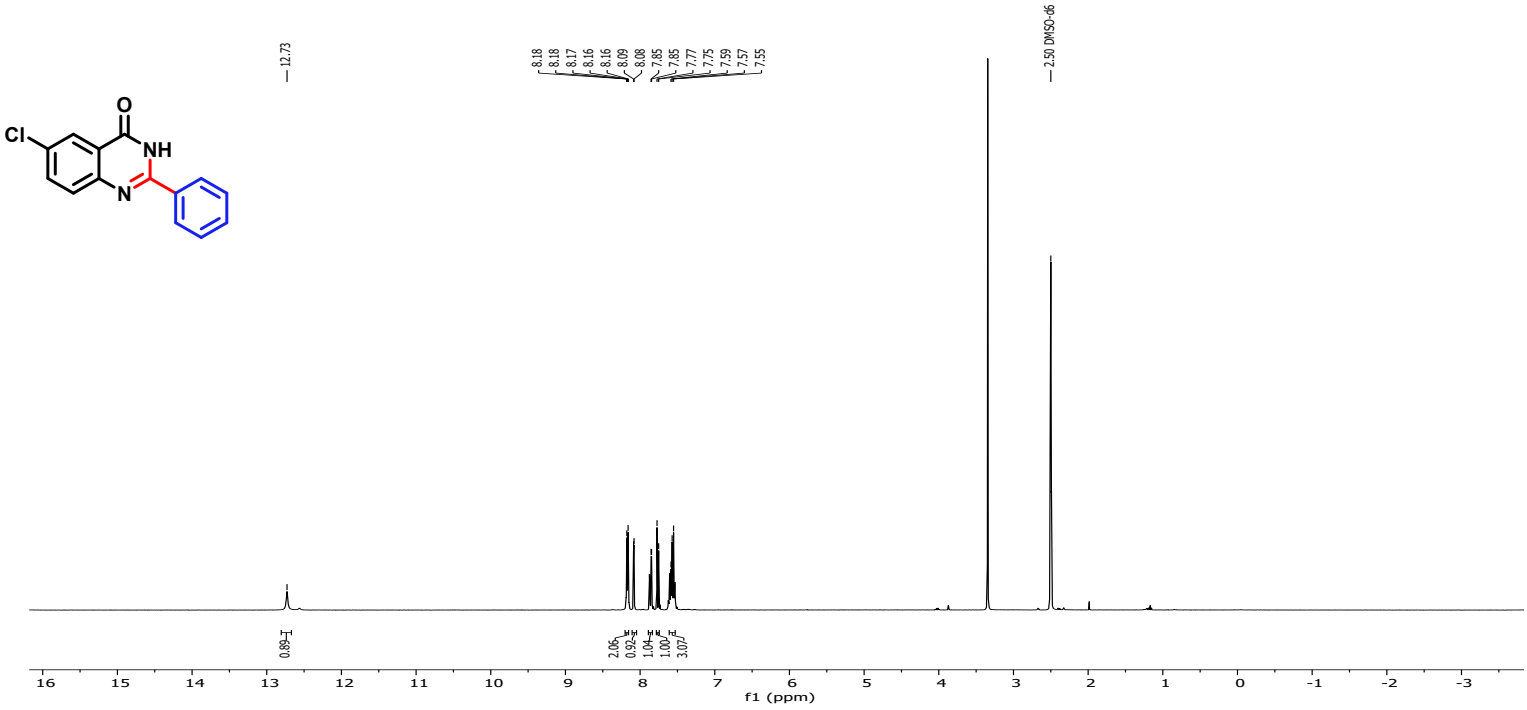


Figure S77. ^{1}H NMR spectrum (400 MHz) of **7a** in DMSO-d_6

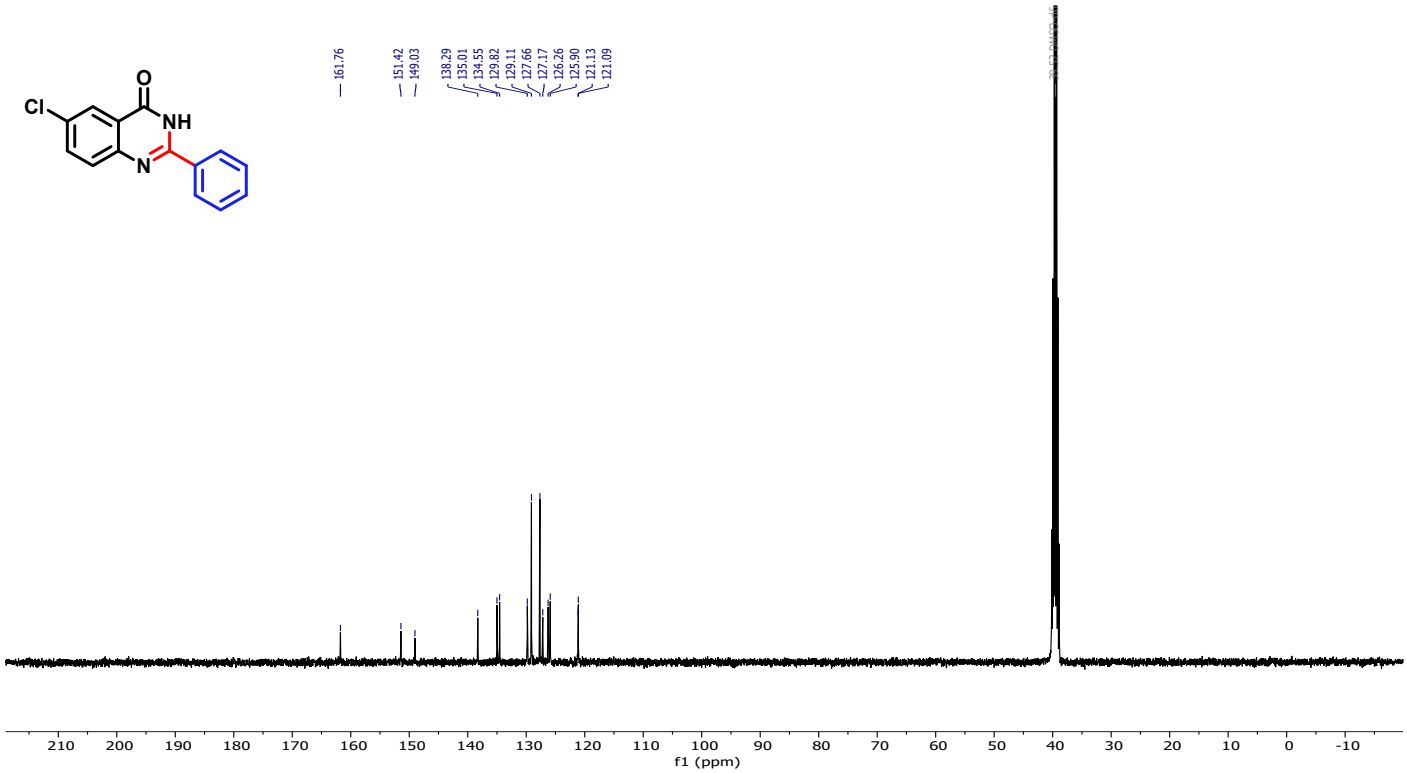


Figure S78. ^{13}C NMR spectrum (100 MHz) of **7a** in DMSO-d_6

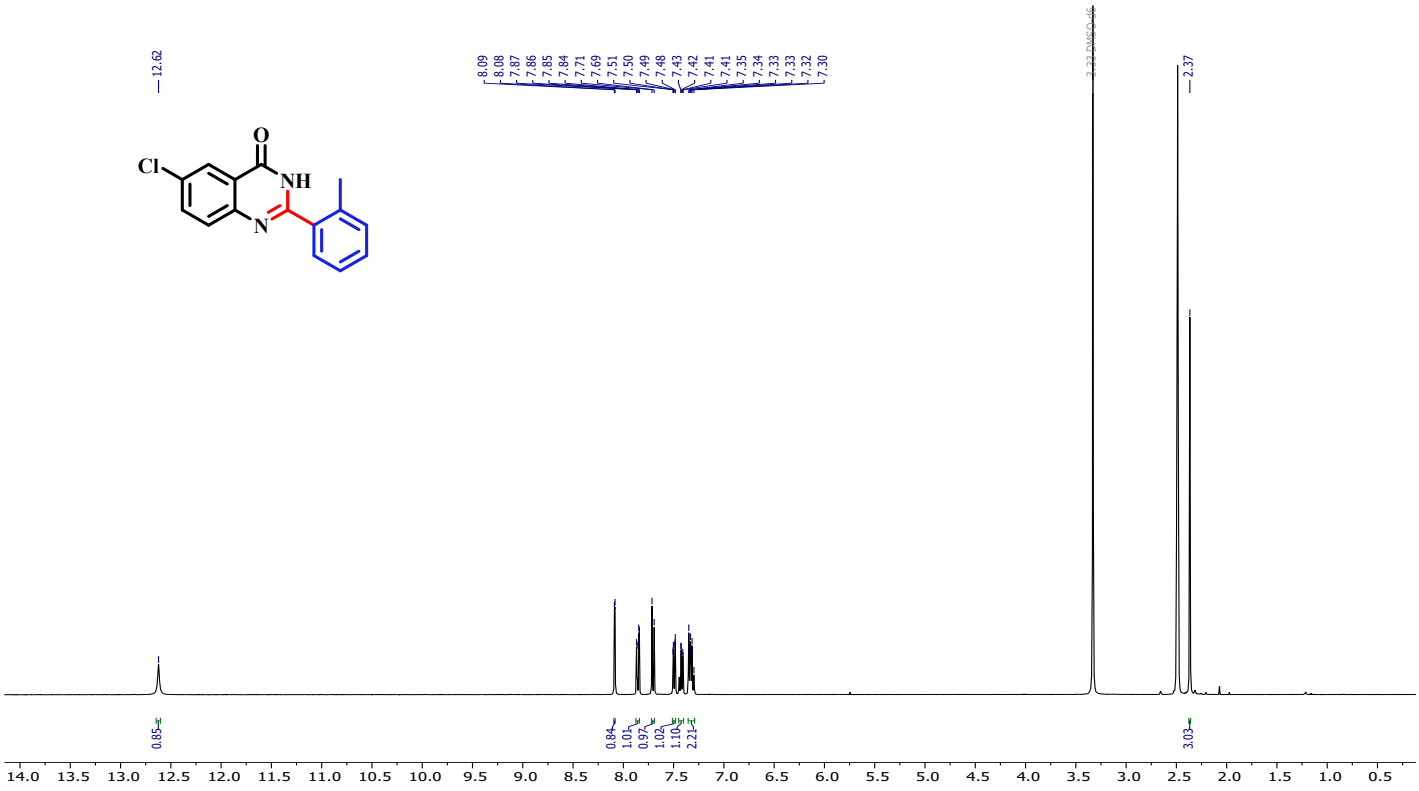


Figure S79. ^{1}H NMR spectrum (400 MHz) of **7b** in DMSO-d_6

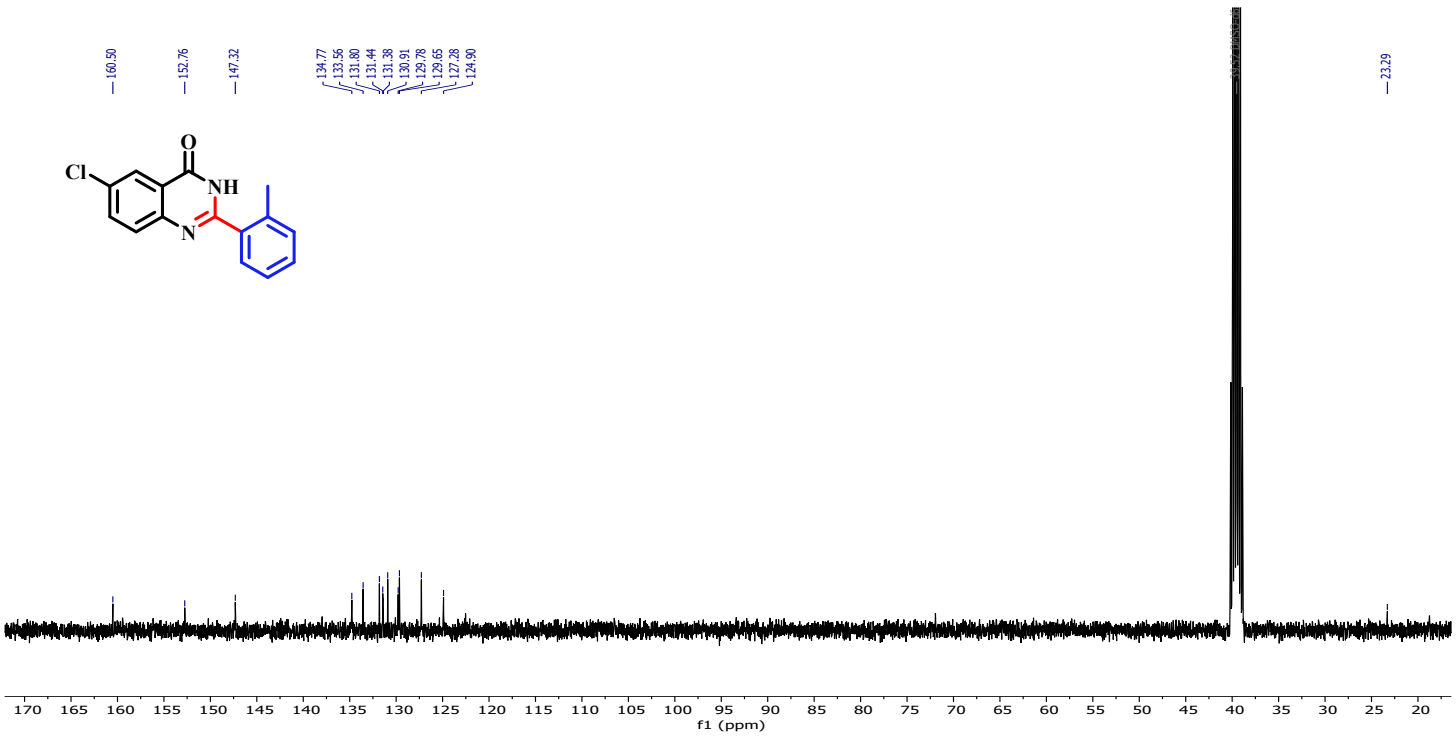


Figure S80. ^{13}C NMR spectrum (100 MHz) of **7b** in DMSO-d_6

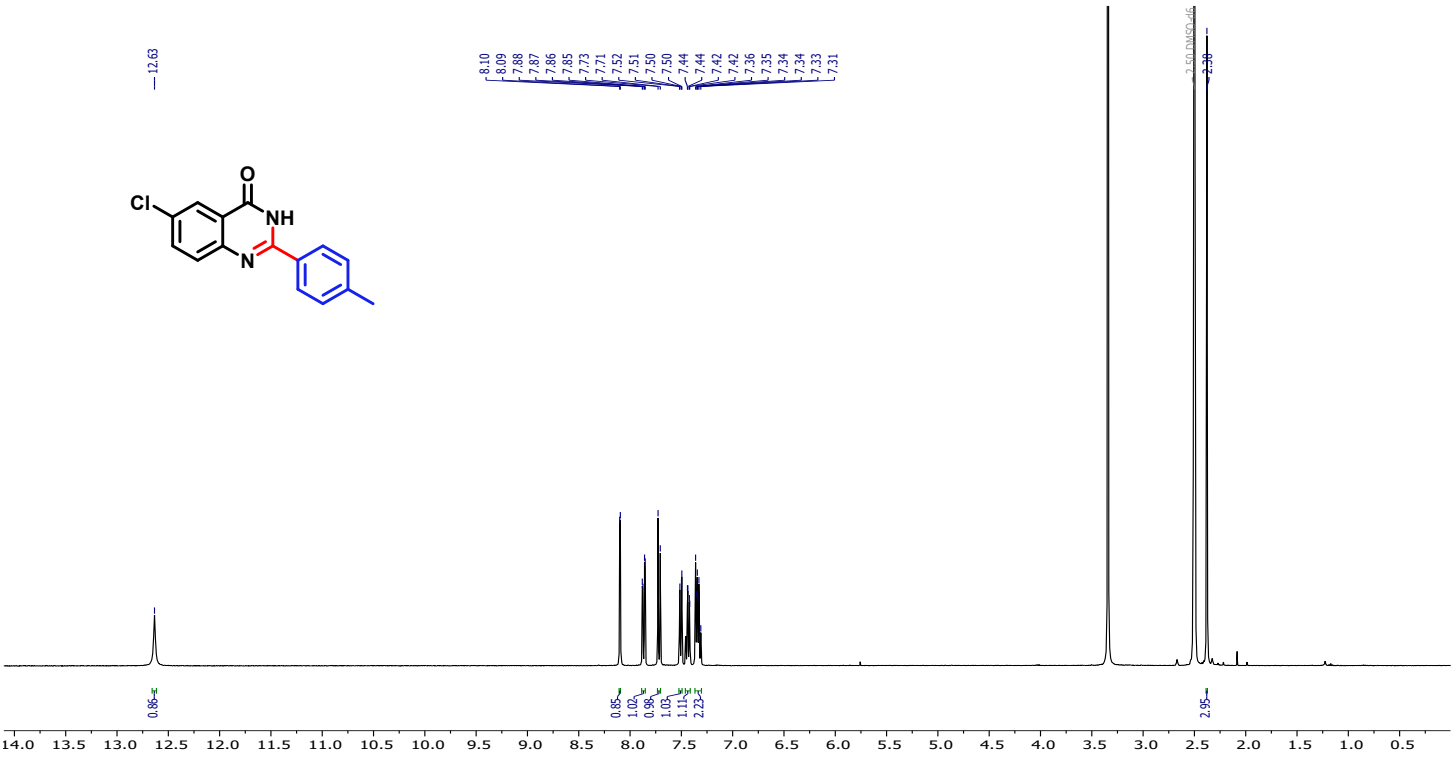


Figure S81. ^{1}H NMR spectrum (400 MHz) of **7c** in DMSO-d_6

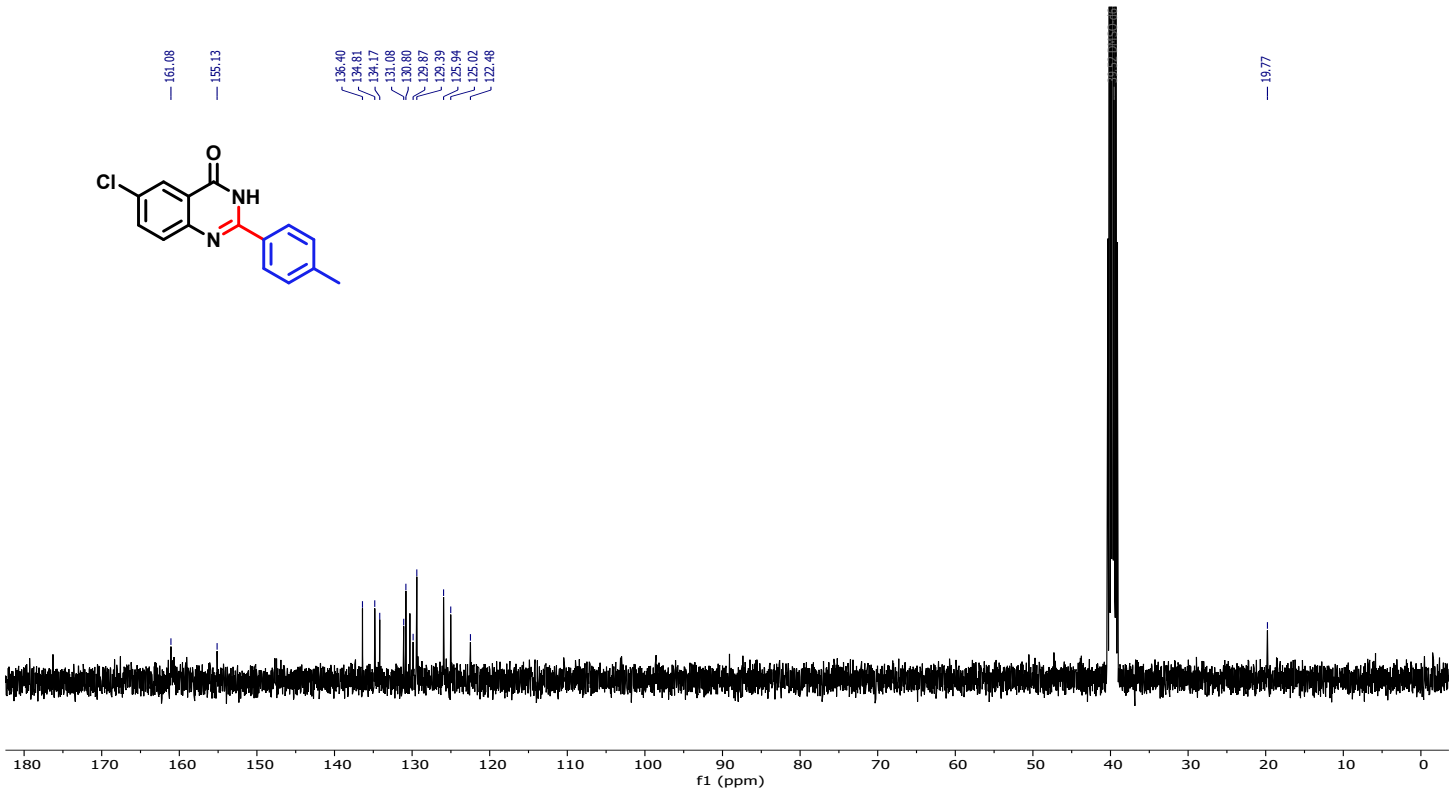


Figure S82. ^{13}C NMR spectrum (100 MHz) of **7c** in DMSO-d_6

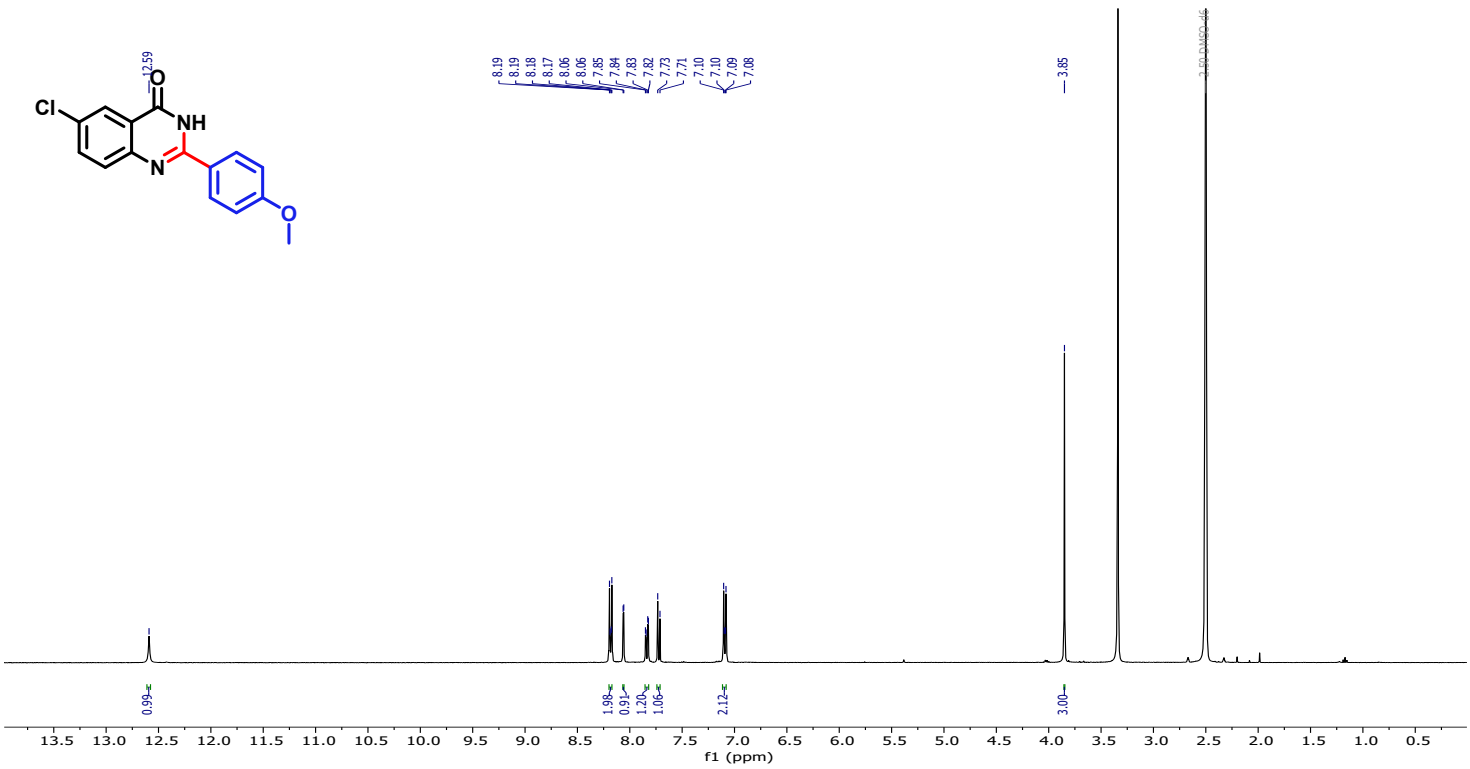


Figure S83. ^{1}H NMR spectrum (400 MHz) of **7d** in DMSO-d_6

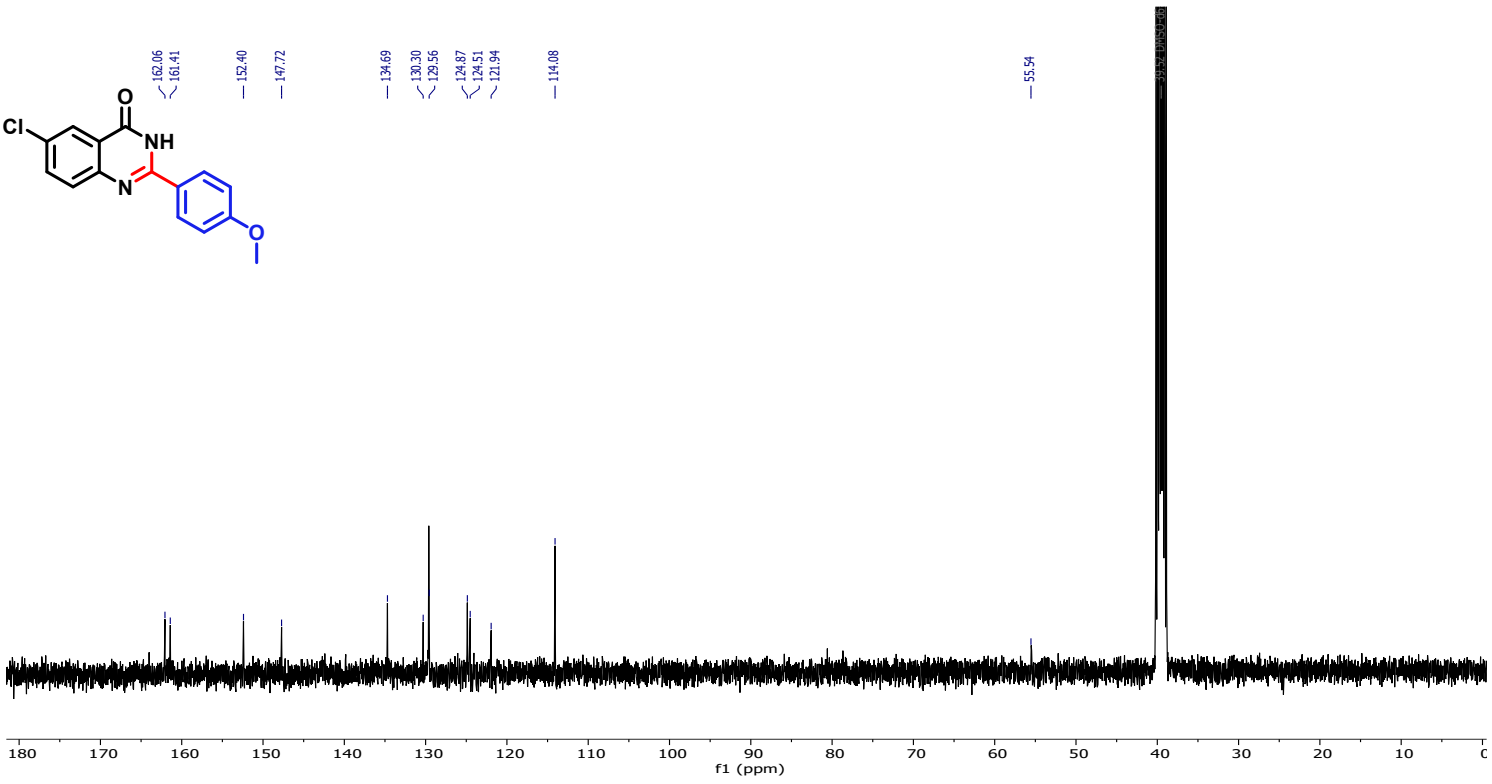


Figure S84. ^{13}C NMR spectrum (100 MHz) of **7d** in DMSO-d_6

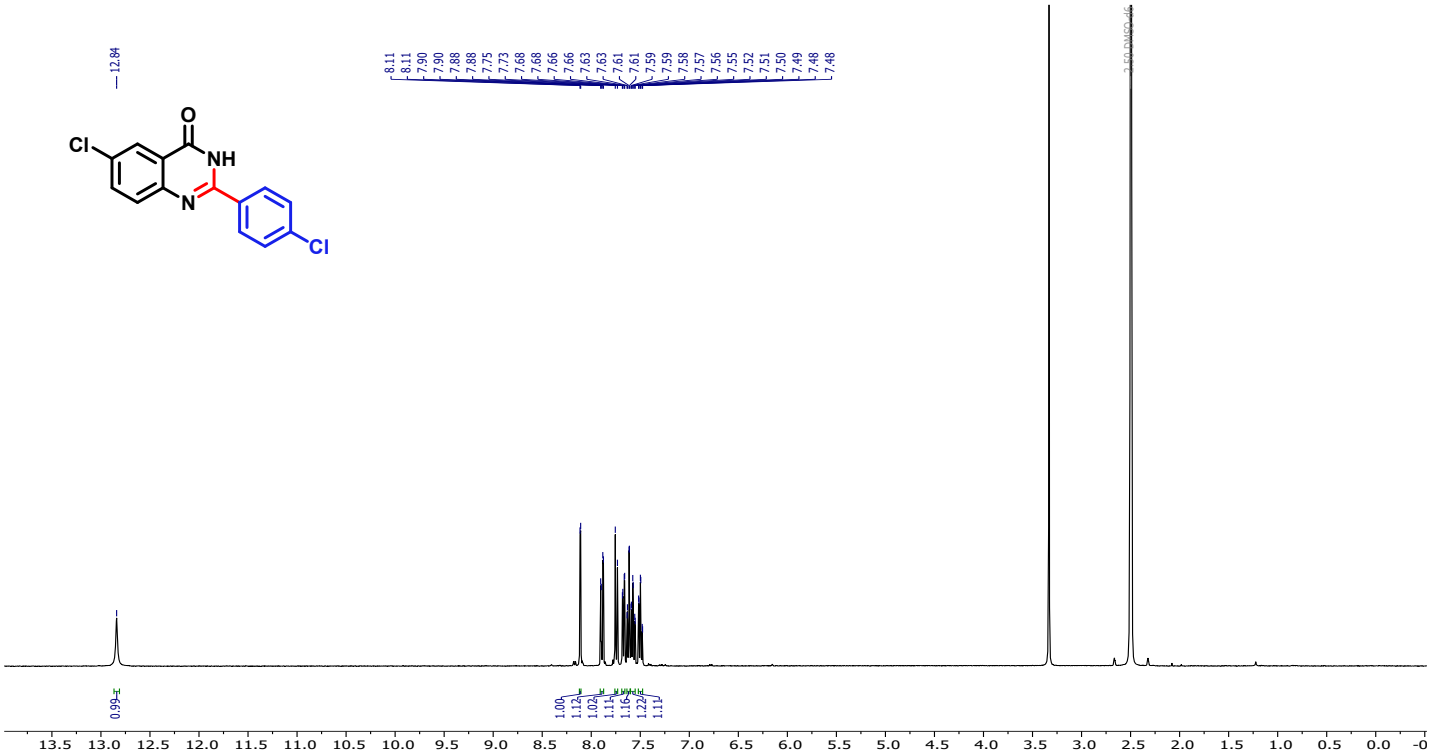


Figure S85. ^{1}H NMR spectrum (400 MHz) of **7e** in DMSO-d_6

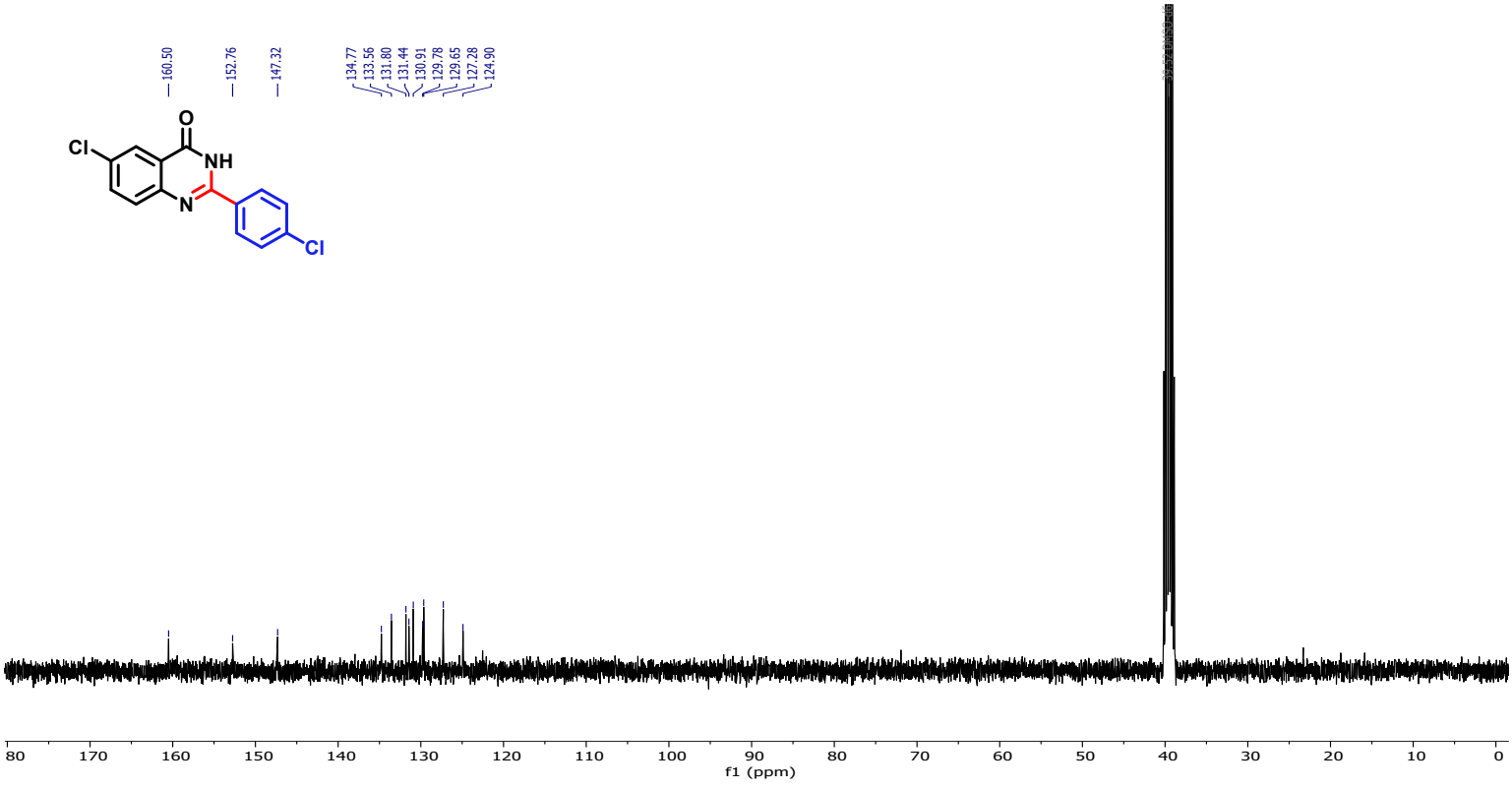


Figure S86. ^{13}C NMR spectrum (100 MHz) of **7e** in DMSO-d_6

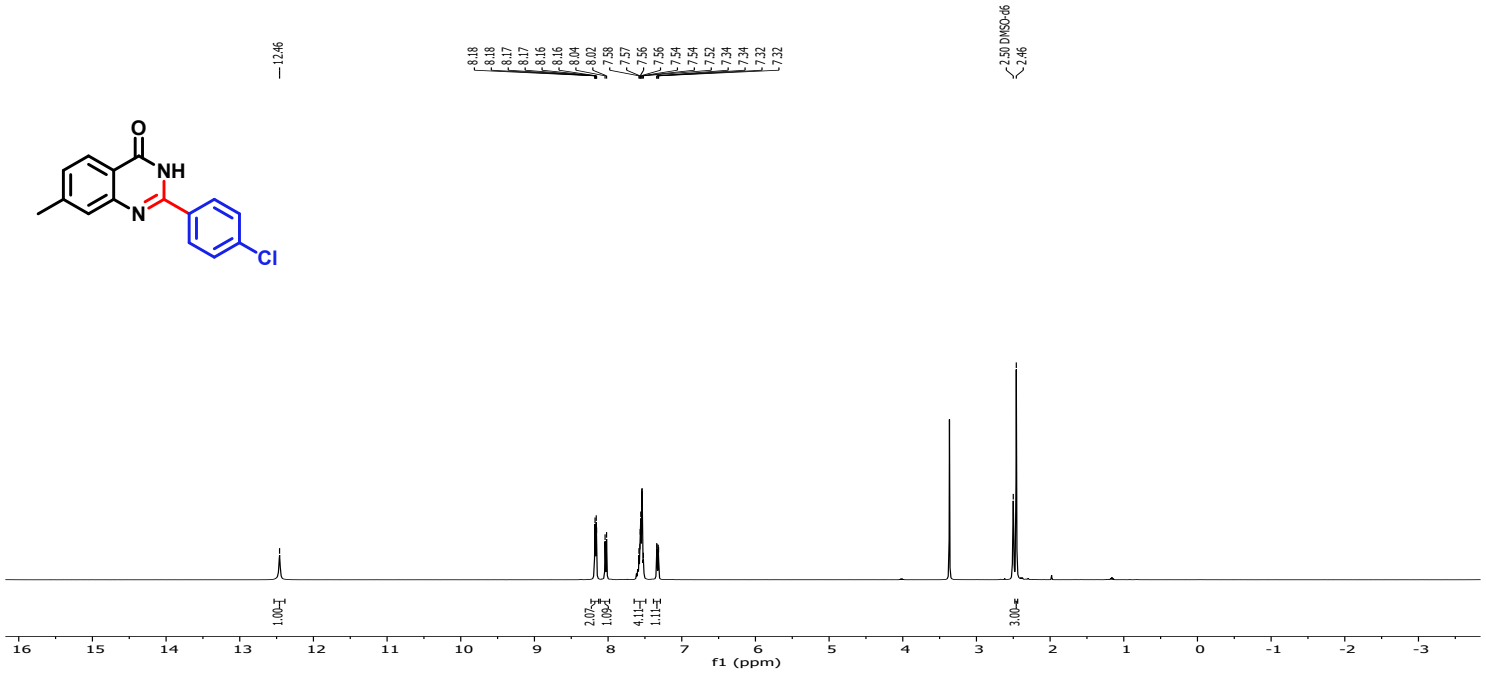


Figure S87. ^{1}H NMR spectrum (400 MHz) of **8a** in DMSO-d_6

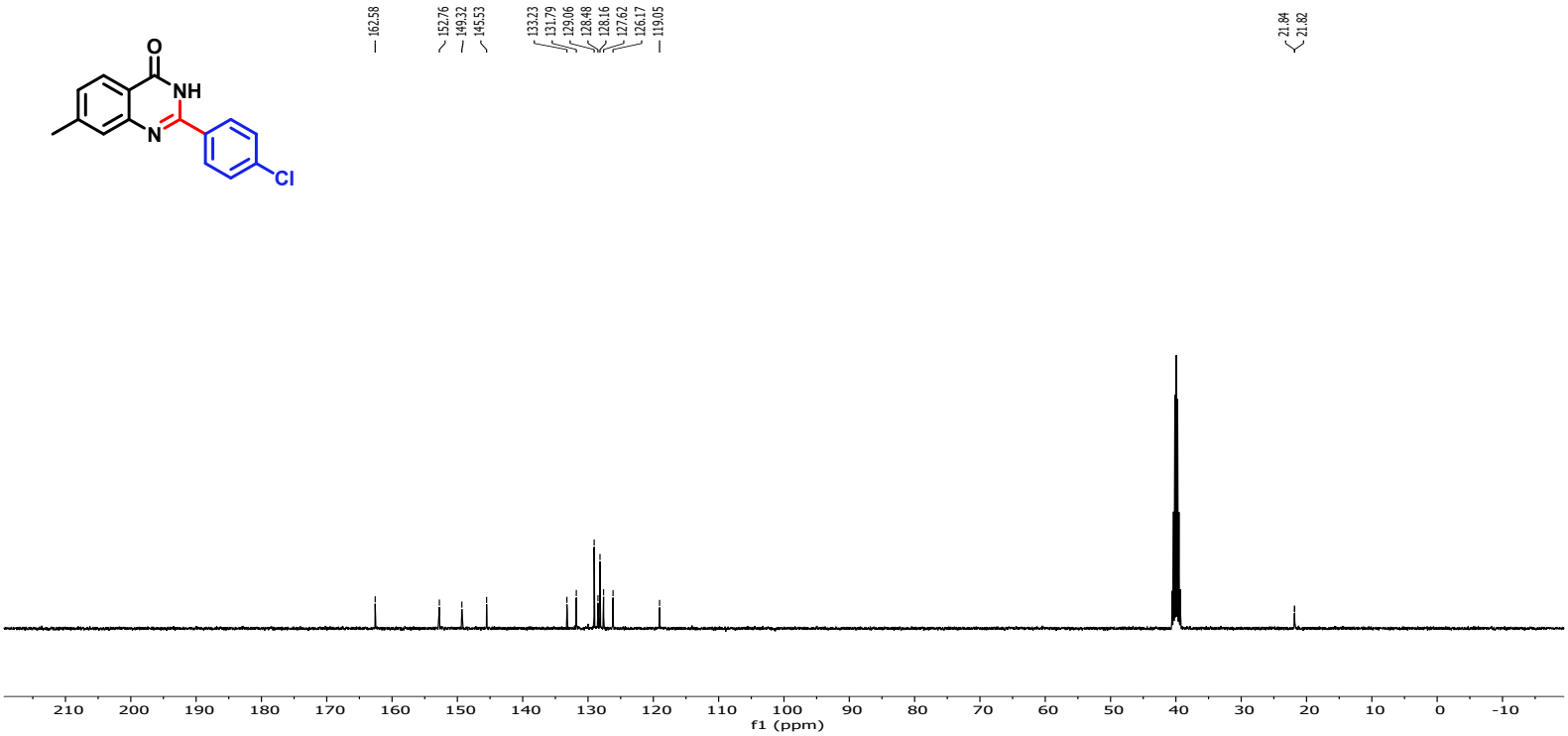


Figure S88. ^{13}C NMR spectrum (100 MHz) of **8a** in DMSO-d_6

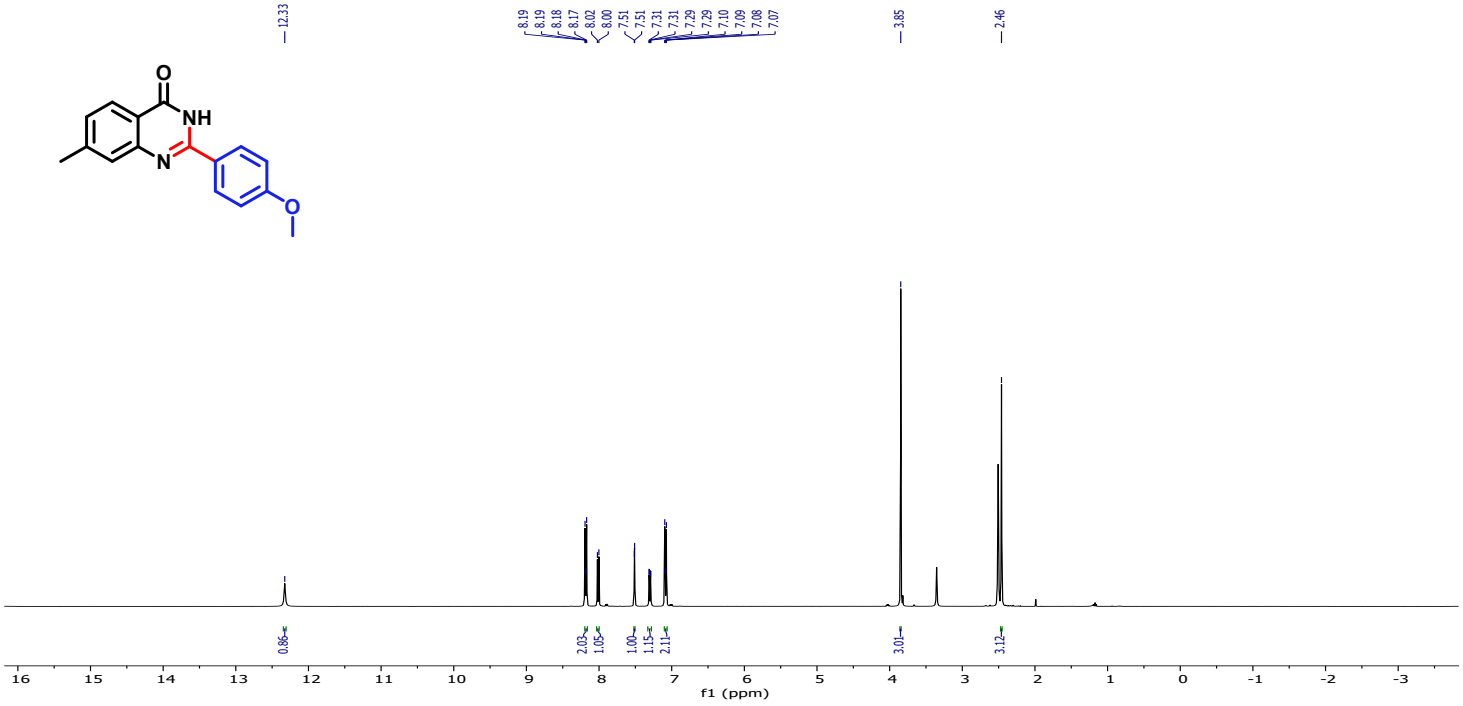


Figure S89. ^{1}H NMR spectrum (400 MHz) of **8b** in DMSO-d_6

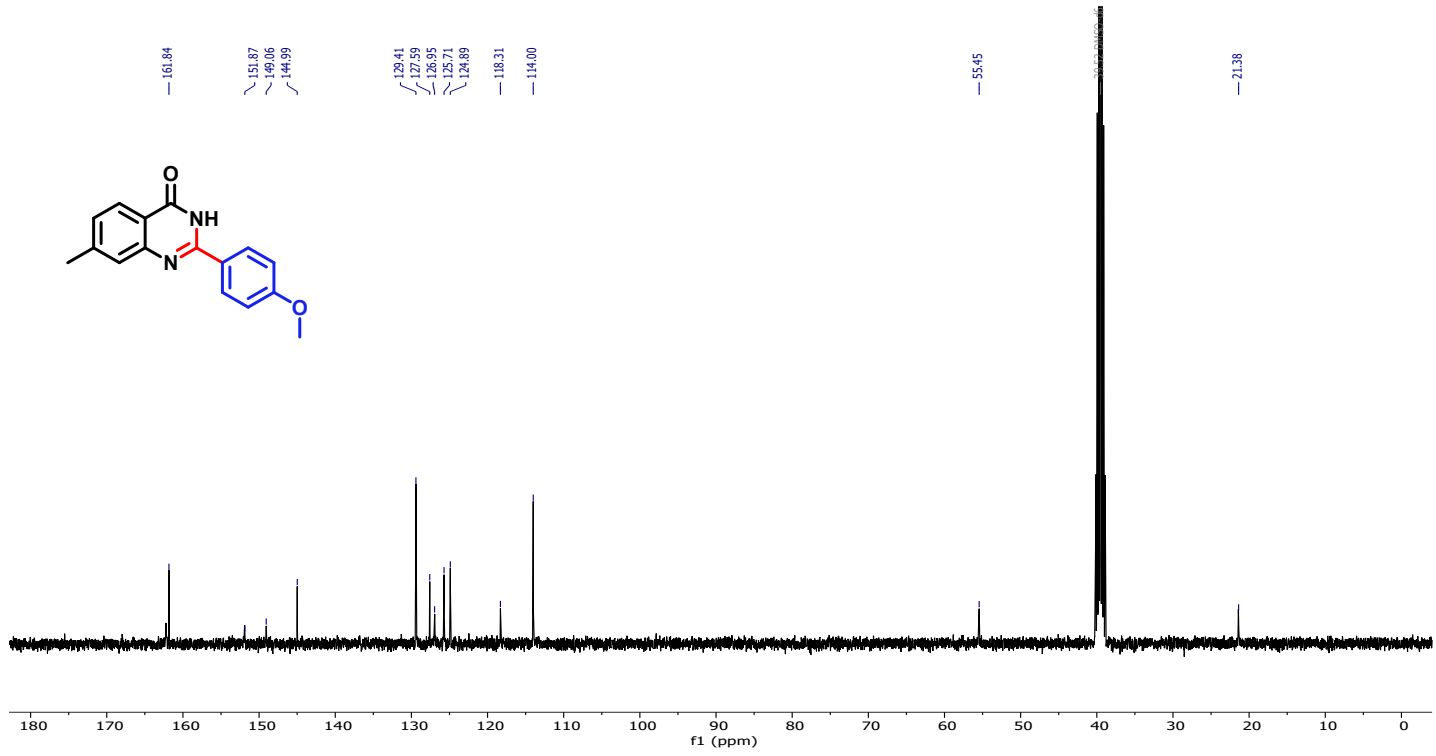


Figure S90. ^{13}C NMR spectrum (100 MHz) of **8b** in DMSO-d_6

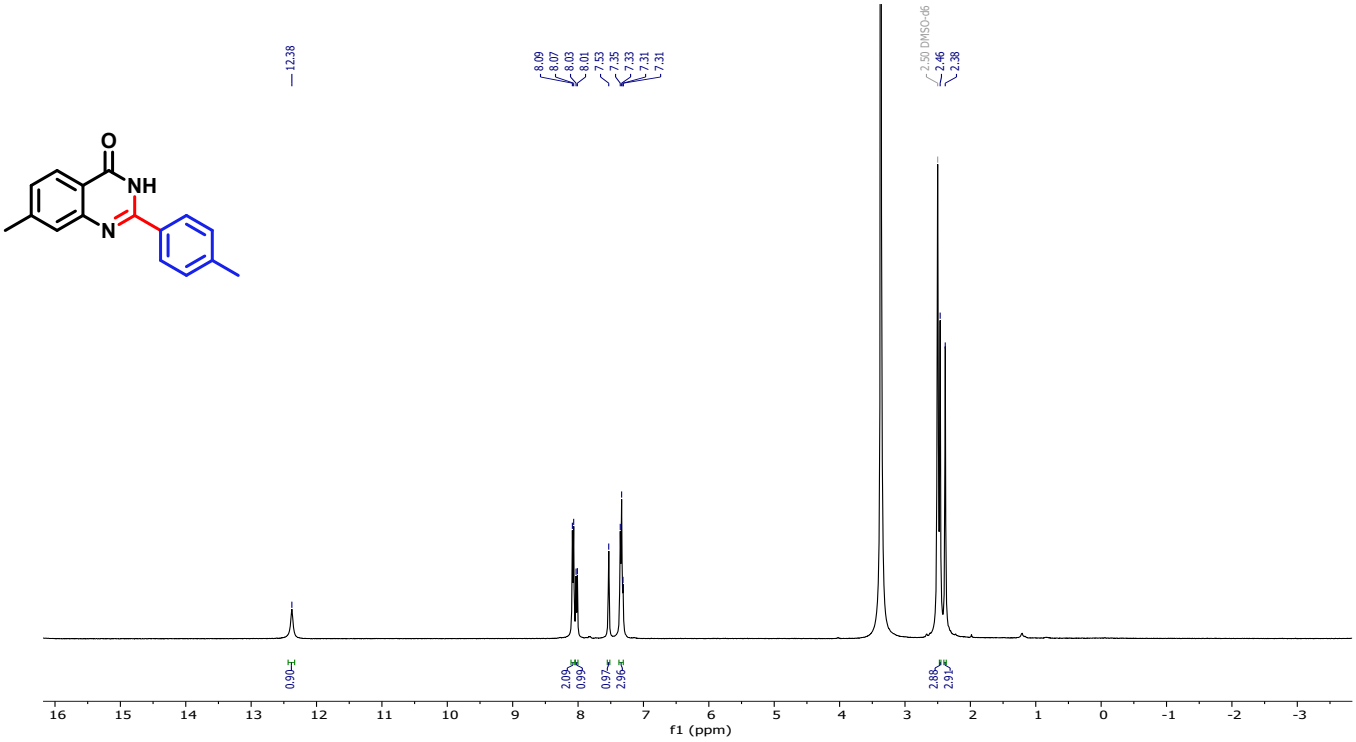


Figure S91. ^{1}H NMR spectrum (400 MHz) of **8c** in DMSO-d_6

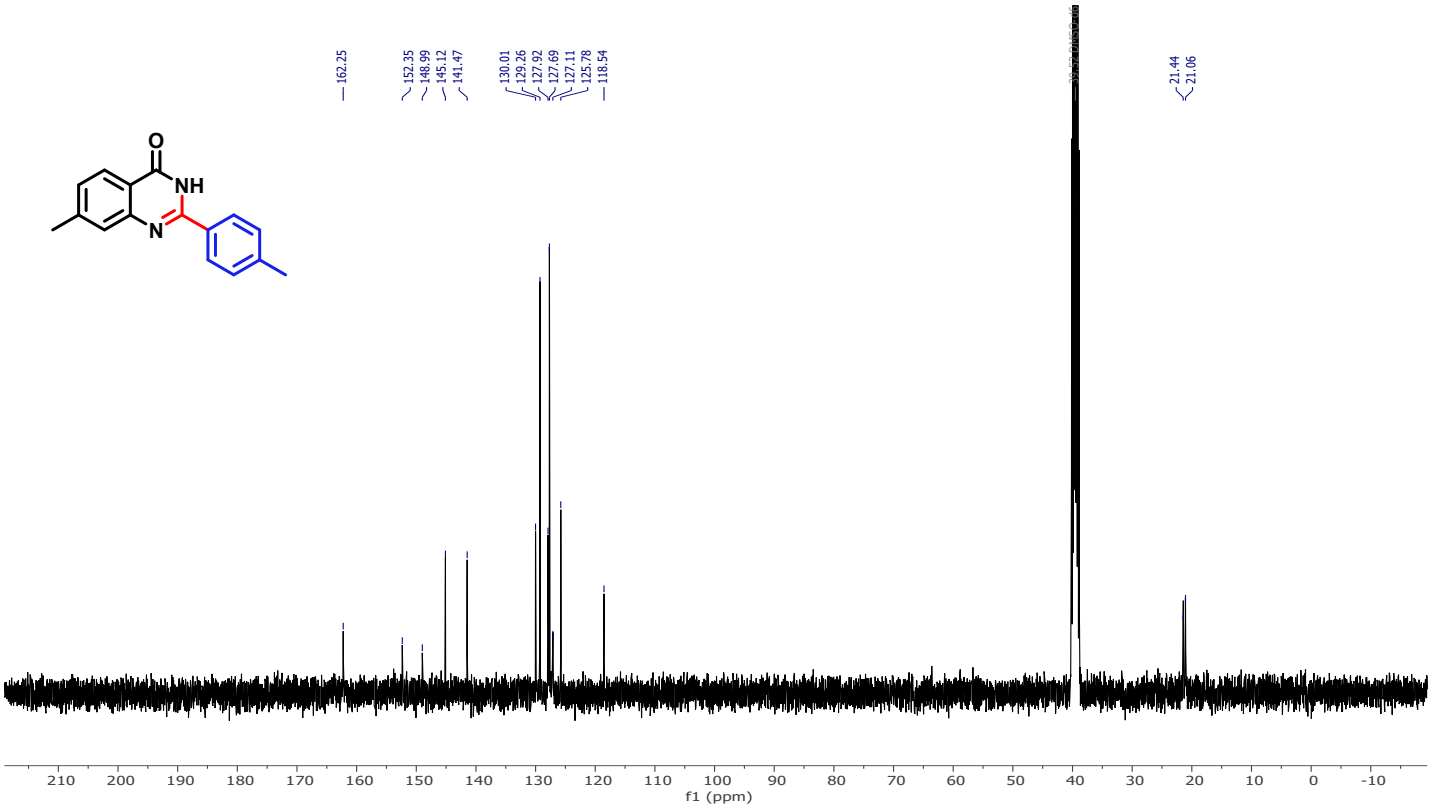


Figure S92. ^{13}C NMR spectrum (100 MHz) of **8c** in DMSO-d_6

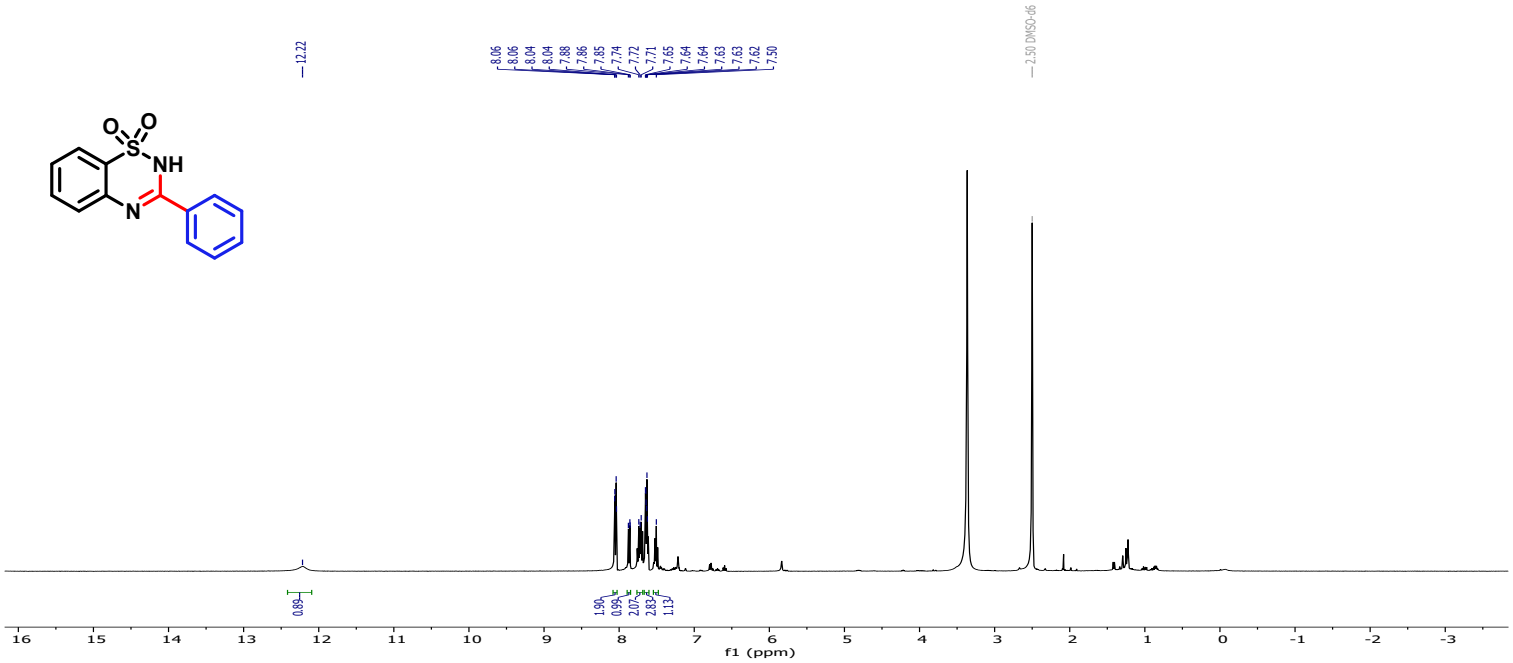


Figure S93. ^{1}H NMR spectrum (400 MHz) of **9a** in DMSO-d_6

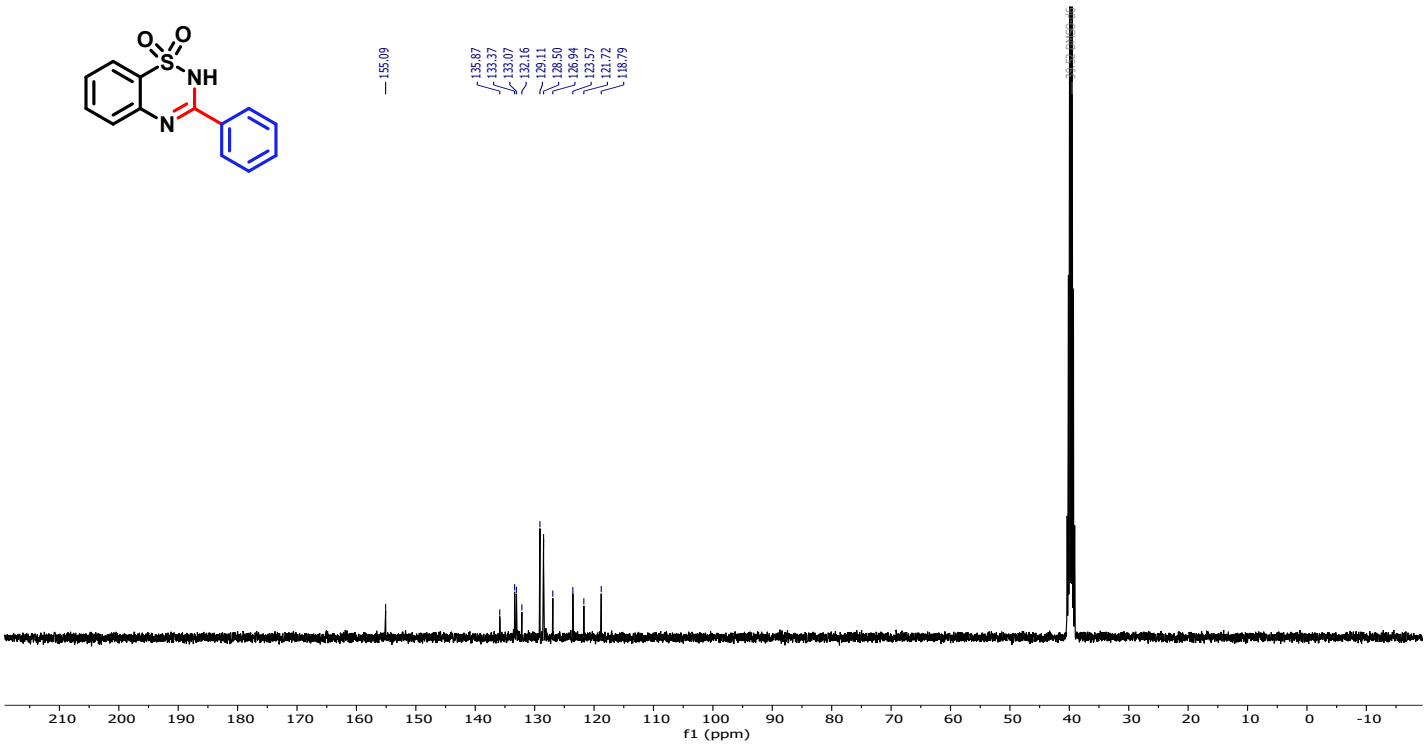


Figure S94. ^{13}C NMR spectrum (100 MHz) of **9a** in DMSO-d_6

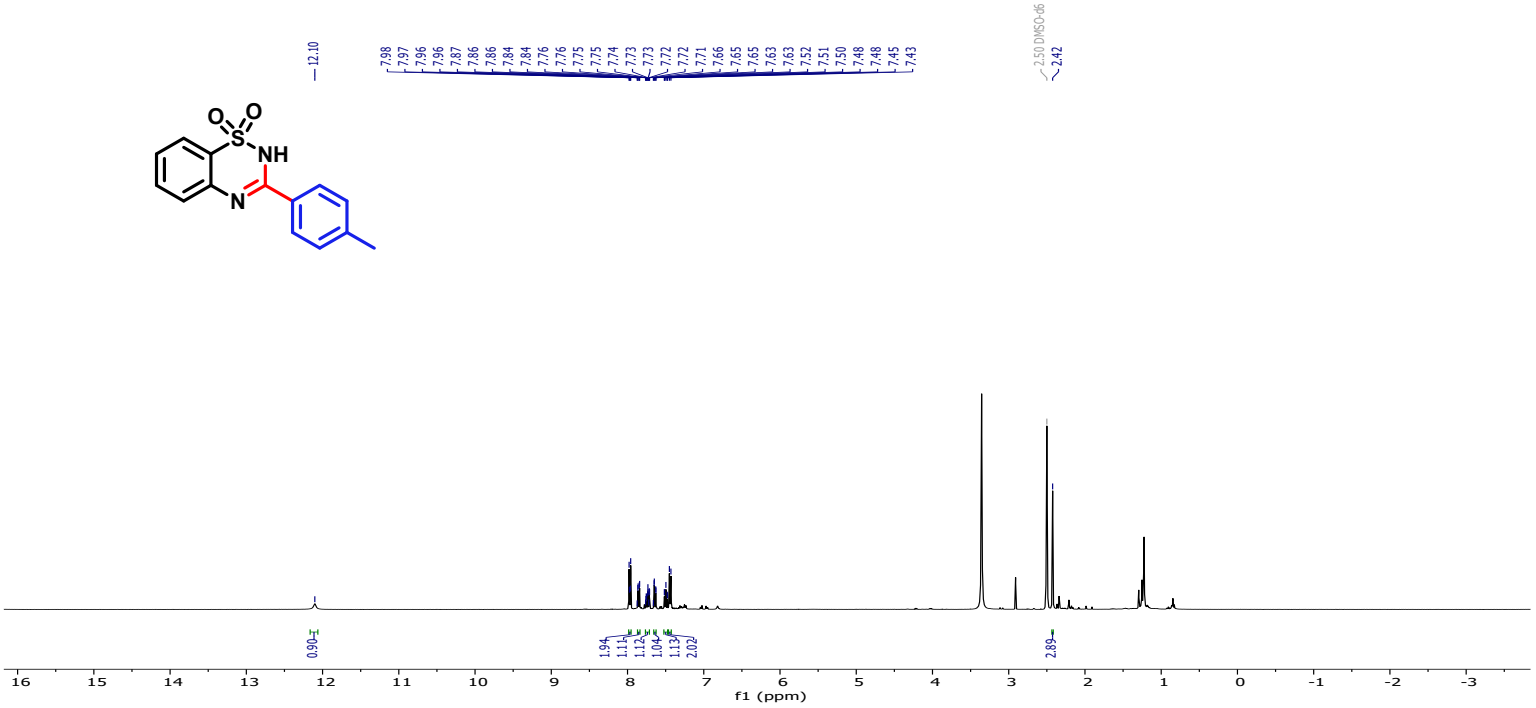


Figure S95. ^{1}H NMR spectrum (400 MHz) of **9b** in DMSO-d_6

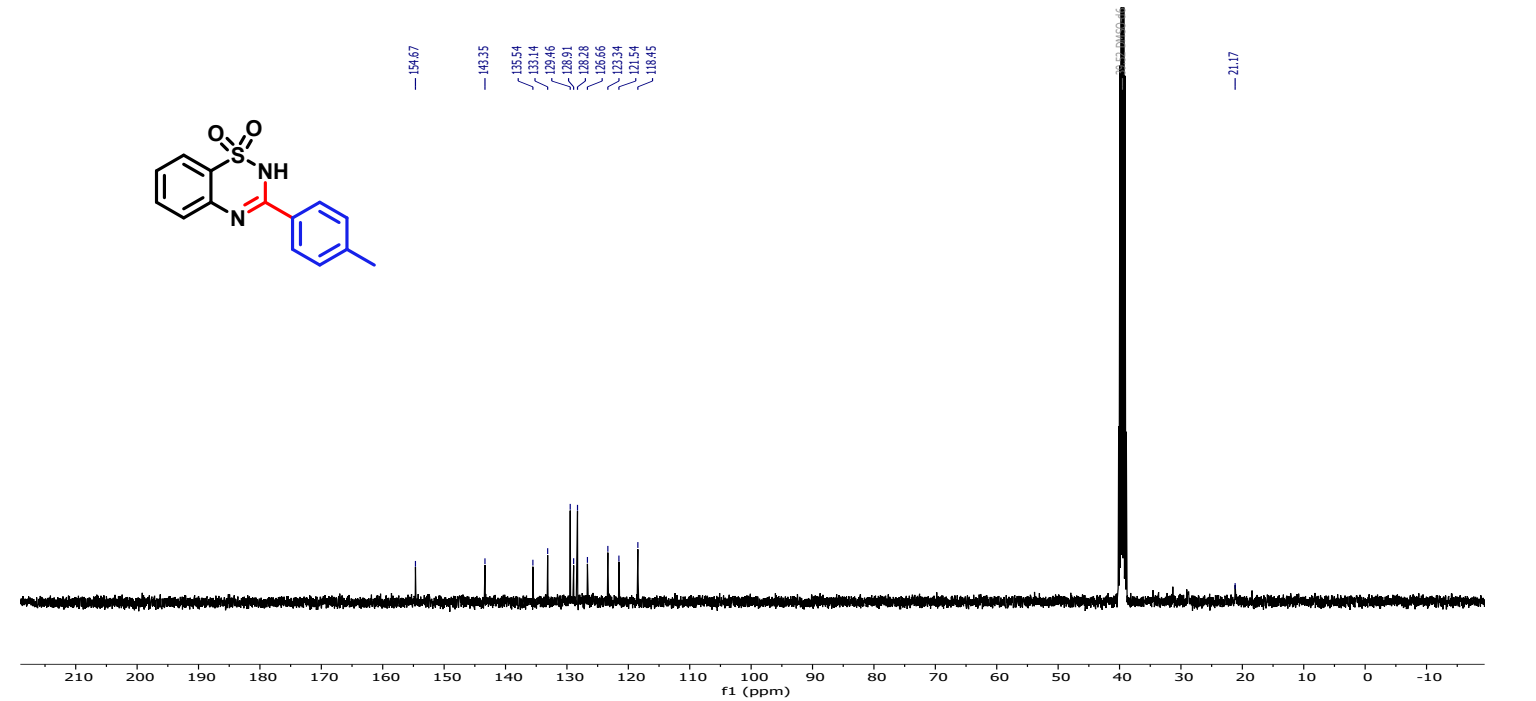


Figure S96. ^{13}C NMR spectrum (100 MHz) of **9b** in DMSO-d_6

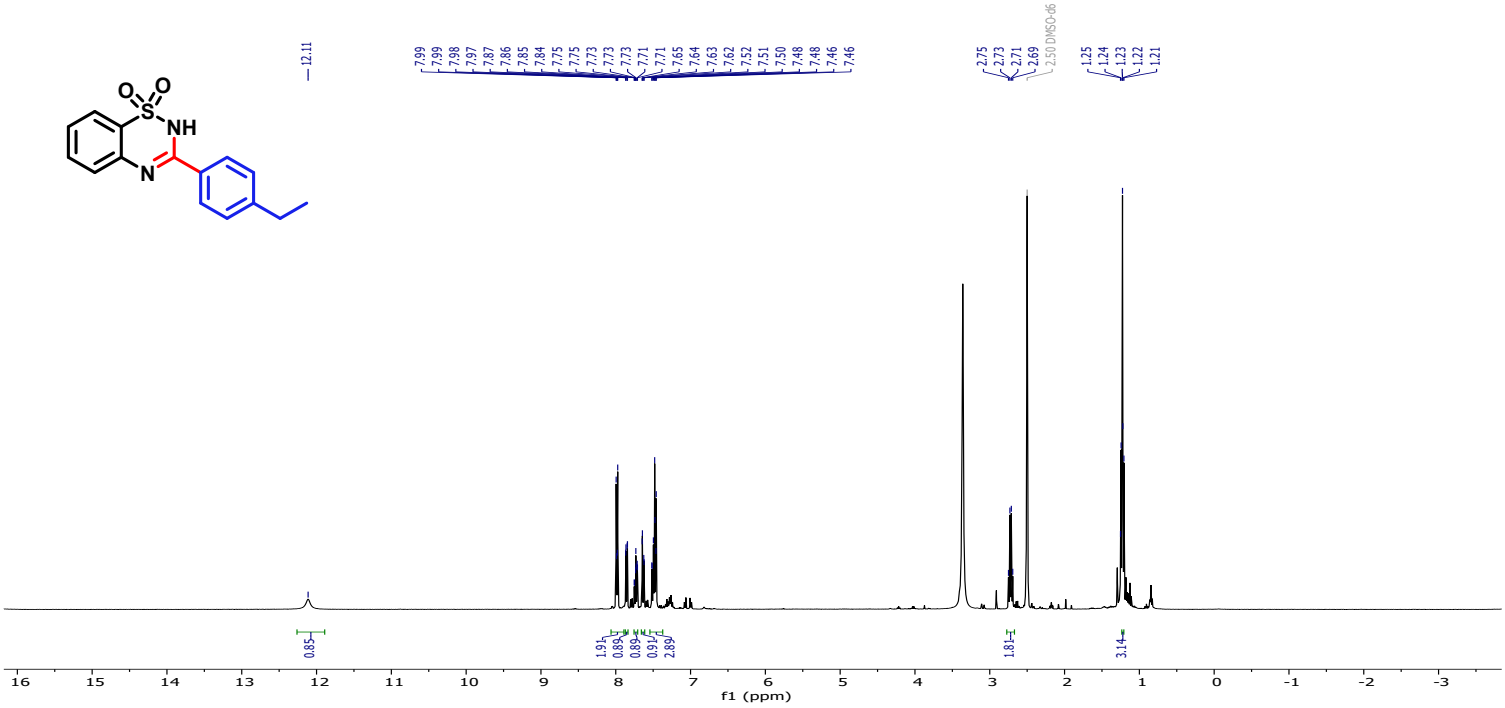


Figure S97. ^{1}H NMR spectrum (400 MHz) of **9c** in DMSO-d_6

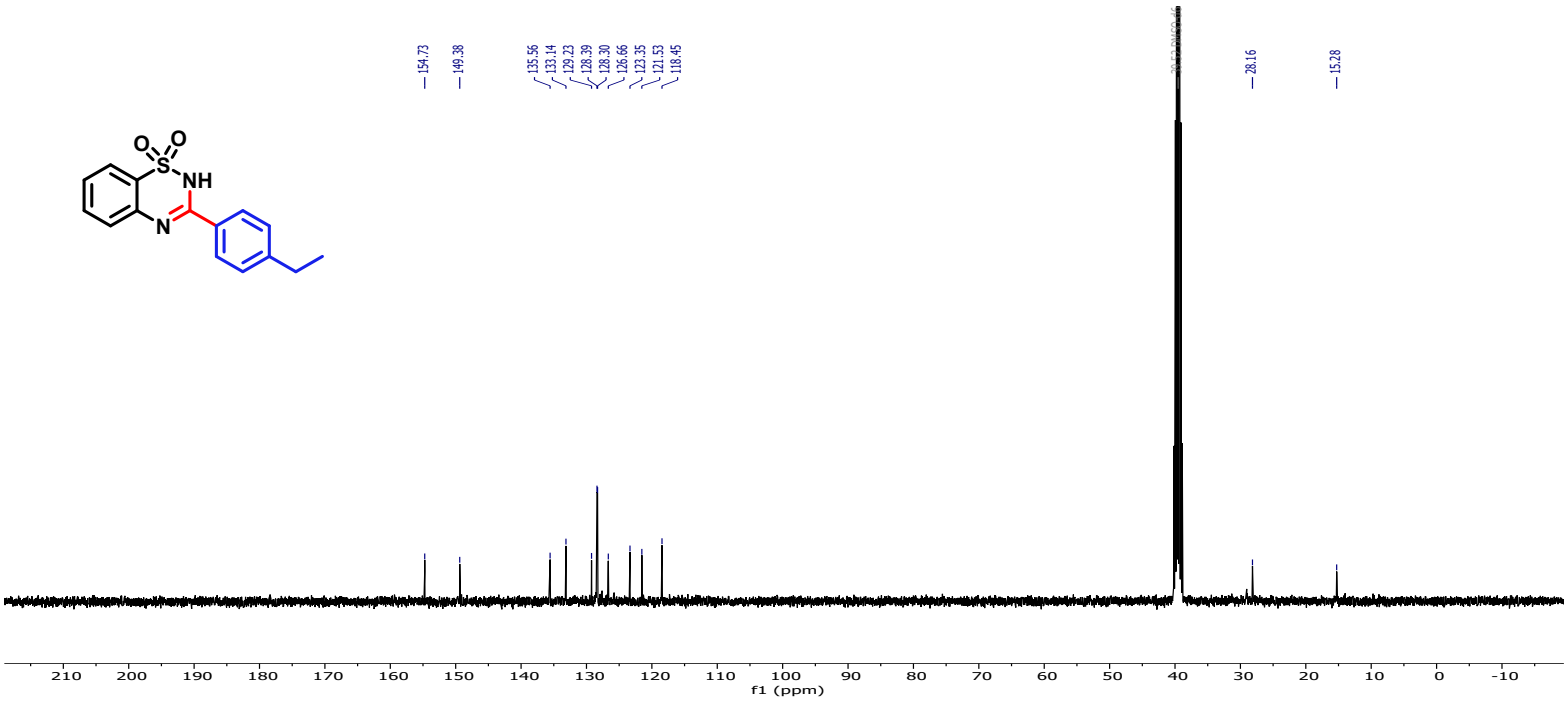


Figure S98. ^{13}C NMR spectrum (100 MHz) of **9c** in DMSO-d6

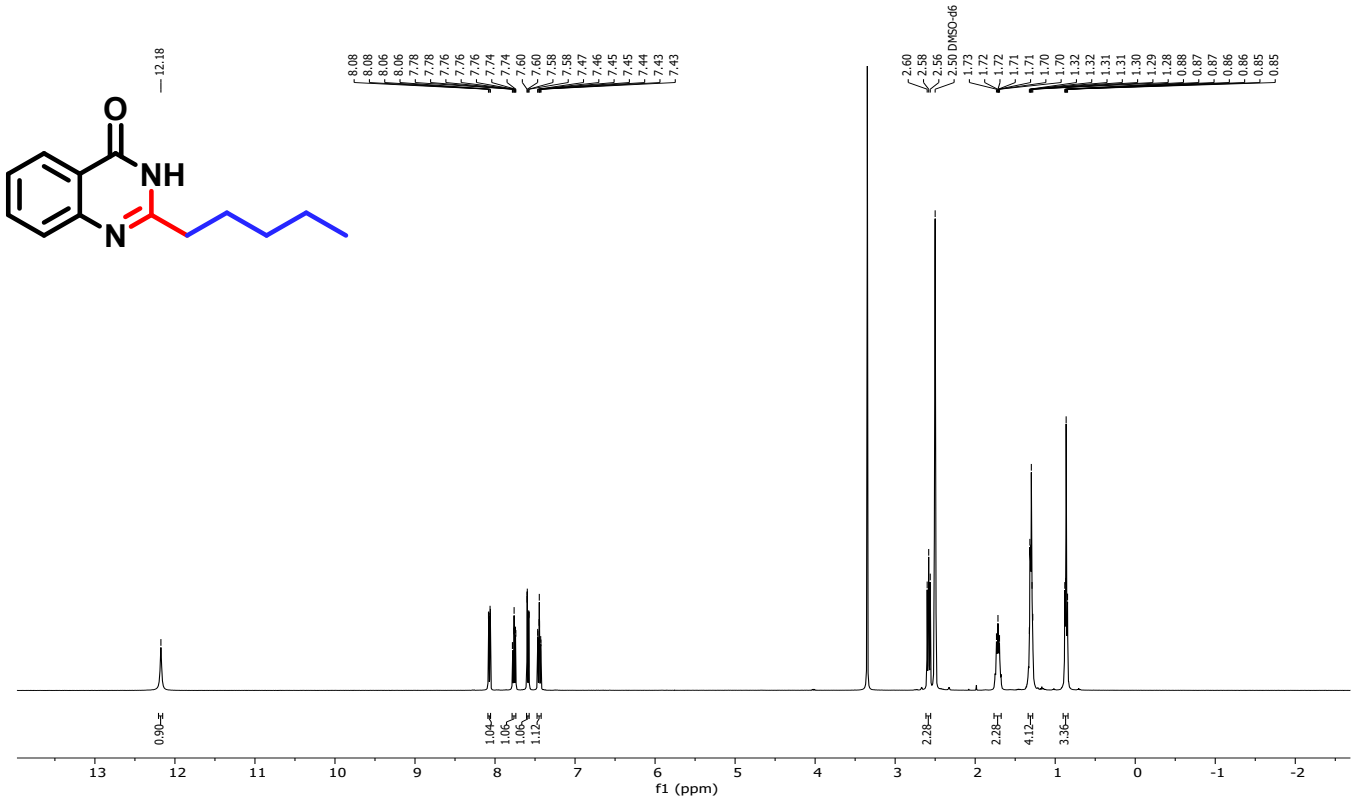


Figure S99. ^{1}H NMR spectrum (400 MHz) of **10a** in DMSO-d_6

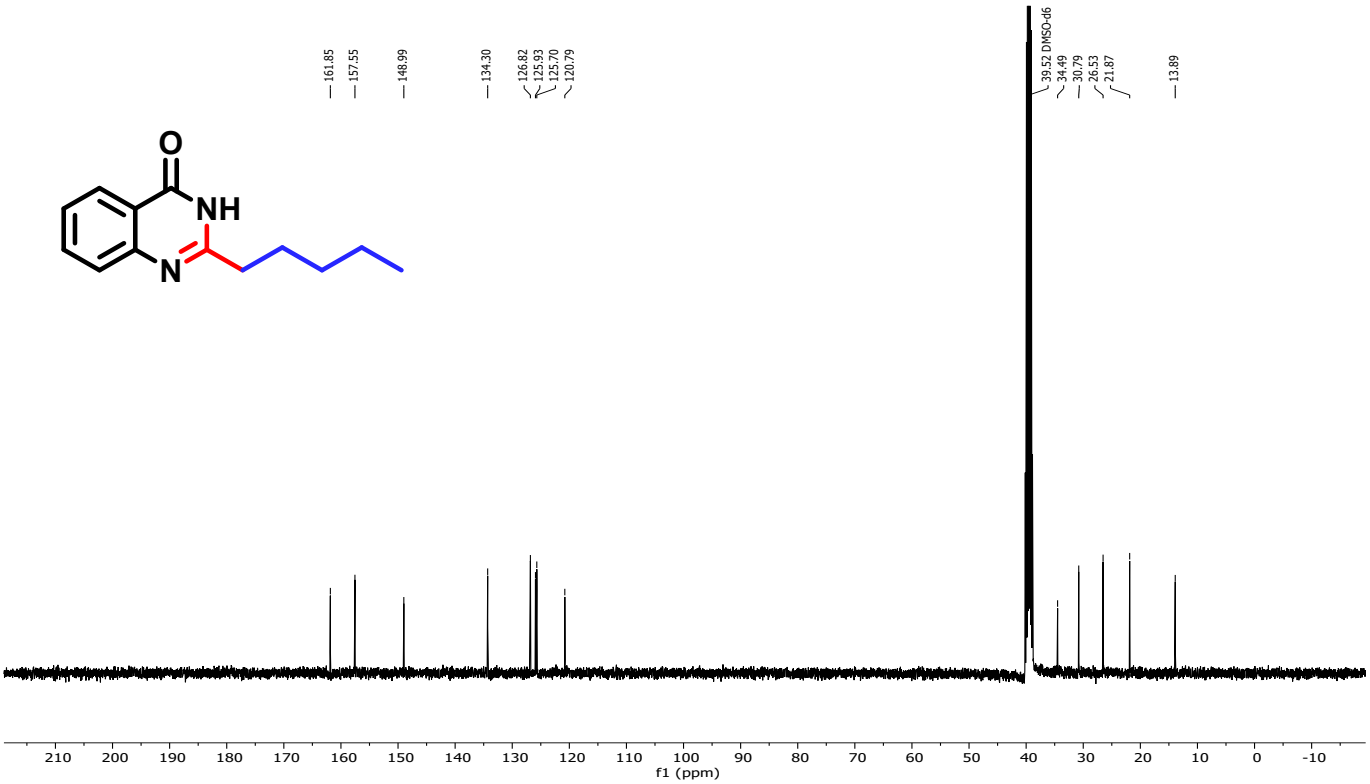


Figure S100. ^{13}C NMR spectrum (100 MHz) of **10a** in DMSO-d_6

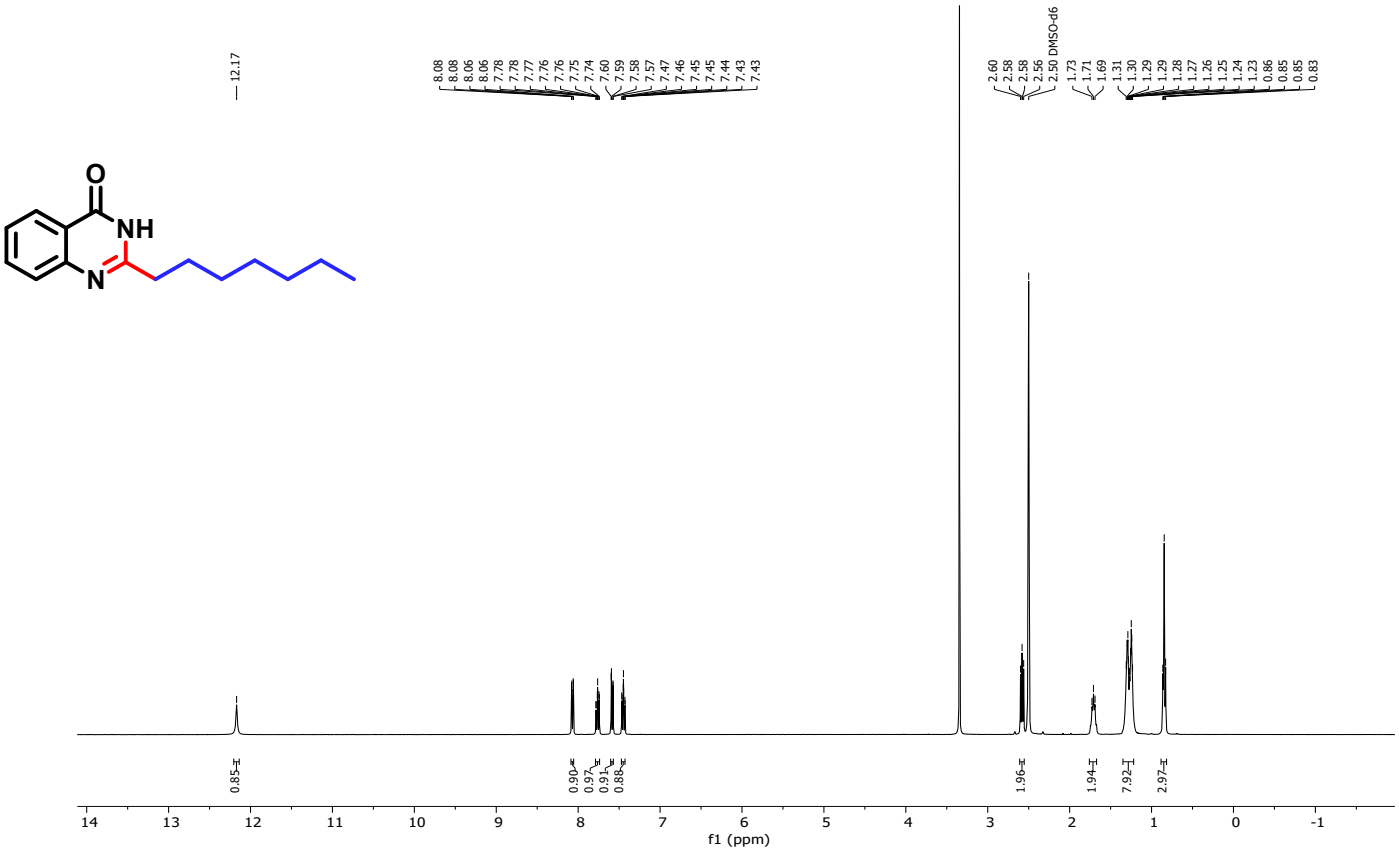


Figure S101. [1]H NMR spectrum (400 MHz) of **10b** in DMSO-d_6

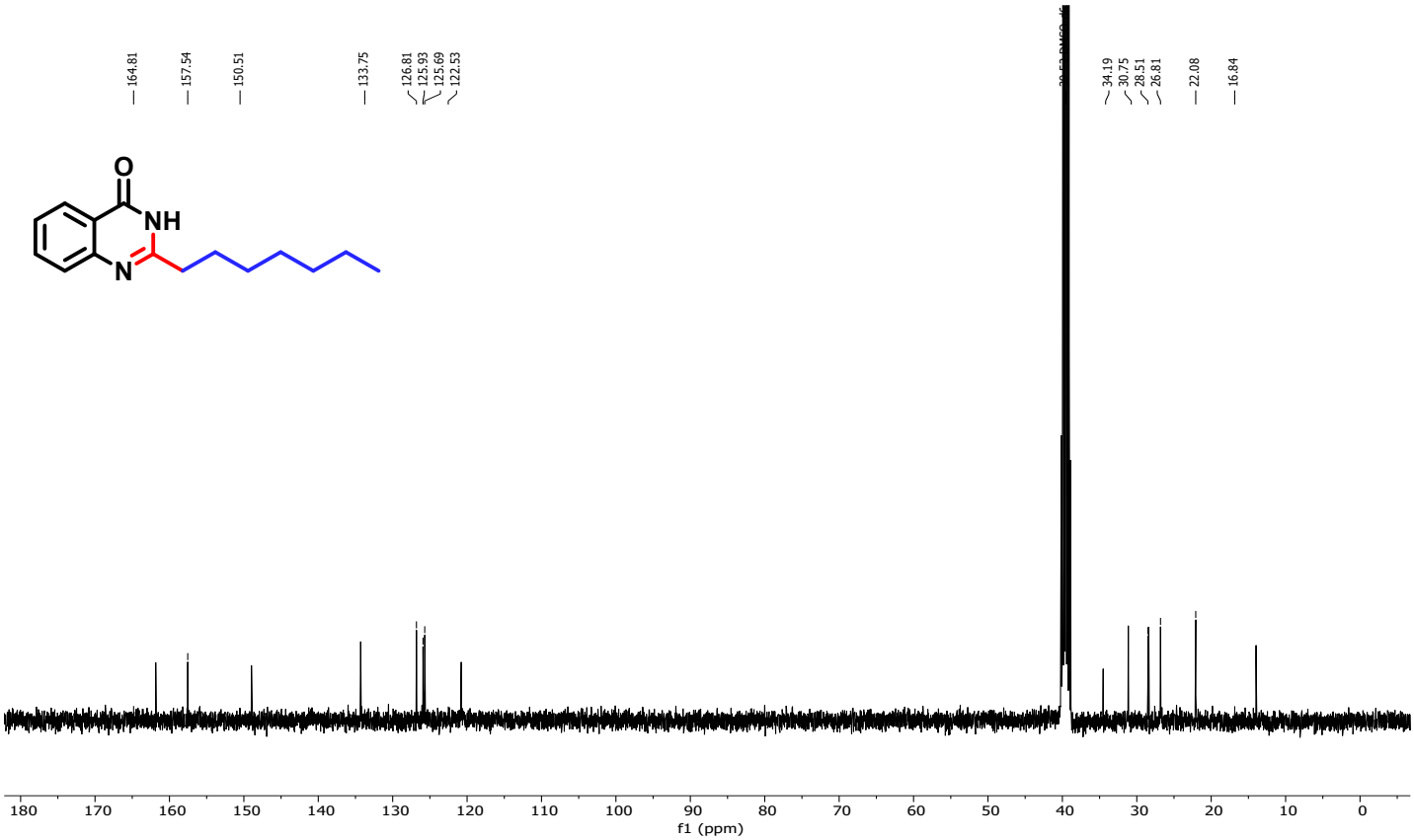


Figure S102. [13]C NMR spectrum (100 MHz) of **10b** in DMSO-d_6

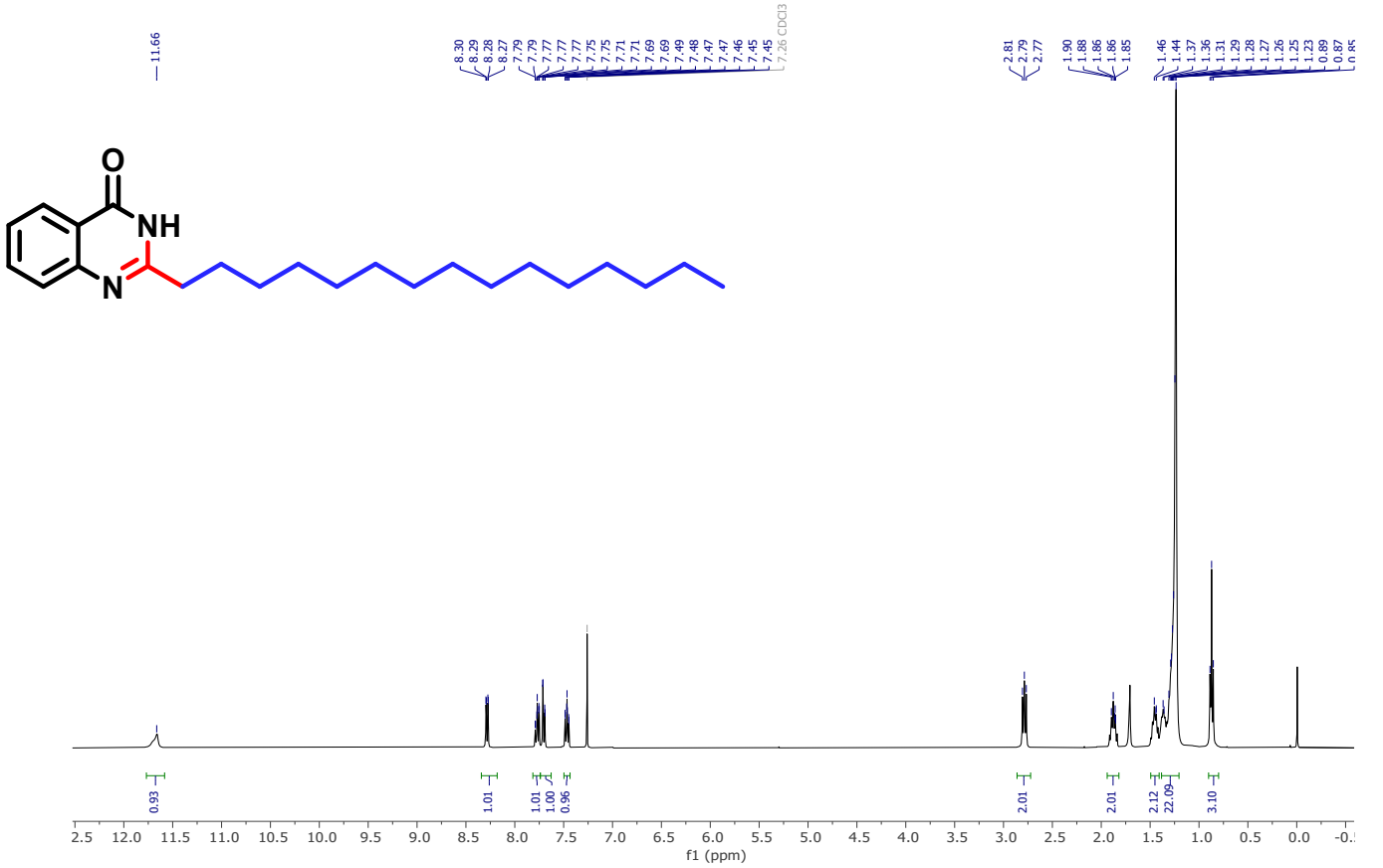


Figure S103. ^{1}H NMR spectrum (400 MHz) of **10c** in DMSO-d_6

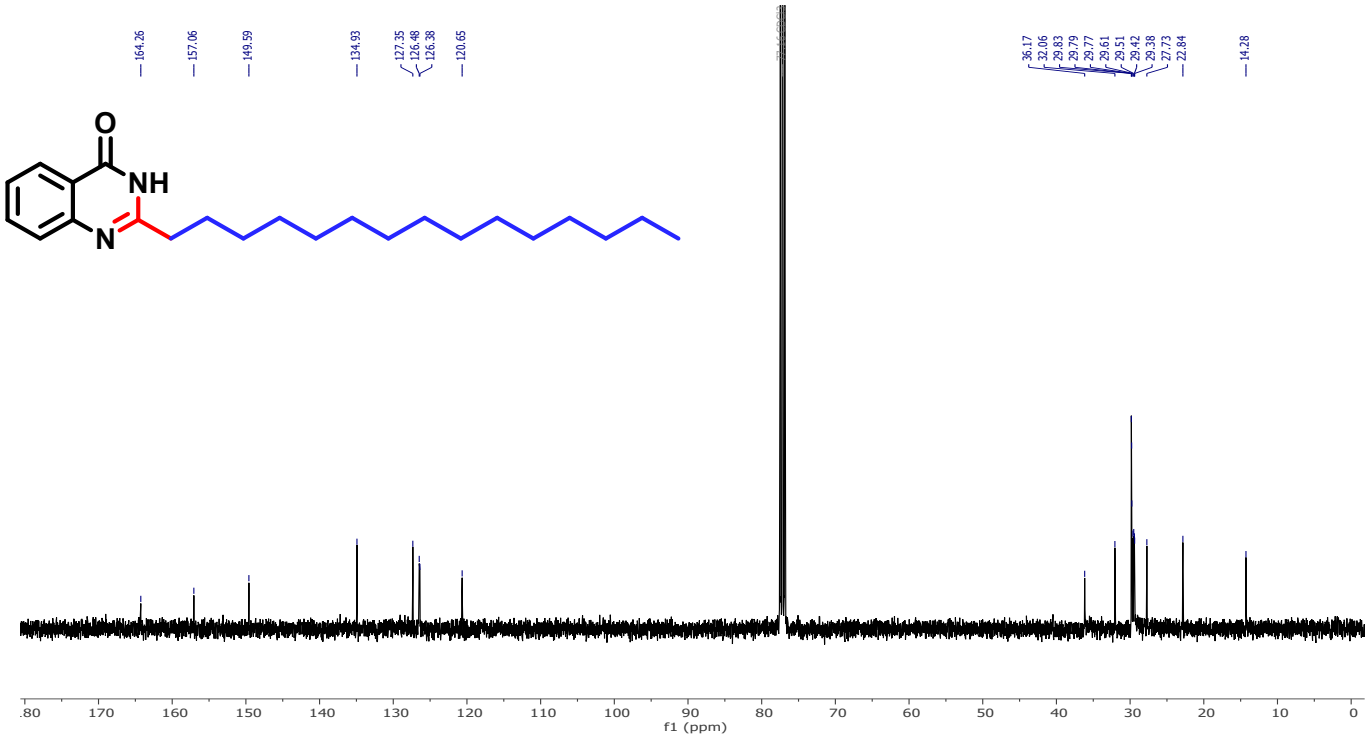


Figure S104. ^{13}C NMR spectrum (100 MHz) of **10c** in DMSO-d_6

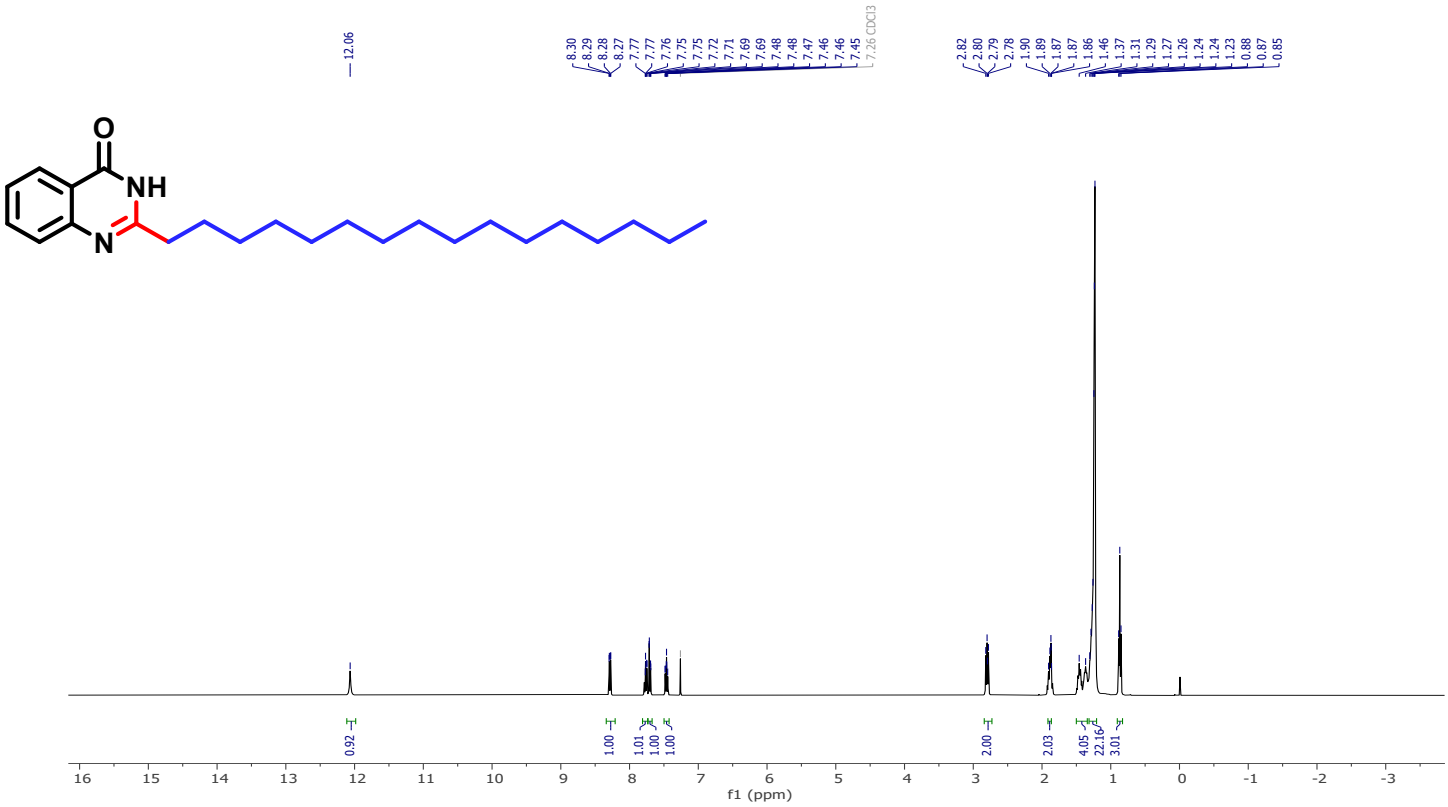


Figure S105. ^{1}H NMR spectrum (400 MHz) of **10d** in DMSO-d_6

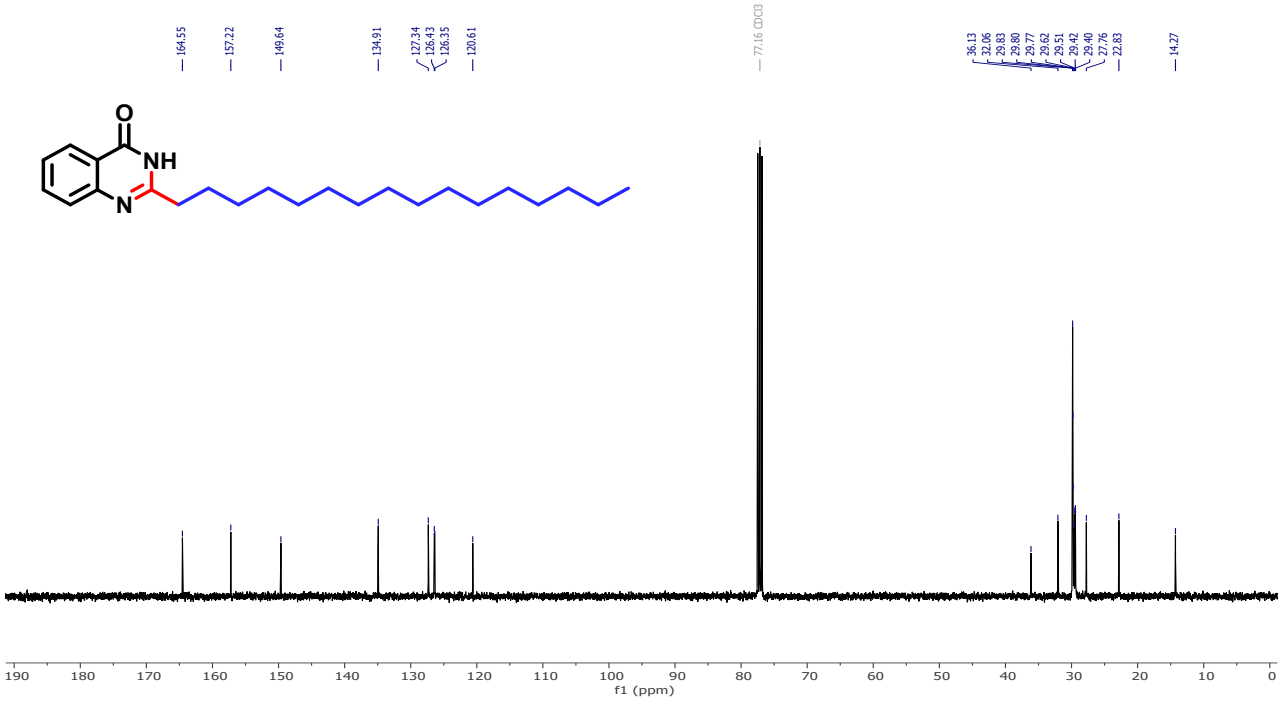


Figure S106. ^{13}C NMR spectrum (100 MHz) of **10d** in DMSO-d_6

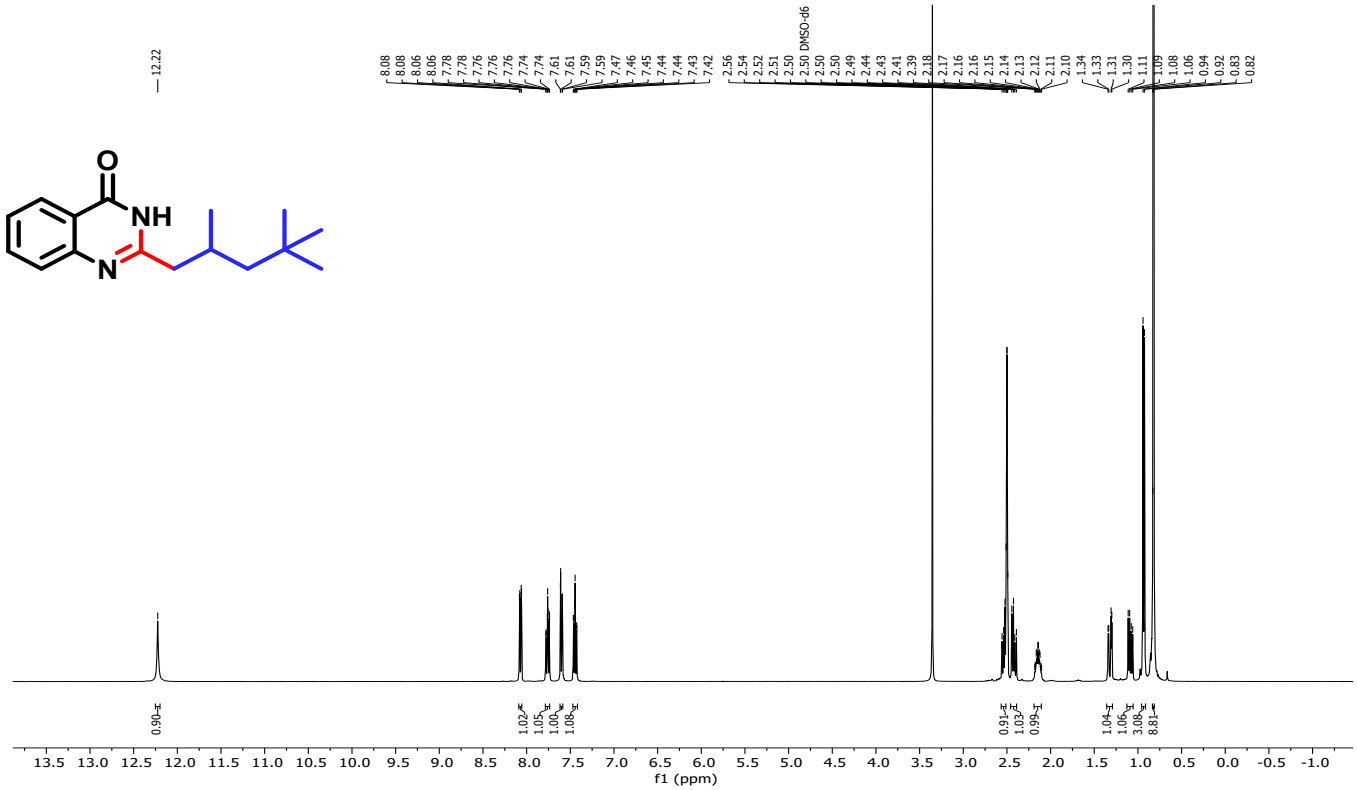


Figure S107. ^{1}H NMR spectrum (400 MHz) of **10e** in DMSO-d_6

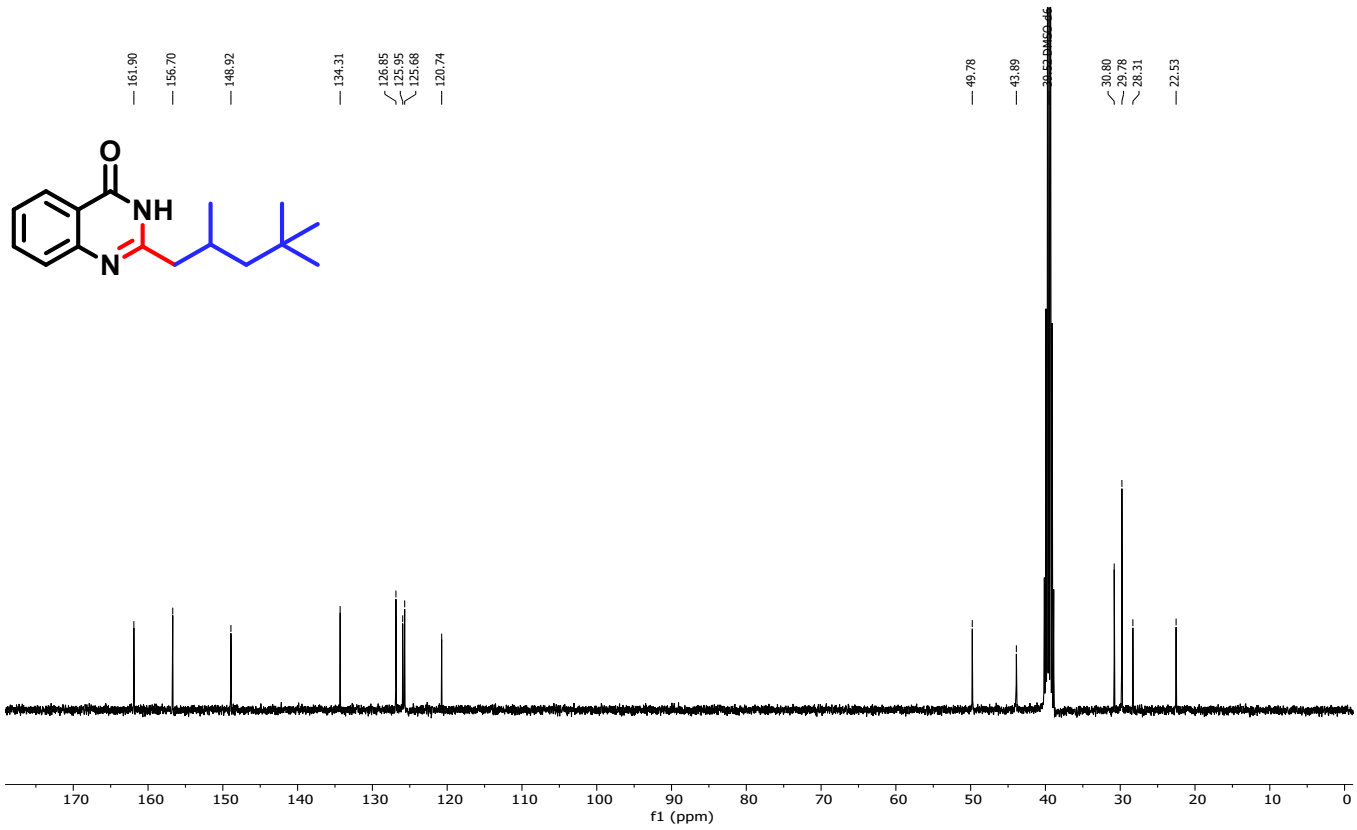


Figure S108. ^{13}C NMR spectrum (100 MHz) of **10e** in DMSO-d_6

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