Supporting Information

Synthesis of Quinazolinone Scaffolds *via* Zinc(II) Stabilized Amidyl Radical Promoted Deaminative Approach

Subarna Manna, Sangita Sahoo, and Arnab Rit*

Department of Chemistry, Indian Institute of Technology Madras, Chennai 600036, India

*E-mail: arnabrit@iitm.ac.in

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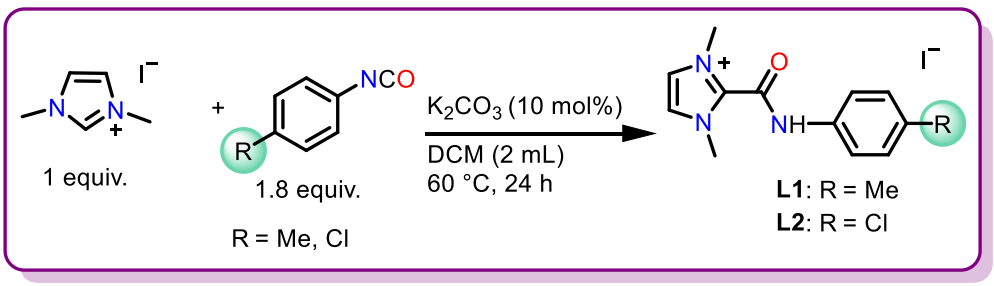
General experimental description:

All the reactions were performed under an argon atmosphere using a glove box and/or standard Schlenk techniques unless stated otherwise. All non-deuterated solvents used for the synthesis were distilled, degassed by standard methods and kept under an inert atmosphere over 4 Å molecular sieves, whereas the deuterated solvents were used as received from the commercial sources. NMR spectra were recorded using the Bruker 400 and 500 MHz FT-NMR spectrometers at ambient temperature and all the $^{1}H/^{13}C\{^{1}H\}$ NMR spectra were referenced internally to the residual solvent signals. ^{19}F NMR spectra were referenced externally to α,α,α -trifluorotoluene (0.05% $CDCl_3$, δ = -63.73 ppm). The ESI-MS spectra were measured with an Agilent 6545A Q-TOF Mass spectrometer. Infrared spectra were recorded on an ATR 4000 Series Spectrometer. UV-vis absorption spectra were recorded on JASCO V-650 spectrometer. Either Metrohm autolab potentiostat or galvanostat MAC90009 instrument was used for the electrochemical analysis. EPR spectra were measured using JES-FA200 ESR Spectrometer. Zinc salts (from TCI) and all other chemicals were purchased from commercial sources and used directly without further purification. Employed amidated salts (**L1-2**) were synthesized according to the literature procedures.[1]

1. General procedure for the synthesis of amidated salts, L1-2

The *N*,*N*-dimethylimidazolium salt and the amidated salts were prepared using the reported procedure.[1] In a pressure tube (25 mL), *N*,*N*-dimethylimidazolium salt (0.669 mmol, 1 equiv.), isocyanate (1.204 mmol, 1.8 equiv.), and K_2CO_3 (0.1 equiv.) were stirred in DCM (2 mL) at 60 °C (oil bath temperature) for 24 h. After completion of the reaction, the reaction mixture was purified by column chromatography using methanol and DCM solvent mixture as eluent to provide the desired C2-amidated imidazolium salts, **L1-2**.[1]

Scheme S1. Synthesis and characterization of amidated salts, L1-2



L1: **L1** was synthesized according to the general procedure using 200 mg of imidazolium salt, 12 mg of K_2CO_3, and 214.0 mg of *p*-tolyl-isocyanate (yield: 280 mg, 0.783 mmol, 87%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.30 (s, 1H), 7.92 (s, 1H), 7.59 (d, J = 10.5 Hz, 1H), 7.25 (d, J = 8.4 Hz, 2H), 3.98 (s, 6H), 2.30 (s, 3H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 150.7, 138.0, 135.0, 134.3, 129.5, 123.9, 120.4, 36.4, 20.6 ppm. IR (KBr): 3428, 1683, and 1530 cm^{-1}.

L2: L2 was synthesized according to the general procedure using 200 mg of imidazolium salt, 12 mg of K_2CO_3, and 205.4 mg of 4-chlorophenyl isocyanate (yield: 274 mg, 0.726 mmol, 81%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.49 (s, 1H), 7.89 (s, 2H), 7.72 (d, J = 8.9 Hz, 2H), 7.52 (d, J = 8.9 Hz, 2H), 3.98 (s, 6H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 151.1, 137.7, 135.9, 129.4, 129.1, 124.1, 122.2, 36.4 ppm. IR (KBr): 3443, 1688, and 1527 cm^{-1}.

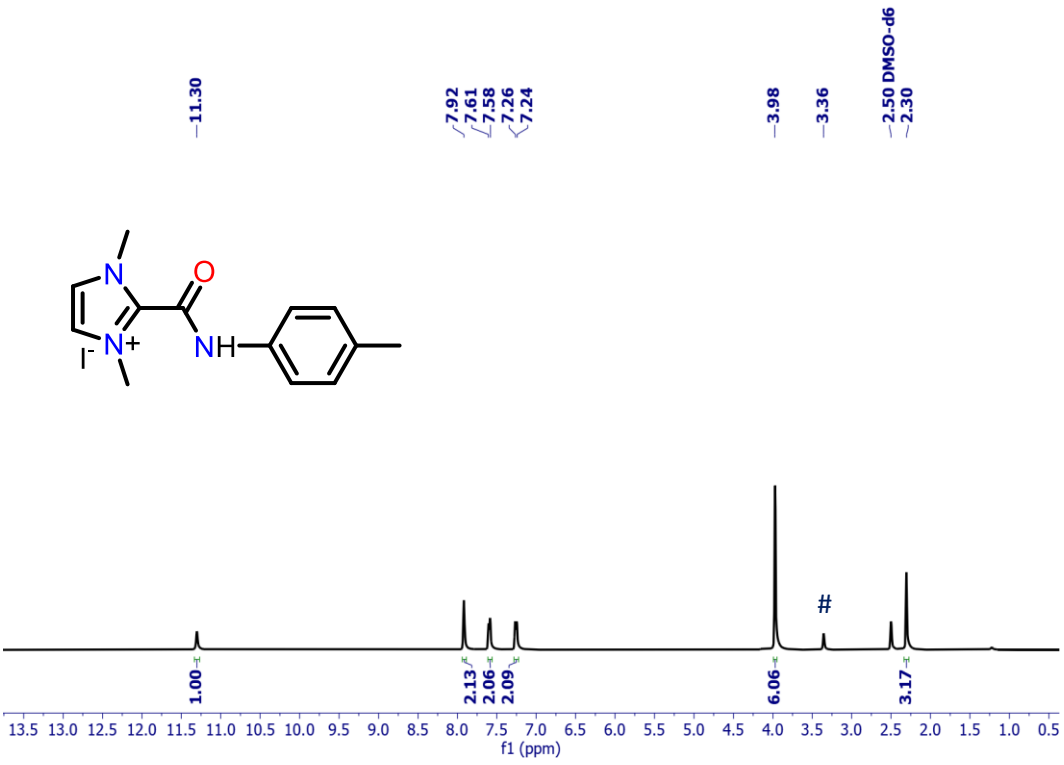


Figure S1. *^{1}H NMR of **L1** in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*

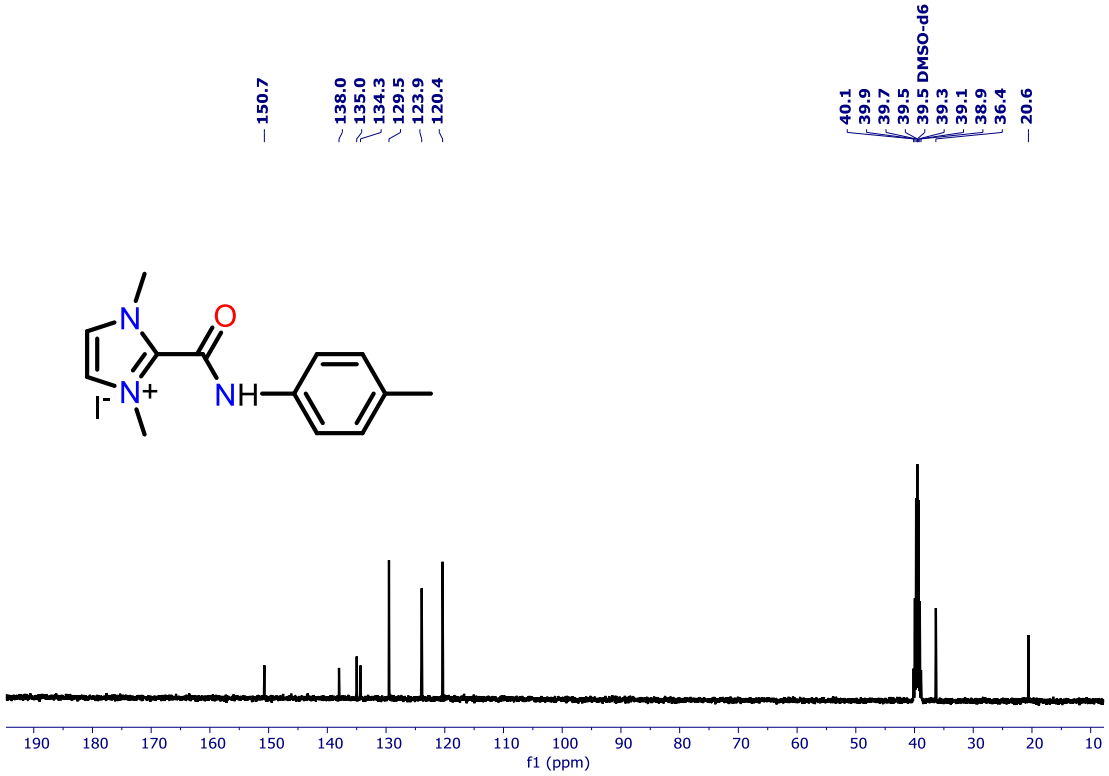


Figure S2. *$^{13}C\{^{1}H\}$ NMR of **L1** in DMSO-d_6*

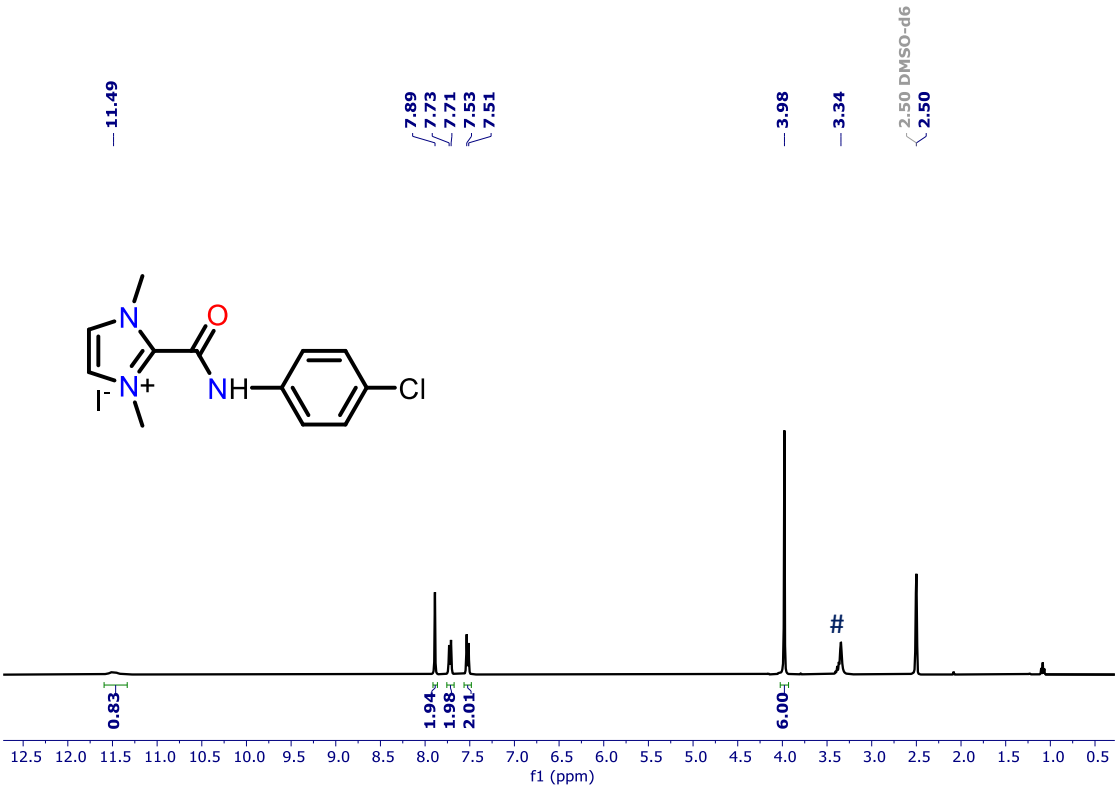


Figure S3. *^{1}H NMR of **L2** in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*

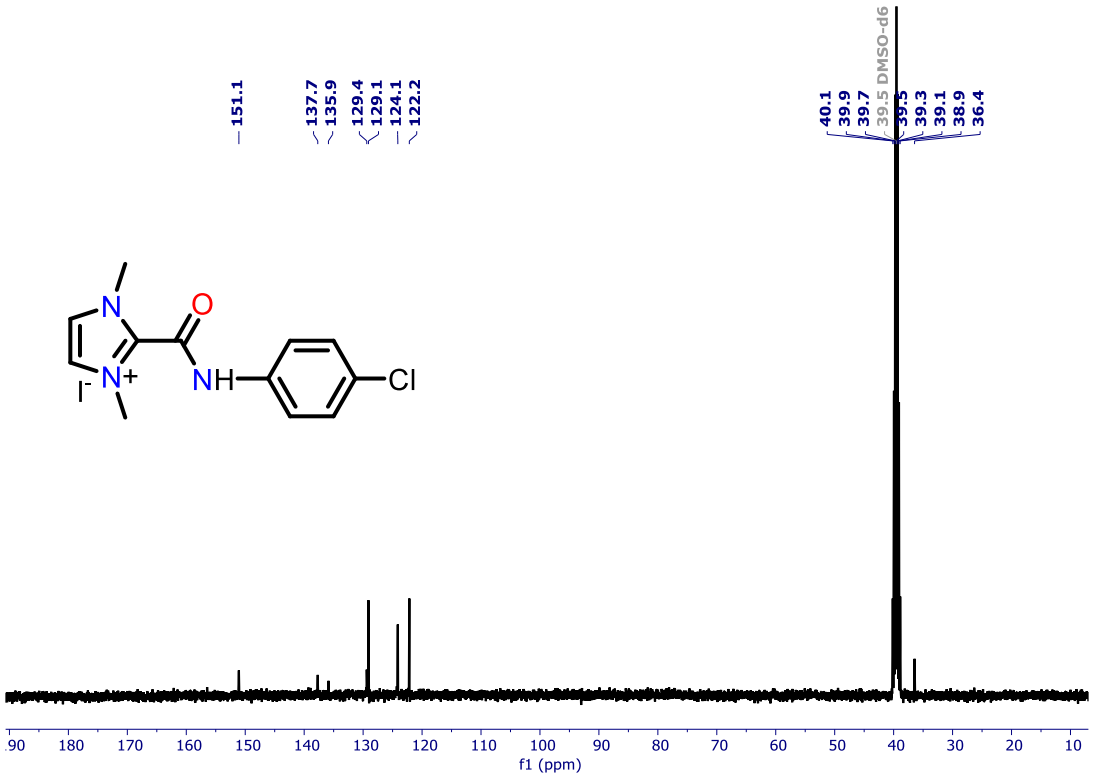


Figure S4. *$^{13}C\{^1H\}$ NMR of **L2** in DMSO-d_6*

2. General Procedure for the synthesis of compounds (1a-b and 1a'-b')

The precursor $ZnBr_2$/ZnI_2 (1 equiv.) and amidated salts, **L1-2** (2 equiv.) were placed in a Schlenk tube containing methanol (2 mL) with constant stirring at ambient temperature for 12 h. After that, all the volatiles were removed under high vacuum and the residue was then dissolved in dichloromethane. After filtration, the filtrate was concentrated and precipitated with diethyl ether. The precipitate was then collected and dried to yield a white solid.

*Compound **1a***. Compound **1a** was synthesized according to the general procedure using 50 mg of **L1** and 16 mg of $ZnBr_2$ (yield: 82.3 mg, 0.087 mmol, 70%). Suitable crystals of **1a** for single-crystal X-ray diffraction study were obtained *via* slow evaporation from a methanolic solution of **1a**. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.32 (s, 2H), 7.88 (s, 4H), 7.59 (d, J = 10.5 Hz, 4H), 7.25 (d, J = 8.4 Hz, 4H), 3.96 (s, 12H), 2.31 (s, 6H) ppm.$^{13}C\{^1H\}$ NMR (101 MHz, DMSO-d_6) δ 150.9, 138.3, 137.5, 134.8, 129.4, 123.8, 120.5, 36.3, 20.6 ppm. IR (KBr): 3447.6, 1685.7, and 1543.3 cm^{-1}.

*Compound **1b***. Compound **1b** was synthesized according to the general procedure using 50 mg of **L2** and 12 mg of $ZnBr_2$ (yield: 75.7 mg, 0.077 mmol, 65%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.54 (s, 2H), 7.90 (s, 4H), 7.74 (d, J = 10.5 Hz, 4H), 7.53 (d, J = 8.4 Hz, 4H), 3.98 (s,

12H) ppm. $^{13}C\{^{1}H\}$ NMR (101 MHz, DMSO-d_6) δ 151.1, 137.7, 135.9, 129.4, 129.1, 124.1, 122.2, 36.4 ppm. IR (KBr): 3451.1, 1694.1, and 1526.9 cm^{-1}.

*Compound **1a'***. Compound **1a'** was synthesized according to the general procedure using 50 mg of **L1** and 22.4 mg of ZnI_2 (yield: 108.15 mg, 0.102 mmol, 75%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.28 (s, 2H), 7.88 (s, 4H), 7.58 (d, J = 10.5 Hz, 4H), 7.25 (d, J = 8.4 Hz, 4H), 3.96 (s, 12H), 2.30 (s, 6H) ppm. $^{13}C\{^{1}H\}$ NMR (101 MHz, DMSO-d_6) δ 150.8, 138.1, 135.1, 134.4, 129.6, 124.0, 120.5, 36.4, 20.7 ppm. IR (KBr): 3460.5, 1688.7, and 1529.8 cm^{-1}.

*Compound **1b'***. Compound **1b'** was synthesized according to the general procedure using 50 mg of **L2** and 21.1 mg of ZnI_2 (yield: 96.4 mg, 0.089 mmol, 68%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.47 (s, 2H), 7.91 (s, 4H), 7.72 (d, J = 10.5 Hz, 4H), 7.53 (d, J = 8.4 Hz, 4H), 3.98 (s, 12H) ppm. $^{13}C\{^{1}H\}$ NMR (101 MHz, DMSO-d_6) δ 151.1, 137.7, 136.0, 129.4, 129.1, 124.2, 122.2, 36.5 ppm. IR (KBr): 3449.2, 1685.6, and 1533.2 cm^{-1}.

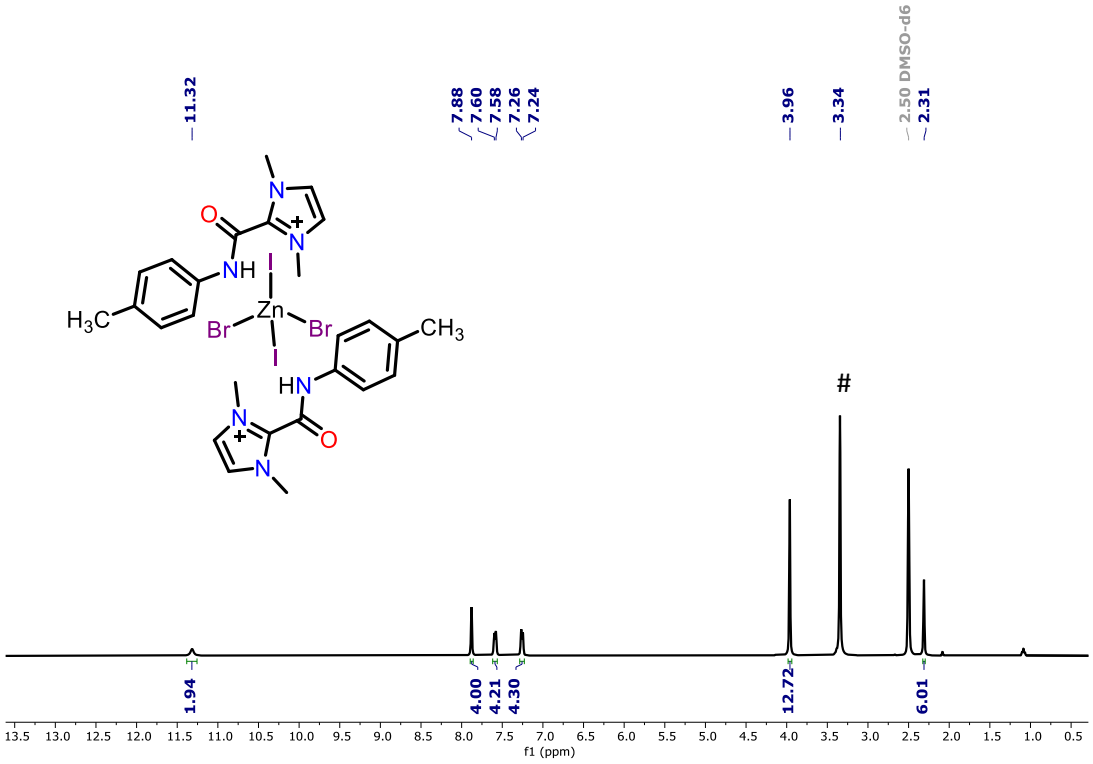


Figure S5. *^{1}H NMR of compound **1a** in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*

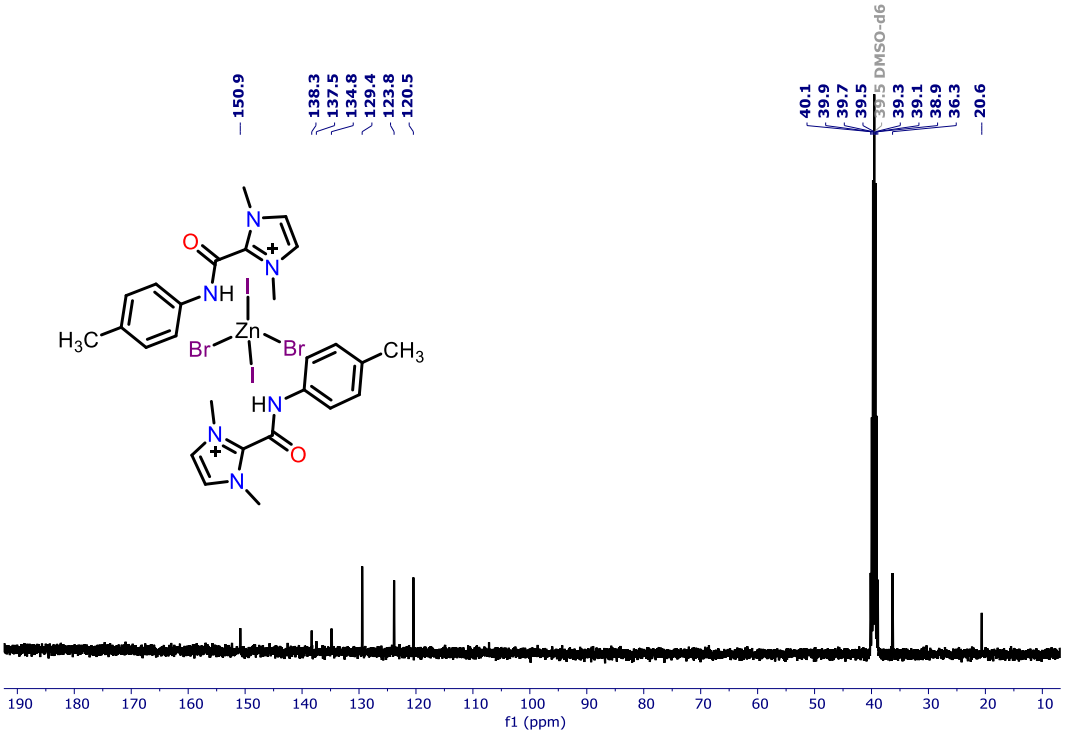


Figure S6. *$^{13}C\{^{1}H\}$ NMR of compound* ***1a*** *in DMSO-d_6*

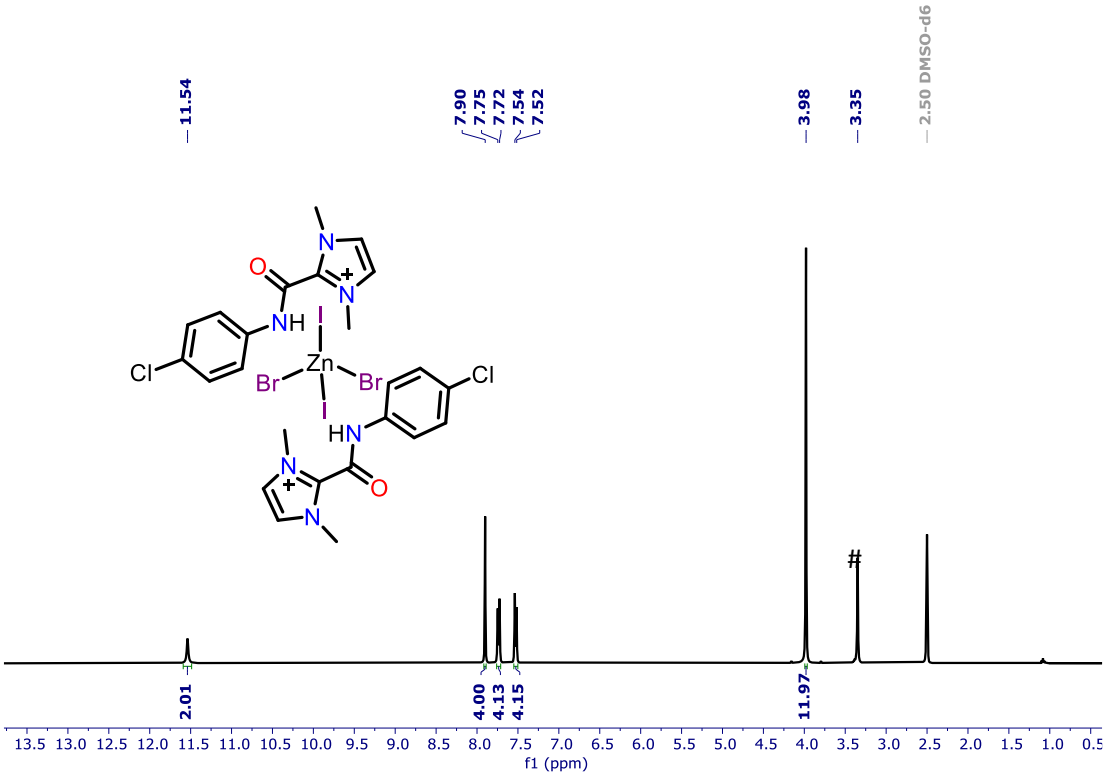


Figure S7. *^{1}H NMR of compound* ***1b*** *in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*

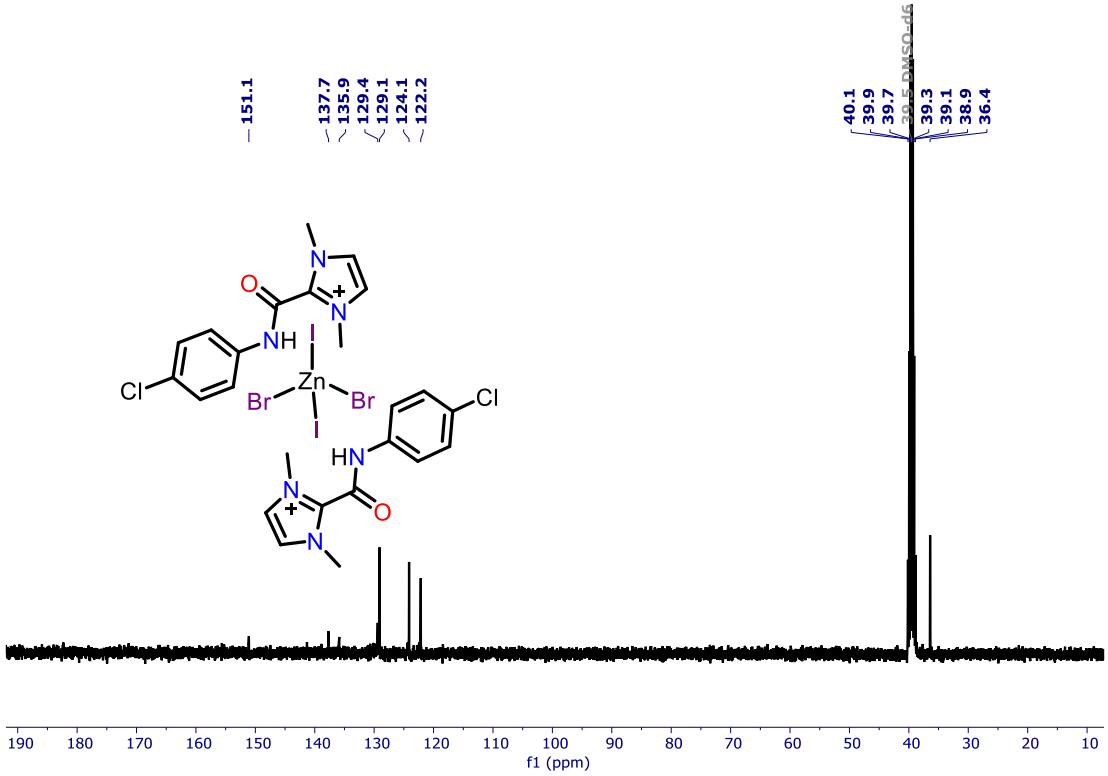


Figure S8. *$^{13}C\{^{1}H\}$ NMR of compound* ***1b*** *in DMSO-d_6*

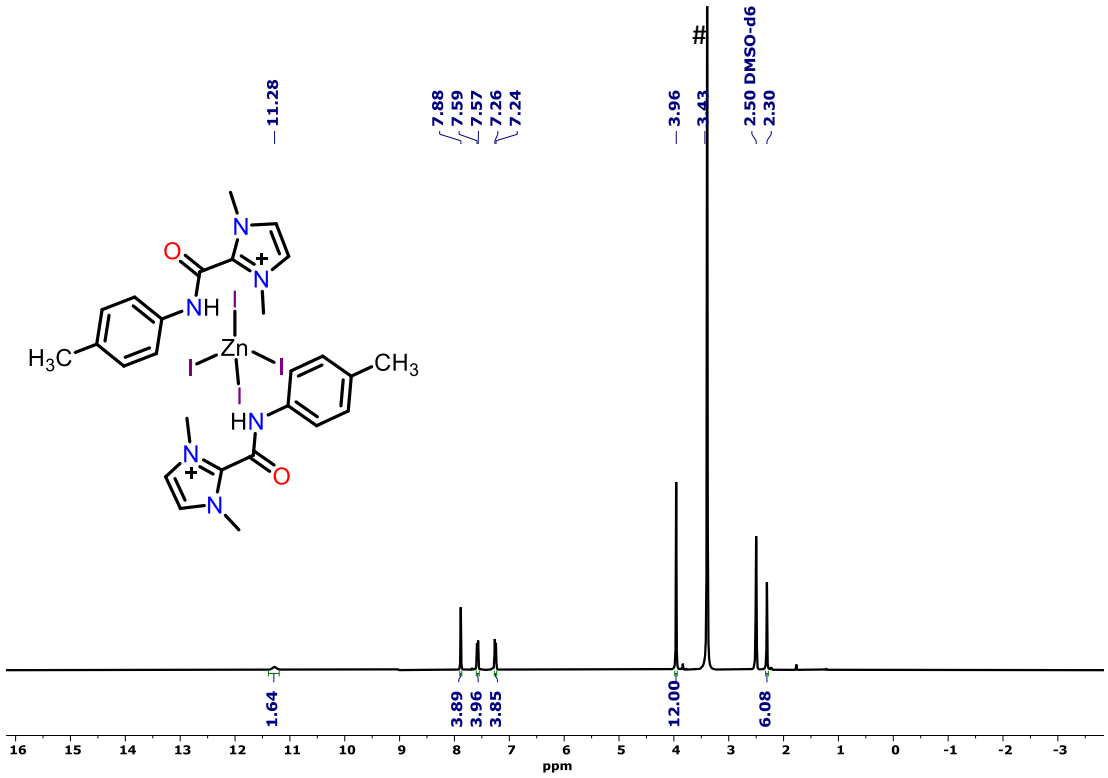


Figure S9. *^{1}H NMR of compound* ***1a'*** *in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*

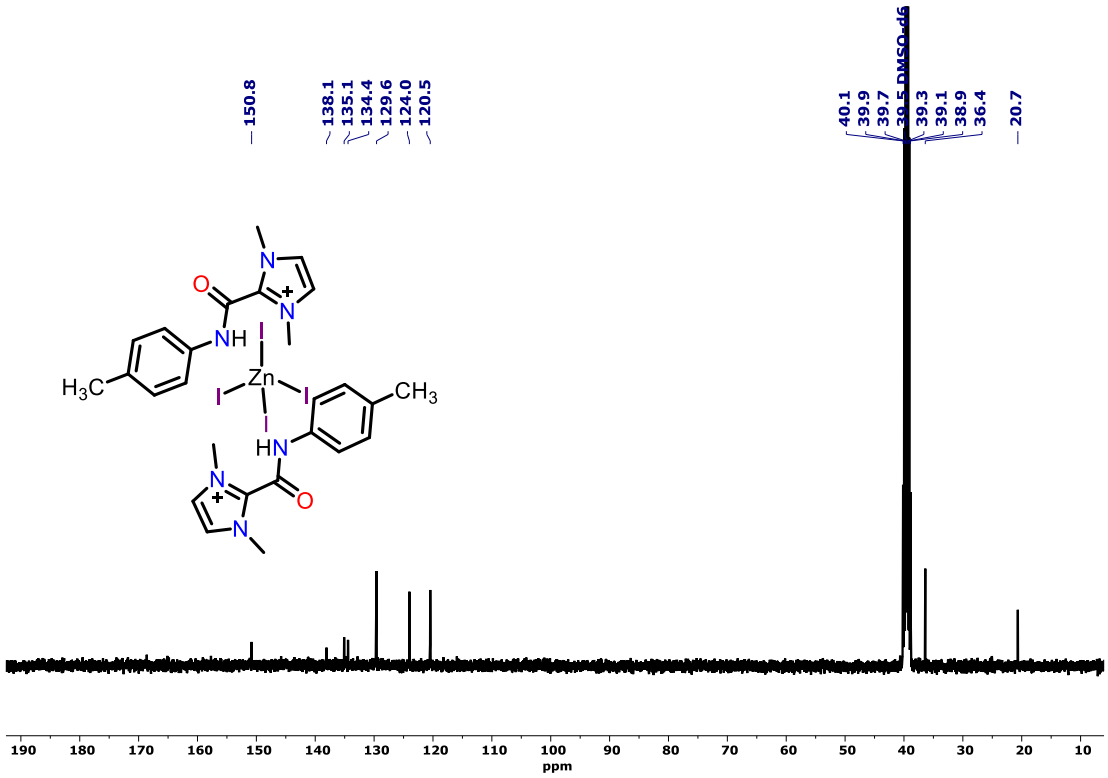


Figure S10. *$^{13}C\{^{1}H\}$ NMR of compound **1a'** in DMSO-d_6*

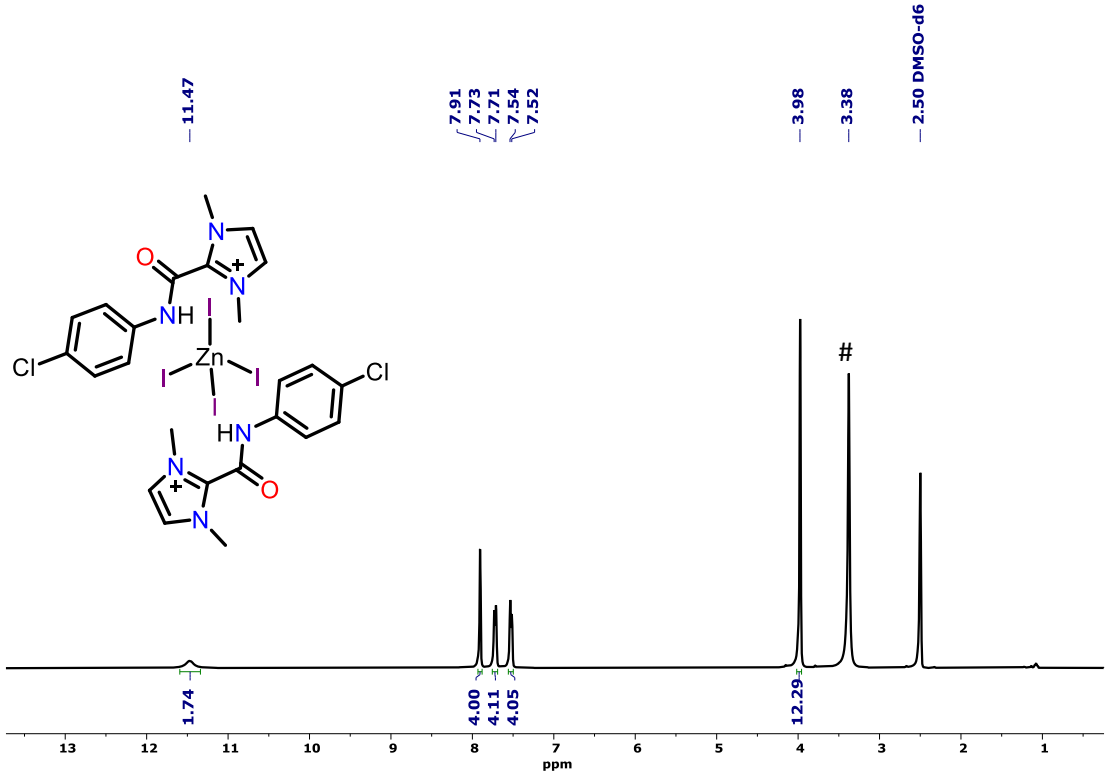


Figure S11. *^{1}H NMR of compound **1b'** in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*

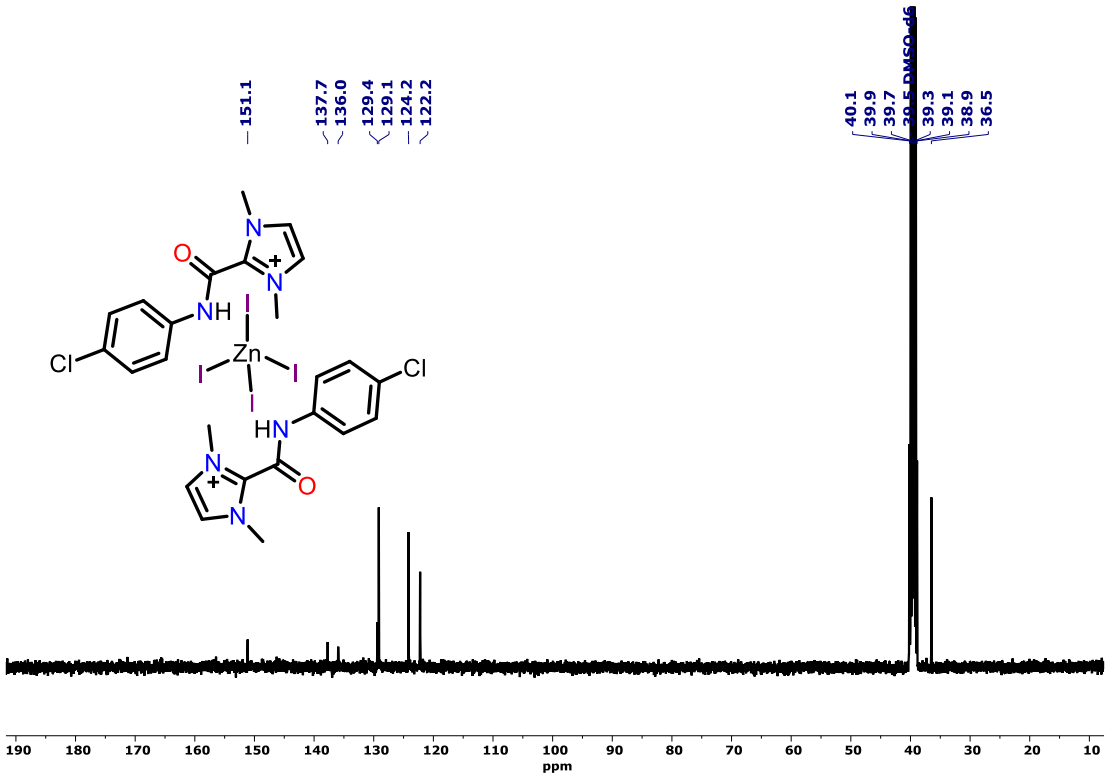
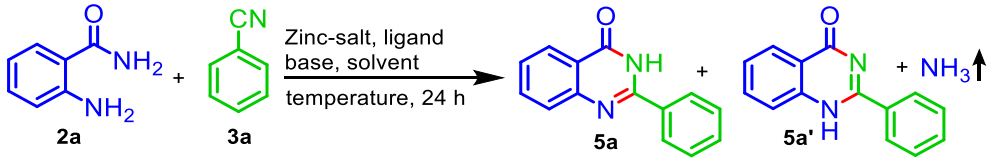


Figure S12. *$^{13}C\{^{1}H\}$ NMR of compound **1b'** in DMSO-d_6*

Table S1. Optimization of the reaction conditions for synthesis of quinazolinone starting from 2-aminobenzamide[a]



Entry	3a	Catalyst	Base	Solvent	Temp	Yield (%) 5a 5a'
1	0.2 mL	$ZnBr_2$+**L1**	LiO^tBu	-	140 °C	75 -
2	0.2 mL	$ZnCl_2$+**L1**	LiO^tBu	-	140 °C	65 -
3	0.2 mL	ZnI_2+**L1**	LiO^tBu	-	140 °C	72 -
4	0.2 mL	$Zn(OAc)_2$/$Zn(NO_3)_2$ + **L1**	LiO^tBu	-	140 °C	15/41 -
5	0.2 mL	**1a/1a'**	LiO^tBu	-	140 °C	81/79 -
6	0.2 mL	**1b/1b'**	LiO^tBu	-	140 °C	55/54 -
7	0.2 mL	**1a/1a'**	LiO^tBu	-	120 °C	86/83 -
8	0.2 mL	**1a**	KO^tBu / NaO^tBu / K_2CO_3	-	120 °C	65/55 27/14 /Trace /N.D.

9	0.2 mL	-	LiO^{t}Bu	-	120 °C	23 -
10	0.2 mL	**1a**	-	-	120 °C	Trace
11[b]	0.2 mL	**L1**	LiO^{t}Bu	-	120 °C	18 -
12	0.2 mL	$ZnBr_2$	-	-	120 °C	Trace
13	0.2 mL	$ZnBr_2$	LiO^{t}Bu	-	120 °C	25 -
14	39 µL (1.5 equiv.)	$ZnBr_2$ + **L1**	LiO^{t}Bu	Toluene/Xylene/ 1,4-dioxane /DMF/DMSO	120 °C	44/50/N.D. /N.D. /N.D.[f] -
15	39 µL (1.5 equiv.)	$ZnBr_2$ + **L1**	LiO^{t}Bu		120 °C	61 -
16	0.2 mL	$Zn(OTf)_2$ + **L1**	LiO^{t}Bu	-	120 °C	32 -
17	0.2 mL	**1a**	NEt_3	-	120 °C	Trace
18[c]	0.2 mL	**1a**	LiO^{t}Bu	-	120 °C	67 -
19[d]	0.2 mL	**1a**	LiO^{t}Bu	-	120 °C	51 -
20[e]	0.2 mL	**1a**	LiO^{t}Bu	-	120 °C	72 -
21	0.2 mL	Zn-dust	LiO^{t}Bu	-	120 °C	22 -

[a]**Reaction conditions**: 2-amino benzamide (**2a**, 0.25 mmol), catalyst (5 mol%), base (0.125 mmol), **3a** (0.2 mL), 120 °C, 24 h, under inert condition. Isolated yield. [b]**L1** (10 mol%), base (0.250 mmol). [c]Base (0.075 mmol). [d]Base (0.050 mmol).[e]**1a** (3 mol%). [f]N.D. = Not detected.

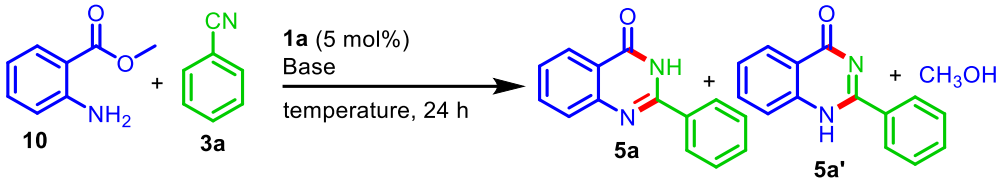
3. General procedure for synthesis of various quinazolinones/2*H*-benzo[1,2,4]thiadiazine 1,1-dioxides from 2-aminobenzamide/ 2-aminobenzenesulfonamide and nitriles

An oven-dried pressure tube (25 mL) was charged with 2-aminobenzamide, **2a**/2-aminobenzenesulfonamide, **2b** (0.25 mmol, 1 equiv.), LiO^{t}Bu (0.125 mmol, 0.50 equiv.), and **1a** (0.025 mmol, 5 mol%) followed by the addition of nitrile (0.2 mL) under inert condition. Then, the tube was kept in an oil bath at 120 °C and heated for 24 h. After completion of the reaction, the desired products were isolated by column chromatography over silica gel using hexane/ethyl acetate as eluent.

4. General procedure for synthesis of various quinazolinone from methyl anthranilate and nitriles

An oven-dried pressure tube (25 mL) was charged with methyl anthranilate (**10**, 0.25 mmol, 1 equiv.), KO^{t}Bu (0.187 mmol, 0.75 equiv.), and **1a** (0.025 mmol, 5 mol%) followed by the addition of nitrile (0.2 mL) under inert condition. Then, the tube was kept in an oil bath at 120 °C and heated for 24 h. After completion of the reaction, the desired products were isolated by column chromatography over silica gel using hexane/ethyl acetate as eluent.

Table S2. Optimization of the reaction conditions for synthesis of quinazolinone starting from methyl anthranilate[a]



Entry	Catalyst	Base	Temp.	Yield (%) 5a	5a'
1[b]	**1a**	LiO^{t}Bu	120 °C	Trace	
2[b]	**1a**	LiO^{t}Bu	140 °C	Trace	
3[b]	**1a**	NaO^{t}Bu	120 °C	42	15
4[b]	**1a**	KO^{t}Bu	120 °C	53	18
5	**1a**	KO^{t}Bu	120 °C	65	21

[a]**Reaction conditions**: Methyl anthranilate (**10**, 0.25 mmol), **1a** (0.0125 mmol), KO^{t}Bu (0.187 mmol), benzonitrile (0.2 mL), 24 h, under inert condition. Isolated yield. [b]KO^{t}Bu (0.125 mmol).

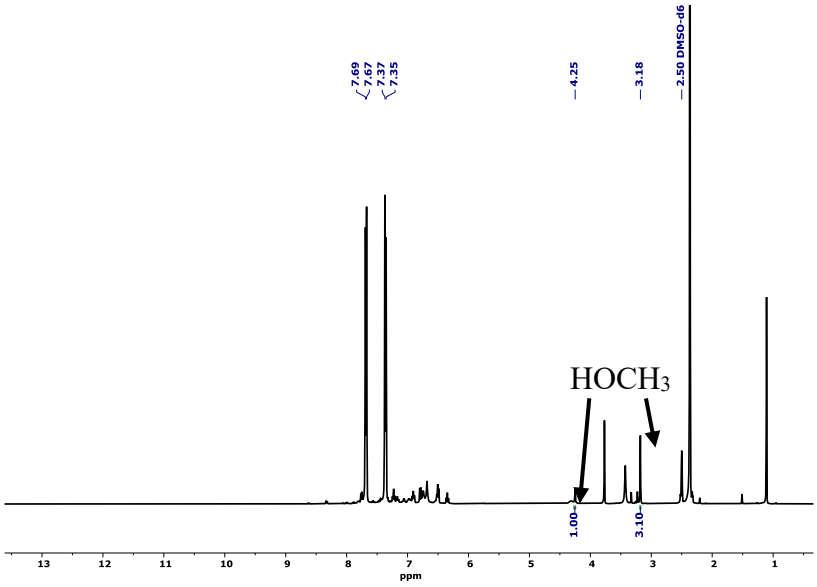
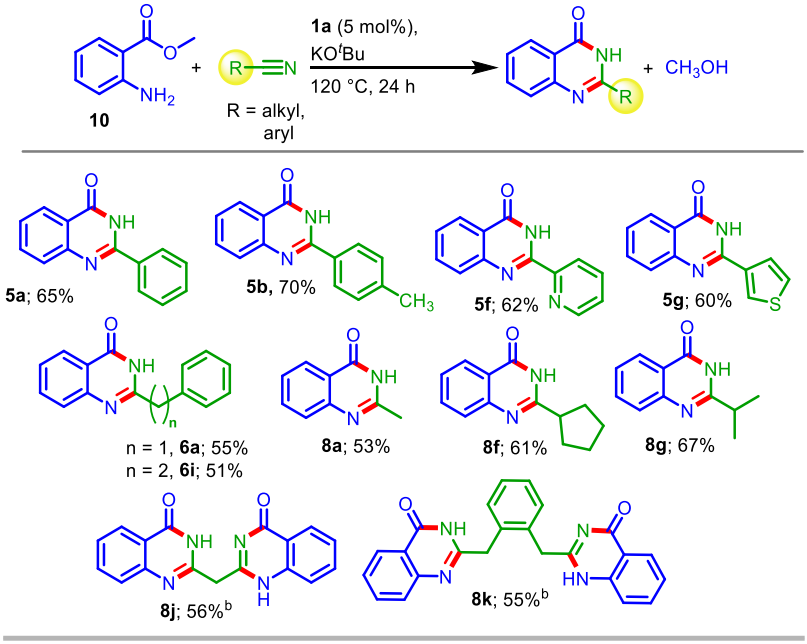


Figure S13: *^{1}H spectra of reaction mixture between methyl anthranilate (**10**) and benzonitrile (**3a**) under standard condition showing removal of methanol (CH_3OH) as a by-product*

Table S3. Substrate scope of nitriles with methyl anthranilate[a]



[a]**Reaction conditions:** Methyl anthranilate (**10**, 0.25 mmol), **1a** (5 mol%), KO^{t}Bu (0.187 mmol), ArCN, 120 °C, 24 h, under inert condition, isolated yield. [b]**1a** (10 mol%), KO^{t}Bu (0.375 mmol).

5. General synthetic method for the synthesis of 2-phenylquinazolin-4(3*H*)-one (5a)/2-methylquinazolin-4(3*H*)-one (8a) in gram scale

An oven-dried pressure tube (25 mL) was charged with 2-aminobenzamide (**2a**, 1g, 7.345 mmol, 1 equiv.), LiO^{t}Bu / KO^{t}Bu (3.673 mmol, 0.50 equiv.), and **1a** (0.367 mmol, 5 mol%) followed by the addition of benzonitrile (3 mL)/acetonitrile (3 mL) under inert condition. Then, the tube was kept in an oil bath at 120 °C and heated for 24 h. After completion of the reaction, the desired products **5a** and **8a** were isolated by column chromatography over silica gel using hexane/ethyl and DCM/MeOH acetate as eluent, respectively.

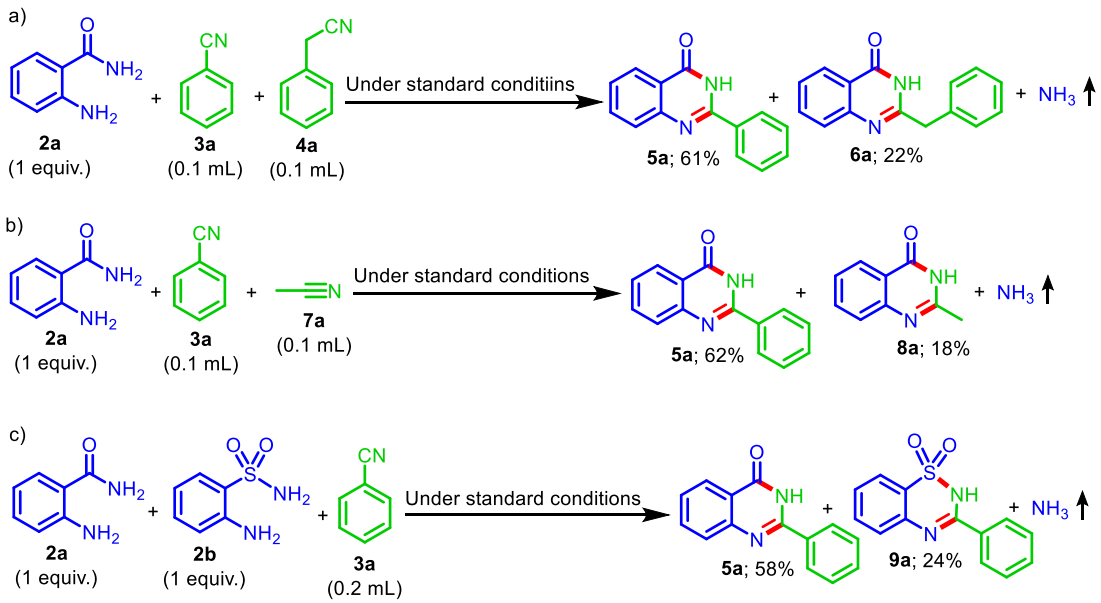
6. Procedure for competitive experiments

(a) Synthesis of quinazolinones via coupling between 2-aminobenzamide, benzonitrile and benzyl cyanide: An oven-dried pressure tube (25 mL) was charged with 2-aminobenzamide (**2a**, 0.25 mmol), LiO^{t}Bu (0.125 mmol, 0.50 equiv.), and **1a** (0.012 mmol, 5 mol%), followed by the addition of benzonitrile (0.1 mL) and benzyl cyanide (0.1 mL). Then, the tube was kept in oil bath at 120 °C and heated for 24 h. After completion of the reaction, the desired products **5a** (yield: 61%, 33.9 mg) and **6a** (yield: 22%, 13 mg) were isolated by column chromatography over silica gel using hexane/ethyl acetate as eluents.

(b) Synthesis of quinazolinones via coupling between 2-aminobenzamide, benzonitrile and acetonitrile: An oven-dried pressure tube (25 mL) was charged with 2-aminobenzamide (**2a**, 0.25 mmol), LiO^{t}Bu (0.125 mmol, 0.50 equiv.), and **1a** (0.012 mmol, 5 mol%), followed by the addition of benzonitrile (0.1 mL) and acetonitrile (0.1 mL). Then, the tube was kept in oil bath at 120 °C and heated for 24 h. After completion of the reaction, the desired products **5a** (yield: 62%, 34.4 mg) and **8a** (yield: 18%, 7.2 mg) were isolated by column chromatography over silica gel using hexane/ethyl acetate and DCM/MeOH as eluents, respectively.

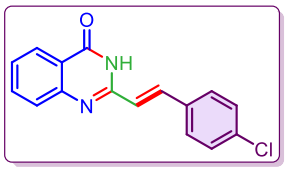
(c) Synthesis of quinazolinones via coupling between 2-aminobenzamide, 2-aminobenzenesulfonamide, and benzonitrile: An oven-dried pressure tube (25 mL) was charged with 2-aminobenzamide (**2a**, 0.25 mmol), 2-aminobenzenesulfonamide (**2b**, 0.25 mmol) LiO^{t}Bu (0.125 mmol, 0.50 equiv.), and **1a** (0.012 mmol, 5 mol%), followed by the addition of benzonitrile (0.2 mL). Then, the tube was kept in oil bath at 120 °C and heated for 24 h. After completion of the reaction, the desired products **5a** (yield: 58%, 32.2 mg) and **9a** (yield: 24%, 15.5 mg) were isolated by column chromatography over silica gel using hexane/ethyl acetate and DCM/MeOH as eluents, respectively.

Scheme S2: Competitive experiments



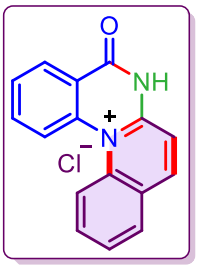
7. Post-synthetic modification of quinazolinones:

(a) Compound **11a** was synthesized following the reported procedure.[2] Equimolar amounts of



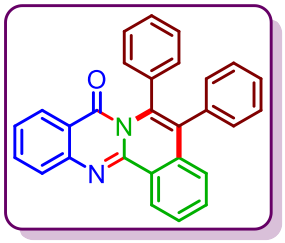
compound **8a** (30 mg, 0.186 mmol) and 4-chlorobenzaldehyde (28 mg, 0.186 mmol) were refluxed in glacial acetic acid (2 mL) for 8 h in presence of anhydrous sodium acetate (0.4 mg, 0.004 mmol). The reaction mixture was allowed to cool then poured onto crushed ice. The obtained product was filtered, washed with water and recrystallized from ethanol to yield compound **11a** (40.9 mg, isolated yield: 78%).

(b) Compound **11b** was synthesized as follows. Equimolar amounts of compound **8a** (30 mg,



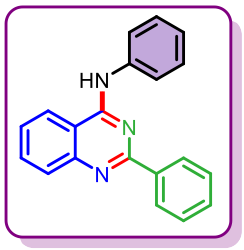
0.186 mmol) and 2-chlorobenzaldehyde (32 µL, 0.186 mmol) were refluxed in glacial acetic acid (2 mL) in presence of anhydrous sodium acetate (0.4 mg, 0.004 mmol) for 8 h. The reaction mixture was allowed to cool then poured onto crushed ice. The obtained solid was filtered off, washed with water and recrystallized from ethanol to yield compound **11b** (37.2 mg, isolated yield: 71%).

(c) Compound **11c** was synthesized following the reported procedure.[3] A mixture of 2-



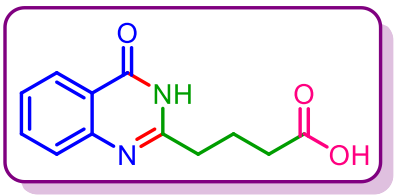
phenylquinazolin-4(3*H*)-one, **5a** (20 mg, 0.089 mmol), diphenyl acetylene (24 mg, 0.135 mmol), $[RuCl_2(p\text{-cymene})]_2$ (5 mol%), Na_2CO_3 (20 mg, 0.179 mmol), $Cu(OAc)_2$ (36 mg, 0.197mmol), and toluene (2 mL) were added to a reaction tube followed by stirring the reaction mixture at 90 °C for 16 h. Upon completion of reaction, the reaction mixture was purified through column chromatography over silica gel using ethyl acetate/hexane as eluent, providing **11c** (26.6 mg, isolated yield: 75%).

(d) Compound **11d** was synthesized following the procedure.[4] 2-phenylquinazolin-4(3*H*)-one



(**5a**, 100 mg) was dissolved in phosphorus oxychloride (2 mL) and heated under reflux to give the intermediate 4-chloro-2-phenylquinazoline. Then the obtained 4-chloro-2-phenylquinazoline (60 mg, 1 mmol) was reacted with aniline (23 µL, 1 mmol) in ethanol under room temperature overnight and completion of the reaction was checked by thin-layer chromatography. Upon completion of the reaction, reaction mixture was purified by column chromatography providing the compound **11d** (52.8 mg, isolated yield: 71%).

(e) Compound **11e** was synthesized as follows. An oven-dried pressure tube (25 mL) was charged with **8c** (20 mg, 0.094 mmol), followed by addition of 0.5 (M) aq. NaOH solution. Then, the tube was kept in oil bath at 100 °C and heated for 24 h. After completion of the reaction, reaction mixture was transferred into a 25 mL round bottom flask, followed by dilution with DCM (5 mL), and $MgSO_4$ was added into the resulted solution, followed by filtration. Afterwards, the organic layer was concentrated under vacuum and then purified through column chromatography over silica gel using MeOH/DCM as eluent, providing **11e** (17.7 mg, isolated yield: 81%).



8. EPR analysis

(a) *Procedure for singly reduced product of compound **1a***:

In a Schlenk tube, 1 equiv. of **1a** and 1 equiv. of LiO^{t}Bu were added followed by the addition of methanol (2 mL). The reaction mixture was stirred for 30 mins. During that time colour of the solution changed to light yellow. Then, EPR measurement of this solution was carried out at room temperature under inert condition.

EPR Detail:

The possible one-electron reduced product generated from **1a** was analysed by X-band EPR (Bruker) at room temperature. The parameters during the data collection were following. Microwave frequency 9.43 GHz; Microwave Power 0.99 MW; Modulation frequency 100 kHz; Modulation amplitude 0.2 mT.

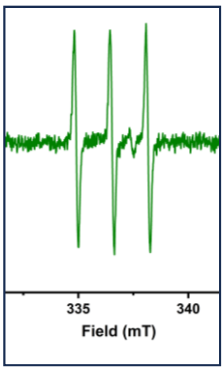


***Figure S14**. EPR signal obtained from singly reduced product of **1a**.*

*(b) Procedure for singly reduced product of **L1***:

In a Schlenk tube, 1 equiv. of **L1**, and 1 equiv. of LiO^{t}Bu were added followed by methanol (2 mL). The reaction mixture was stirred for 30 mins, no change in colour was observed. Then

the EPR measurement of this solution was carried out both at room temperature and liquid nitrogen temperature under inert condition. No signal was observed.

EPR details:

The resultant solution was analysed by X-band EPR (Bruker) at room temperature. The parameters during the data collection were following. Microwave frequency 9.43 GHz; Microwave Power 2 MW; Modulation frequency 100 kHz; Modulation amplitude 0.35 mT.

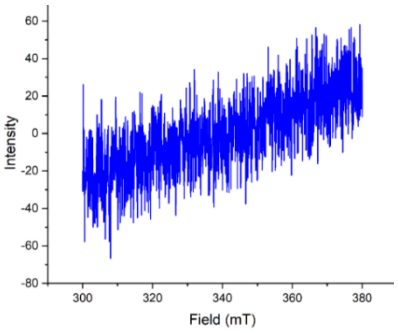
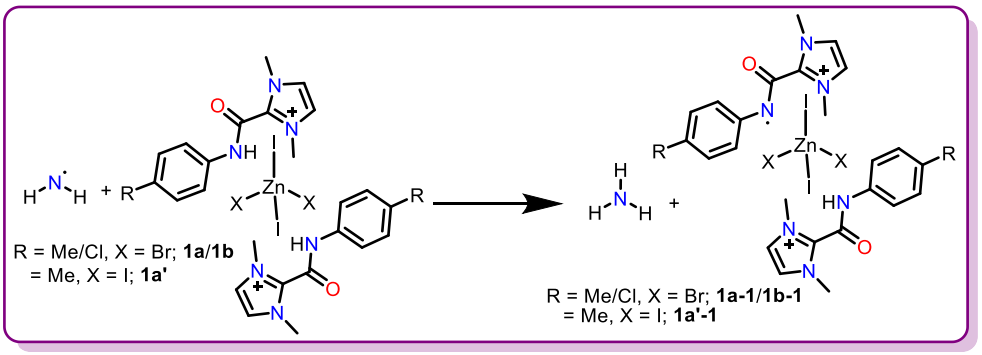


Figure S15. *EPR spectrum obtained from* ***L1*** *and base*.

9. Calculation of Bond-Dissociation Enthalpy (BDE)

The BDE (N-H) values of amidated compound (**1a-b, 1a'**) were estimated following the theoretical scheme reported by Zipse *et al*.[5] The stabilities of amidyl radicals (**1a-1/1b-1 /1a'-1)** relative to the reference aminyl radical ($\cdot NH_2$) were calculated as the reaction enthalpies at 298.15 K for the hydrogen atom transfer reaction shown below (ΔH_{rxn}). We could estimate the BDE of **1a-b/1a'** by adding the calculated reaction enthalpy to the experimentally determined BDE value of ammonia (450.1 kJ mol^{-1} = 107.6 kcal mol^{-1}).



Geometry optimizations of amidated compound (**1a** and **1a'**) and their corresponding radical forms (**1a-1, 1b-1** and **1a'-1** radicals) were performed at the B3LYP/6-31G(d). Thermochemical corrections to 298.15 K with a scaling factor of 0.9806 were used to obtain an enthalpy of the systems at same level of theory. The components of the calculations are

summarized in Table **S3**. The Gaussian 16, Revision B.01 program was used for all calculations.

Table S4. Enthalpies and BDE data for **1a-b** and **1a'** systems in reaction

	H_{298}/Hf
NH_3	-56.519520
NH_2•	-55.856231
1a	-6719.847896
1a-1	-6719.203457

ΔH_{rxn} = -11.828 kcal mol^{-1}

BDE of N-H in **1a** = 95.7 kcal mol^{-1}

	H_{298}/Hf
NH_3	-56.519520
NH_2•	-55.856231
1a'	-1599.793429
1a'-1	-1599.149366

ΔH_{rxn} = -12.067 kcal mol^{-1}

BDE of N-H in **1a'** = 95.5 kcal mol^{-1}

	H_{298}/Hf
NH_3	-56.519520
NH_2•	-55.856231
1b	-2443.986198
1b-1	-2443.338296

ΔH_{rxn} = -9.657 kcal mol^{-1}

BDE of N-H in **1b** = 97.9 kcal mol^{-1}

10. Electrochemical analysis of L1 and **1a**:

The electrochemical measurements, cyclic voltammetry (CV), of the synthesized salt **L1** and compound **1a** were carried out at ambient temperature with Metrohm auto lab potentiostat and galvanostat MAC90009 instrument, respectively. The measurements of salt **L1** and **1a** were performed at a sweep rate of 100 mV/sec with three-electrode configuration with auxiliary electrode: Pt wire; working electrode: Glassy carbon; reference electrode: Ag/Ag^+. All the measurements were calibrated externally using Ferrocene ($E_{1/2}$, Fc/Fc^+ = 0.22 volts *vs*. Ag/Ag^+).

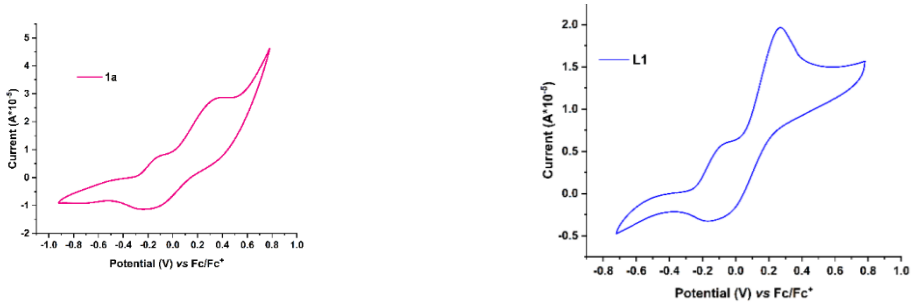


Figure S16. Cyclic voltammogram of **L1** and **1a** in acetonitrile using auxiliary electrode: Pt wire; working electrode: Glassy carbon; reference electrode: Ag/Ag^+. All the measurements were calibrated externally using Ferrocene ($E_{1/2}$, Fc/Fc^+ = 0.22 volts *vs*. Ag/Ag^+).

11. Control experiments for establishing radical mediated pathway

(a) Radical scavenger experiments:

(i) An oven-dried pressure tube (25 mL) was charged with 2-aminobenzamide, **2a**/2-aminobenzenesulfonamide, **2b** (0.25 mmol, 1 equiv.), LiO^{t}Bu (0.125 mmol, 0.50 equiv.), and **1a** (0.025 mmol, 5 mol%), and radical scavenger, BHT (0.25 mmol)/ galvinoxyl (0.125 mmol)/$CuCl_2$ (0.25 mmol) followed by the addition of benzonitrile (0.2 mL) under inert condition. Then, the tube was kept in an oil bath at 120 °C/140 °C and heated for 24 h. After completion of the reaction, the desired products were isolated by column chromatography over silica gel using hexane/ethyl acetate as eluent.

(ii) An oven-dried pressure tube (25 mL) was charged with 2-aminobenzamide (**2a**, 0.25 mmol, 1 equiv.), LiO^{t}Bu (0.125 mmol, 0.50 equiv.), and **1a** (0.025 mmol, 5 mol%), and radical scavenger, BHT (0.25 mmol) followed by the addition of xylene (2 mL). Then, the tube was kept in an oil bath at 120 °C and heated for 24 h. After completion of the reaction, an aliquot of reaction mixture was taken in a mass vial and diluted with methanol, and then subjected to HRMS analysis.

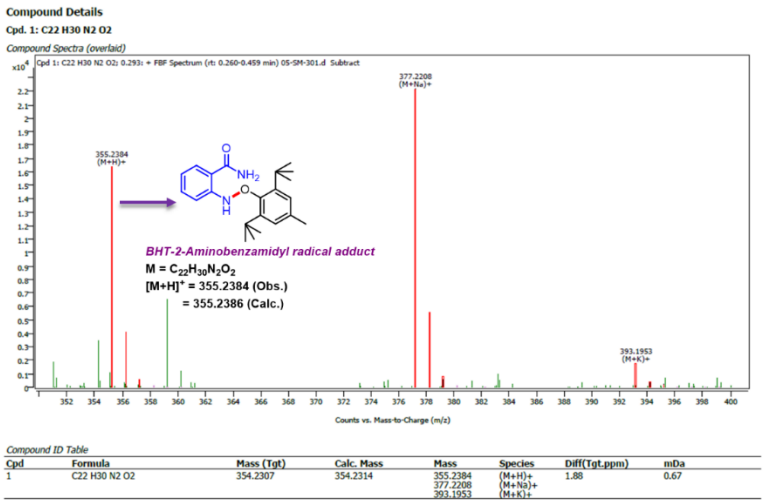


***Figure S17**: HRMS of BHT-2-aminobenzamidyl radical adduct. M corresponds to 2-aminobenzamide radical trapped with BHT*

(iii) An oven-dried pressure tube (25 mL) was charged with methyl anthranilate (**10**, 0.25 mmol, 1 equiv.), KO^{t}Bu (0.187 mmol, 0.75 equiv.), and **1a** (0.025 mmol, 5 mol%), and radical scavenger, BHT (0.25 mmol)/TEMPO (0.25 mmol)/$CuCl_2$ (0.25 mmol) followed by the addition of benzonitrile (0.2 mL). Then, the tube was kept in an oil bath at 120 °C and heated for 24 h. After completion of the reaction, an aliquot of reaction mixture was diluted with dichloromethane and subjected to HRMS analysis.

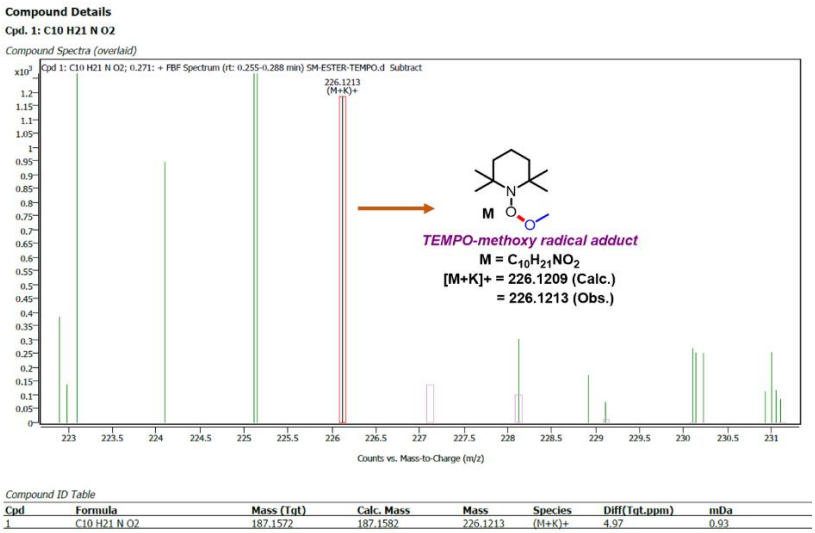


***Figure S18**: HRMS of TEMPO-Methoxy radical adduct. M corresponds to methoxy radical trapped with TEMPO*

(b) (i) Experiment for detection of CH_3NH_2:

An oven-dried pressure tube (25 mL) was charged with 2-amino-*N*-methylbenzamide (**2c**, 0.25 mmol, 1 equiv.), LiO^{t}Bu (0.125 mmol, 0.50 equiv.), and **1a** (0.025 mmol, 5 mol%), followed by the addition of benzonitrile (0.2 mL). Then, the tube was kept in an oil bath at 120 °C and heated for 24 h. After completion of the reaction, the reaction mixture was taken in DMSO-d_6 and analyzed by ^{1}H NMR spectroscopy.

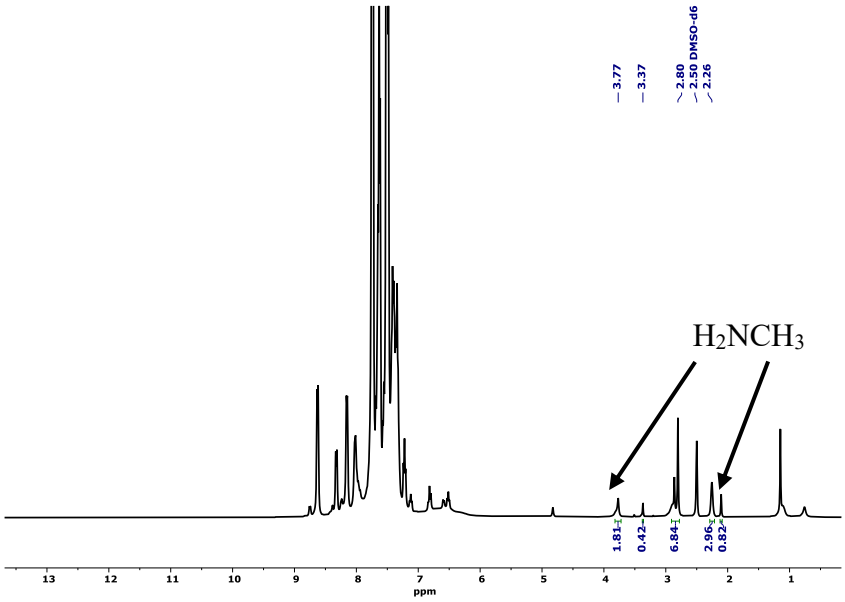


***Figure S19**: ^{1}H NMR spectrum of reaction mixture between 2-amino-N-methylbenzamide (**2c**) and benzonitrile (**3a**) under standard condition showing removal of methylamine (CH_3NH_2) as a by-product*

(ii) *Experiment for detection of NH_3*:

An oven-dried pressure tube (25 mL) was charged with 2-aminobenzamide (**2a**, 0.25 mmol, 1 equiv.), LiO^tBu (0.187 mmol, 0.75 equiv.), and **1a** (0.025 mmol, 5 mol%), followed by the addition of benzonitrile (0.2 mL). Then, the tube was kept in an oil bath at 120 °C and heated for 24 h. After completion of reaction, a glass rod dipped in conc. HCl was held near the mouth of pressure tube containing reaction mixture, which resulted in the formation of a dense white fume as well as white solid of NH_4Cl on glass rod. Subsequently, this white solid was dissolved in distilled water and the solution was added dropwise to $AgNO_3$ solution, yielding white color AgCl ppt.

12. Kinetics analysis

(a) Procedure to find out the order of reaction with respect to catalyst loading, 2-aminobenzamide, and acetonitrile

To find out the order of our present catalytic reaction with respect to catalyst **1a**, different sets of reactions were carried out by varying the amount of catalyst (3-6 mol%)/2-aminobenzamide (**2a**, 0.2-0.35 mmol)/acetonitrile (**7a**, 0.2-0.35 mL) keeping the other factors constant. An aliquot of the reaction mixture from each set was then taken after a certain time interval and amount of product **8a** formed over time was calculated (from GC-MS analysis) in each case. Then, the obtained rates were plotted against the amount of catalyst/**2a**/acetonitrile, and the obtained straight lines indicated that the reaction is pseudo first order w. r. t. catalyst **1a** and **2a**. However, it is zeroth order w. r. t. nitrile.

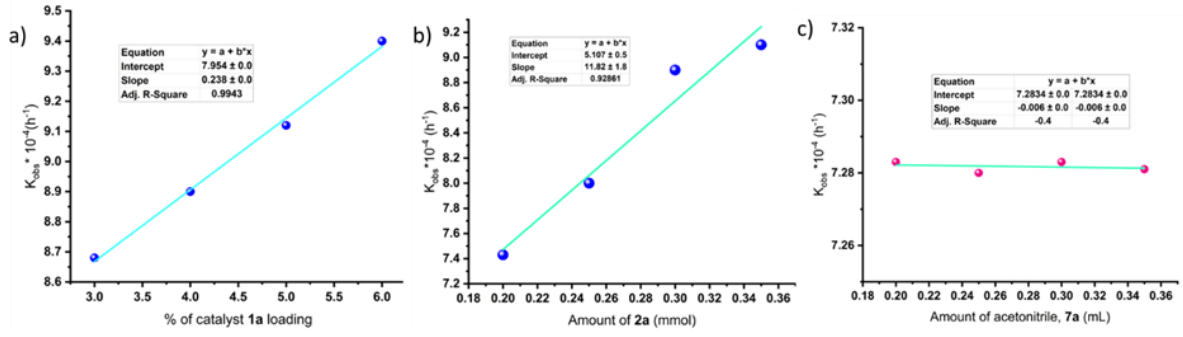
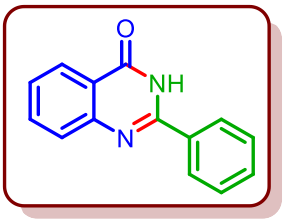


***Figure S20**: (a) K_{obs} vs catalyst loading. Reaction conditions: **2a** (0.25 mmol), acetonitrile (**7a**, 0.2 mL), **1a** (variable catalyst loading, 3-6 mol%), KO^{t}Bu (0.125 mmol), 120 °C, (b) Plot of K_{obs} vs amount of **2a**. Reaction conditions: **2a** (variable amount, 0.20-0.35 mmol), acetonitrile (**7a**, 0.2 mL), **1a** (5 mol%), KO^{t}Bu (0.125 mmol), 120 °C, (c) Plot of K_{obs} vs amount of acetonitrile (**7a**). Reaction conditions: **2a** (0.25 mmol), acetonitrile (variable amount, 0.2-0.35 mL), **1a** (5 mol%), KO^{t}Bu (0.125 mmol), 120 °C.*

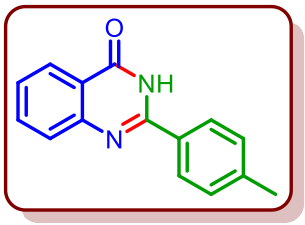
14. Analytical data:

2-phenylquinazolin-4(3H)-one (Compound-5a):[6] Following the general procedure, the titled



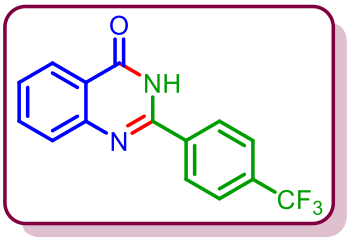
compound was isolated as white solid (48.3 mg, 0.217 mmol, 87% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.55 (s, 1H), 8.17 (m, 3H), 7.83 (t, J = 7.6 Hz, 1H), 7.74 (d, J = 7.9 Hz, 1H), 7.60-7.50 (m, 4H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 162.3, 152.4, 148.7, 134.6, 132.8, 131.4, 128.6, 127.8, 127.5, 126.6, 125.9, 121.0 ppm.

2-(p-tolyl)quinazolin-4(3H)-one (Compound-5b):[6] Following the general procedure, the titled



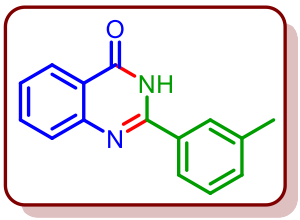
compound was isolated as white solid (45.4 mg, 0.192 mmol, 77% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.47 (s, 1H), 8.14 (d, J = 8.2 Hz, 1H), 8.09 (d, J = 7.8 Hz, 2H), 7.82 (t, J = 8.0 Hz, 1H), 7.72 (d, J = 8.7 Hz, 1H), 7.50 (t, J = 8.0 Hz, 1H), 7.34 (d, J = 8.1 Hz, 2H), 2.38 (s, 3H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 162.3, 152.3, 148.9, 141.5, 134.7, 129.9, 129.3, 127.7, 127.5, 126.5, 125.9, 120.9, 21.1 ppm.

2-(4-(trifluoromethyl)phenyl)quinazolin-4(3H)-one (Compound-5c):[7] Following the general



procedure, the titled compound was isolated as white solid (48.3 mg, 0.217 mmol, 65% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.75 (s, 1H), 8.37 (d, J = 8.2 Hz, 2H), 8.17 (d, J = 7.9 Hz, 1H), 7.92 (d, J = 8.3 Hz, 2H), 7.86 (t, J = 7.7 Hz, 1H), 7.77 (d, J = 8.1 Hz, 1H), 7.56 (t, J = 7.5 Hz, 1H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 162.2, 151.2, 148.5, 136.6, 134.8, 128.8, 127.7, 127.2, 125.9, 125.6, 125.5, 122.6, 121.2 ppm. ^{19}F NMR (471 MHz, DMSO-d_6) δ -61.33 ppm.

2-(m-tolyl)quinazolin-4(3H)-one (Compound-5d):[6] Following the general procedure, the titled



compound was isolated as white solid (41.3 mg, 0.174 mmol, 70% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.46 (s, 1H), 8.15 (d, J = 7.9 Hz, 1H), 8.02 (s, 1H), 7.96 (d, J = 7.5 Hz, 1H), 7.83 (t, J = 7.6 Hz, 1H), 7.74 (d, J = 8.2 Hz, 1H), 7.51 (t, J = 7.5 Hz, 1H), 7.44-7.38 (m, 2H), 2.40 (s, 3H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 162.3, 152.5, 138.0, 134.7, 132.7, 132.1, 128.6, 128.3, 127.5, 126.6, 125.9, 124.9, 121.0, 21.0 ppm.

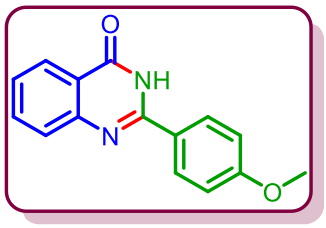
2-(naphthalen-2-yl)quinazolin-4(3H)-one (Compound-5e):[6] Following the general procedure, the titled compound was isolated as white solid (41.5 mg, 0.152 mmol, 61% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.68 (s, 1H), 8.82 (s, 1H), 8.30 (d, J = 8.6 Hz, 1H), 8.19 (d, J = 7.8 Hz, 1H), 8.09-8.05 (m, 2H), 8.02 (d, J = 9.3 Hz, 1H), 7.87 (t, J = 7.6 Hz, 1H), 7.80 (d, J = 8.1 Hz, 1H), 7.67-7.61 (m, 2H), 7.55 (t, J = 7.5 Hz, 1H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 162.3, 152.3, 148.8, 148.0, 134.8, 134.2, 132.3, 130.0, 129.0, 128.2, 128.2, 128.0, 127.7, 127.6, 127.0, 126.8, 126.0, 124.6, 121.1 ppm.

2-(pyridin-2-yl)quinazolin-4(3H)-one (Compound-5f):[6] Following the general procedure, the titled compound was isolated as white solid (40.2 mg, 0.180 mmol, 72% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.79 (s, 1H), 8.75 (s, 1H), 8.44 (d, J = 8.1 Hz, 1H), 8.18 (d, J = 8.2 Hz, 1H), 8.06 (t, J = 8.4 Hz, 1H), 7.86 (t, J = 7.8 Hz, 1H), 7.79 (d, J = 8.4 Hz, 1H), 7.65 (s, 1H), 7.56 (t, J = 7.8 Hz, 1H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 160.8, 149.9, 149.0, 148.7, 148.4, 138.0, 134.7, 127.7, 127.3, 126.6, 126.1, 122.2, 122.0 ppm.

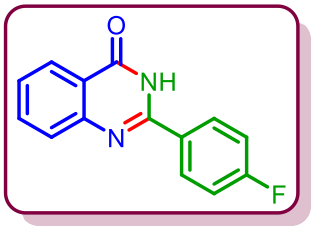
2-(thiophen-3-yl)quinazolin-4(3H)-one (Compound-5g):[6] Following the general procedure, the titled compound was isolated as white solid (42.8 mg, 0.191 mmol, 75% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.46 (s, 1H), 8.60 (s, 1H), 8.13 (d, J = 7.9 Hz, 1H), 7.87 (d, J = 5.1 Hz, 1H), 7.80 (t, J = 7.7 Hz, 1H), 7.70-7.68 (m, 2H), 7.49 (t, J = 7.5 Hz, 1H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 162.1, 148.9, 148.3, 135.4, 134.6, 128.7, 127.4, 127.3, 127.1, 126.4, 125.9, 121.0 ppm.

2-(pyridin-4-yl)quinazolin-4(3H)*-one *(Compound-5h):[8] Following the general procedure, the titled compound was isolated as white solid (26.23 mg, 0.117 mmol, 47% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.77 (s, 1H), 8.78 (d, J = 6.1 Hz, 2H), 8.18 (d, J = 7.9 Hz, 1H), 8.11 (d, J = 2.4 Hz, 2H), 7.87 (t, J = 7.6 Hz, 1H), 7.79 (d, J = 8.4 Hz, 1H), 7.58 (t, J = 7.5 Hz, 1H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 162.2, 150.7, 150.3, 148.3, 140.0, 134.8, 127.8, 127.5, 126.0, 121.7, 121.5 ppm.

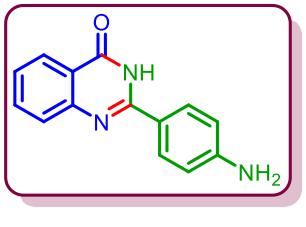
2-(4-methoxyphenyl)quinazolin-4(3H)-one (Compound-5i):[8] Following the general procedure, the titled compound was isolated as white solid (32.8 mg, 0.130 mmol, 52% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.41 (s, 1H), 8.19 (d, J = 7.1 Hz, 2H), 8.13 (d, J = 7.9 Hz, 1H), 7.81 (t, J = 7.6 Hz, 1H), 7.70 (d, J = 8.1 Hz, 1H), 7.48 (t, J = 7.5 Hz, 1H), 7.08 (d, J = 7.0 Hz, 2H), 3.85 (s, 3H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 162.4, 161.9, 151.9, 149.0, 134.6, 129.5, 127.3, 126.2, 125.9, 124.8, 120.7, 114.0, 55.5 ppm.



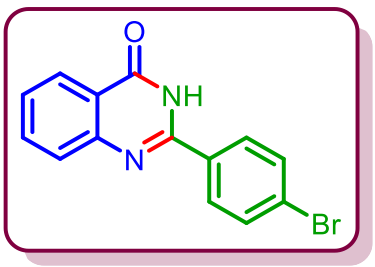
2-(4-fluorophenyl)quinazolin-4(3H)-one (Compound-5j):[6] Following the general procedure, the titled compound was isolated as white solid (25.8 mg, 0.103 mmol, 41% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.57 (s, 1H), 8.26-8.22 (m, 2H), 8.15 (d, J = 7.8 Hz, 1H), 7.84 (t, J = 8.2 Hz, 1H), 7.73 (d, J = 8.2 Hz, 1H), 7.52 (t, J = 7.1 Hz, 1H), 7.39 (t, J = 8.9 Hz, 2H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 162.2, 150.7, 150.3, 148.3, 140.0, 134.8, 127.8, 127.5, 126.0, 121.7, 121.5 ppm. ^{19}F NMR (471 MHz, DMSO-d_6) δ -108.86 ppm.



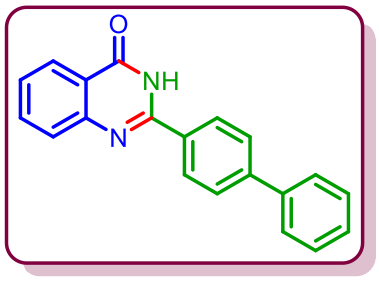
2-(4-aminophenyl)quinazolin-4(3H)-one (Compound-5k): Following the general procedure, the titled compound was isolated as yellow solid (26.1 mg, 0.110 mmol, 44% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.07 (s, 1H), 8.08 (d, J = 7.9 Hz, 1H), 7.96 (d, J = 8.4 Hz, 2H), 7.76 (t, J = 7.6 Hz, 1H), 7.62 (d, J = 8.1 Hz, 1H), 7.40 (t, J = 7.5 Hz, 1H), 6.63 (d, J = 8.6 Hz, 2H), 5.84 (s, 2H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 162.4, 152.5, 152.2, 149.4, 134.4, 129.2, 127.0, 125.8, 125.3, 120.3, 118.8, 113.1 ppm. HRMS (ESI) *m/z*: $[M + H]^+$: Calcd. for $C_{14}H_{11}N_3O$ 238.0910; Found 238.0911.



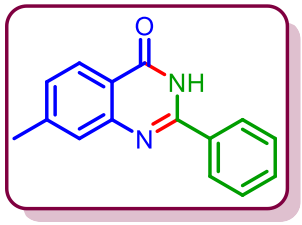
2-(4-bromophenyl)quinazolin-4(3H)-one (Compound-5l):[6] Following the general procedure, the titled compound was isolated as white solid (34.6 mg, 0.115 mmol, 46% yield).^{1}H NMR (400 MHz, DMSO-d_6) δ 12.59 (s, 1H), 8.16-8.11 (m, 3H), 7.85 (t, J = 7.9 Hz, 1H), 7.77-7.73 (m, 3H), 7.54 (t, J = 7.8 Hz, 1H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 162.3, 148.6, 134.7, 131.7, 129.9, 128.7, 127.8, 127.5, 126.8, 126.6, 125.9, 121.0 ppm.



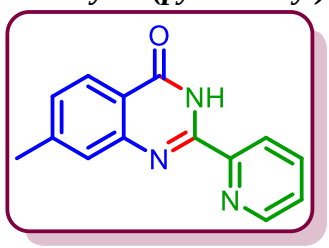
2-([1,1'-biphenyl]-4-yl)quinazolin-4(3H)-one (Compound-5m):[6] Following the general procedure, the titled compound was isolated as white solid (41.0 mg, 0.137 mmol, 55% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.57 (s, 1H), 8.64 (s, 1H), 8.30 (d, J = 8.4 Hz, 1H), 8.17 (d, J = 7.9 Hz, 1H), 7.88-7.75 (m, 5H), 7.55-7.50 (m, 2H), 7.44-7.41 (m, 1H), 6.55 (s, 2H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 162.5, 152.2, 149.8, 143.0, 139.1, 134.8, 131.7, 129.2, 128.5, 128.3, 127.5, 127.0, 126.9, 126.7, 126.0, 121.1, 115.8 ppm.



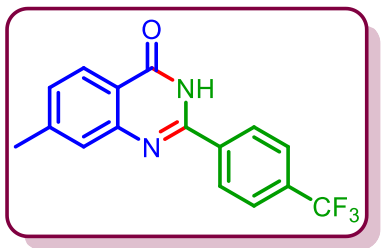
7-methyl-2-phenylquinazolin-4(3H)-one (Compound-5n):[9] Following the general procedure, the titled compound was isolated as white solid (54.3 mg, 0.230 mmol, 92% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.43 (s, 1H), 8.17 (d, J = 9.8 Hz, 2H), 8.03 (d, J = 8.1 Hz, 1H), 7.60-7.52 (m, 4H), 7.33 (d, J = 8.1 Hz, 1H), 2.46 (s, 3H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 162.1, 152.3, 148.9, 145.1, 132.8, 131.3, 128.6, 128.0, 127.7, 127.2, 125.7, 118.6, 21.4 ppm.



7-methyl-2-(pyridin-2-yl)quinazolin-4(3H)-one (Compound-5o): Following the general procedure, the titled compound was isolated as white solid (52.8 mg, 0.222 mmol, 89% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.67 (s, 1H), 8.75 (d, J = 5.9 Hz, 1H), 8.43 (d, J = 7.9 Hz, 1H), 8.09-8.05 (m, 2H), 7.67-7.64 (m, 1H), 7.60 (s, 1H), 7.39 (d, J = 8.1 Hz, 1H), 2.48 (s, 3H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 160.6, 149.9, 149.0, 148.7, 148.5, 145.2, 138.0, 128.7, 127.4, 126.5, 125.9, 122.0, 119.6, 21.3 ppm. HRMS (ESI) *m/z*: [M + H]$^{+}$: Calcd. for $C_{14}H_{12}N_2O$ 238.0936; Found 238.0926.



7-methyl-2-(4-(trifluoromethyl)phenyl)quinazolin-4(3H)-one (Compound-5p): Following the general procedure, the titled compound was isolated as white solid (50.9 mg, 0.167 mmol, 67% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.65 (s, 1H), 8.35 (d, J = 8.2 Hz, 2H), 8.05 (d, J = 7.9 Hz, 1H), 7.91 (d, J = 7.9 Hz, 2H), 7.58 (s, 1H), 7.38 (d, J = 8.1 Hz, 1H), 2.47 (s, 3H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 162.1, 151.2, 145.3, 136.7, 128.7, 128.6, 127.3, 125.8, 125.5, 125.5, 125.3, 122.6, 118.8, 115.7, 21.4 ppm. ^{19}F NMR (471 MHz, DMSO-d_6) δ -61.03 ppm.



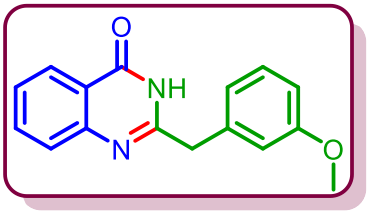
8-amino-2-phenylquinazolin-4(3H)-one (Compound-5q): Following the general procedure, the titled compound was isolated as white solid (49.8 mg, 0.209 mmol, 84% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.32 (s, 1H), 8.30 (d, J = 8.2 Hz, 2H), 7.57-7.50 (m, 3H), 7.28 (d, J = 7.8 Hz, 1H), 7.19 (t, J = 7.8 Hz, 1H), 7.00 (d, J = 9.3 Hz, 1H), 5.86 (s, 2H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 162.6, 149.0, 145.1, 135.6, 132.8, 131.0, 128.5, 127.6, 127.2, 121.2, 115.7, 111.5 ppm. HRMS (ESI) *m/z*: [M + Na]$^{+}$: Calcd. for $C_{14}H_{11}N_3ONa$ 260.0799; Found 260.0793.

7-nitro-2-phenylquinazolin-4(3H)-one (Compound-5r):[10] Following the general procedure, the titled compound was isolated as yellow solid (31.4 mg, 0.118 mmol, 47% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.42 (s, 1H), 8.36 (d, J = 8.7 Hz, 2H), 8.21 (d, J = 6.7 Hz, 3H), 7.63-7.55 (m, 3H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 161.8, 155.0, 151.3, 149.3, 132.4, 131.9, 128.7, 128.2, 128.1, 125.3, 122.3, 119.9 ppm. HRMS (ESI) *m/z*: [M + NH_4]$^{+}$: Calcd. for $C_{14}H_{13}N_4O_3$ 285.0988; Found 285.0998.

6-methoxy-2-phenylquinazolin-4(3H)-one (Compound-5s):[11] Following the general procedure, the titled compound was isolated as white solid (47.3 mg, 0.187 mmol, 75% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.48 (s, 1H), 8.17-8.14 (m, 2H), 7.70 (d, J = 8.9 Hz, 1H), 7.57-7.52 (m, 4H), 7.44 (dd, J = 8.9, 3.0 Hz, 1H), 3.89 (s, 3H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 162.1, 157.8, 150.2, 143.2, 132.8, 131.1, 129.3, 128.6, 127.5, 124.1, 121.8, 105.9, 55.7 ppm. HRMS (ESI) *m/z*: [M + H]$^{+}$: Calcd. for $C_{15}H_{13}N_2O_2$ 253.0977; Found 253.0977.

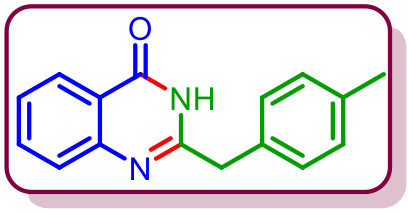
2-benzylquinazolin-4(3H)-one (Compound-6a):[6] Following the general procedure, the titled compound was isolated as white solid (40.2 mg, 0.170 mmol, 68% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.42 (s, 1H), 8.07 (d, J = 6.5 Hz, 1H), 7.77 (t, J = 7.7 Hz, 1H), 7.60 (d, J = 8.2 Hz, 1H), 7.46 (t, J = 7.5 Hz, 1H), 7.38 (d, J = 7.1 Hz, 2H), 7.32 (t, J = 7.3 Hz, 2H), 7.24 (t, J = 7.2 Hz, 1H), 3.93 (s, 2H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 161.9, 156.0, 148.9, 136.6, 134.4, 128.9, 128.5, 127.0, 126.8, 126.3, 125.7, 120.8, 40.8 ppm.

2-(3-methoxybenzyl)quinazolin-4(3H)-one (Compound-6b):[12] Following the general procedure, the titled compound was isolated as white solid (43.3 mg, 0.162 mmol, 65% yield).



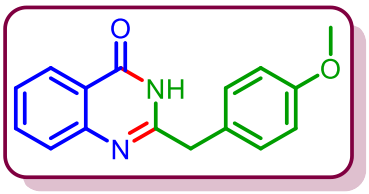
^{1}H NMR (400 MHz, DMSO-d_6) δ 12.40 (s, 1H), 8.07 (d, J = 7.8 Hz, 1H), 7.77 (t, J = 7.6 Hz, 1H), 7.61 (d, J = 8.1 Hz, 1H), 7.46 (t, J = 7.6 Hz, 1H), 7.22 (t, J = 8.0 Hz, 1H), 6.97 (s, 1H), 6.93 (d, J = 7.6 Hz, 1H), 6.81 (d, J = 8.2 Hz, 1H), 3.89 (s, 2H), 3.72 (s, 3H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 162.1, 159.4, 156.1, 149.0, 138.1, 134.7, 129.8, 127.1, 126.5, 125.9, 121.2, 120.8, 115.0, 112.3, 55.2, 40.9 ppm.

2-(4-methylbenzyl)quinazolin-4(3H)-one (Compound-6c): Following the general procedure,



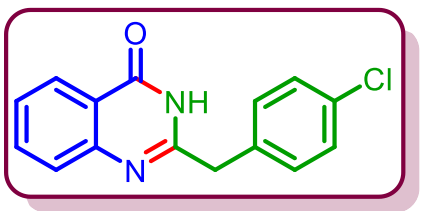
the titled compound was isolated as white solid (40.0 mg, 0.160 mmol, 64% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.38 (s, 1H), 8.06 (d, J = 7.9 Hz, 1H), 7.76 (t, J = 7.6 Hz, 1H), 7.60 (d, J = 8.2 Hz, 1H), 7.46 (t, J = 7.5 Hz, 1H), 7.26 (d, J = 8.1 Hz, 2H), 7.12 (d, J = 8.1 Hz, 2H), 3.87 (s, 2H), 2.24 (s, 3H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 162.0, 156.3, 149.0, 136.0, 134.5, 133.5, 129.1, 128.8, 127.0, 126.3, 125.8, 120.8, 40.5, 20.7 ppm. HRMS (ESI) *m/z*: $[M + H]^+$: Calcd. for $C_{16}H_{15}N_2O$ 251.1195; Found 251.1194.

2-(4-methoxybenzyl)quinazolin-4(3H)-one (Compound-6d):[13] Following the general

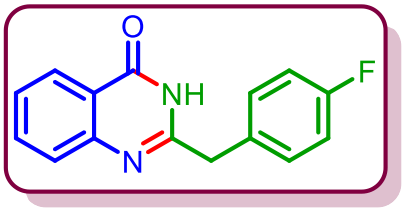


procedure, the titled compound was isolated as white solid (32.6 mg, 0.122 mmol, 49% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.34 (s, 1H), 8.06 (d, J = 8.6 Hz, 1H), 7.76 (t, J = 8.6 Hz, 1H), 7.60 (d, J = 8.1 Hz, 1H), 7.45 (t, J = 8.6 Hz, 1H), 7.30 (d, J = 8.9 Hz, 2H), 6.88 (d, J = 8.8 Hz, 2H), 3.85 (s, 2H), 3.71 (s, 3H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 161.9, 158.2, 156.4, 149.0, 142.7, 134.5, 130.0, 128.4, 126.9, 126.2, 125.7, 114.0, 55.1 ppm.

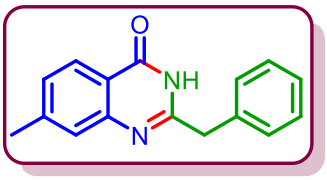
2-(4-chlorobenzyl)quinazolin-4(3H)-one (Compound-6e):[14] Following the general procedure,



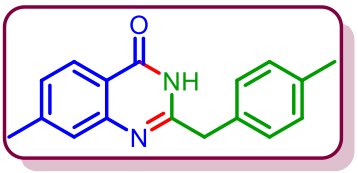
the titled compound was isolated as white solid (42.6 mg, 0.157 mmol, 63% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.40 (s, 1H), 8.07 (d, J = 9.7 Hz, 1H), 7.78-7.74 (m, 1H), 7.58 (d, J = 7.2 Hz, 1H), 7.48-7.44 (m, 1H), 7.41-7.36 (m, 4H), 3.93 (s, 2H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 161.9, 155.6, 148.8, 135.5, 134.4, 131.6, 130.9, 128.4, 126.9, 126.3, 125.7, 120.8, 40.1 ppm.

2-(4-fluorobenzyl)quinazolin-4(3H)-one (Compound-6f):[14] Following the general procedure, 

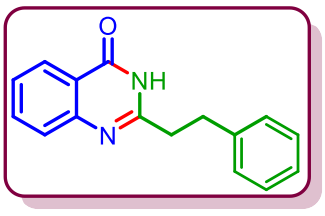
the titled compound was isolated as white solid (38.1 mg, 0.150 mmol, 60% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.06 (d, J = 7.9 Hz, 1H), 7.74 (t, J = 6.8 Hz, 1H), 7.57 (d, J = 8.1 Hz, 1H), 7.45-7.40 (m, 3H), 7.13 (t, J = 8.9 Hz, 2H), 3.92 (s, 2H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 162.4, 160.0, 134.2, 133.0, 130.9, 130.8, 126.8, 126.1, 125.8, 120.8, 115.3, 115.1, 40.1 ppm. ^{19}F NMR (471 MHz, DMSO-d_6) δ -116.10 ppm.

2-benzyl-7-methylquinazolin-4(3H)-one (Compound-6g): Following the general procedure, 

the titled compound was isolated as white solid (51.3 mg, 0.205 mmol, 82% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.31 (s, 1H), 7.96 (d, J = 8.2 Hz, 1H), 7.45-7.22 (m, 7H), 3.93 (s, 2H), 2.42 (s, 3H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 161.8, 156.0, 149.1, 144.9, 136.7, 129.9, 128.9, 128.5, 127.6, 126.8, 126.7, 125.6, 118.4, 40.8, 21.3 ppm. HRMS (ESI) m/z: [M + H]$^{+}$: Calcd. for $C_{16}H_{15}N_2O$ 251.1140; Found 251.1149.

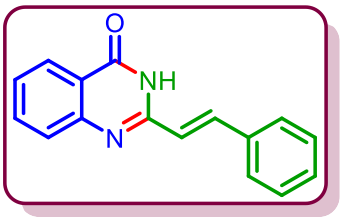
7-methyl-2-(4-methylbenzyl)quinazolin-4(3H)-one (Compound 6h): Following the general 

procedure, the titled compound was isolated as white solid (56.2 mg, 0.212 mmol, 85% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.27 (s, 1H), 7.94 (d, J = 8.1 Hz, 1H), 7.40 (s, 1H), 7.26 (t, J = 7.8 Hz, 3H), 7.11 (d, J = 7.2 Hz, 2H), 3.85 (s, 2H), 2.41 (s, 3H), 2.24 (s, 3H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 161.9, 156.3, 149.1, 144.9, 135.9, 133.6, 129.1, 128.8, 127.6, 126.6, 125.6, 118.3, 40.4, 21.4, 20.7 ppm. HRMS (ESI) m/z: [M + H]$^{+}$: Calcd. for $C_{17}H_{17}N_2O$ 265.1323; Found 265.1314.

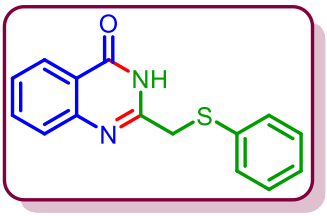
2-phenethylquinazolin-4(3H)-one (Compound-6i):[9] Following the general procedure, the 

titled compound was isolated as white solid (43.8 mg, 0.175 mmol, 70% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.24 (s, 1H), 8.08 (dd, J = 7.9, 1.7 Hz, 1H), 7.79-7.75 (m, 1H), 7.62 (d, J = 7.2 Hz, 1H), 7.48-7.44 (m, 1H), 7.28-7.27 (m, 4H), 7.20-7.16 (m, 1H), 3.07-3.03 (m, 2H), 2.92-2.88 (m, 2H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 161.8, 156.6, 148.9, 140.8, 134.3, 128.4, 128.3, 126.8, 126.1, 126.0, 125.7, 120.9, 36.3, 32.5 ppm.

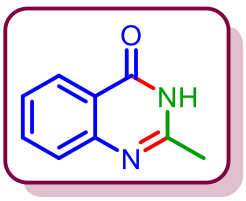
(E)-2-styrylquinazolin-4(3H)-one (Compound-6j):[9] Following the general procedure, the titled compound was isolated as white solid (37.2 mg, 0.150 mmol, 60% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.35 (s, 1H), 8.11 (d, J = 7.9 Hz, 1H), 7.95 (d, J = 16.3 Hz, 1H), 7.80 (t, J = 7.6 Hz, 1H), 7.69-7.65 (m, 3H), 7.50-7.39 (m, 4H), 7.01 (d, J = 16.3 Hz, 1H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 162.1, 161.8, 151.5, 138.3, 135.0, 134.6, 129.8, 129.1, 129.1, 127.7, 127.1, 126.3, 125.9, 121.1 ppm.



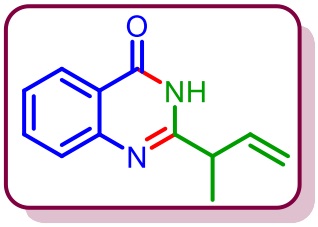
2-((phenylthio)methyl)quinazolin-4(3H)-one (Compound-6k): Following the general procedure, the titled compound was isolated as white solid (47.8 mg, 0.178 mmol, 71% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.39 (s, 1H), 8.09 (dd, J = 7.9, 1.6 Hz, 1H), 7.79-7.75 (m, 1H), 7.58 (d, J = 9.5 Hz, 1H), 7.50-7.44 (m, 3H), 7.30 (t, J = 7.6 Hz, 2H), 7.22-7.18 (m, 1H), 4.14 (s, 2H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 161.6, 153.9, 148.4, 135.0, 134.5, 129.1, 129.0, 127.0, 126.6, 126.5, 125.8, 120.9, 36.4 ppm. HRMS (ESI) *m/z*: [M + H]$^{+}$: Calcd. for $C_{15}H_{13}N_2OS$ 269.0749; Found 269.0748.



2-methylquinazolin-4(3H)-one (Compound-8a):[8] Following the general procedure, the titled compound was isolated as light-yellow solid (28.4 mg, 0.178 mmol, 71% yield). ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.19 (s, 1H), 8.06 (dd, J = 7.9, 1.8 Hz, 1H), 7.77-7.74 (m, 1H), 7.56 (d, J = 7.3 Hz, 1H), 7.46-7.43 (m, 1H), 2.34 (s, 3H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 161.7, 154.3, 149.0, 134.3, 126.6, 125.9, 125.7, 120.6, 21.4 ppm. HRMS (ESI) *m/z*: [M + H]$^{+}$: Calcd. for $C_9H_9N_2O$ 161.0714; Found 161.0717.



2-(but-3-en-2-yl)quinazolin-4(3H)-one (Compound-8b): Following the general procedure, the titled compound was isolated as white solid (27.53 mg, 0.137 mmol, 55% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.93 (s, 1H), 8.08 (d, J = 7.8 Hz, 1H), 7.79-7.76 (m, 1H), 7.62 (d, J = 8.2 Hz, 1H), 7.46 (t, J = 7.5 Hz, 1H), 6.66-6.61 (m, 1H), 2.03 (s, 3H), 1.85-1.82 (m, 3H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 162.1, 154.3, 148.7, 134.5, 131.8, 130.3, 127.4, 126.3, 125.8, 120.9, 14.5, 13.2 ppm. HRMS (ESI) *m/z*: [M + H]$^{+}$: Calcd. for $C_{12}H_{13}N_2O$ 201.1027; Found 201.1029.



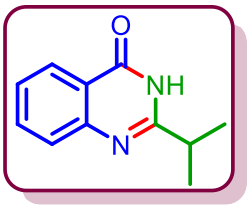
4-(4-oxo-3,4-dihydroquinazolin-2-yl)butanenitrile (Compound-8c): Following the general procedure, the titled compound was isolated as white solid (36.23 mg, 0.170 mmol, 68% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.20 (s, 1H), 8.08 (d, J = 8.1 Hz, 1H), 7.77 (t, J = 7.7 Hz, 1H), 7.60 (d, J = 8.2 Hz, 1H), 7.46 (t, J = 7.4 Hz, 1H), 2.72 (t, J = 7.5 Hz, 2H), 2.62 (t, J = 7.2 Hz, 2H), 2.09-2.01 (m, 2H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 161.7, 155.8, 148.7, 134.3, 126.9, 126.1, 125.7, 121.0, 120.3, 32.9, 22.0, 15.7 ppm. HRMS (ESI) *m/z*: [M + H]$^{+}$: Calcd. for $C_{12}H_{12}N_3O$ 214.0980; Found 214.0981.

2-nonylquinazolin-4(3H)-one (Compound-8d):[15] Following the general procedure, the titled compound was isolated as white solid (41.67 mg, 0.153 mmol, 61% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.14 (s, 1H), 8.07 (d, J = 8.2 Hz, 1H), 7.76 (t, J = 8.3 Hz, 1H), 7.58 (d, J = 8.3 Hz, 1H), 7.44 (t, J = 7.8 Hz, 1H), 2.58 (t, J = 7.9 Hz, 2H), 1.72-1.69 (m, 2H), 1.28 (s, 3H), 1.22 (s, 9H), 0.85-0.81 (br., 3H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 161.9, 157.5, 149.0, 134.3, 126.8, 125.9, 125.7, 120.8, 34.5, 31.3, 28.8, 28.7, 28.7, 28.5, 26.8, 22.1, 14.0 ppm. HRMS (ESI) *m/z*: [M + Na]$^{+}$: Calcd. for $C_{17}H_{24}N_2ONa$ 295.1786; Found 295.1778.

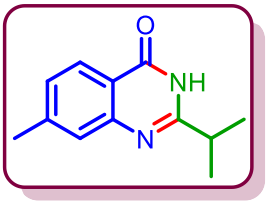
2-ethylquinazolin-4(3H)-one (Compound-8e):[16] Following the general procedure, the titled compound was isolated as white solid (27.4 mg, 0.158 mmol, 63% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.17 (s, 1H), 8.08 (d, J = 8.1 Hz, 1H), 7.77 (t, J = 7.7 Hz, 1H), 7.60 (d, J = 8.1 Hz, 1H), 7.46 (t, J = 7.4 Hz, 1H), 2.65-2.60 (m, 2H), 1.24 (t, J = 7.6 Hz, 3H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 161.8, 158.4, 149.0, 134.3, 126.8, 125.9, 125.7, 120.8, 27.9, 11.3 ppm. HRMS (ESI) *m/z*: [M + Na]$^{+}$: Calcd. for $C_{10}H_{10}N_2ONa$ 197.0690; Found 197.0681.

2-cyclopentylquinazolin-4(3H)-one (Compound-8f):[6] Following the general procedure, the titled compound was isolated as white solid (33.2 mg, 0.155 mmol, 62% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.06 (d, J = 7.9 Hz, 1H), 7.75 (d, J = 8.1 Hz, 1H), 7.58 (d, J = 8.1 Hz, 1H), 7.44 (m, 1H), 3.06-2.98 (m, 1H), 1.96 (br., 2H), 1.88 (br., 2H), 1.74 (br., 2H), 1.59 (br., 1H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 162.2, 160.7, 148.8, 134.5, 126.9, 126.1, 125.8, 120.9, 43.9, 31.0, 25.5 ppm. HRMS (ESI) *m/z*: [M + H]$^{+}$: Calcd. for $C_{13}H_{15}N_2O$ 215.1184; Found 251.1170.

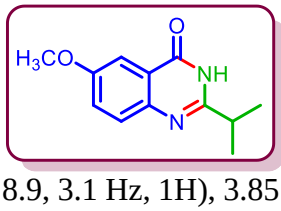
2-isopropylquinazolin-4(3H)-one (Compound-8g):[17] Following the general procedure, the titled compound was isolated as white solid (33.8 mg, 0.180 mmol, 72% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.12 (s, 1H), 8.08 (d, J = 7.8 Hz, 1H), 7.76 (t, J = 7.6 Hz, 1H), 7.60 (d, J = 8.2 Hz, 1H), 7.45 (t, J = 7.5 Hz, 1H), 2.93-2.83 (m, 1H), 1.25 (d, J = 6.8 Hz, 6H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 162.0, 161.6, 148.9, 134.3, 127.0, 126.0, 125.7, 121.0, 33.3, 20.4 ppm. HRMS (ESI) *m/z*: $[M + H]^+$: Calcd. for $C_{11}H_{13}N_2O$ 189.1030; Found 189.1020.



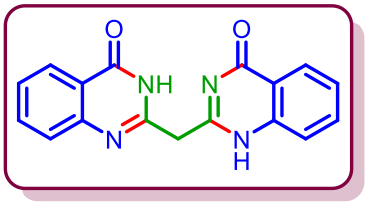
2-isopropyl-7-methylquinazolin-4(3H)-one (Compound-8h): Following the general procedure, the titled compound was isolated as white solid (44 mg, 0.217 mmol, 87% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.00 (s, 1H), 7.95 (d, J = 8.1 Hz, 1H), 7.41 (s, 1H), 7.26 (d, J = 9.9 Hz, 1H), 2.90-2.80 (m, 1H), 2.42 (s, 3H), 1.24 (d, J = 6.8 Hz, 6H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 161.9, 161.6, 149.0, 144.7, 127.4, 126.7, 125.5, 118.5, 33.3, 21.3, 20.4 ppm. HRMS (ESI) *m/z*: $[M + H]^+$: Calcd. for $C_{12}H_{15}N_2O$ 203.1184; Found 203.1170.



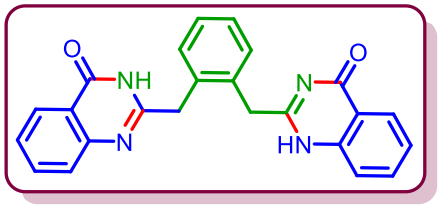
2-isopropyl-6-methoxyquinazolin-4(3H)-one (Compound-8i): Following the general procedure, the titled compound was isolated as white solid (44.2 mg, 0.203 mmol, 81% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.06 (s, 1H), 7.55 (d, J = 8.9 Hz, 1H), 7.47 (d, J = 3.1 Hz, 2H), 7.36 (dd, J = 8.9, 3.1 Hz, 1H), 3.85 (s, 3H), 2.89-2.82 (m, 1H), 1.24 (d, J = 6.8 Hz, 6H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 161.8, 159.2, 157.2, 143.3, 128.6, 123.7, 121.6, 105.7, 55.6, 33.1, 20.4 ppm. HRMS (ESI) *m/z*: $[M + H]^+$: Calcd. for $C_{12}H_{15}N_2O_2$ 219.1134; Found 219.1126.



2-((4-oxo-1,4-dihydroquinazolin-2-yl)methyl)quinazolin-4(3H)-one (Compound-8j): Following the general procedure, the titled compound was isolated as white solid (21.3 mg, 0.069 mmol, 56% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.39 (s, 1H), 8.51 (d, J = 8.6 Hz, 1H), 8.00 (d, J = 8.1 Hz, 1H), 7.67-7.60 (m, 2H), 7.27-7.19 (m, 2H), 6.80 (d, J = 8.4 Hz, 1H), 6.64 (t, J = 7.6 Hz, 1H), 6.56 (s, 1H), 3.88 (s, 2H) ppm. ^{13}C NMR (101 MHz, DMSO-d_6) δ 168.2, 167.5, 150.5, 140.6, 134.3, 132.9, 130.7, 127.4, 123.0, 120.8, 117.1, 116.8, 115.3, 113.9, 52.7 ppm. HRMS (ESI) *m/z*: $[M + NH_4]^+$: Calcd. for $C_{19}H_{20}N_5O_2$ 350.1617; Found 350.1686.

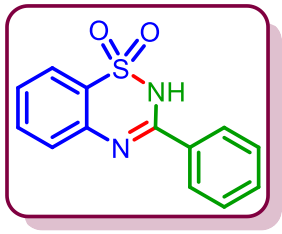


2-((4-oxo-1,4-dihydroquinazolin-2-yl)methyl)quinazolin-4(3H)-one (Compound-8k):



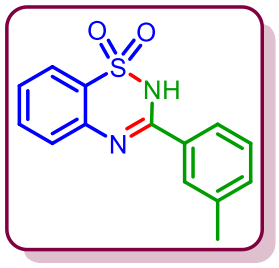
Following the general procedure, the titled compound was isolated as white solid (54.2 mg, 0.137 mmol, 55% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.39 (s, 1H), 8.52 (d, J = 8.3 Hz, 1H), 8.00 (d, J = 7.1 Hz, 1H), 7.67-7.61 (m, 2H), 7.27-7.19 (m, 3H), 6.80 (d, J = 8.2 Hz, 1H), 6.65 (t, J = 7.4 Hz, 1H), 6.56 (s, 2H), 3.88 (s, 3H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 168.1, 167.4, 150.5, 140.6, 134.2, 132.8, 130.7, 127.4, 122.9, 120.7, 117.1, 116.8, 115.2, 113.9, 52.6 ppm. HRMS (ESI) *m/z*: [M + NH_4]$^{+}$: Calcd. for $C_{24}H_{22}N_5O_2$ 412.1821; Found 412.1828.

3-phenyl-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (Compound-9a):[6] Following the general



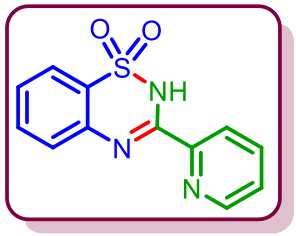
procedure, the titled compound was isolated as white solid (45.8 mg, 0.117 mmol, 71% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.21 (s, 1H), 8.05 (d, J = 7.5 Hz, 2H), 7.86 (d, J = 7.9 Hz, 1H), 7.76-7.69 (m, 2H), 7.65-7.61 (m, 3H), 7.51 (t, J = 7.6 Hz, 1H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 155.1, 135.8, 133.4, 133.1, 132.1, 129.1, 128.5, 127.0, 123.6, 121.7, 118.7 ppm.

3-(m-tolyl)-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (Compound-9b):[18] Following the



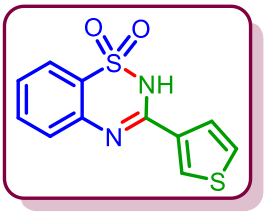
general procedure, the titled compound was isolated as white solid (38.8 mg, 0.143 mmol, 57% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87-7.84 (m, 3H), 7.76-7.69 (m, 1H), 7.64 (d, J = 8.3 Hz, 1H), 7.52-7.50 (m, 3H) ppm. ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 154.9, 138.4, 135.5, 133.5, 133.1, 131.8, 128.8, 128.6, 126.7, 125.4, 123.3, 121.5, 118.4, 20.9 ppm.

3-(pyridin-2-yl)-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (Compound-9c): Following the



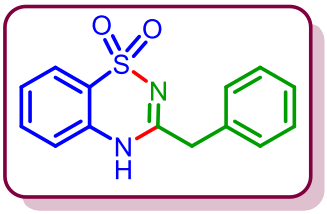
general procedure, the titled compound was isolated as white solid (40.2 mg, 0.155 mmol, 62% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.58 (s, 1H), 8.85 (d, J = 4.8 Hz, 1H), 8.32 (d, J = 7.8 Hz, 1H), 8.15-8.11 (m, 1H), 7.95 (d, J = 7.7 Hz, 1H), 7.88 (d, J = 7.9 Hz, 1H), 7.78-7.71 (m, 2H), 7.52 (t, J = 7.6 Hz, 1H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 151.8, 149.2, 147.6, 138.6, 135.0, 133.2, 127.8, 127.0, 123.3, 123.1, 121.7, 119.2 ppm. HRMS (ESI) *m/z*: [M + NH_4]$^{+}$: Calcd. for $C_{12}H_{15}N_4O_2S$ 279.0915; Found 279.0914.

3-(thiophen-3-yl)-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (Compound-9d):[18] Following



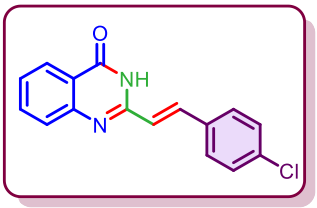
the general procedure, the titled compound was isolated as white solid (51.5 mg, 0.195 mmol, 78% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.03 (s, 1H), 8.58 (s, 1H), 7.84 (d, J = 7.8 Hz, 1H), 7.77-7.70 (m, 3H), 7.62 (d, J = 10.9 Hz, 1H), 7.48 (t, J = 8.9 Hz, 1H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 150.1, 135.5, 134.0, 133.2, 131.9, 128.2, 126.9, 126.6, 123.4, 121.6, 118.3 ppm.

3-benzyl-4H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (Compound-9e):[19] Following the general



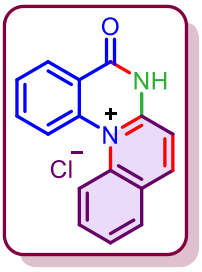
procedure, the titled compound was isolated as white solid (44.3 mg, 0.163 mmol, 65% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.47-7.37 (m, 2H), 7.33 (d, J = 7.9 Hz, 1H), 7.27 (t, J = 7.3 Hz, 1H), 7.20-7.10 (m, 4H), 6.95 (d, J = 7.7 Hz, 1H), 6.07 (br.s, 1H), 3.92 (s, 1H), 3.62 (s, 1H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 167.3, 163.3, 162.6, 139.5, 139.4, 134.8, 130.4, 129.6, 129.4, 129.0, 128.6, 128.5, 126.5, 126.4, 114.8, 45.5 ppm.

(E)-2-(4-chlorostyryl)quinazolin-4(3H)-one (Compound-11a):[2] Following the general



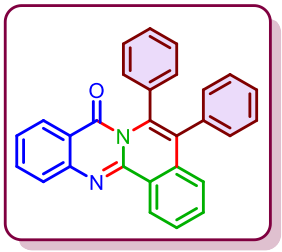
procedure, the titled compound was isolated as white solid (41 mg, 0.145 mmol, 78% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.11 (d, J = 7.9 Hz, 1H), 7.93 (d, J = 16.3 Hz, 1H), 7.81 (t, J = 7.8 Hz, 1H), 7.69-7.66 (m, 3H), 7.53-7.46 (m, 3H), 7.02 (d, J = 16.3 Hz, 1H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 161.8, 151.3, 148.9, 136.9, 134.6, 134.2, 134.0, 129.3, 129.1, 127.1, 126.4, 125.9, 121.9, 121.1 ppm.

5-oxo-5,6-dihydroquinolino[1,2-a]quinazolin-13-ium chloride (Compound-11b): Following

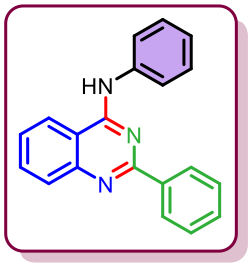


the general procedure, the titled compound was isolated as white solid (37.3 mg, 0.132 mmol, 71% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.49 (s, 1H), 8.23 (d, J = 16.0 Hz, 1H), 8.12 (dd, J = 7.9, 1.6 Hz, 1H), 7.84-7.80 (m, 2H), 7.71 (d, J = 8.3 Hz, 1H), 7.57-7.54 (m, 1H), 7.52-7.47 (m, 1H), 7.46-7.42 (m, 2H), 7.06 (d, J = 16.0 Hz, 1H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 161.7, 151.0, 148.8, 138.1, 134.6, 133.4, 132.9, 131.1, 130.1, 127.9, 127.6, 127.3, 126.5, 125.9, 124.2, 121.2 ppm. HRMS (ESI) *m/z*: $[M + H]^+$: Calcd. for $C_{16}H_{11}ClN_2Na$ 305.0434; Found 305.0408.

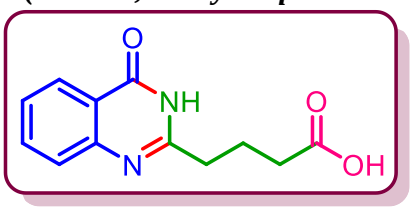
5,6-diphenyl-8H-isoquinolino[1,2-b]quinazolin-8-one (Compound-11c):[3] Following the general procedure, the titled compound was isolated as white solid (26.6 mg, 0.067 mmol, 75% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.13 (d, J = 7.9 Hz, 1H), 8.17 (d, J = 7.9 Hz, 1H), 7.89 (d, J = 8.1 Hz, 1H), 7.82 (t, J = 7.0 Hz, 1H), 7.63 (t, J = 7.4 Hz, 1H), 7.57 (t, J = 7.4 Hz, 1H), 7.41 (t, J = 7.5 Hz, 1H), 7.28 (s, 3H), 7.19 (d, J = 7.9 Hz, 1H), 7.13-7.12 (m, 3H), 7.10-7.08 (m, 4H) ppm. ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 161.4, 147.6, 147.0, 137.1, 135.6, 135.3, 134.6, 134.1, 132.1, 131.3, 128.6, 128.5, 128.2, 127.9, 127.4, 127.4, 127.3, 127.3, 127.3, 127.0, 127.0, 126.4, 125.8, 120.4 ppm. HRMS (ESI) *m/z*: [M + Na]$^{+}$: Calcd. for $C_{28}H_{18}N_2ONa$ 421.1317; Found 421.1324.



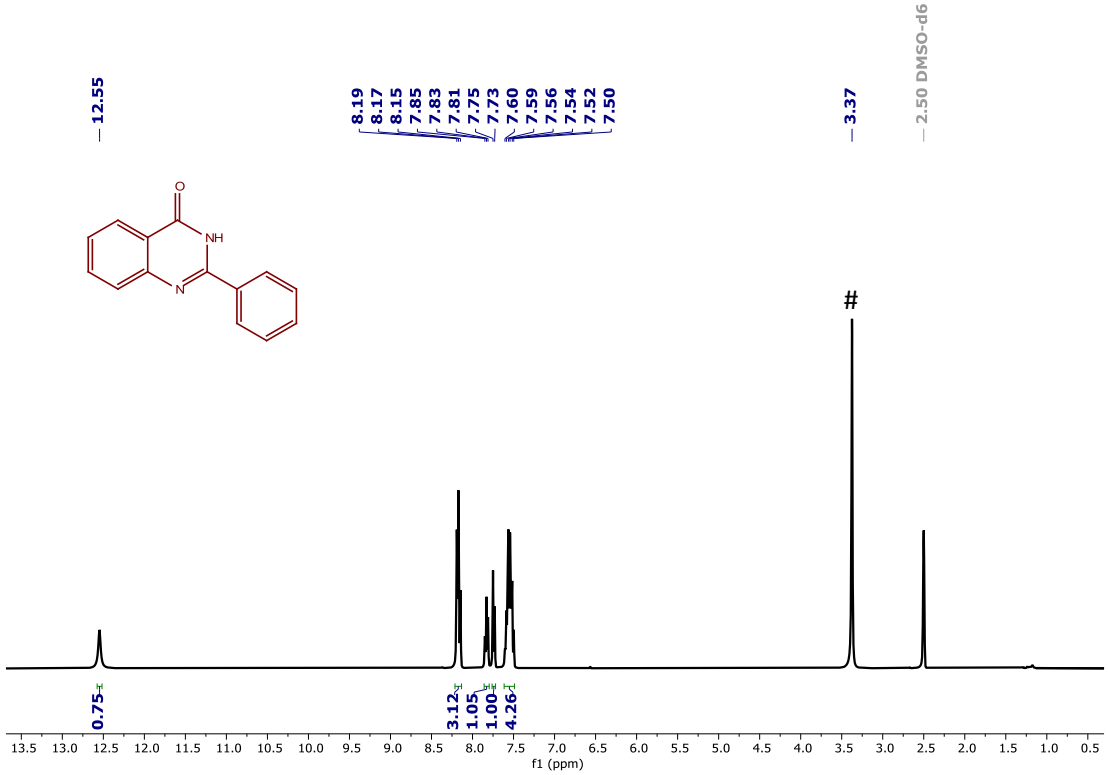
N,2-diphenylquinazolin-4-amine (Compound-11d):[4] Following the general procedure, the titled compound was isolated as white solid (52.8 mg, 0.177 mmol, 71% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.56 (dd, J = 8.1, 1.7 Hz, 2H), 8.01 (d, J = 8.4 Hz, 1H), 7.92-7.88 (m, 3H), 7.80 (t, J = 8.4 Hz, 1H), 7.55-7.46 (m, 7H), 7.20 (t, J = 8.4 Hz, 1H) ppm. ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 160.6, 157.5, 151.3, 138.9, 133.0, 130.4, 129.6, 128.7, 128.5, 126.2, 124.2, 121.5, 120.3, 114.0 ppm.



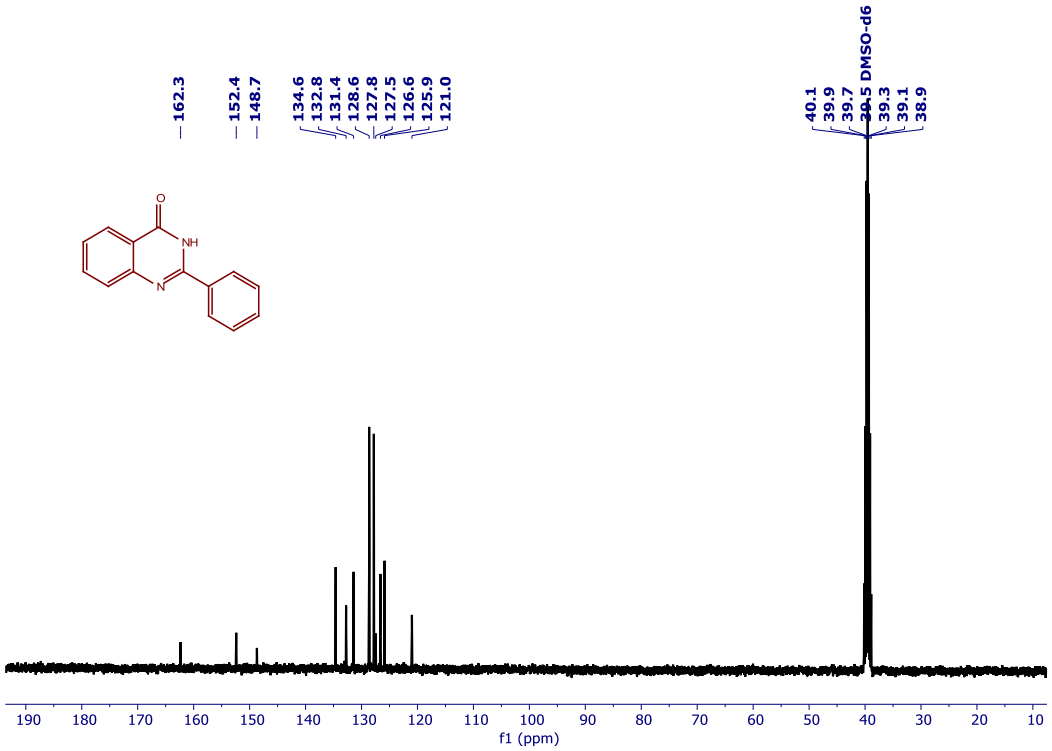
4-(4-oxo-3,4-dihydroquinazolin-2-yl)butanoic acid (Compound-11e):[20] Following the general procedure, the titled compound was isolated as white solid (17.6 mg, 0.076 mmol, 81% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.17 (s, 1H), 8.07 (d, J = 7.8 Hz, 1H), 7.76 (t, J = 7.6 Hz, 1H), 7.59 (d, J = 8.2 Hz, 1H), 7.45 (t, J = 7.6 Hz, 1H), 2.63 (t, J = 7.5 Hz, 2H), 2.31 (t, J = 7.4 Hz, 2H), 1.99-1.92 (m, 2H) ppm. ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) δ 174.2, 161.9, 156.9, 148.8, 134.3, 126.8, 126.0, 125.7, 120.9, 33.6, 32.9, 21.9 ppm. HRMS (ESI) *m/z*: [M + Na]$^{+}$: Calcd. for $C_{12}H_{12}N_2O_3Na$ 255.0746; Found 255.0735.



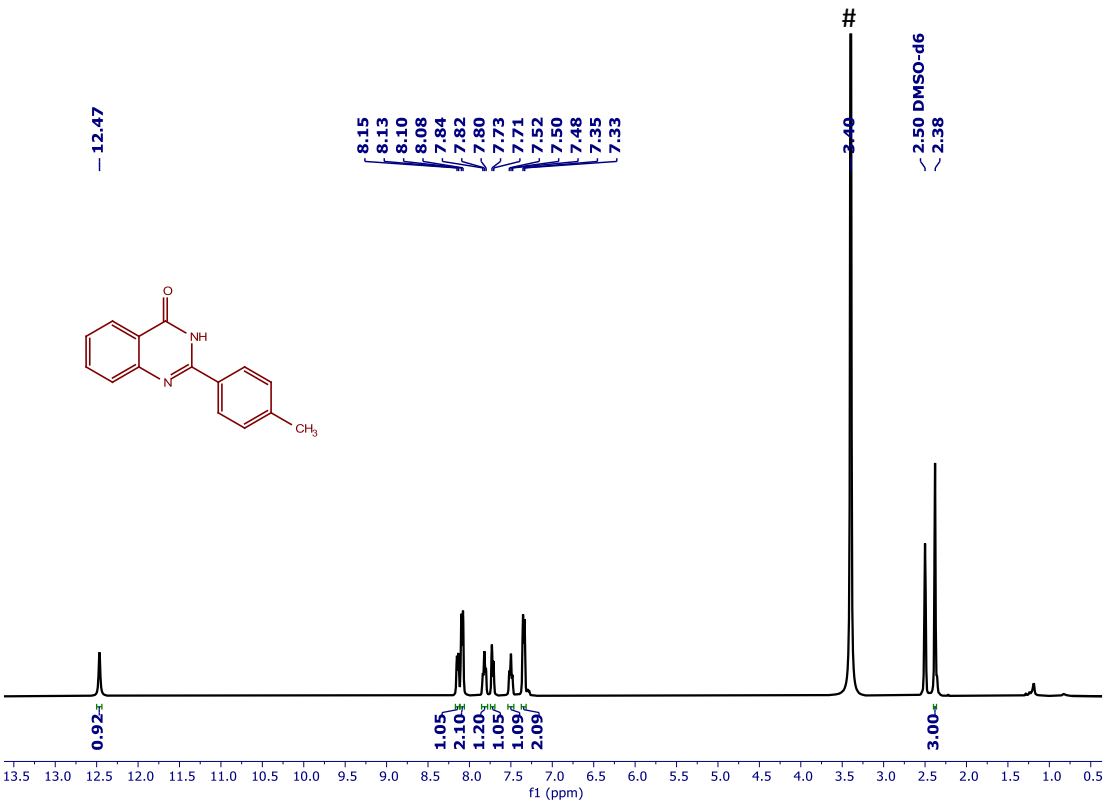
15. ^{1}H and $^{13}C\{^{1}H\}$ spectra for desired products:



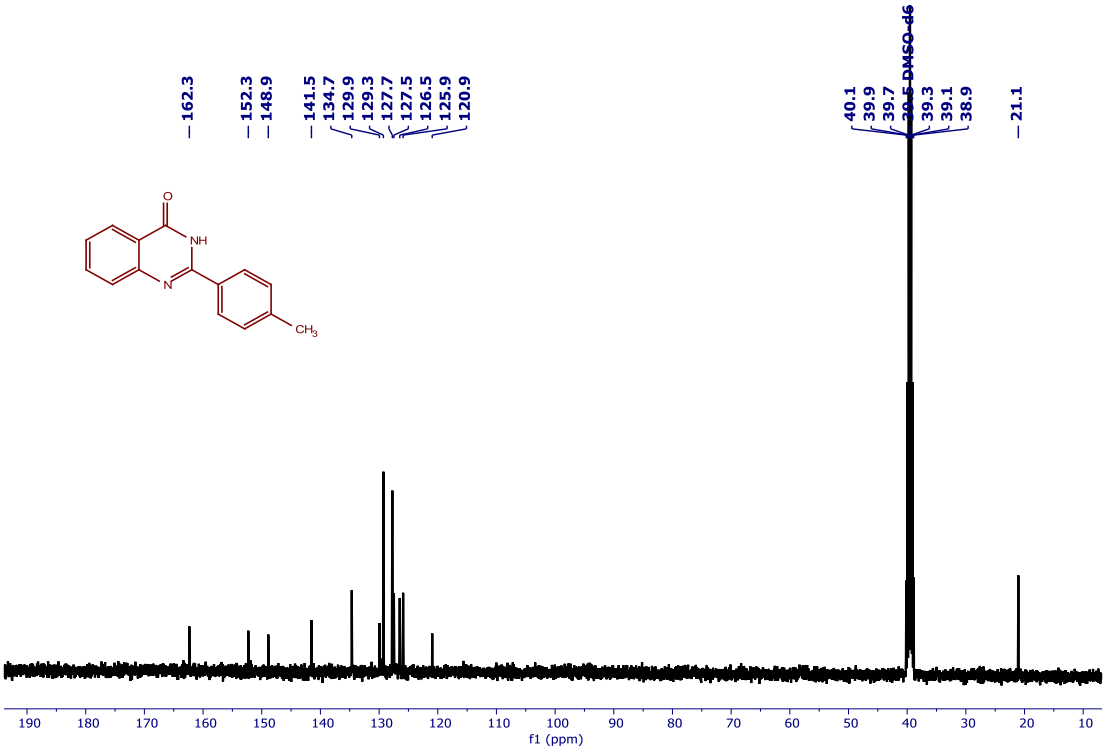
*^{1}H NMR of 2-phenylquinazolin-4(3H)-one (Compound-**5a**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



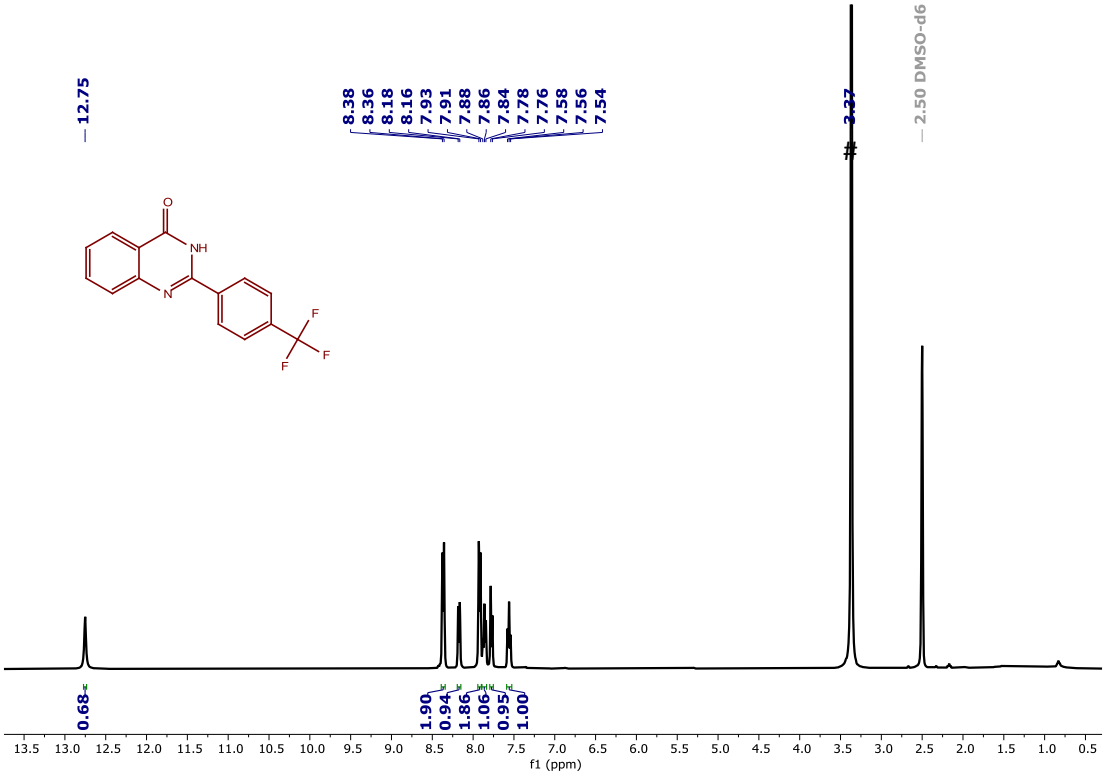
*$^{13}C\{^{1}H\}$ NMR of 2-phenylquinazolin-4(3H)-one (Compound-**5a**) in DMSO-d_6*



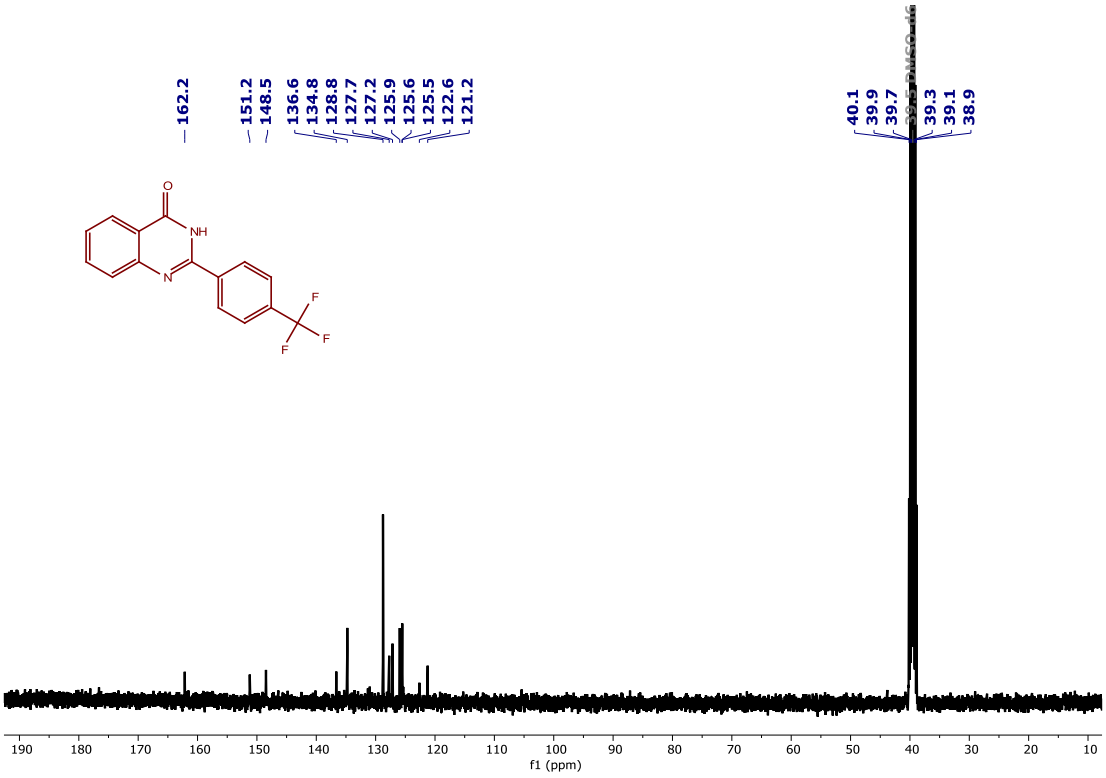
*[1]H NMR of 2-(p-tolyl)quinazolin-4(3H)-one (Compound-**5b**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



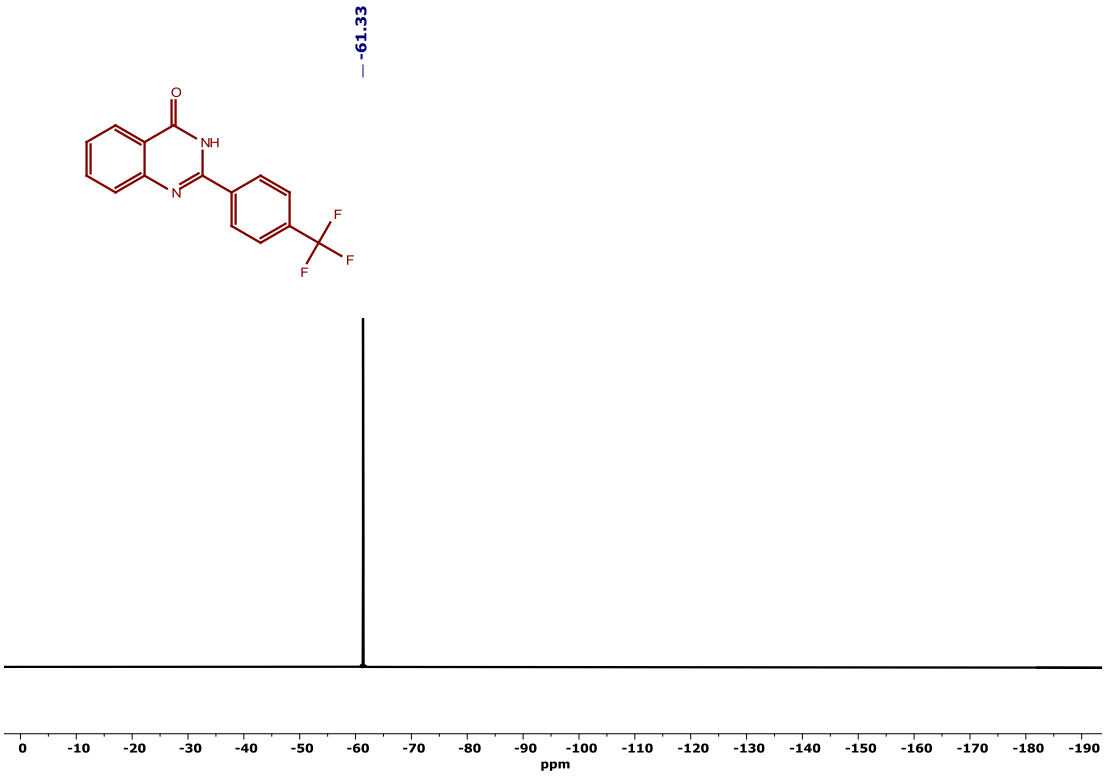
*[13]C{[1]H} NMR of 2-(p-tolyl)quinazolin-4(3H)-one (Compound-**5b**) in DMSO-d_6*



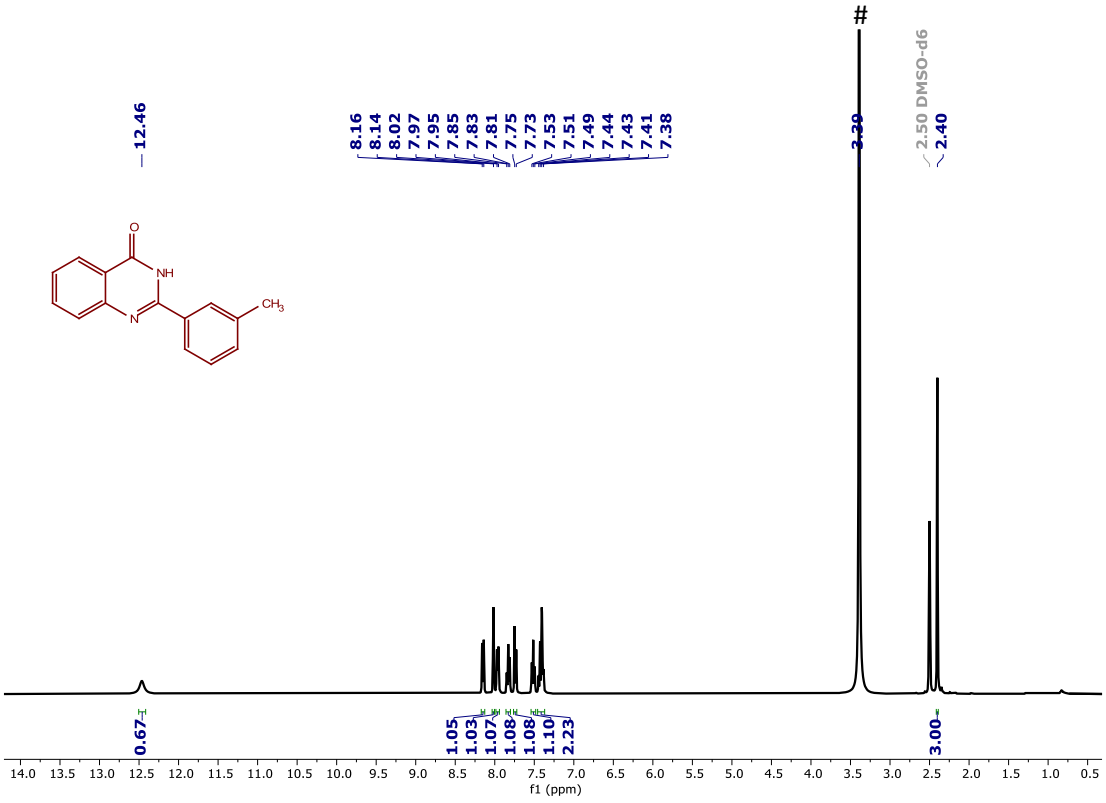
*[1]H NMR of 2-(4-(trifluoromethyl)phenyl)quinazolin-4(3H)-one (Compound-**5c**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



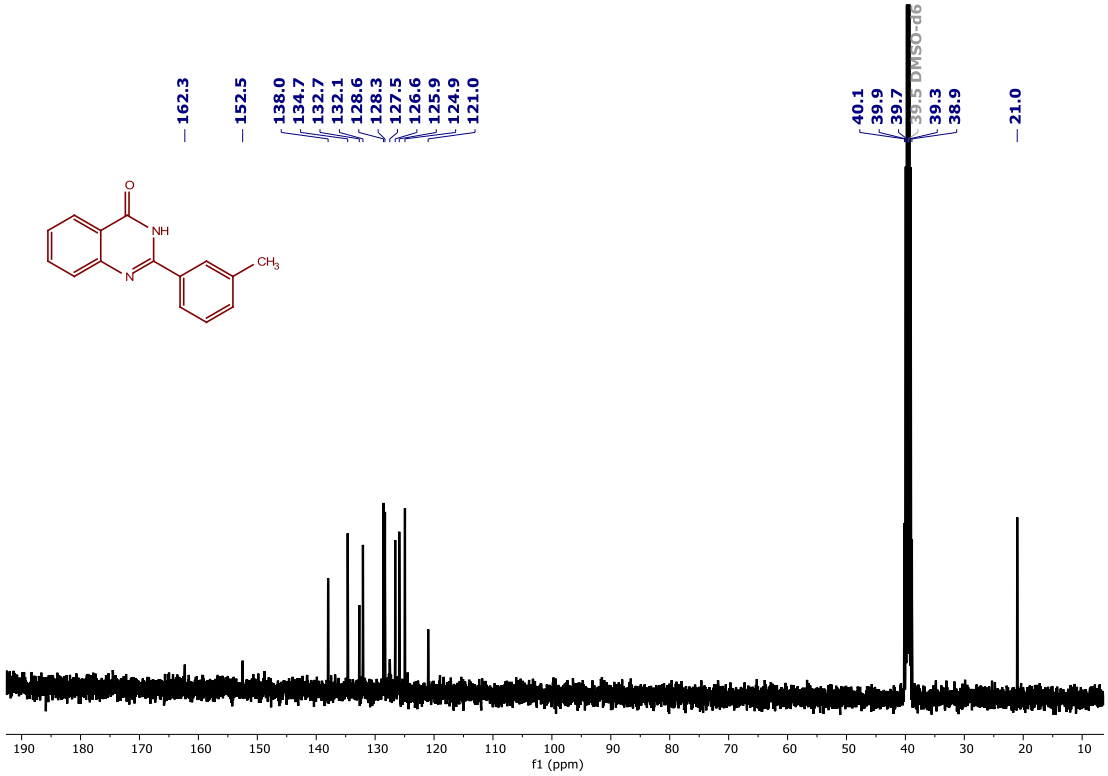
*[13]C{[1]H} NMR of 2-(4-(trifluoromethyl)phenyl)quinazolin-4(3H)-one (Compound-**5c**) in DMSO-d_6*



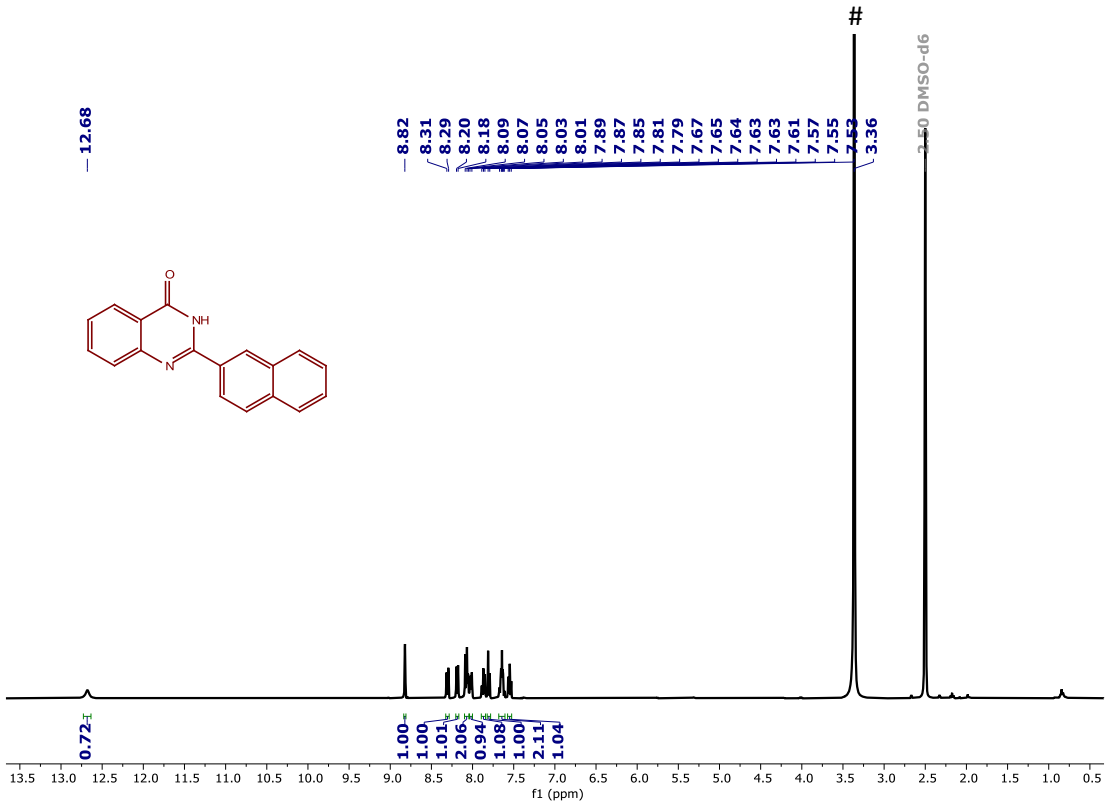
*[19]F NMR of 2-(4-(trifluoromethyl)phenyl)quinazolin-4(3H)-one (Compound-**5c**) in DMSO-d6*



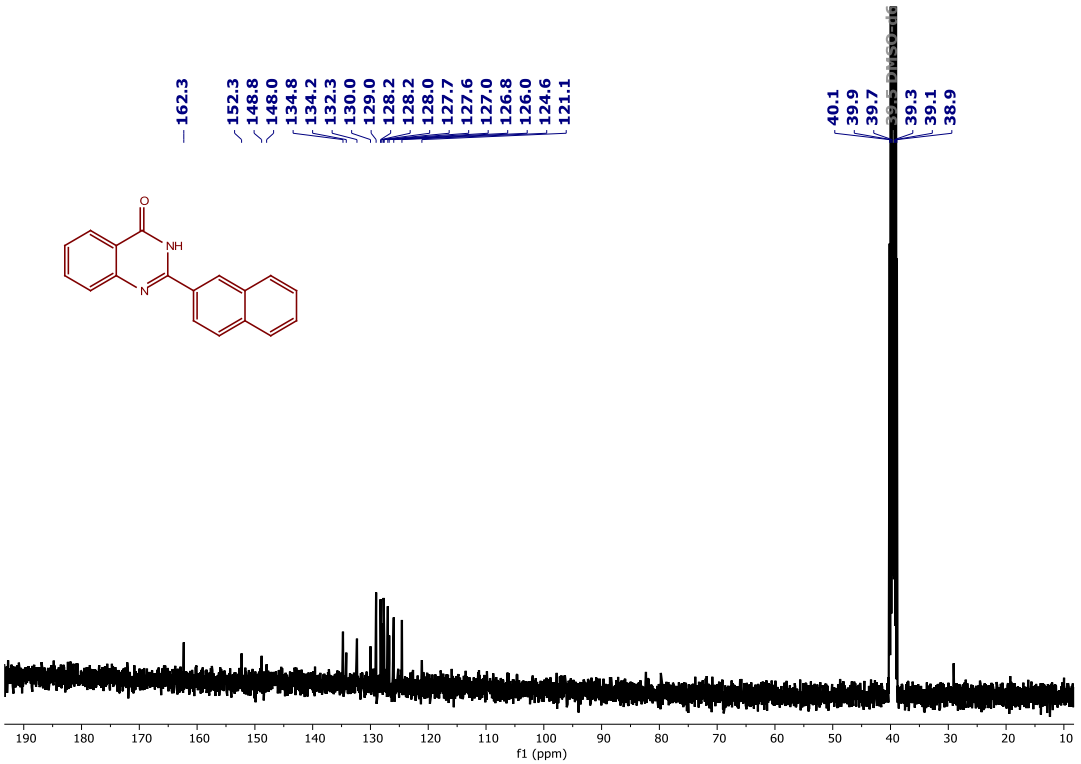
*[1]H NMR of 2-(m-tolyl)quinazolin-4(3H)-one (Compound-**5d**) in DMSO-d6. # indicates the solvent impurity of H_2O in DMSO-d6*



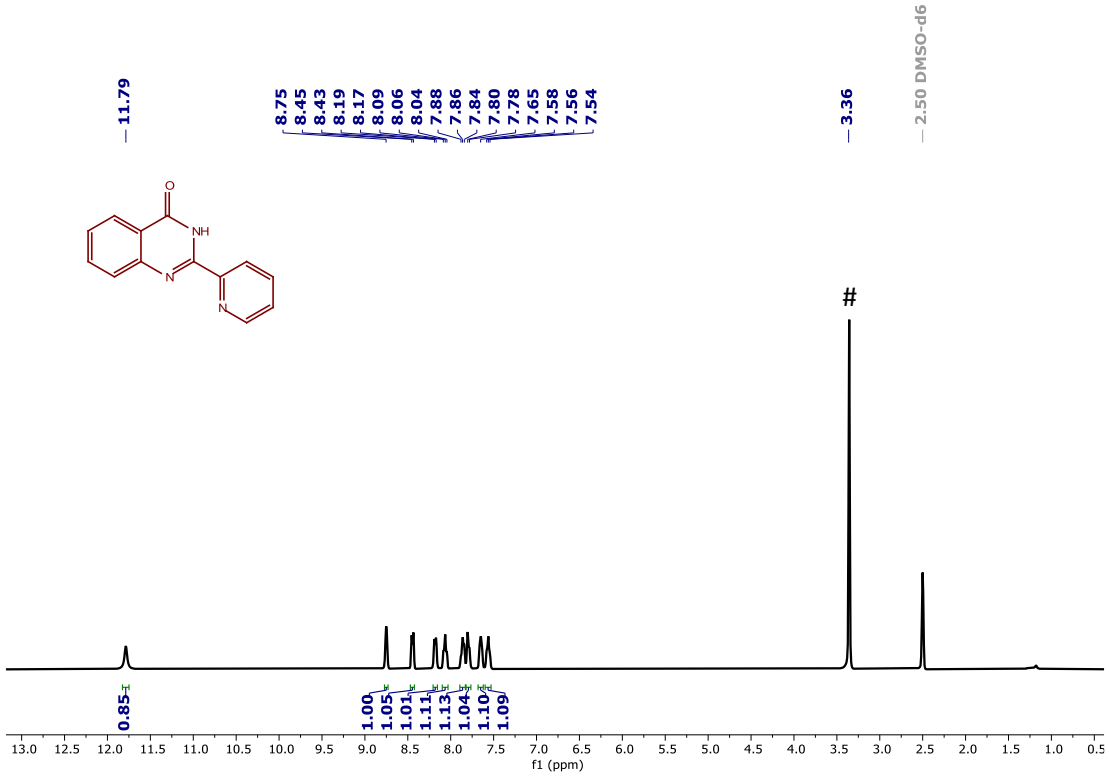
*$^{13}C\{^{1}H\}$ NMR of 2-(m-tolyl)quinazolin-4(3H)-one(Compound-**5d**) in DMSO-d_6*



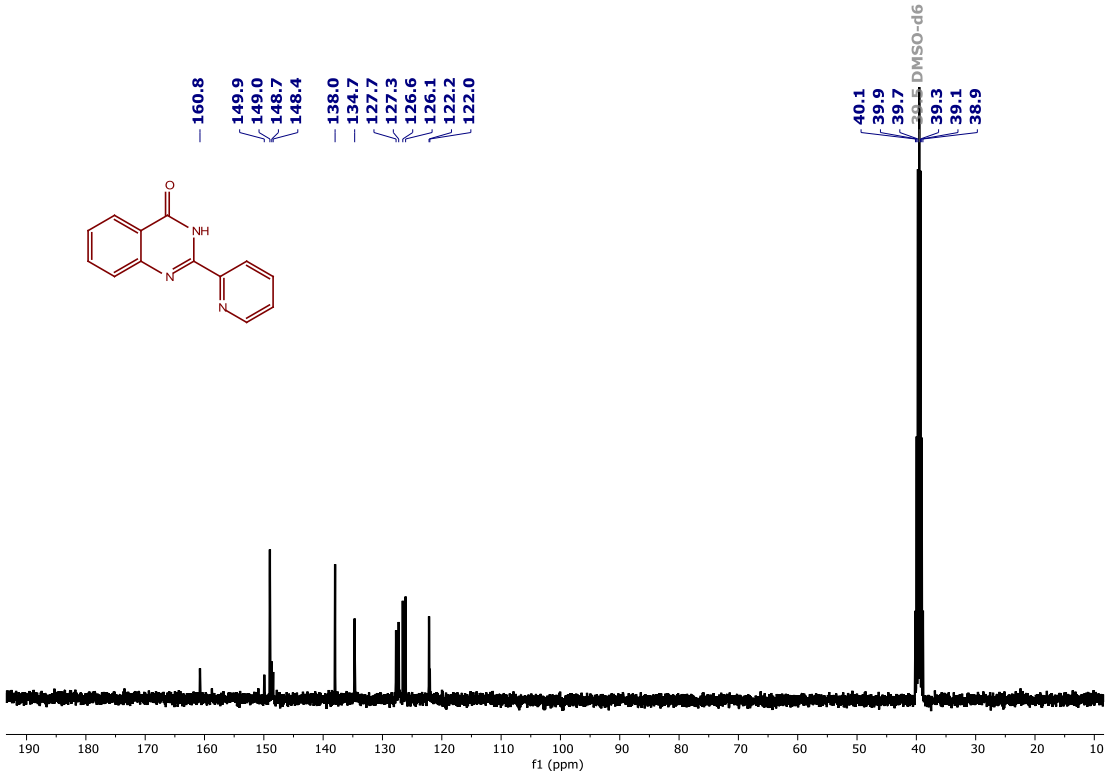
*^{1}H NMR of 2-(naphthalen-2-yl)quinazolin-4(3H)-one (Compound-**5e**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



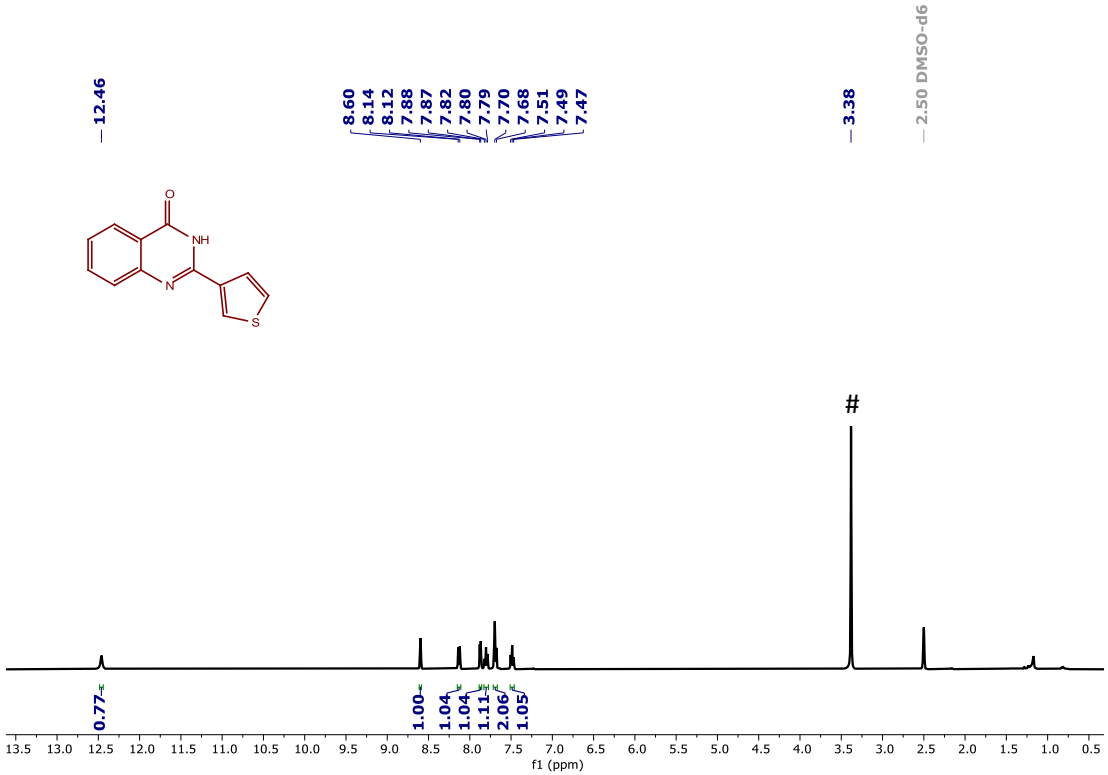
*$^{13}C\{^{1}H\}$ NMR of 2-(naphthalen-2-yl)quinazolin-4(3H)-one (Compound-**5e**) in DMSO-d_6. Intensity of the signals are low due to poor solubility of the compound.*



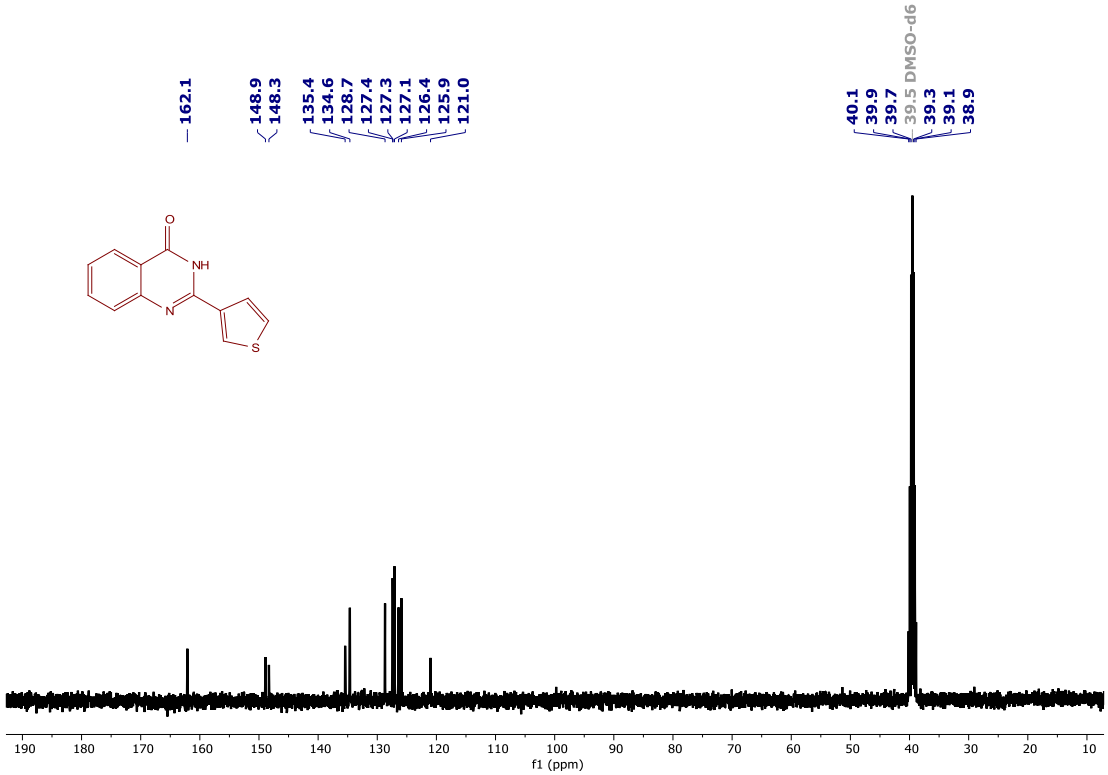
*^{1}H NMR of 2-(pyridin-2-yl)quinazolin-4(3H)-one (Compound-**5f**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



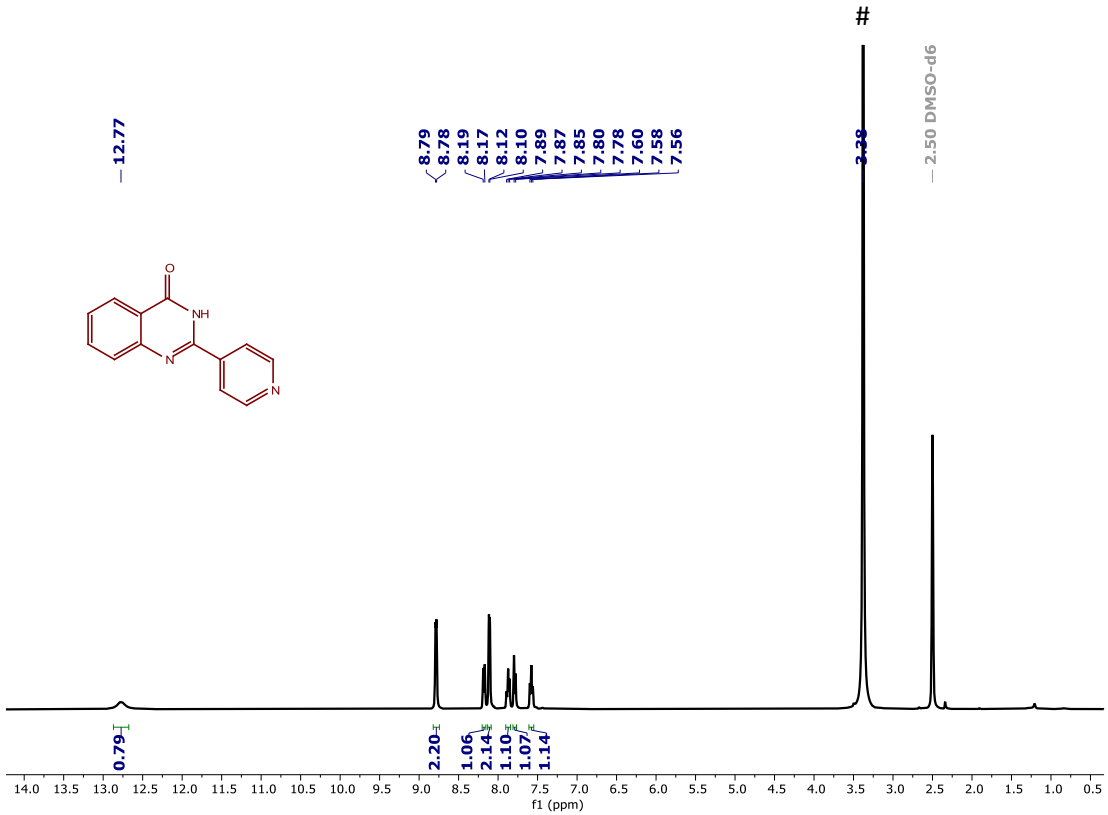
*$^{13}C\{^{1}H\}$ NMR of 2-(pyridin-2-yl)quinazolin-4(3H)-one (Compound-**5f**) in DMSO-d_6*



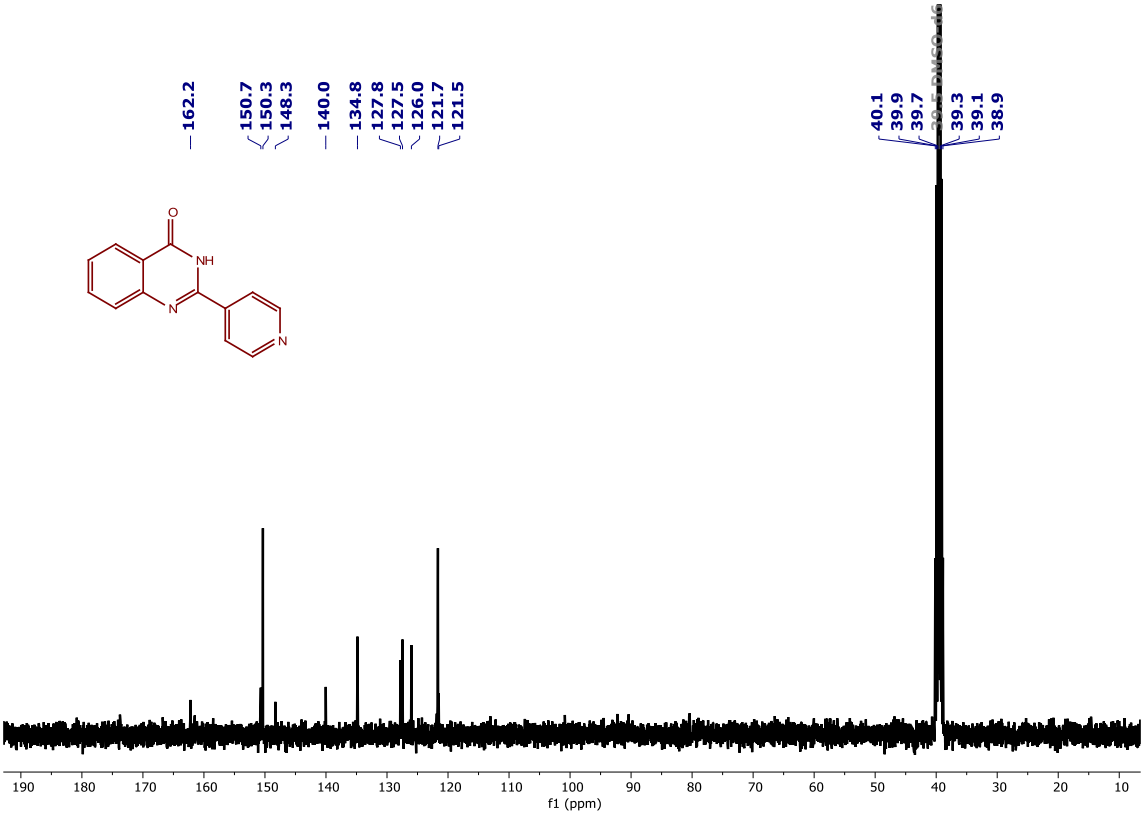
*^{1}H NMR of 2-(thiophen-3-yl)quinazolin-4(3H)-one (Compound-**5g**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



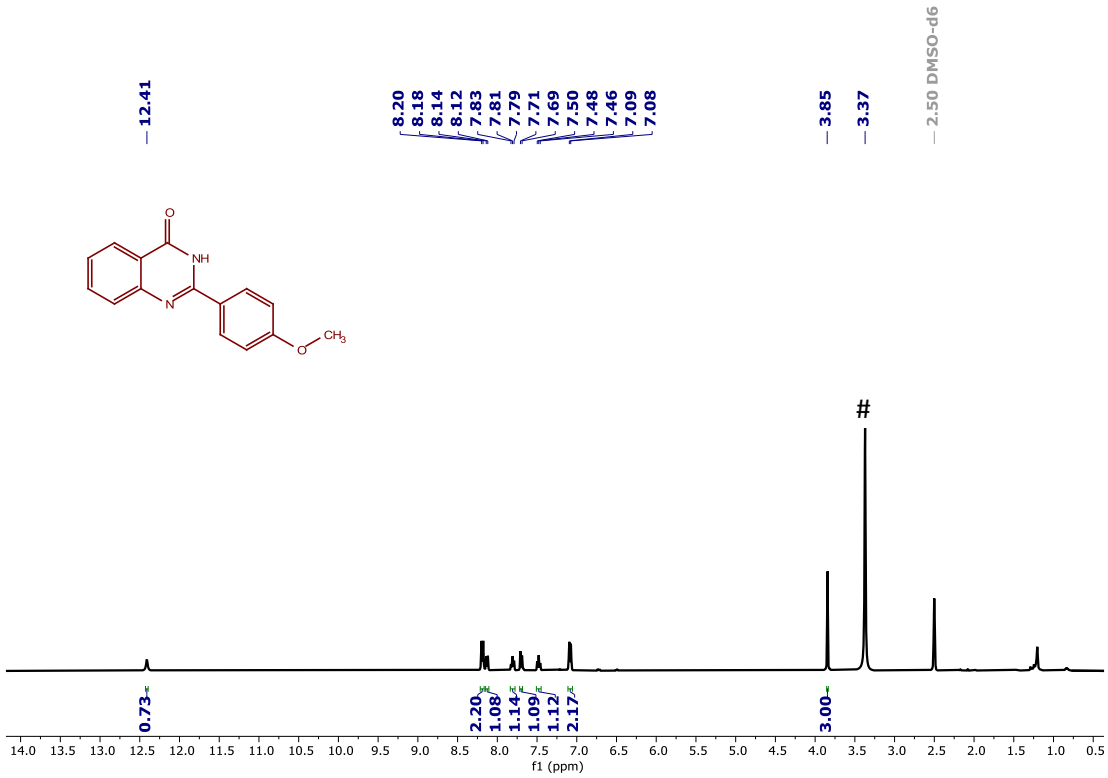
*$^{13}C\{^{1}H\}$ NMR of 2-(thiophen-3-yl)quinazolin-4(3H)-one (Compound-**5g**) in DMSO-d_6*



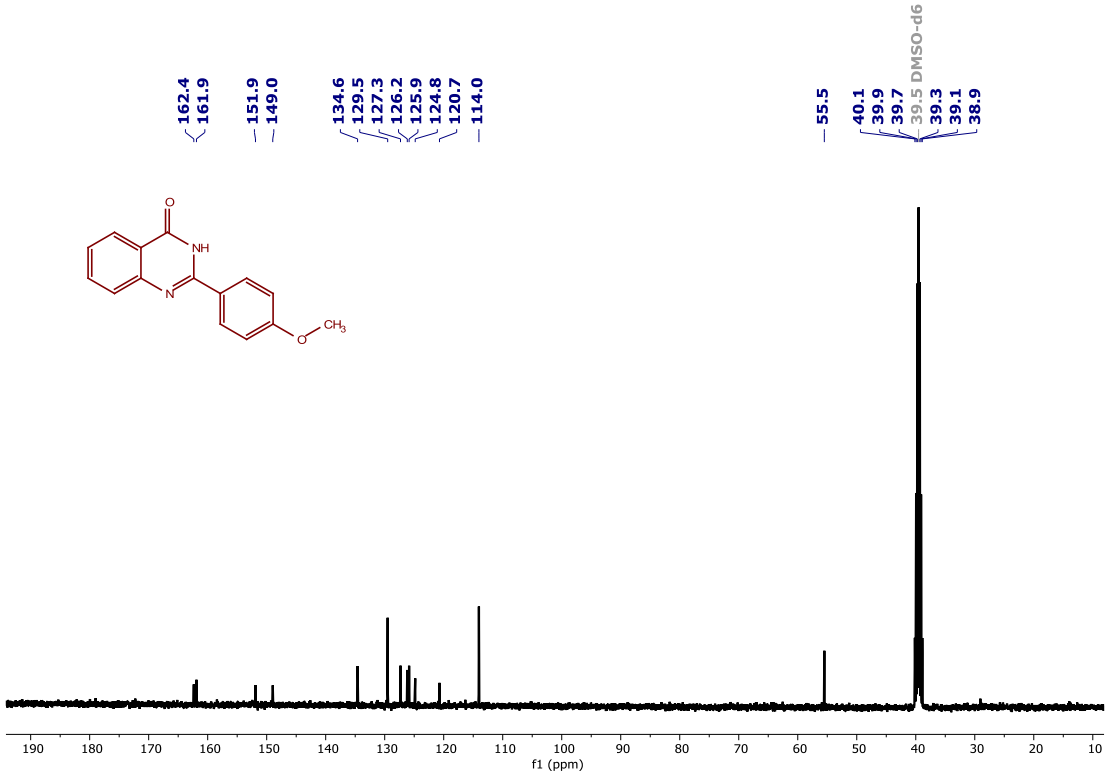
*^{1}H NMR of 2-(pyridin-4-yl)quinazolin-4(3H)-one (Compound-**5h**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



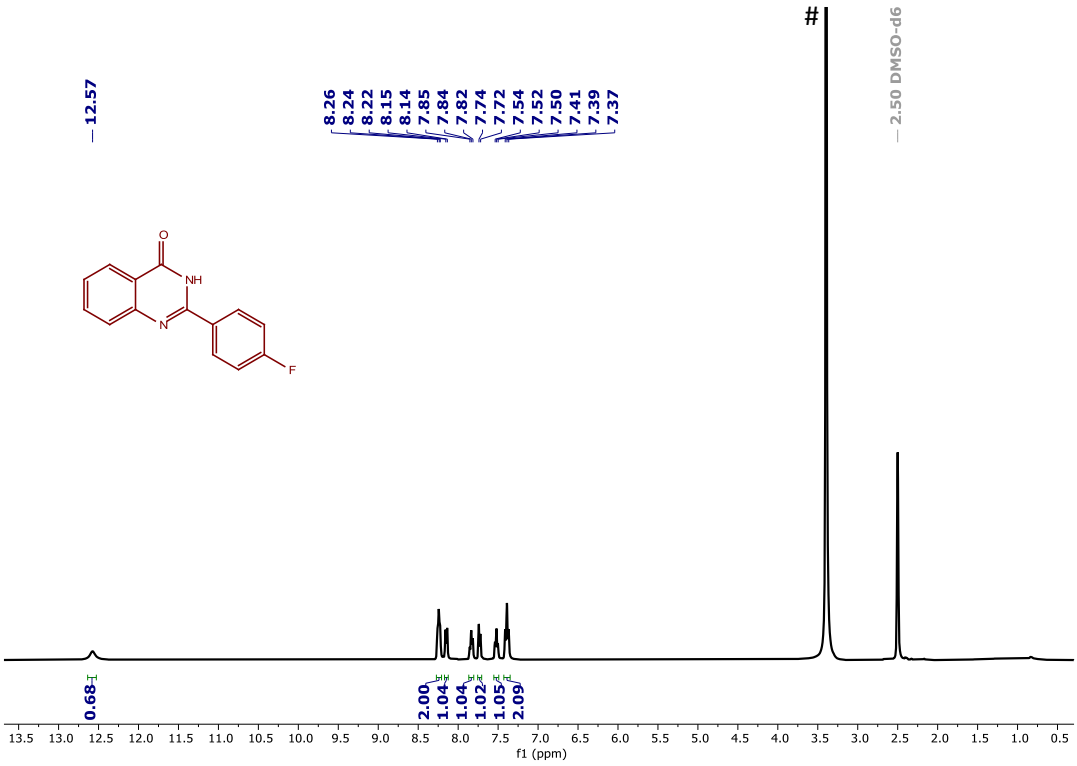
*$^{13}C\{^{1}H\}$ NMR of 2-(pyridin-4-yl)quinazolin-4(3H)-one (Compound-**5h**) in DMSO-d_6*



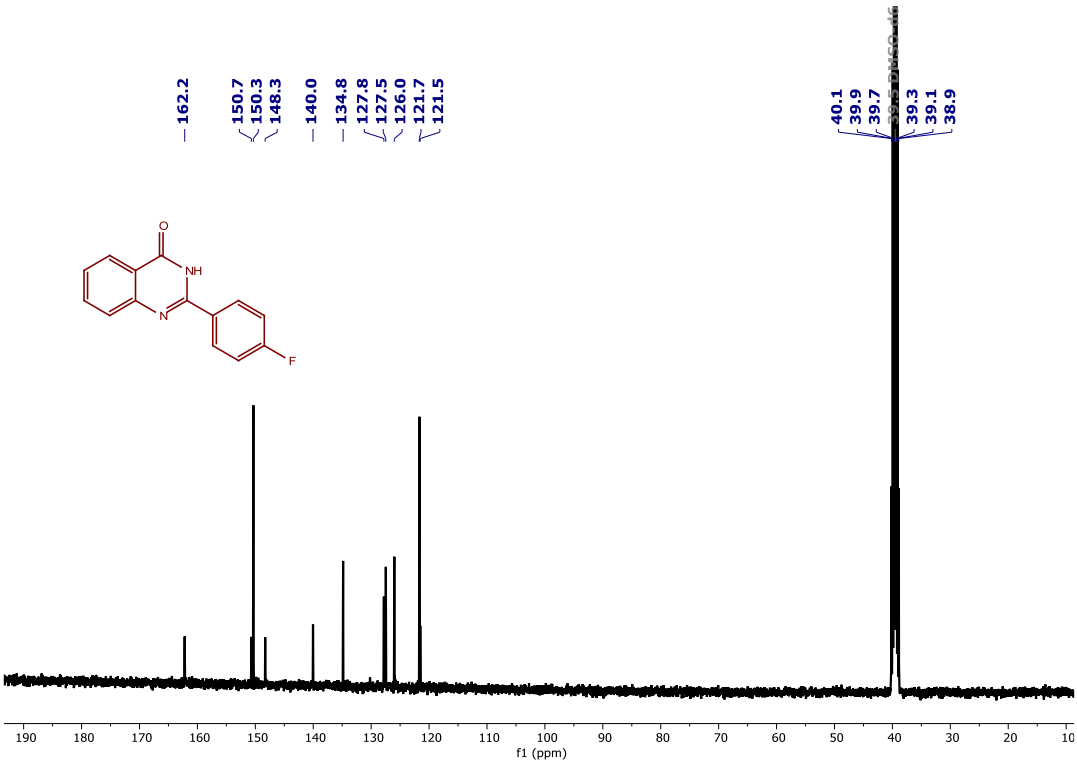
*^{1}H NMR of 2-(4-methoxyphenyl)quinazolin-4(3H)-one (Compound-**5i**) in DMSO-d_6. # and $ indicates the solvent impurity of H_2O and grease in DMSO-d_6*



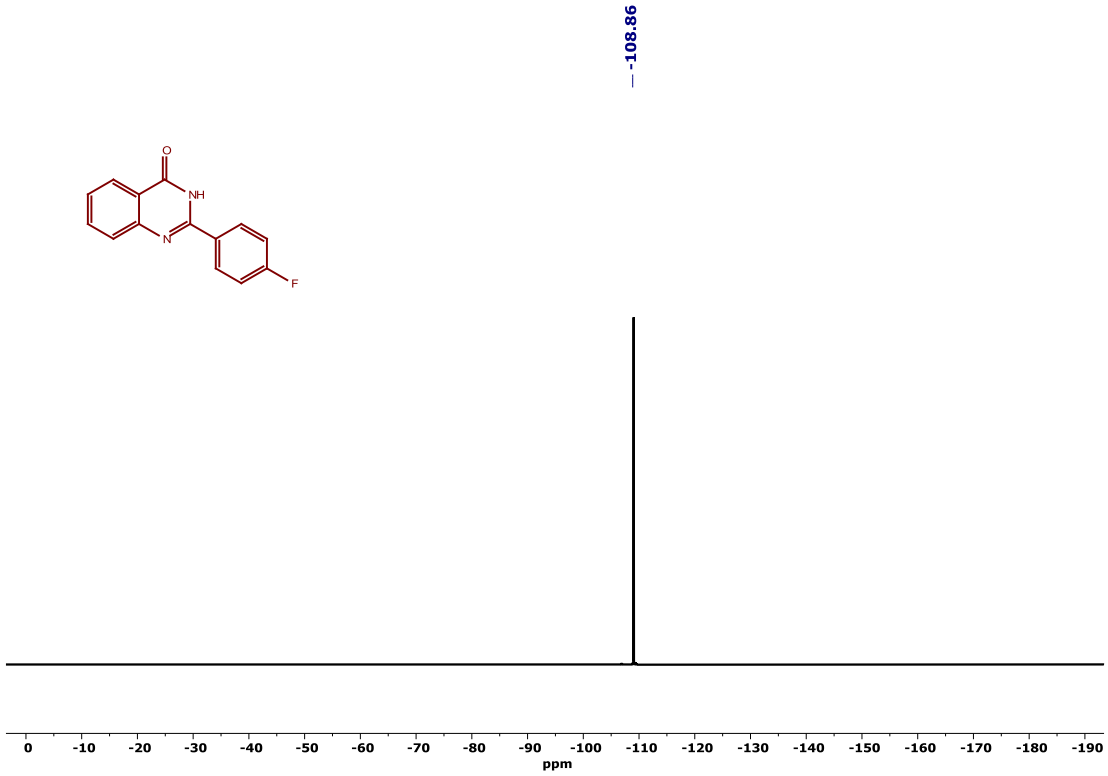
*$^{13}C\{^{1}H\}$ NMR of 2-(4-methoxyphenyl)quinazolin-4(3H)-one (Compound-**5i**) in DMSO-d_6*



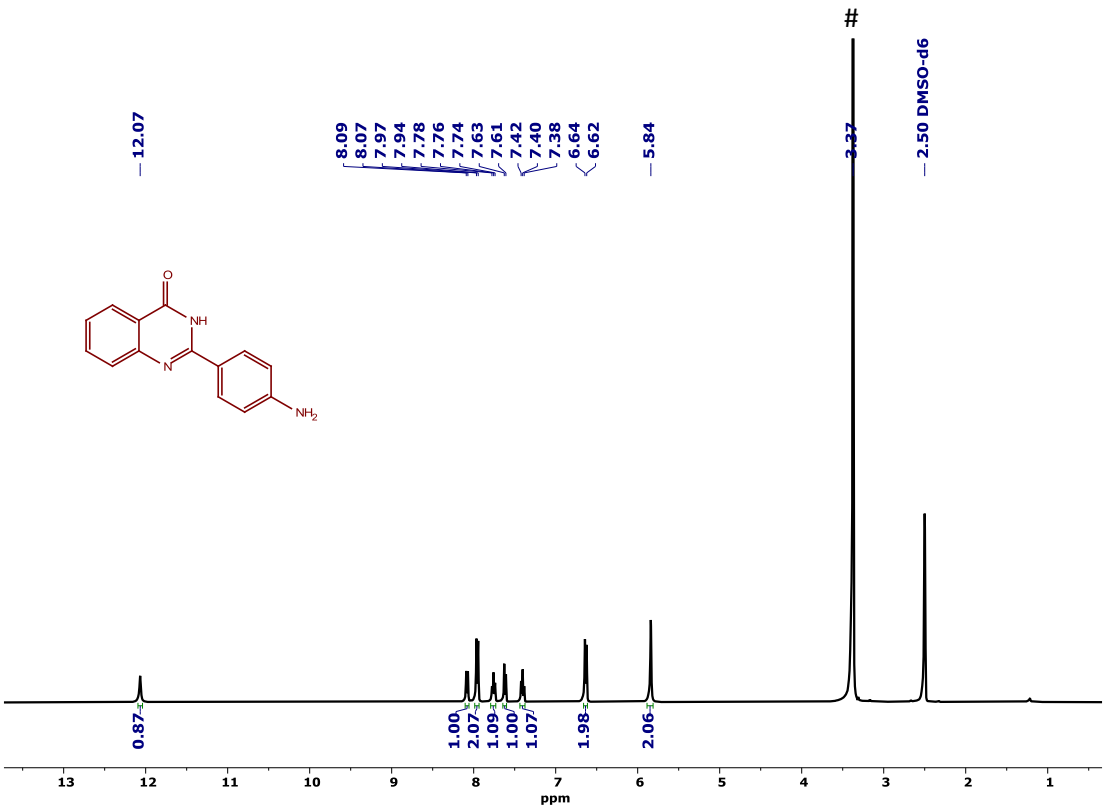
*^{1}H NMR of 2-(4-fluorophenyl)quinazolin-4(3H)-one (Compound-**5j**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



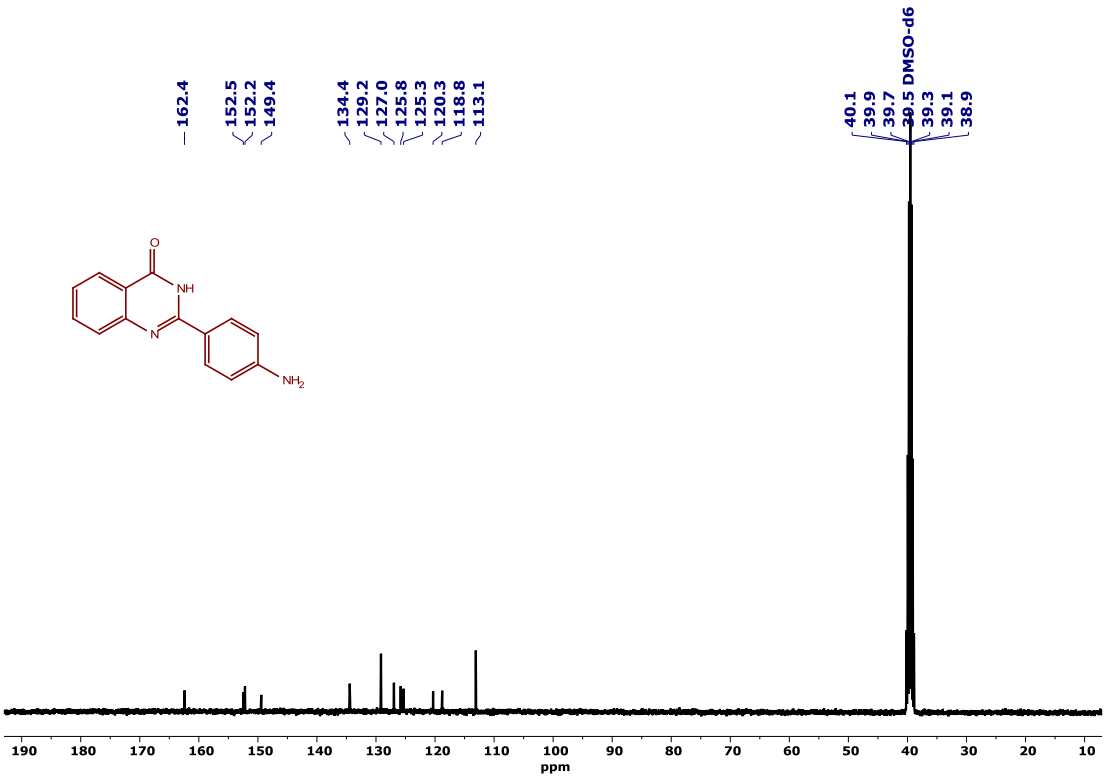
*$^{13}C\{^{1}H\}$ NMR of 2-(4-fluorophenyl)quinazolin-4(3H)-one (Compound-**5j**) in DMSO-d_6*



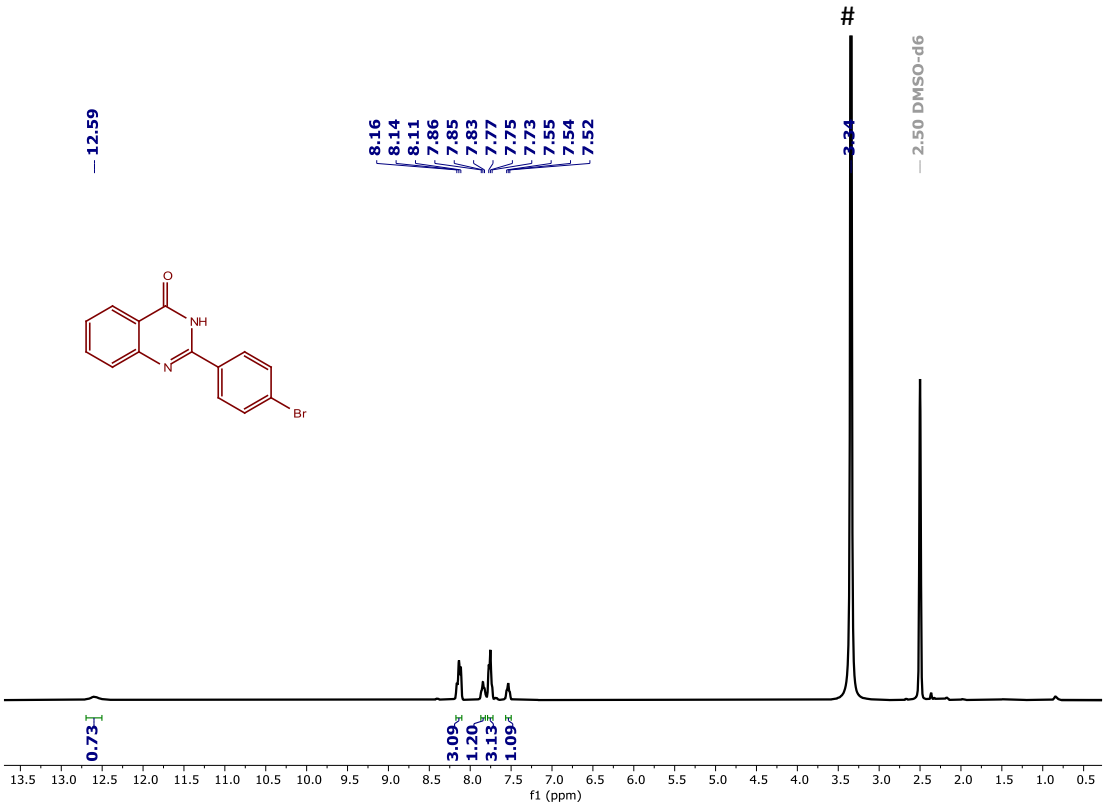
*^{19}F NMR of 2-(4-fluorophenyl)quinazolin-4(3H)-one (Compound-**5j**) in DMSO-d_6*



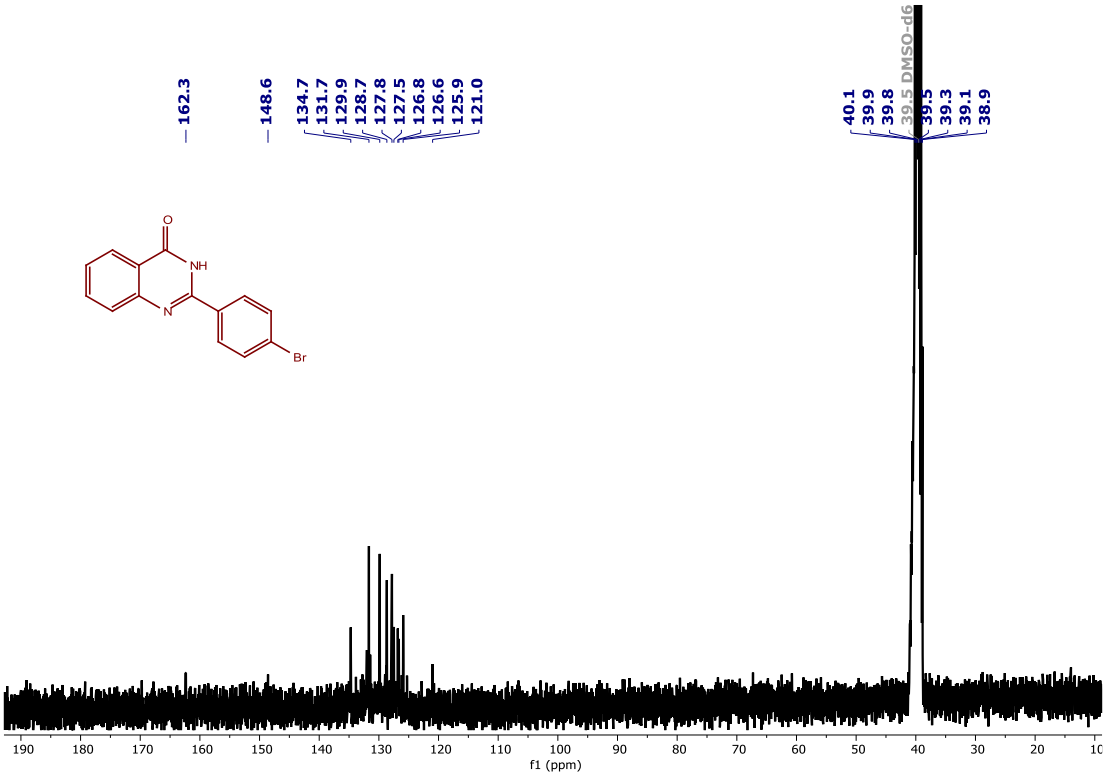
*[1]H NMR of 2-(4-aminophenyl)quinazolin-4(3H)-one (Compound-**5l**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



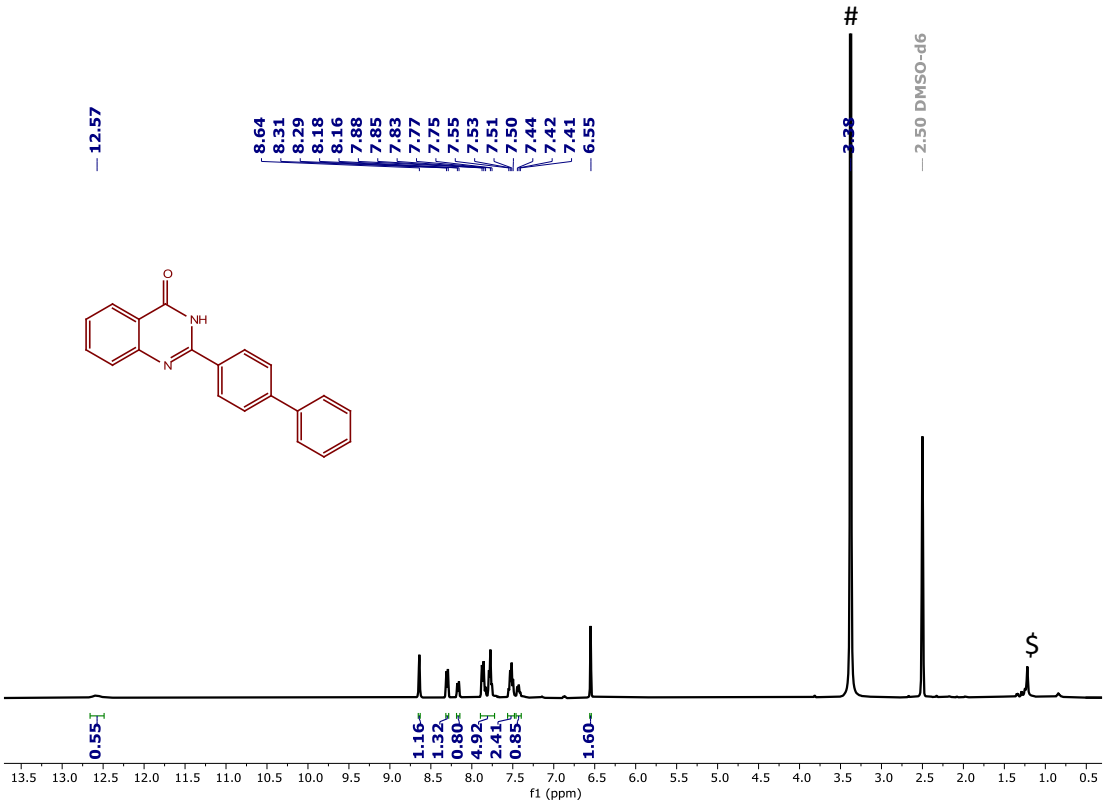
*[13]C{[1]H} NMR of 2-(4-aminophenyl)quinazolin-4(3H)-one (Compound-**5l**) in DMSO-d_6*



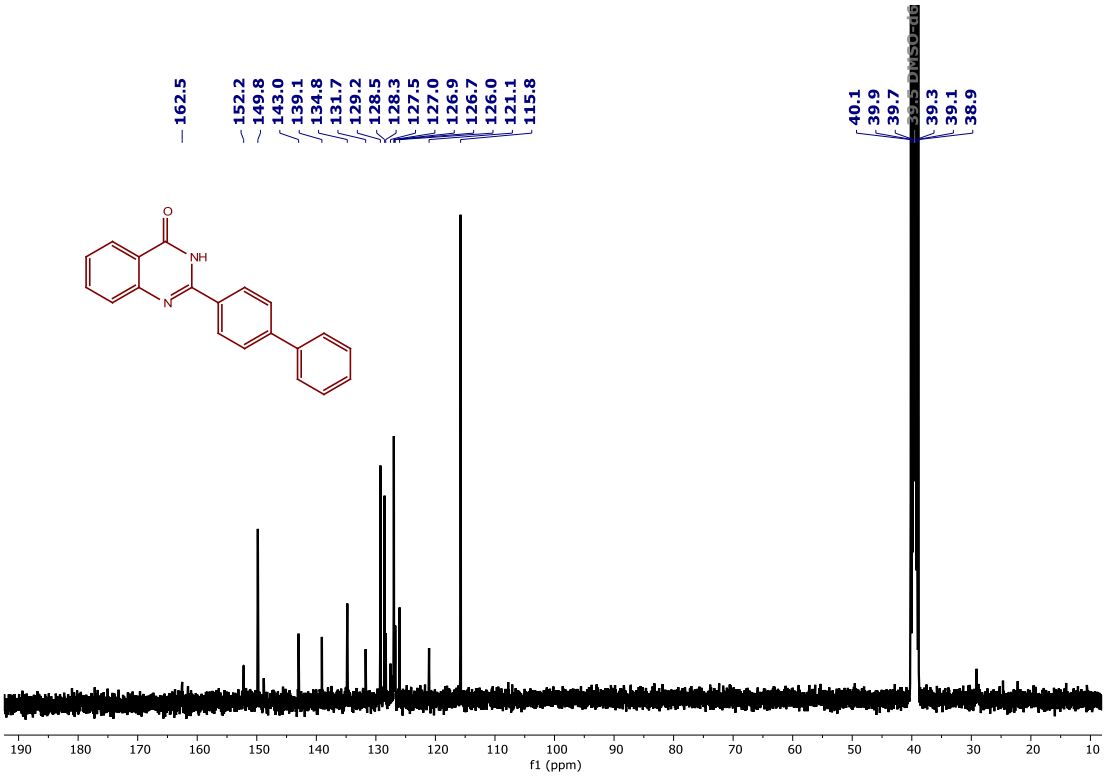
*[1]H NMR of 2-(4-bromophenyl)quinazolin-4(3H)-one (Compound-**5k**) in DMSO-d6. # indicates the solvent impurity of H_2O in DMSO-d6*



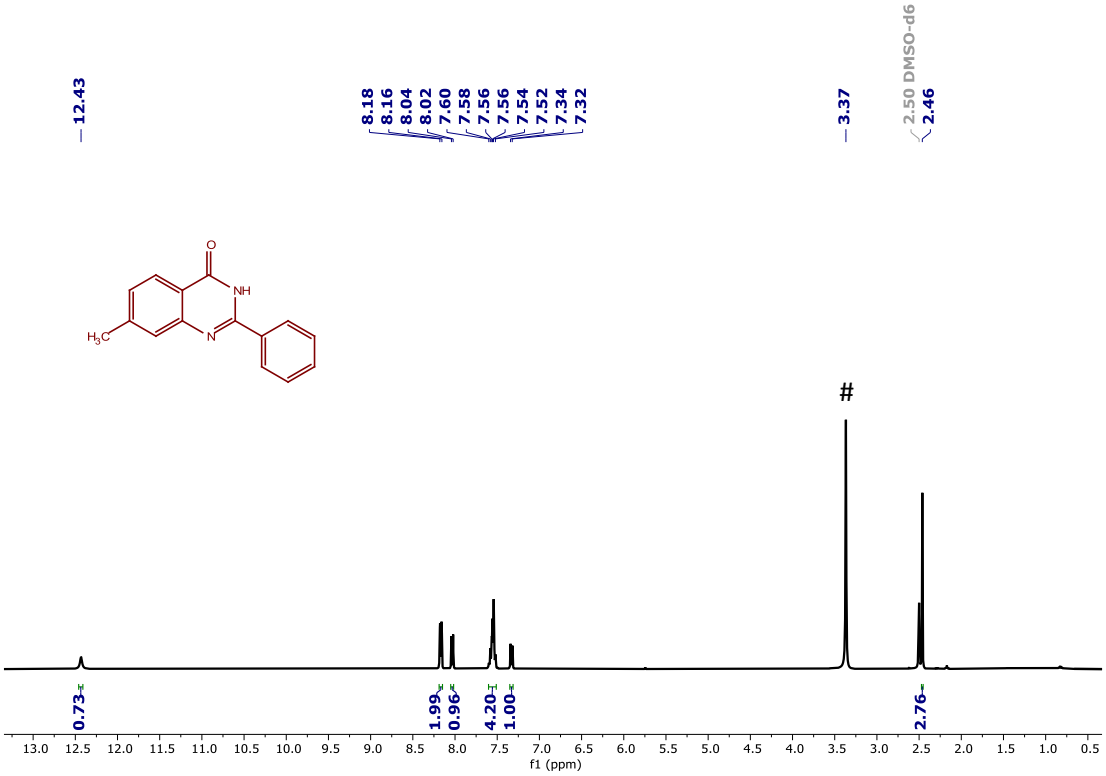
*[13]C{[1]H} NMR of 2-(4-bromophenyl)quinazolin-4(3H)-one (Compound-**5k**) in DMSO-d6. Intensity of the signals are low due to poor solubility of the compound.*



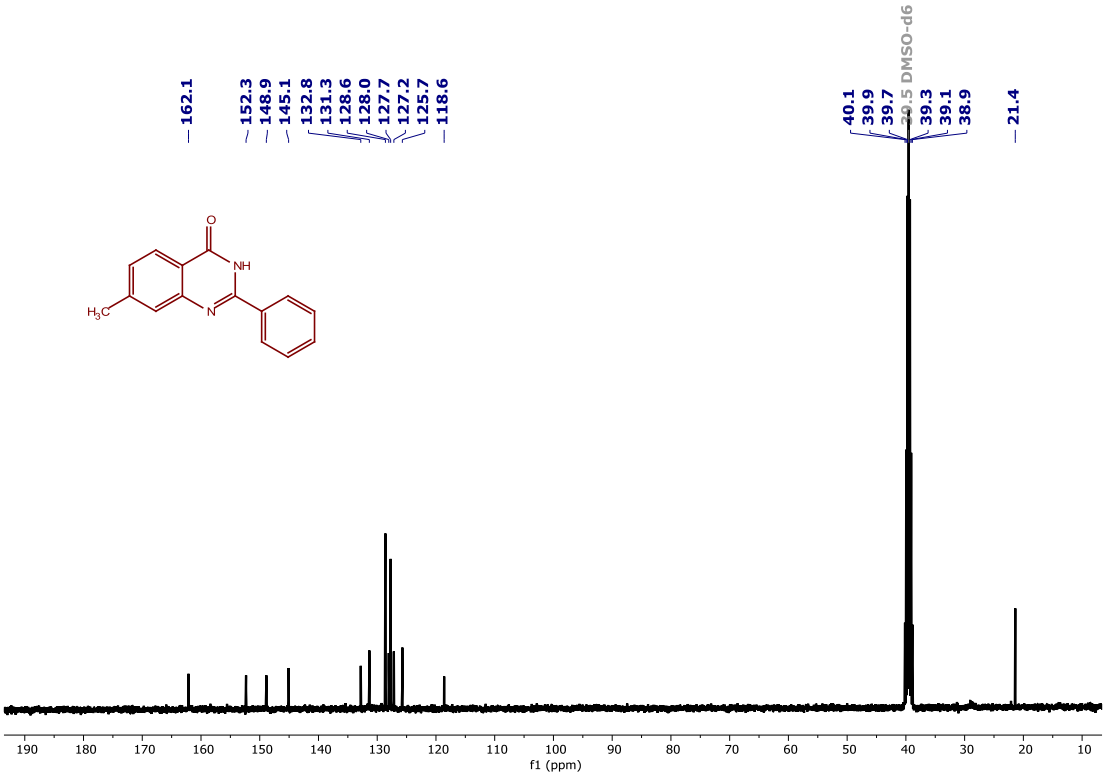
*^{1}H NMR of 2-([1,1'-biphenyl]-4-yl)quinazolin-4(3H)-one (Compound-**5m**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6. $ indicates grease.*



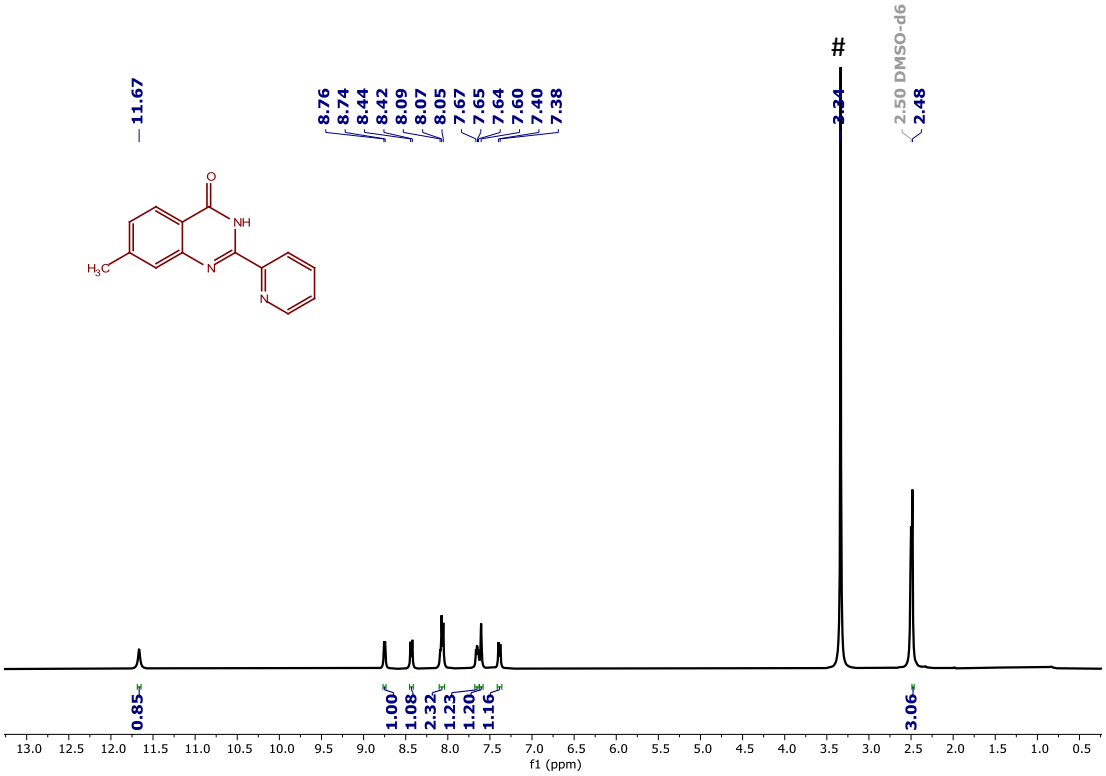
*^{13}C{^{1}H} NMR of 2-([1,1'-biphenyl]-4-yl)quinazolin-4(3H)-one (Compound-**5m**) in DMSO-d_6*



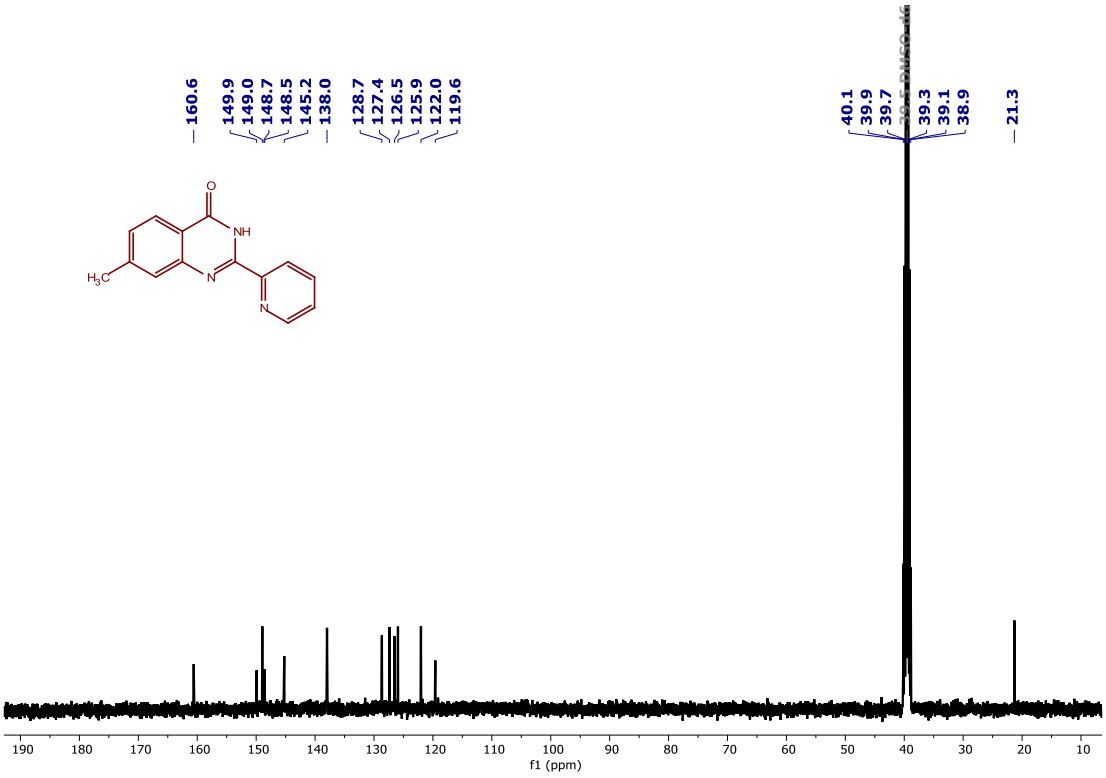
*[1]H NMR of 7-methyl-2-phenylquinazolin-4(3H)-one (Compound-**5n**) in DMSO-d6. # indicates the solvent impurity of H_2O in DMSO-d_6*



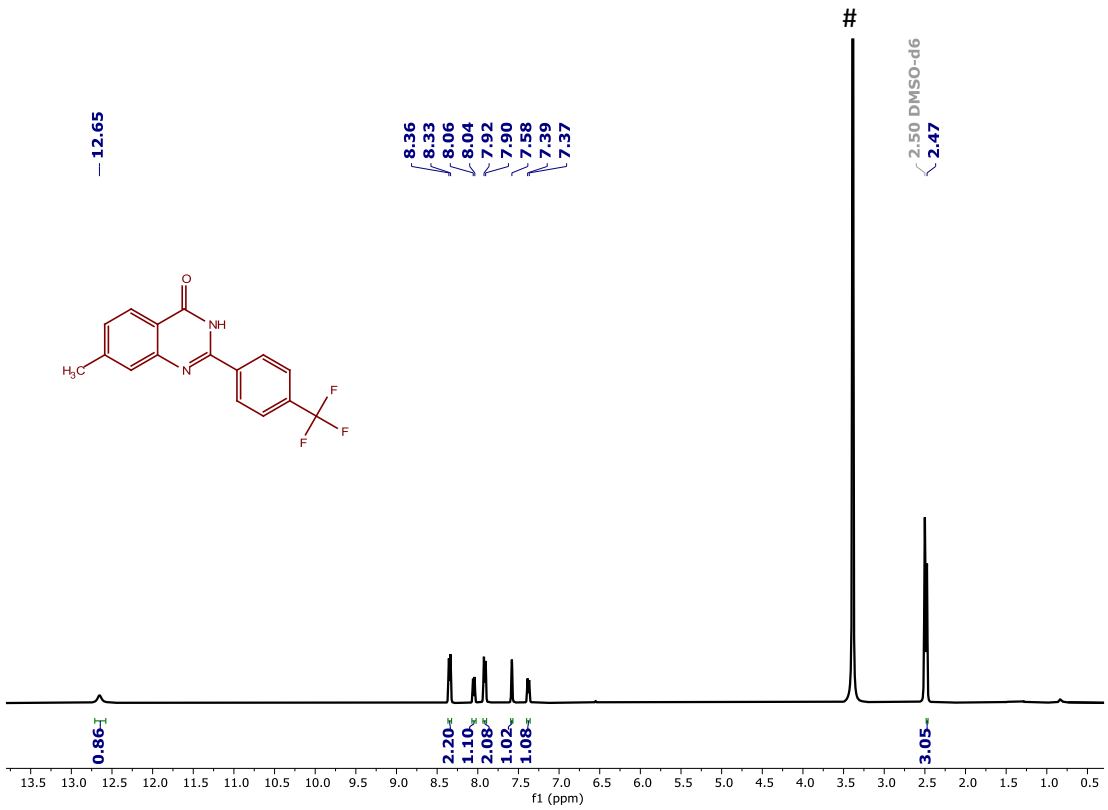
*[13]C{[1]H} NMR of 7-methyl-2-phenylquinazolin-4(3H)-one (Compound-**5n**) in DMSO-d_6*



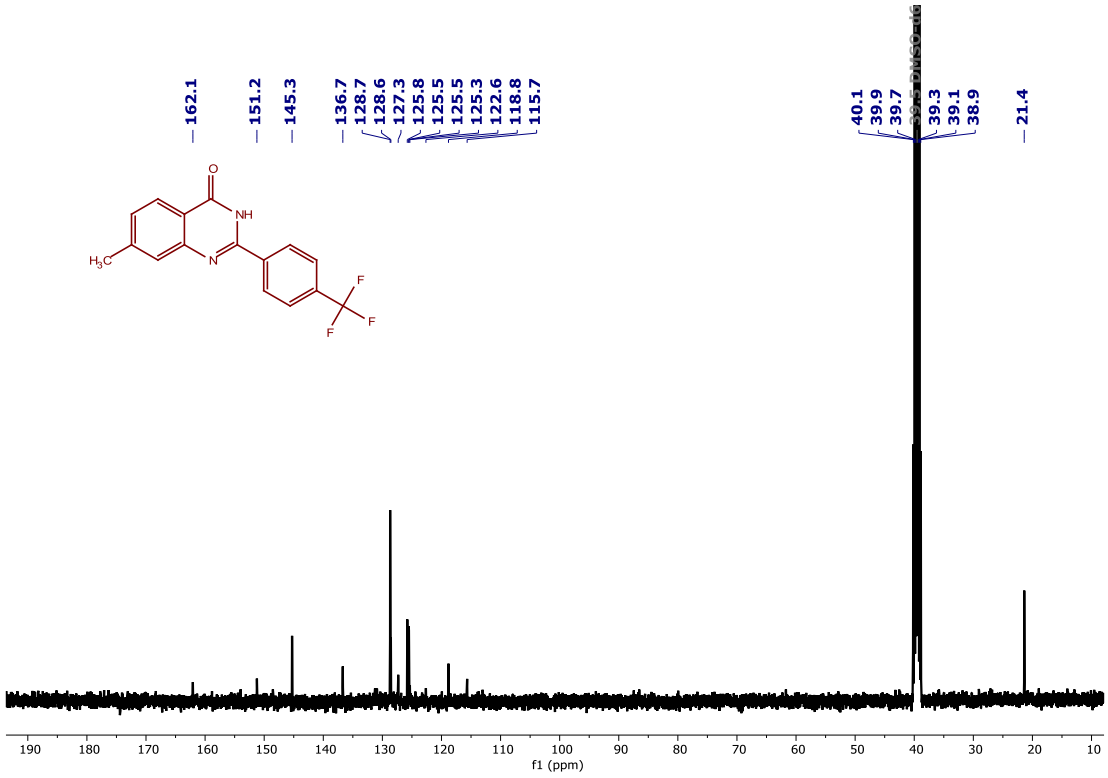
*^{1}H NMR of 7-methyl-2-(pyridin-2-yl)quinazolin-4(3H)-one (Compound-**5o**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



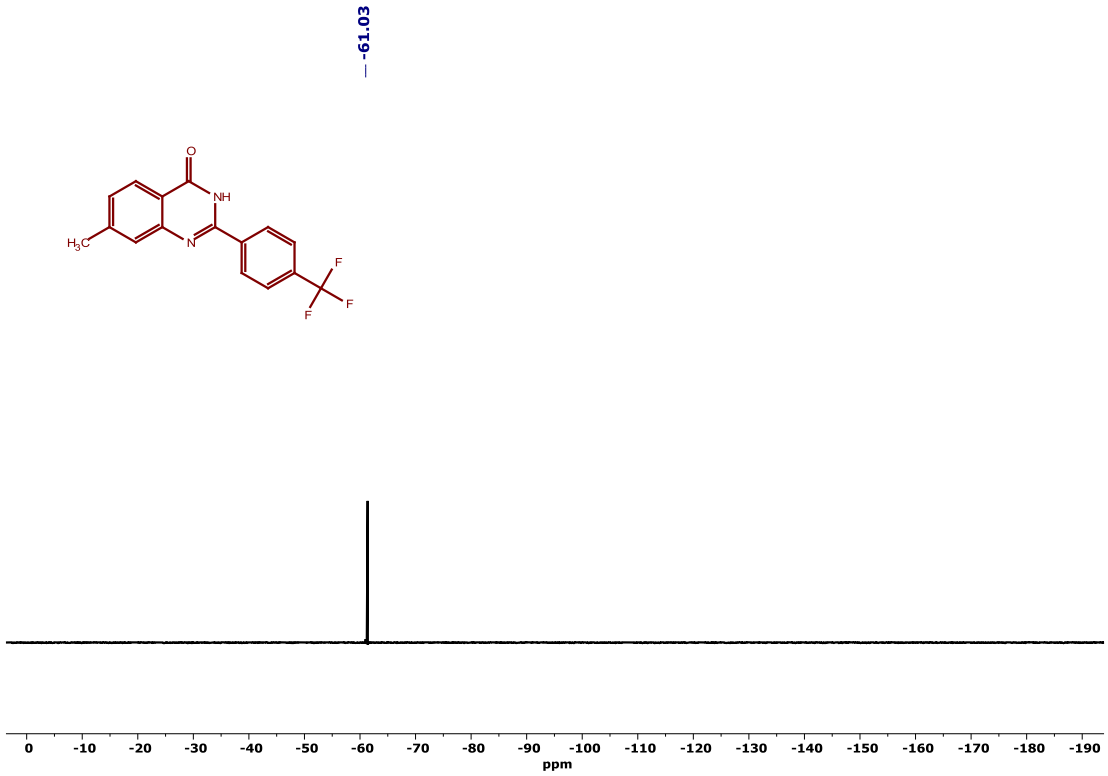
*$^{13}C\{^{1}H\}$ NMR of 7-methyl-2-(pyridin-2-yl)quinazolin-4(3H)-one (Compound-**5o**) in DMSO-d_6*



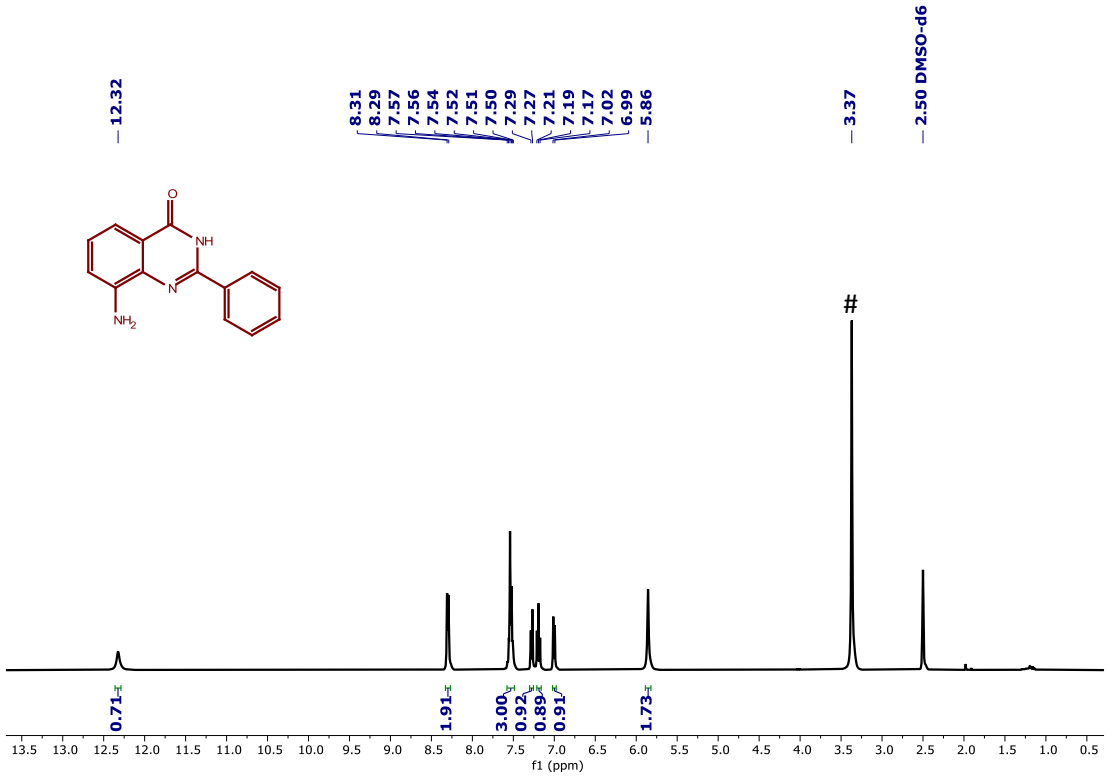
*[1]H NMR of 7-methyl-2-(4-(trifluoromethyl)phenyl)quinazolin-4(3H)-one (Compound-**5p**) in DMSO-d6. # indicates the solvent impurity of H_2O in DMSO-d6*



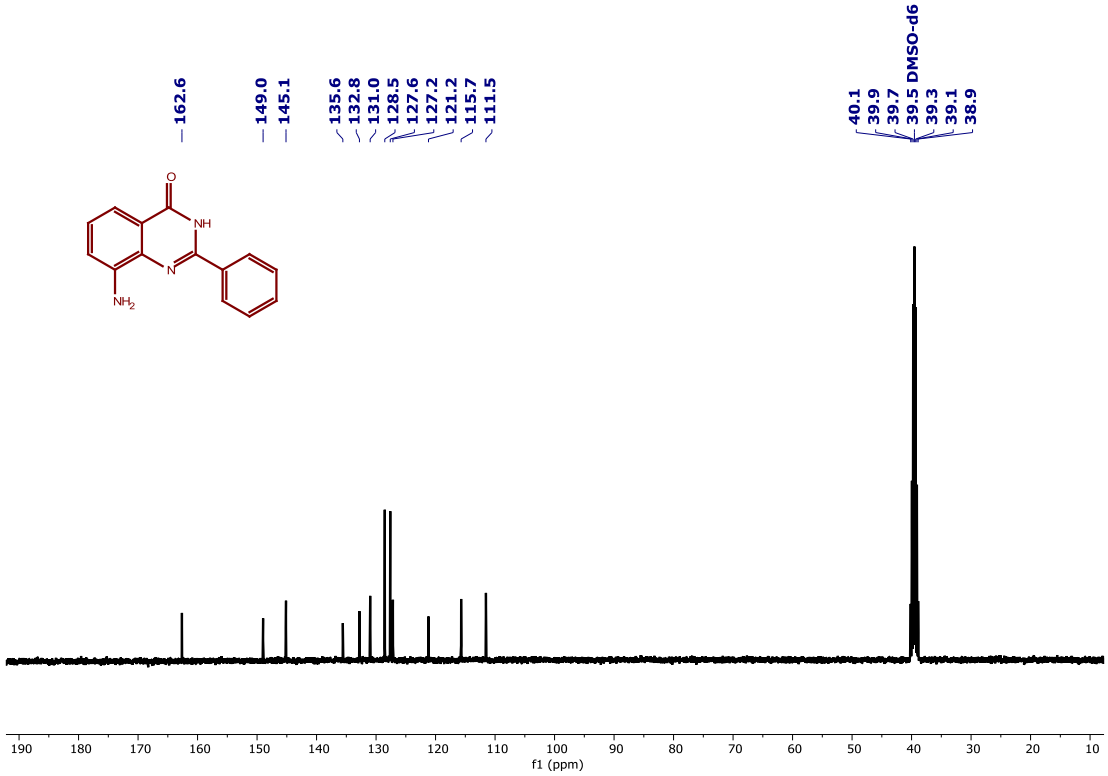
*[13]C{[1]H} NMR of 7-methyl-2-(4-(trifluoromethyl)phenyl)quinazolin-4(3H)-one (Compound-**5p**) in DMSO-d6*



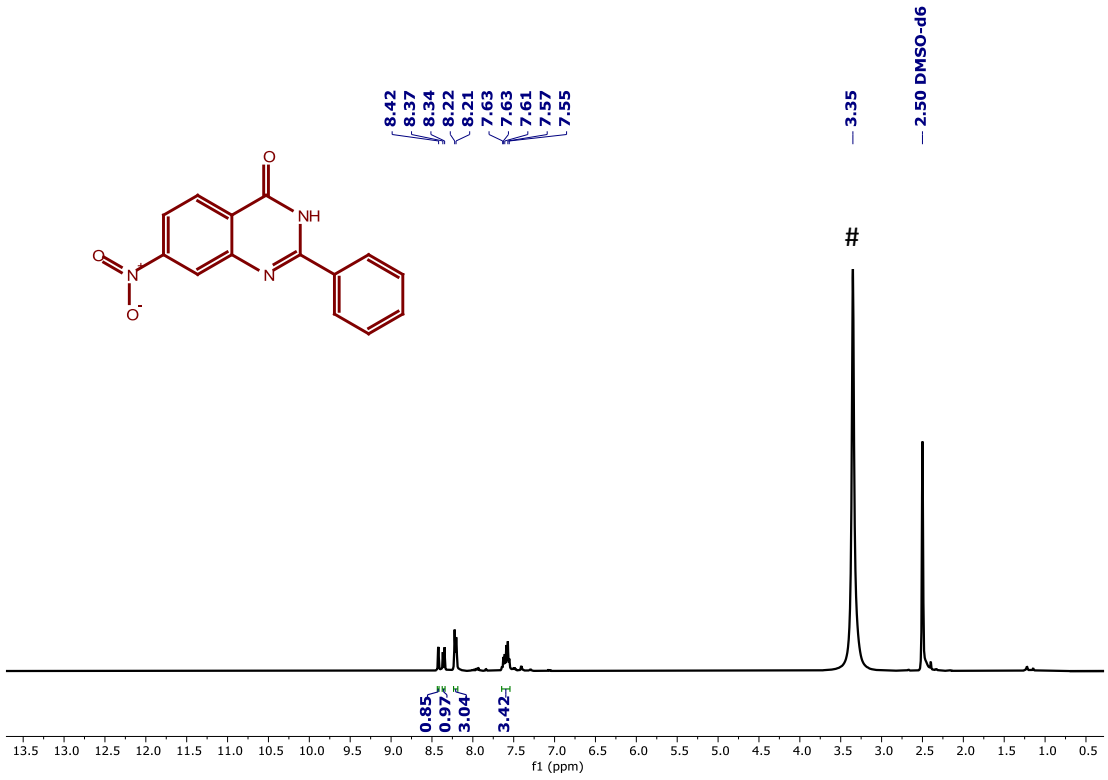
*[19]F NMR of 7-methyl-2-(4-(trifluoromethyl)phenyl)quinazolin-4(3H)-one (Compound-**5p**) in DMSO-d6*



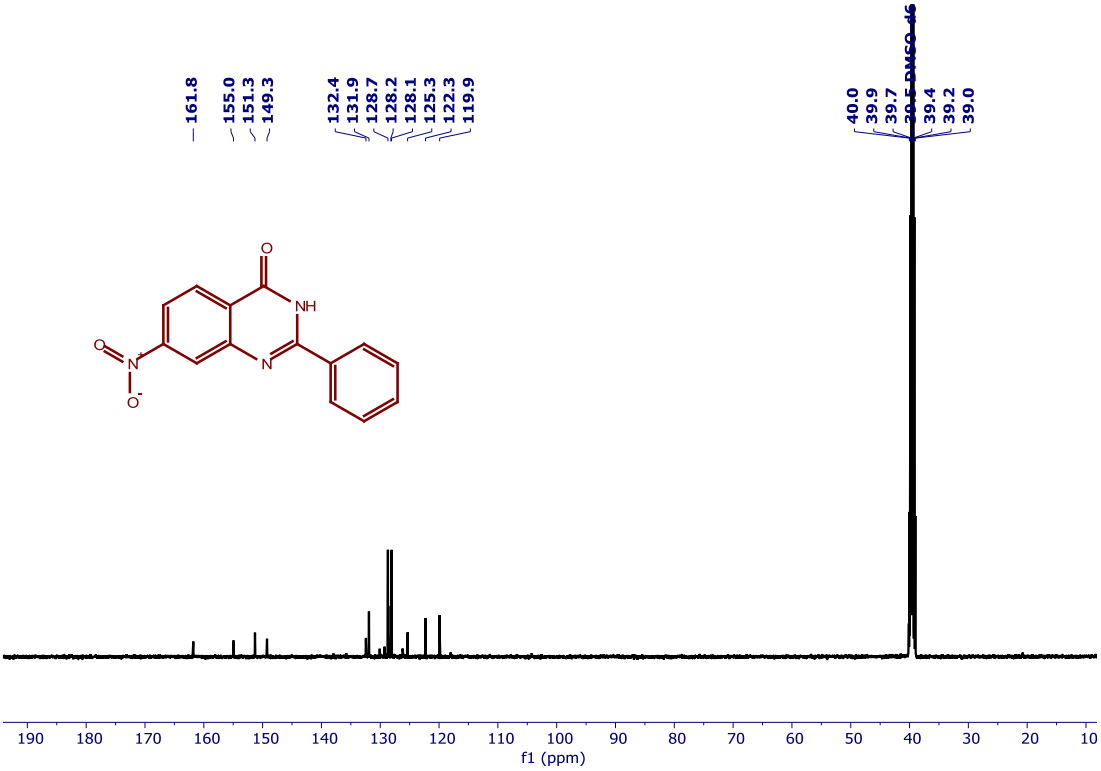
*[1]H NMR of 8-amino-2-phenylquinazolin-4(3H)-one (Compound-**5q**) in DMSO-d6. # indicates the solvent impurity of H2O in DMSO-d6*



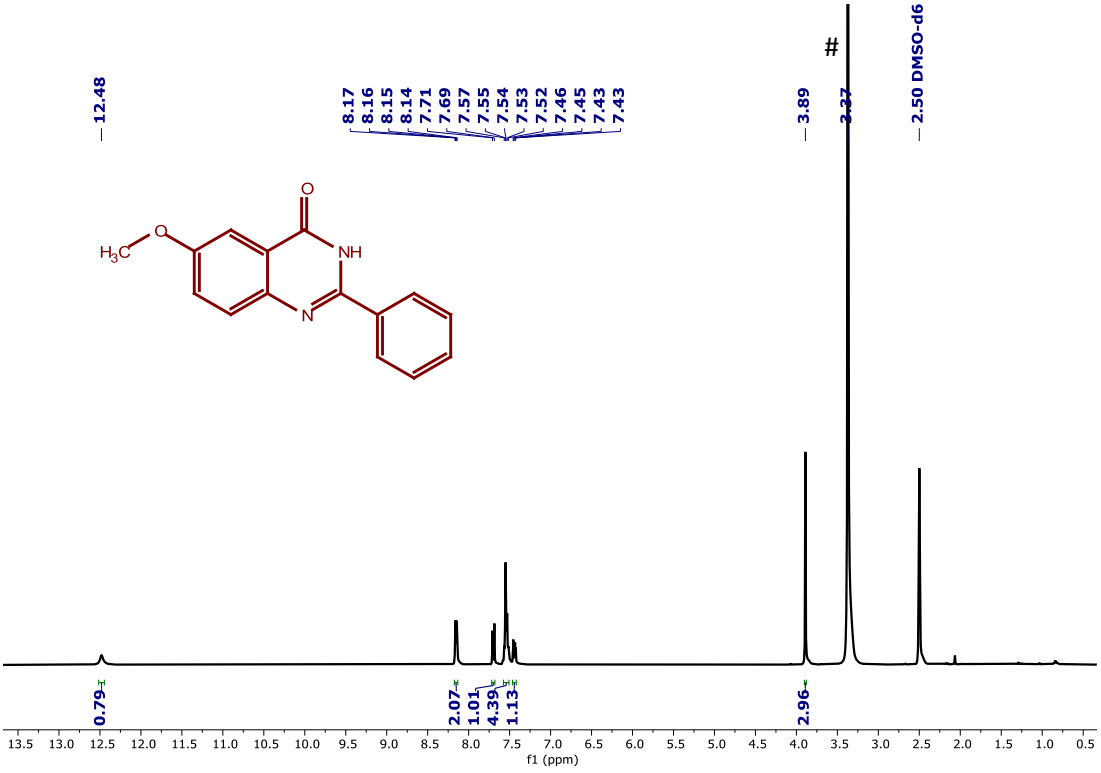
*$^{13}C\{^{1}H\}$ NMR of 8-amino-2-phenylquinazolin-4(3H)-one (Compound-**5q**) in DMSO-d_6*



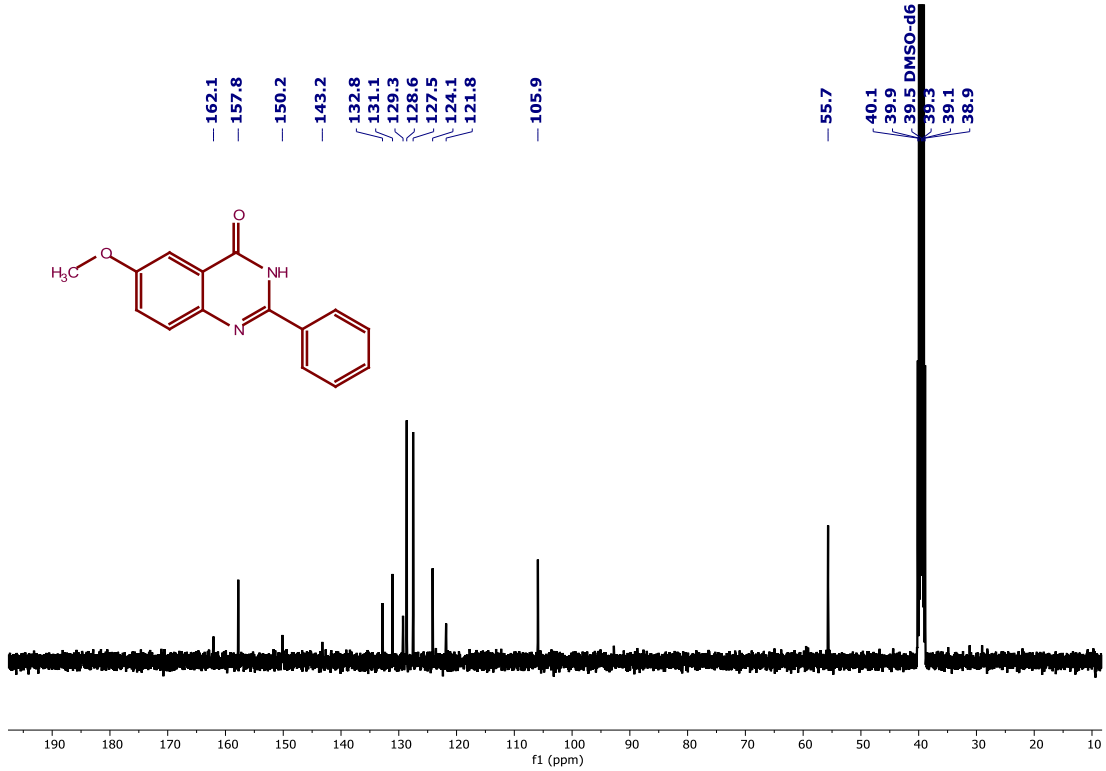
*^{1}H NMR of 7-nitro-2-phenylquinazolin-4(3H)-one (Compound-**5r**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



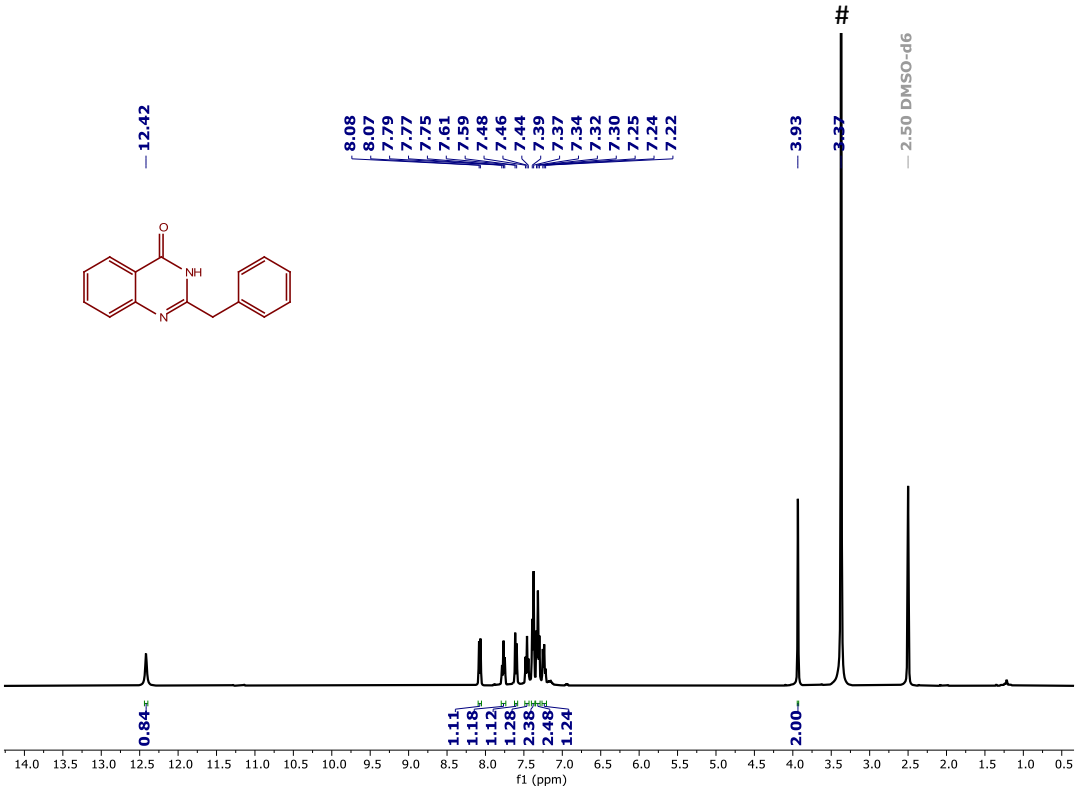
*$^{13}C\{^{1}H\}$ NMR of 7-nitro-2-phenylquinazolin-4(3H)-one (Compound-**5r**) in DMSO-d_6*



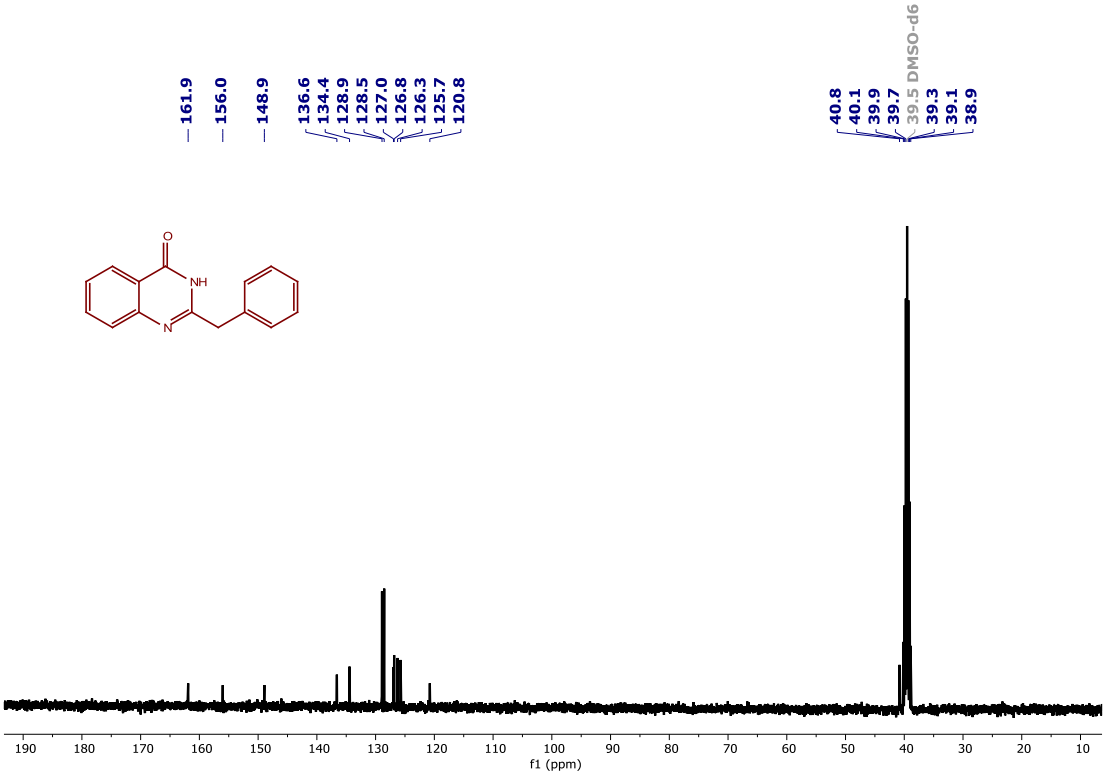
*^{1}H NMR of 6-methoxy-2-phenylquinazolin-4(3H)-one (Compound-**5s**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



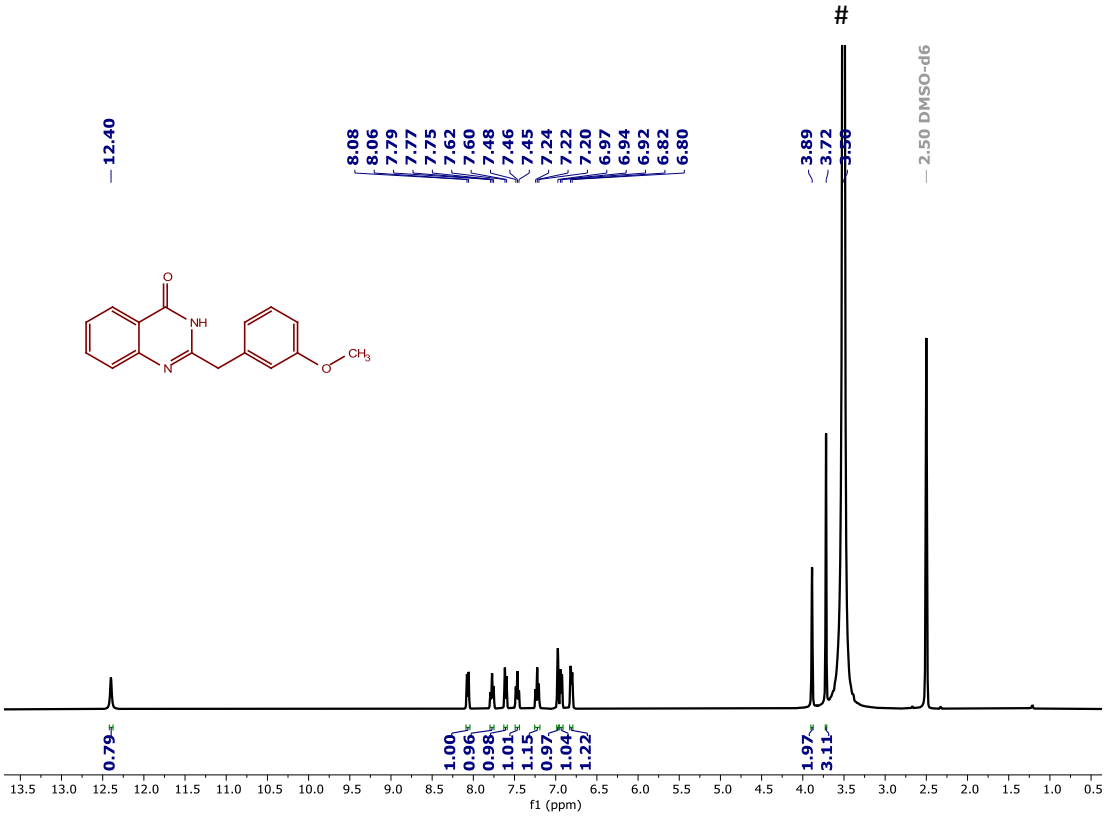
*$^{13}C\{^{1}H\}$ NMR of 6-methoxy-2-phenylquinazolin-4(3H)-one (Compound-**5s**) in DMSO-d_6.*



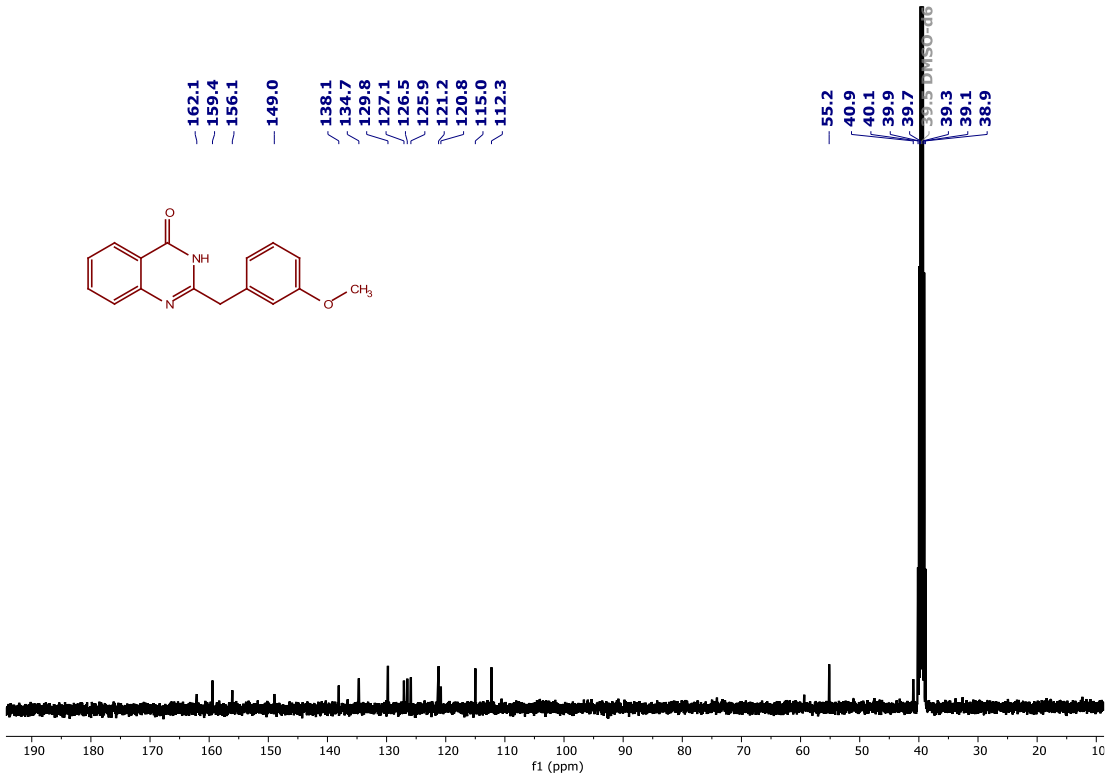
*^{1}H NMR of 2-benzylquinazolin-4(3H)-one (Compound-**6a**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



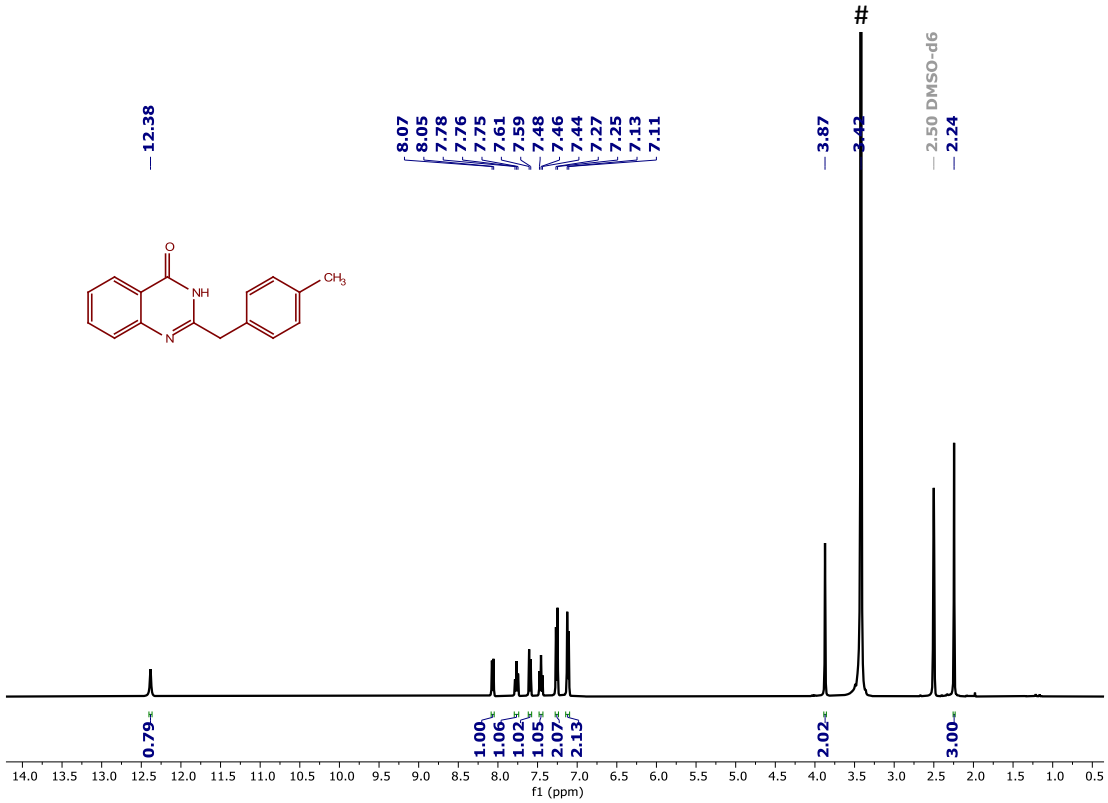
*$^{13}C\{^{1}H\}$ NMR of 2-benzylquinazolin-4(3H)-one (Compound-**6a**) in DMSO-d_6*



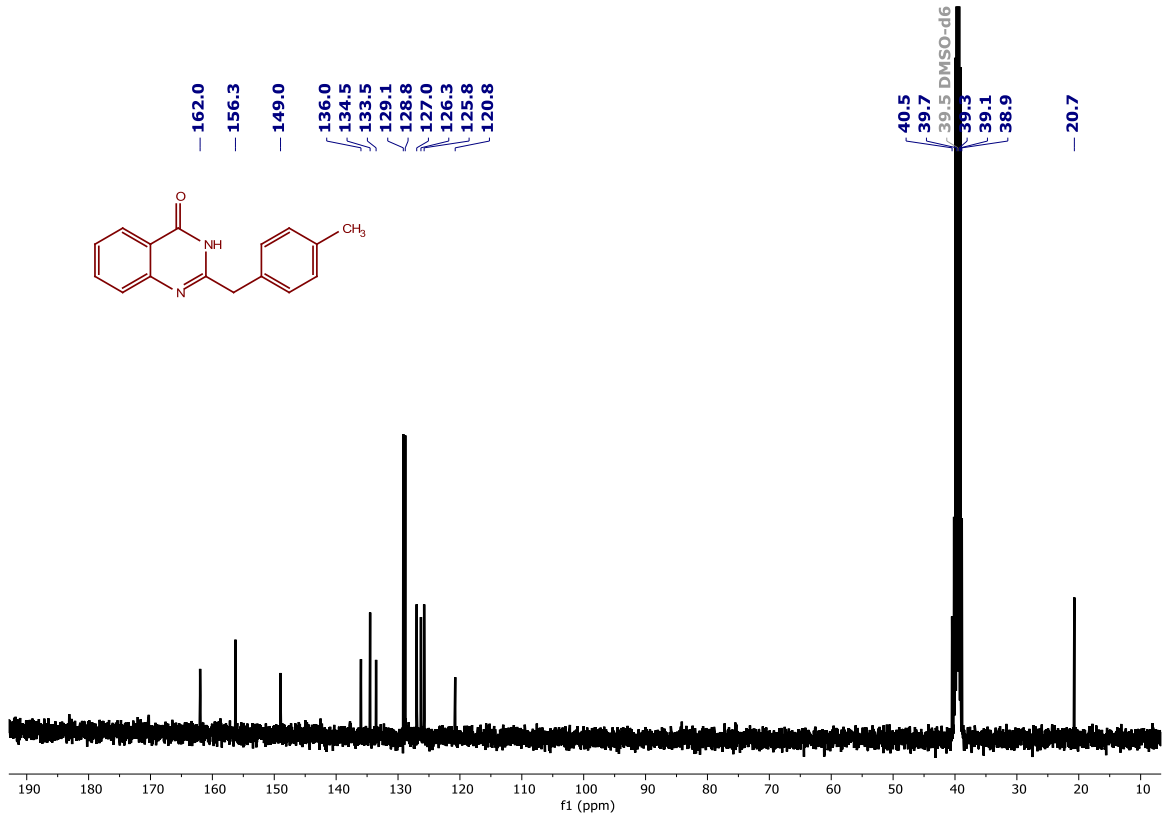
*^{1}H NMR of 2-(3-methoxybenzyl)quinazolin-4(3H)-one (Compound-**6b**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



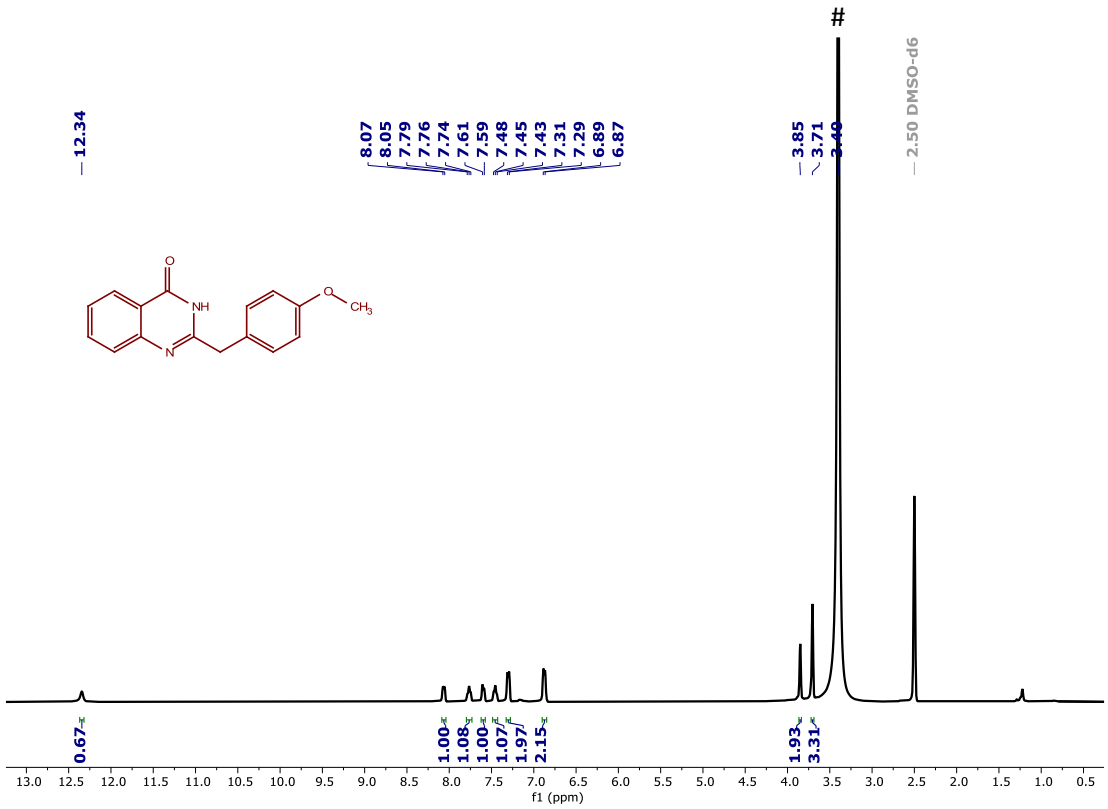
*$^{13}C\{^{1}H\}$ NMR of 2-(3-methoxybenzyl)quinazolin-4(3H)-one (Compound-**6b**) in DMSO-d_6*



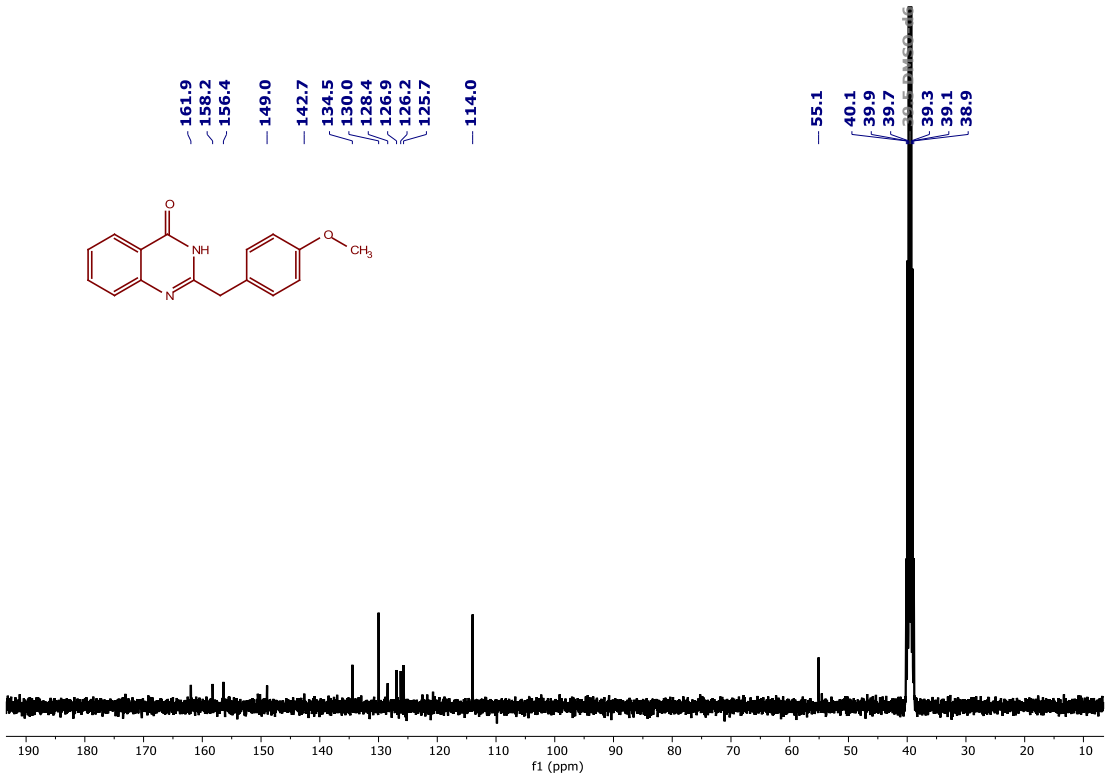
*^{1}H NMR of 2-(4-methylbenzyl)quinazolin-4(3H)-one (Compound-**6c**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



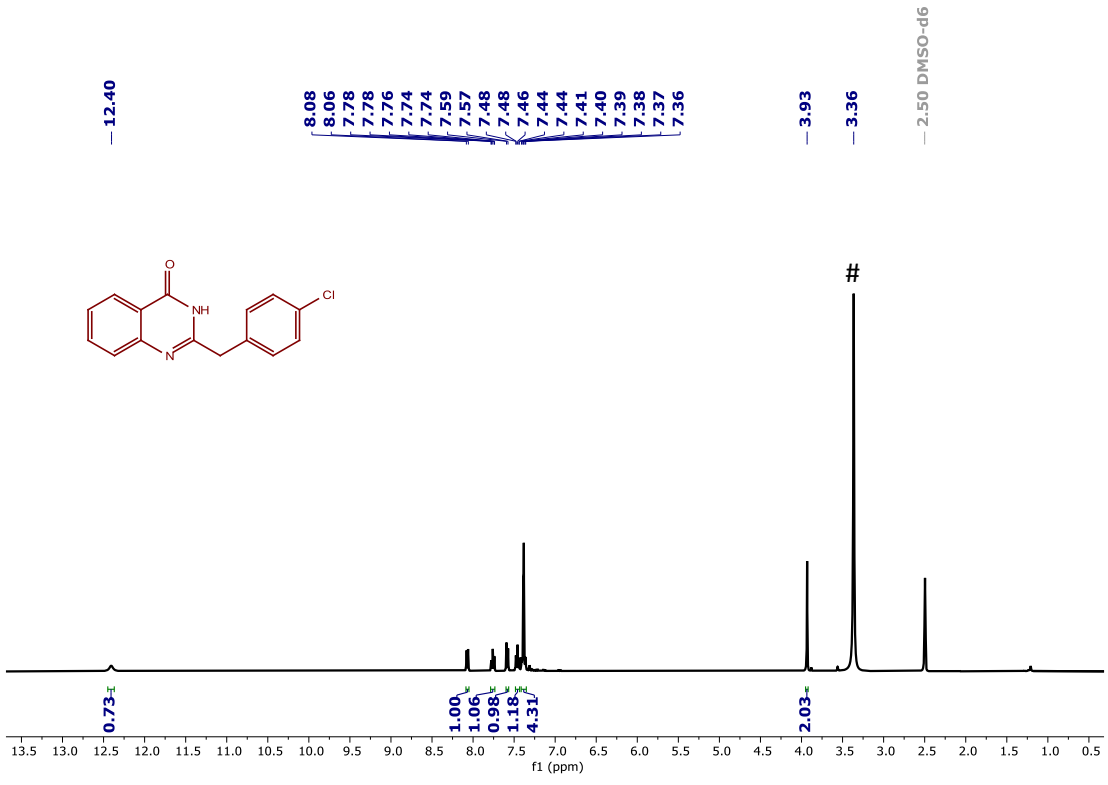
*$^{13}C\{^{1}H\}$ NMR of 2-(4-methylbenzyl)quinazolin-4(3H)-one (Compound-**6c**) in DMSO-d_6*



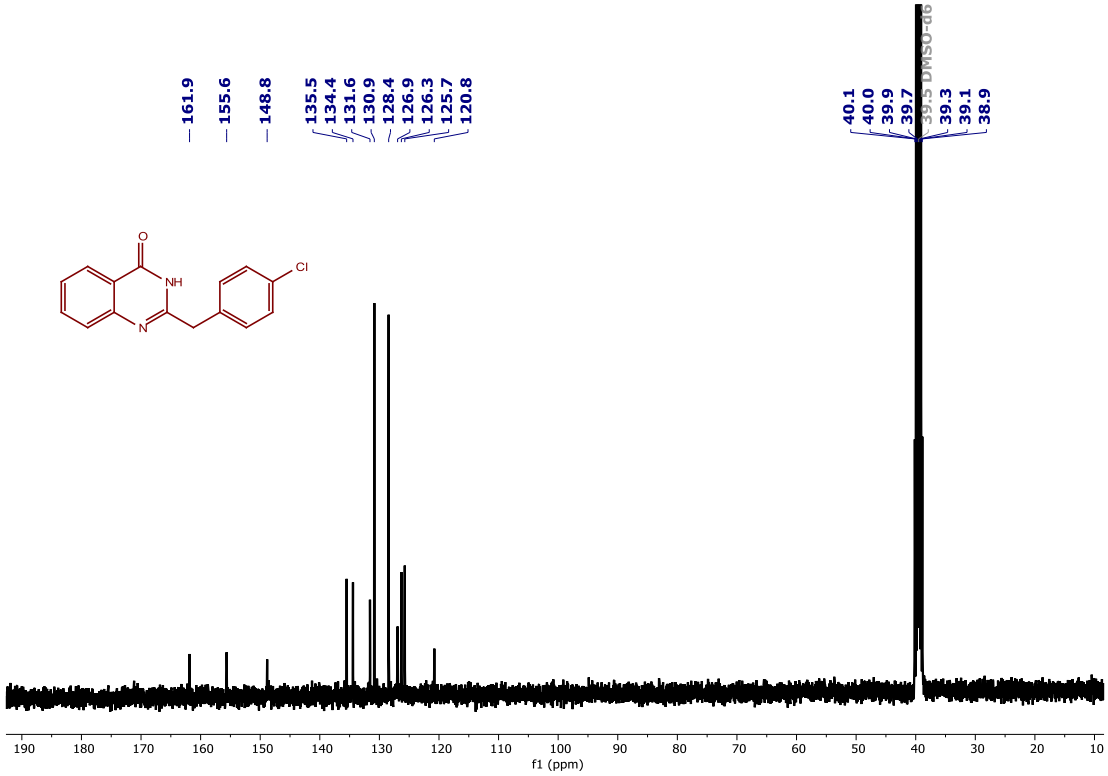
*^{1}H NMR of 2-(4-methoxybenzyl)quinazolin-4(3H)-one (Compound-**6d**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



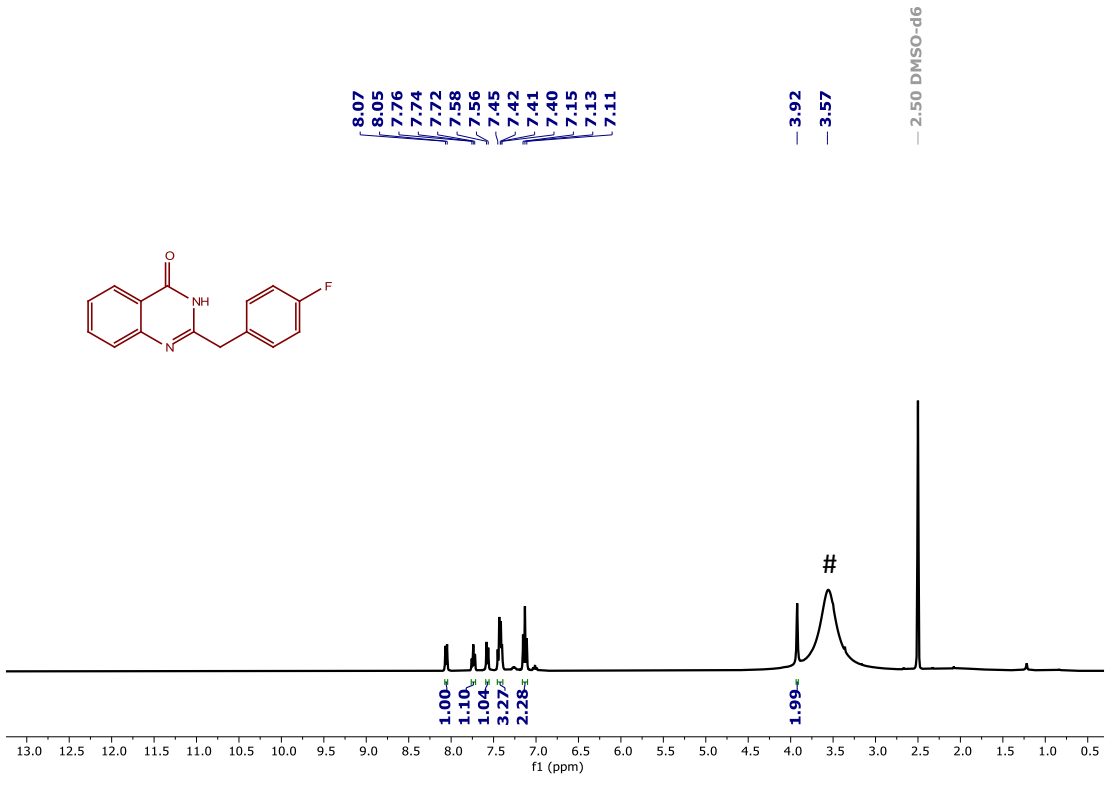
*$^{13}C\{^{1}H\}$ NMR of 2-(4-methoxybenzyl)quinazolin-4(3H)-one (Compound-**6d**) in DMSO-d_6*



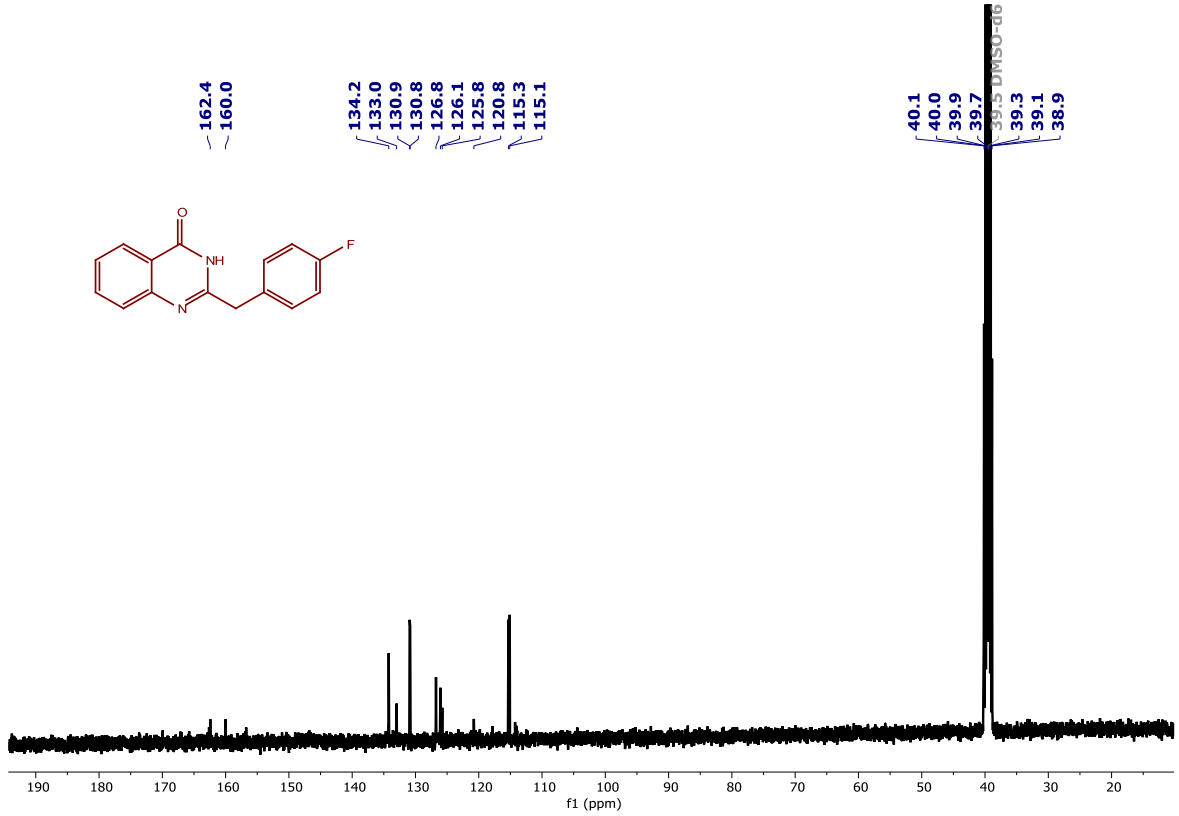
*^{1}H NMR of 2-(4-chlorobenzyl)quinazolin-4(3H)-one (Compound-**6e**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



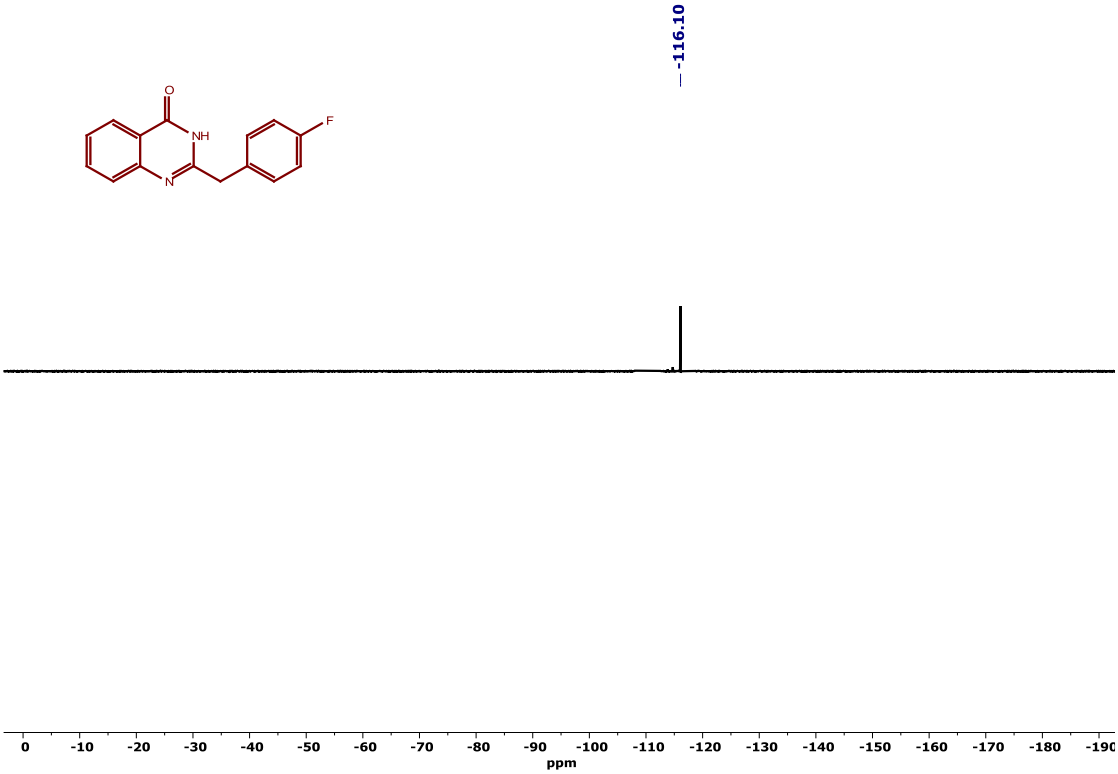
*$^{13}C\{^{1}H\}$ NMR of 2-(4-chlorobenzyl)quinazolin-4(3H)-one (Compound-**6e**) in DMSO-d_6*



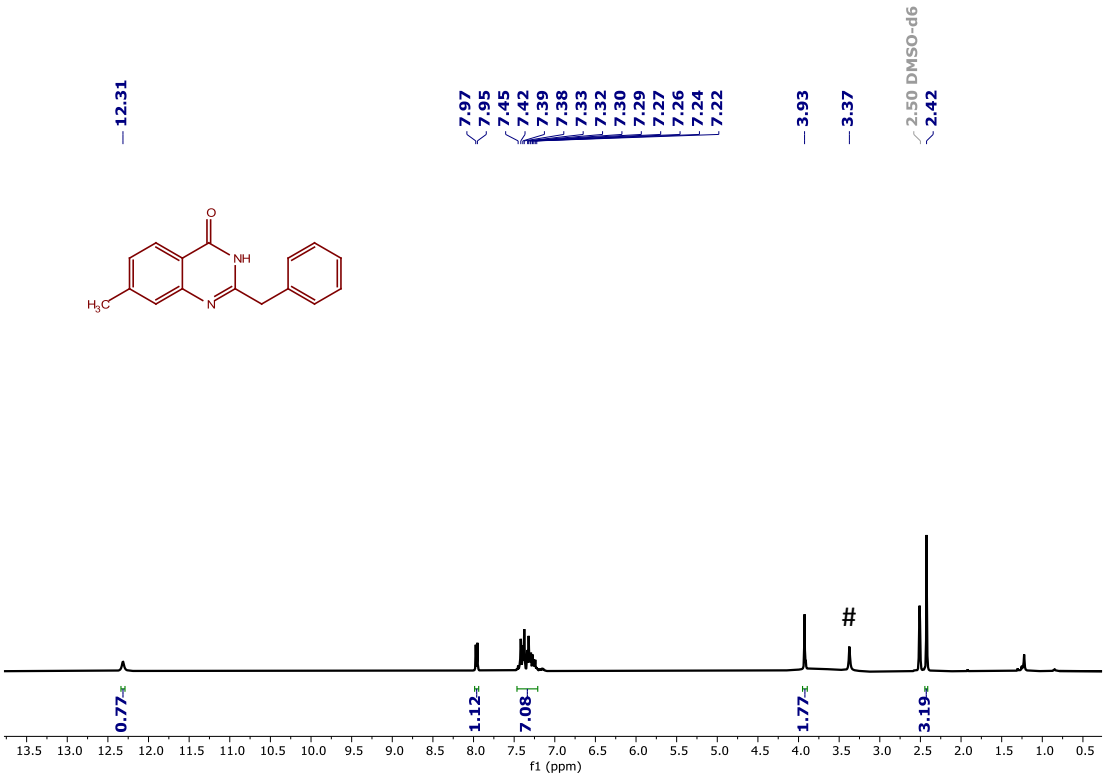
*^{1}H NMR of 2-(4-fluorobenzyl)quinazolin-4(3H)-one (Compound-**6f**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



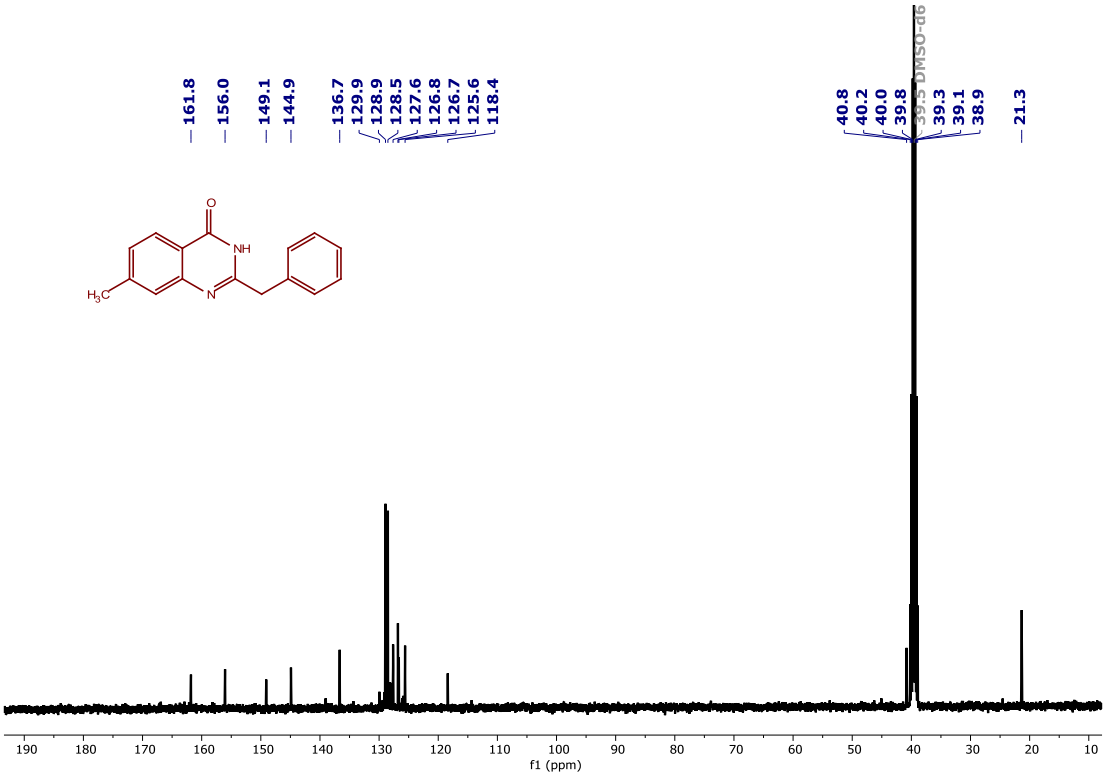
*$^{13}C\{^{1}H\}$ NMR of 2-(4-fluorobenzyl)quinazolin-4(3H)-one (Compound-**6f**) in DMSO-d_6*



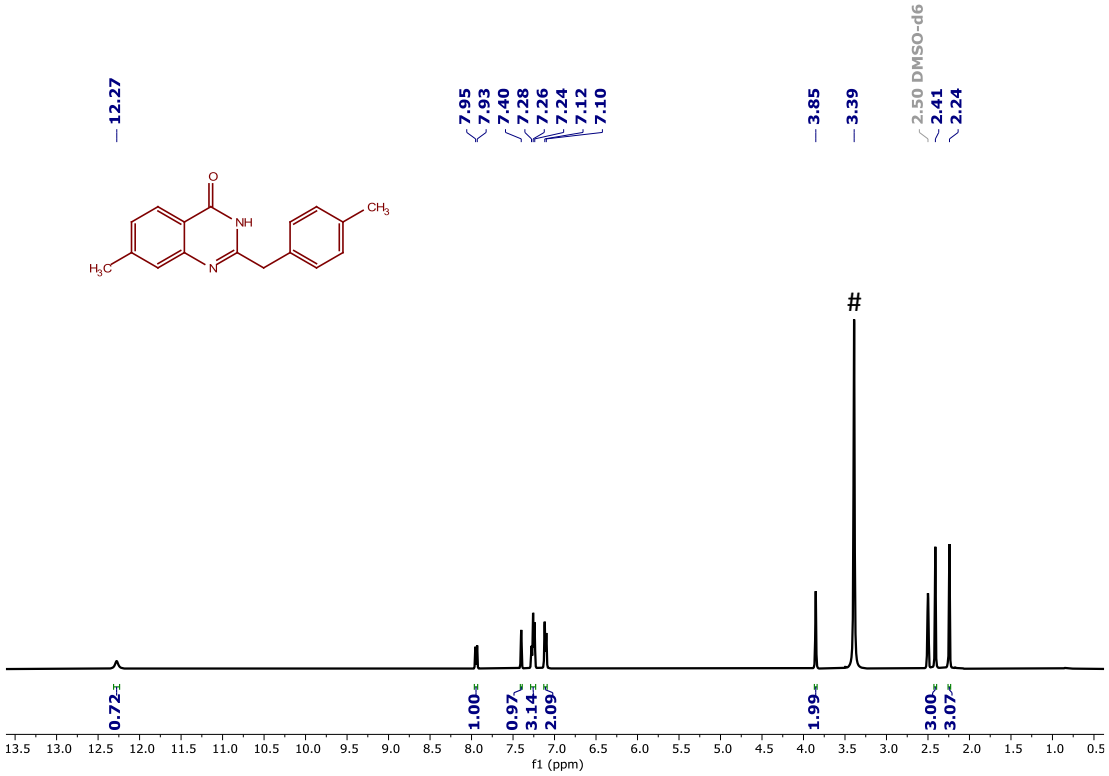
*^{19}F NMR of 2-(4-fluorobenzyl)quinazolin-4(3H)-one (Compound-**6f**) in DMSO-d_6*



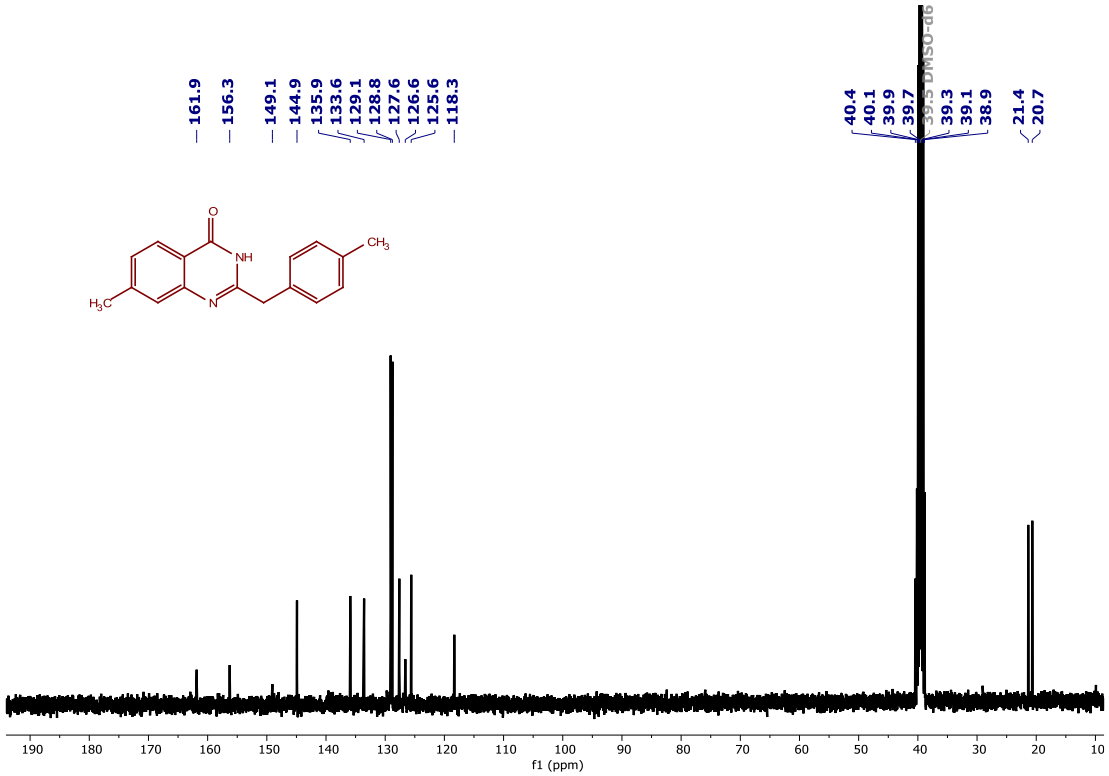
*[1]H NMR of 2-benzyl-7-methylquinazolin-4(3H)-one (Compound-**6g**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



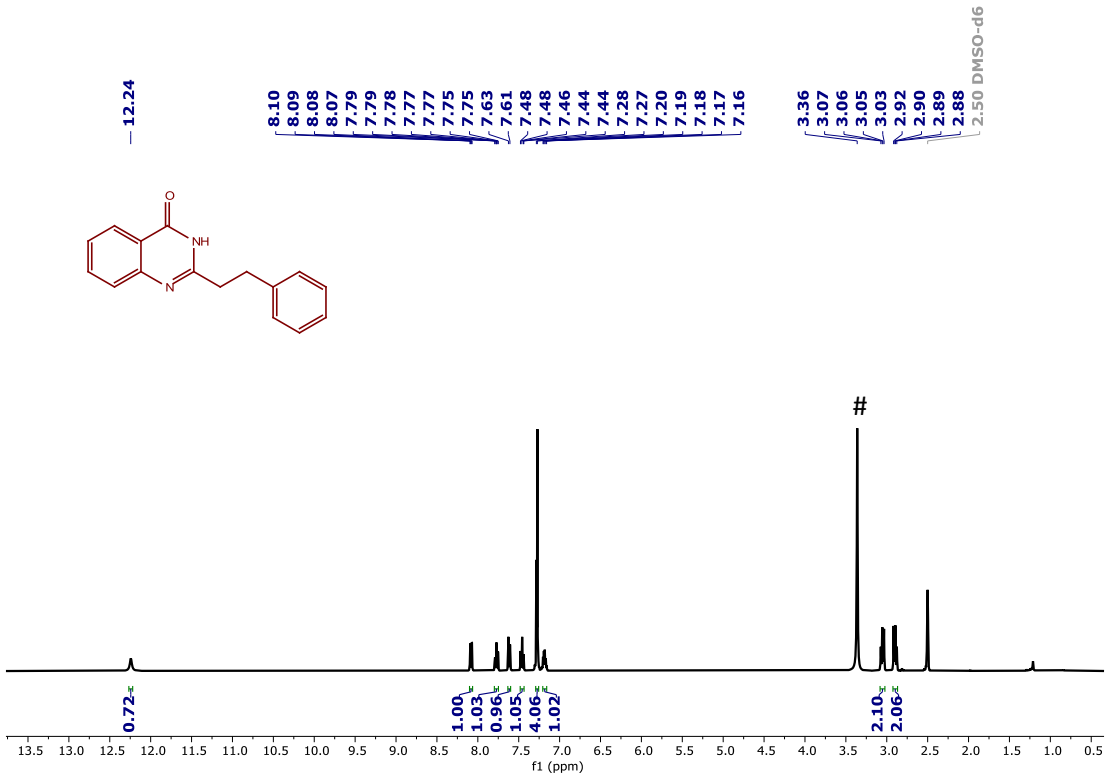
*[13]C{[1]H} NMR of 2-benzyl-7-methylquinazolin-4(3H)-one (Compound-**6g**) in DMSO-d_6*



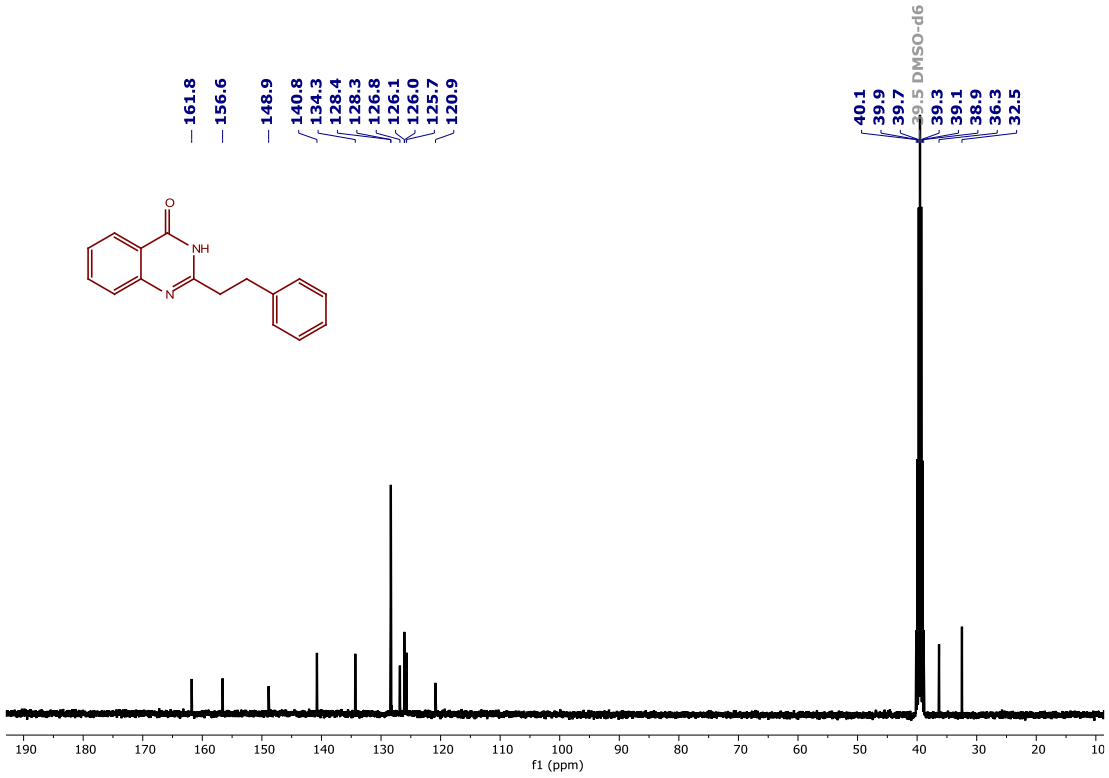
*[1]H NMR of 7-methyl-2-(4-methylbenzyl)quinazolin-4(3H)-one (Compound-**6h**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



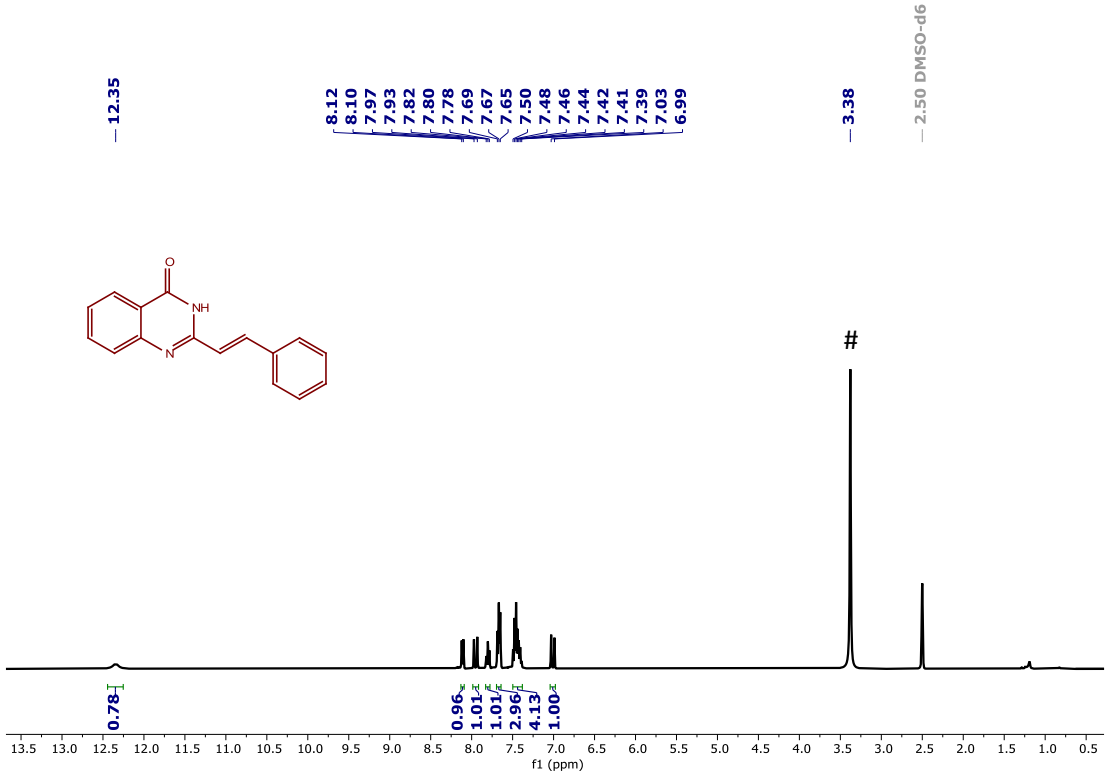
*[13]C{[1]H} NMR of 7-methyl-2-(4-methylbenzyl)quinazolin-4(3H)-one (Compound-**6h**) in DMSO-d_6*



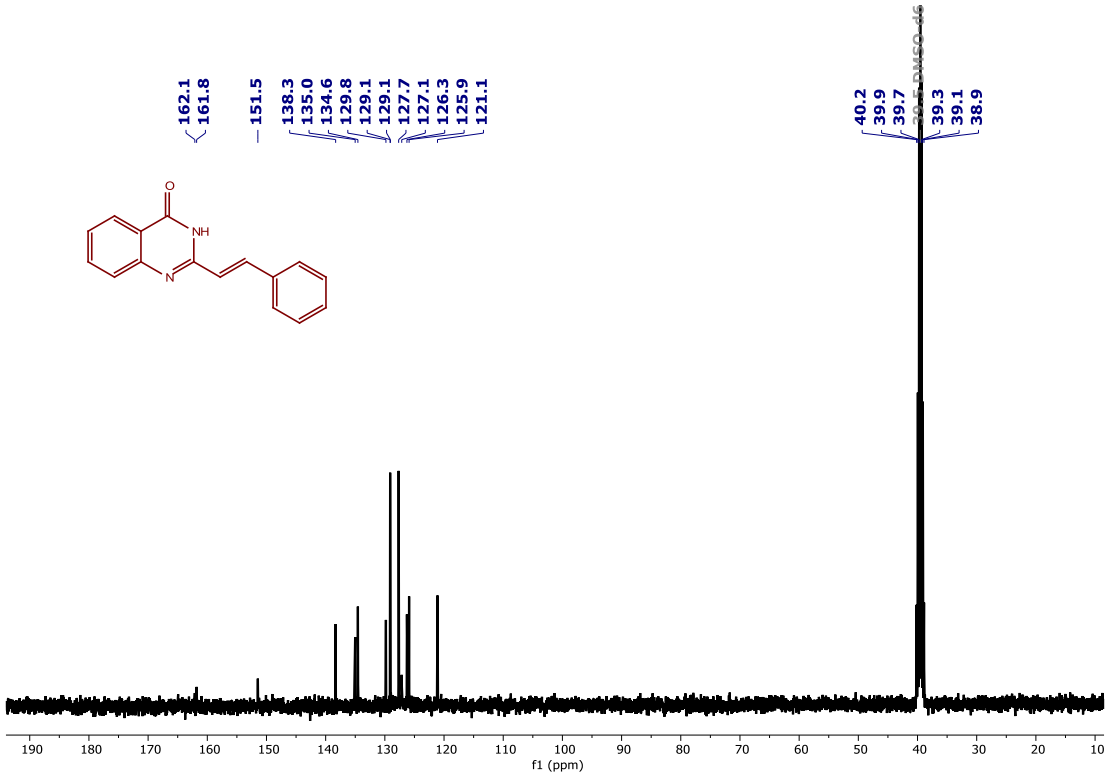
*[1]H NMR of 2-phenethylquinazolin-4(3H)-one (Compound-**6i**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



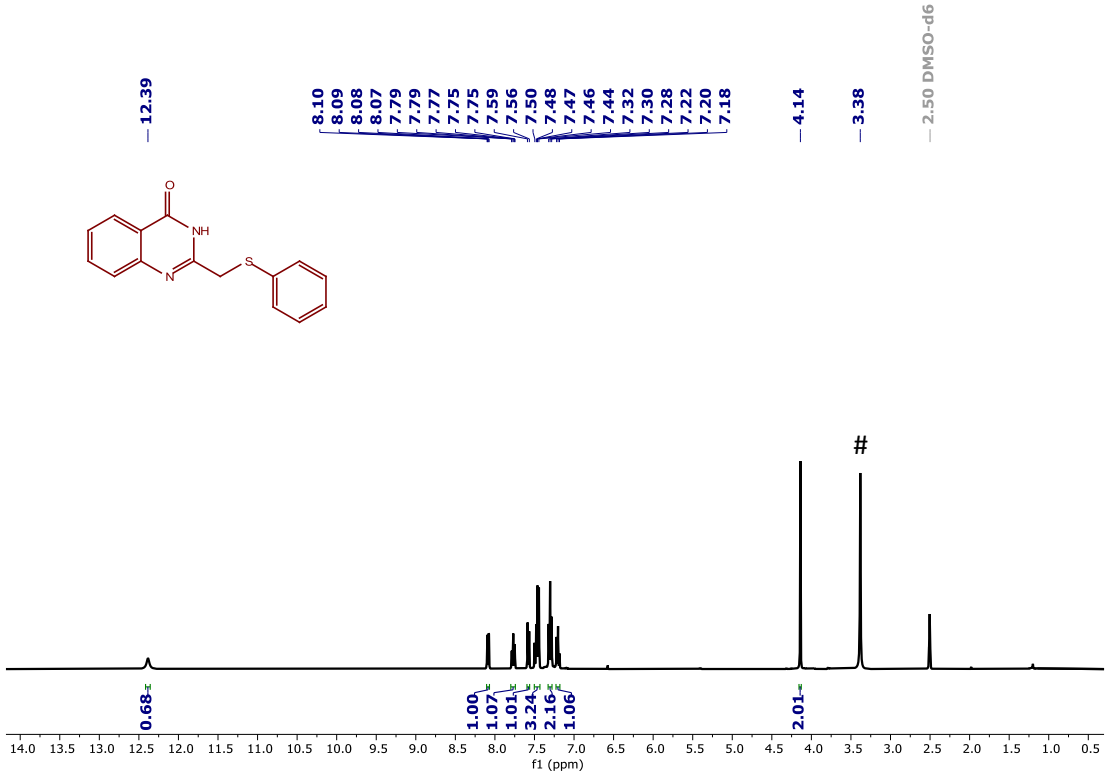
*[13]C{[1]H} NMR of 2-phenethylquinazolin-4(3H)-one (Compound-**6i**) in DMSO-d_6*



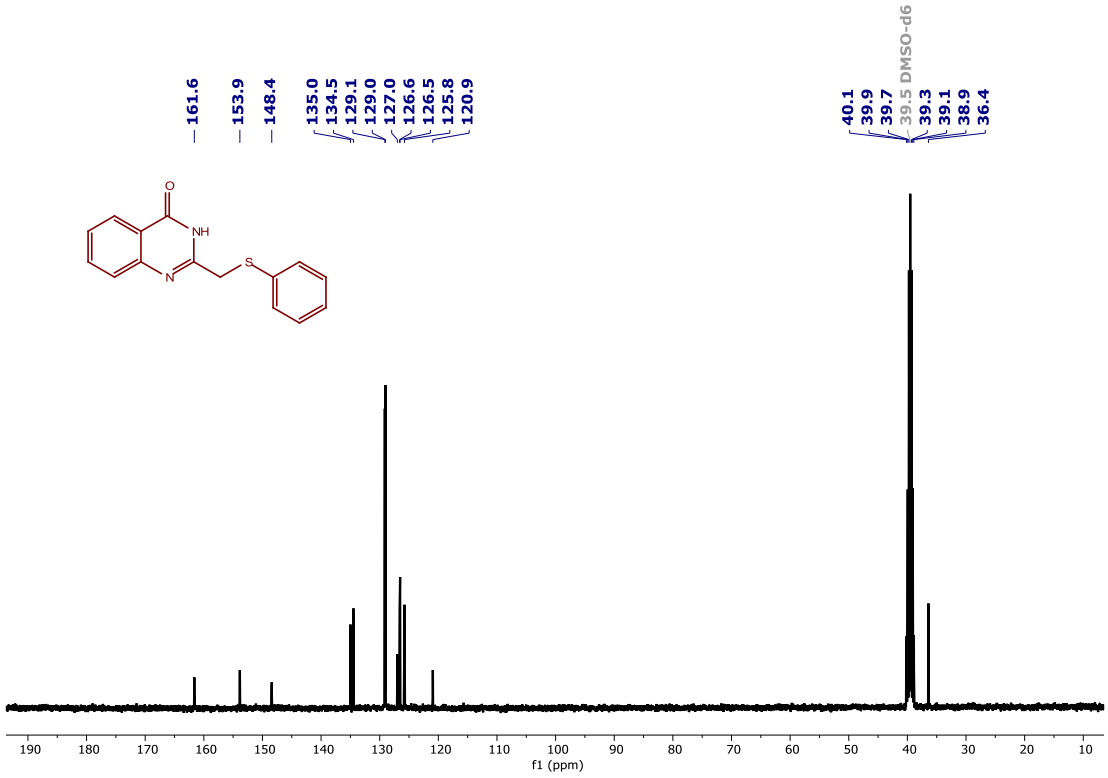
*[1]H NMR of (E)-2-styrylquinazolin-4(3H)-one (Compound-**6j**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



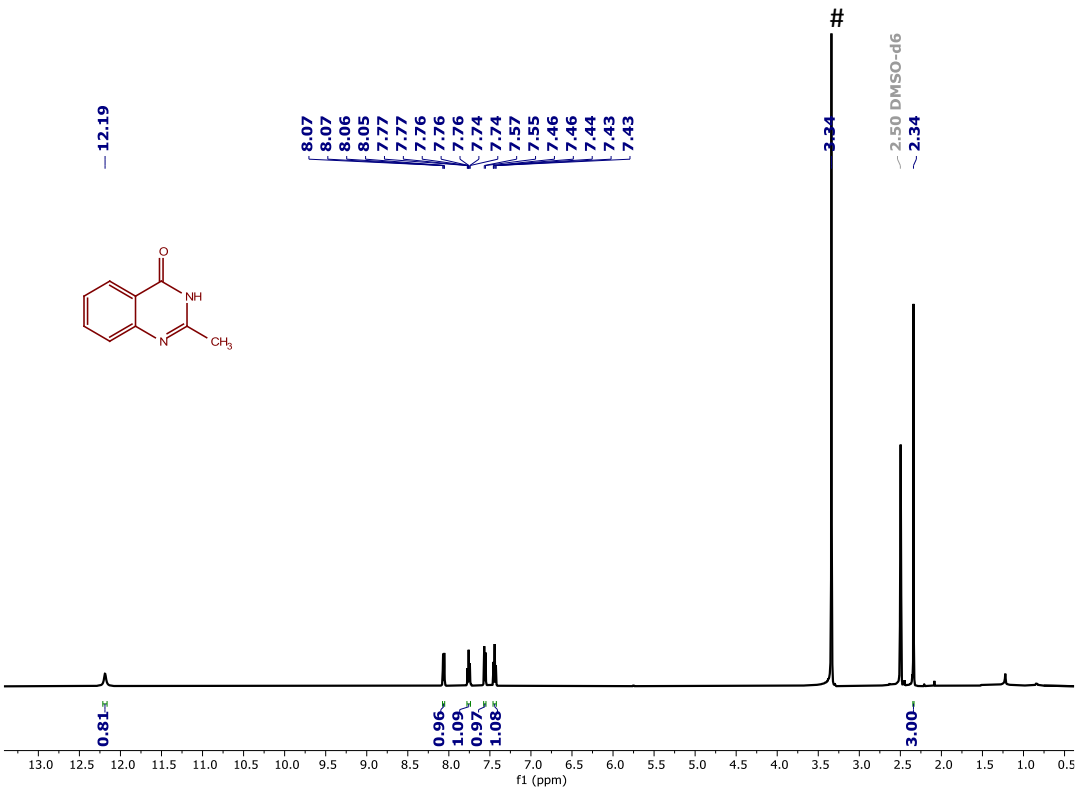
*[13]C{[1]H} NMR of (E)-2-styrylquinazolin-4(3H)-one (Compound-**6j**) in DMSO-d_6*



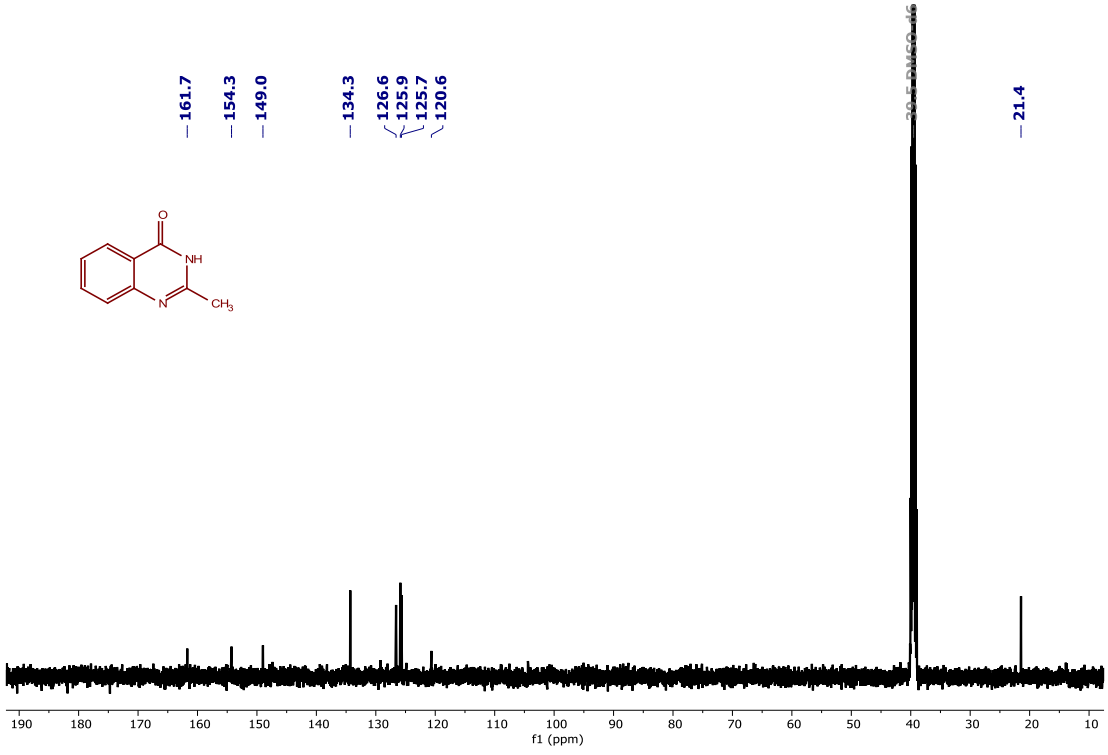
*[1]H NMR of 2-((phenylthio)methyl)quinazolin-4(3H)-one (Compound-**6k**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



*[13]C{[1]H} NMR of 2-((phenylthio)methyl)quinazolin-4(3H)-one (Compound-**6k**) in DMSO-d_6*

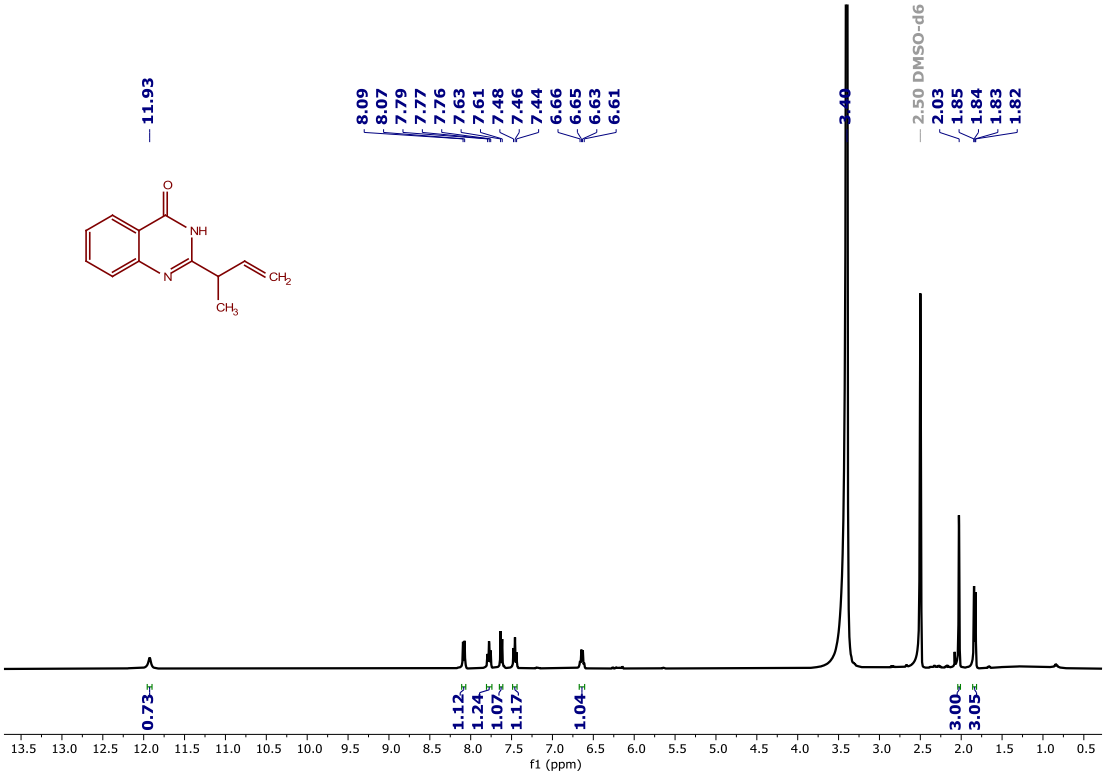


*[1]H NMR of 2-methylquinazolin-4(3H)-one (Compound-**8a**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*

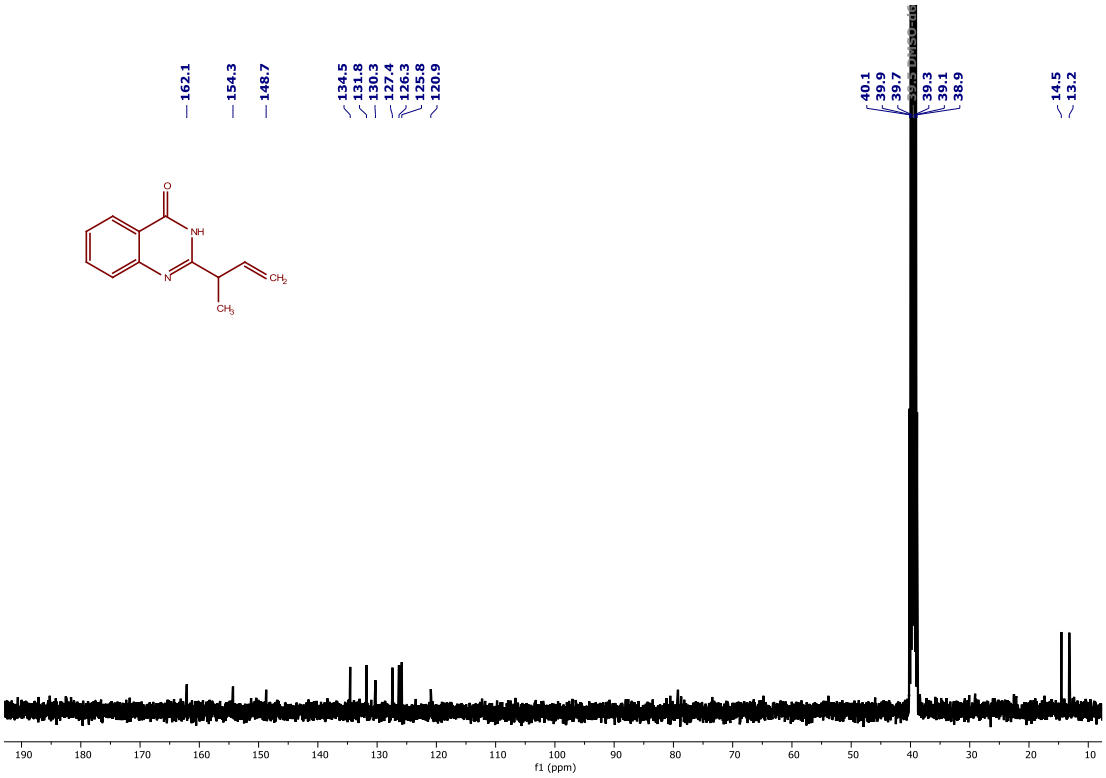


*[13]C{[1]H} NMR of 2-methylquinazolin-4(3H)-one (Compound-**8a**) in DMSO-d_6*

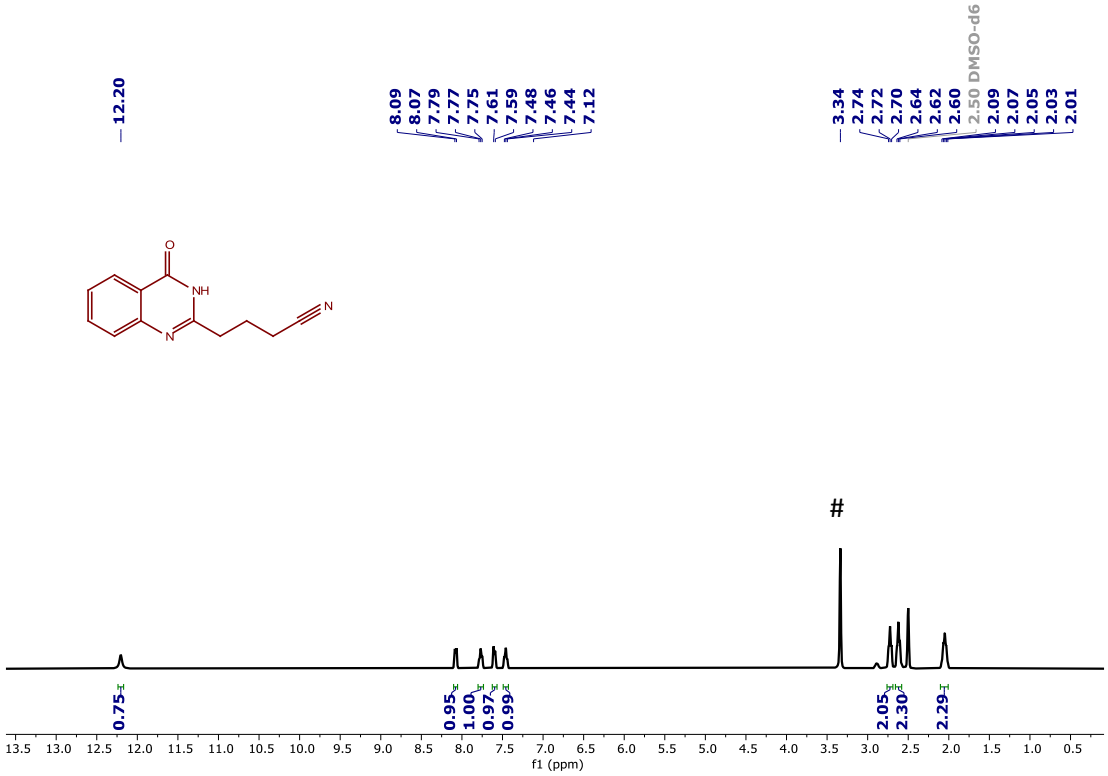
#



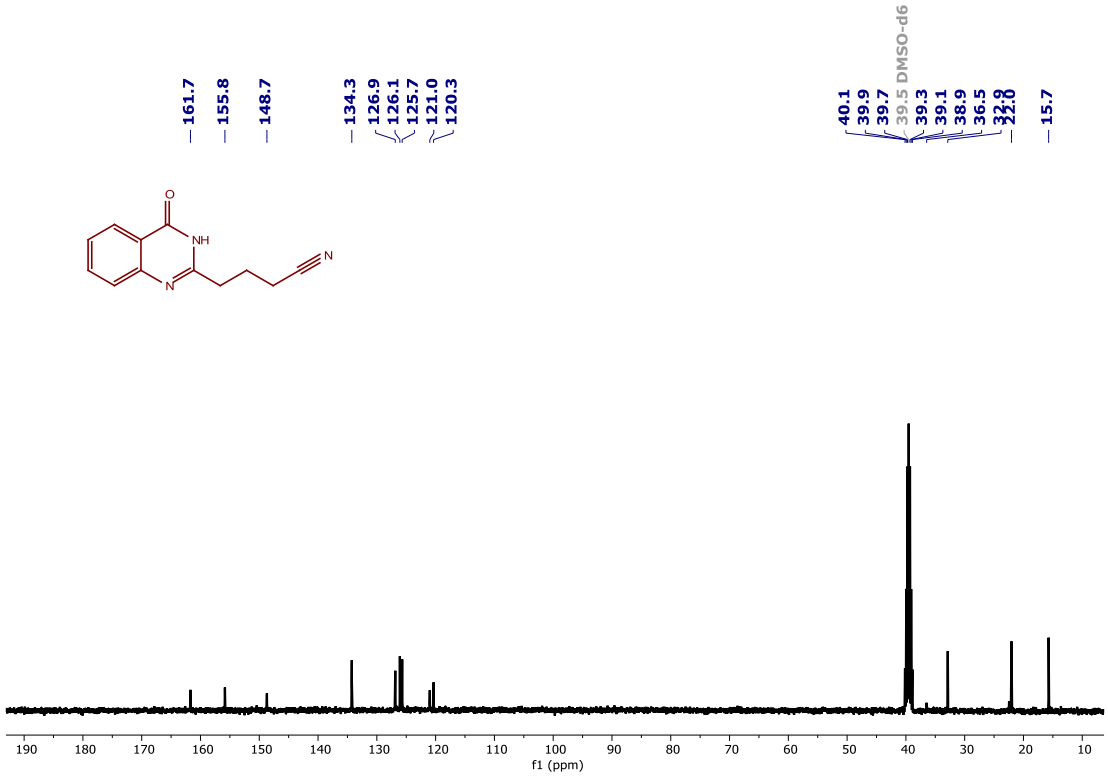
*^{1}H NMR of 2-(but-3-en-2-yl)quinazolin-4(3H)-one (Compound-**8b**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



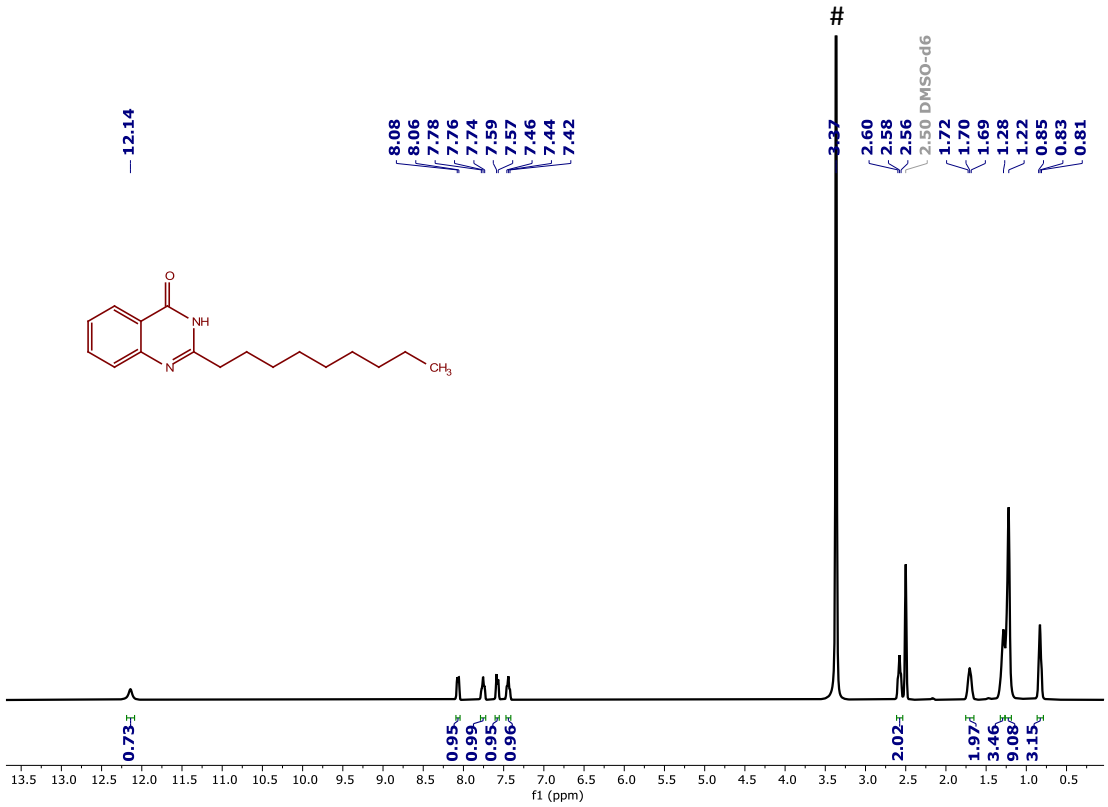
*$^{13}C\{^{1}H\}$ NMR of 2-(but-3-en-2-yl)quinazolin-4(3H)-one (Compound-**8b**) in DMSO-d_6*



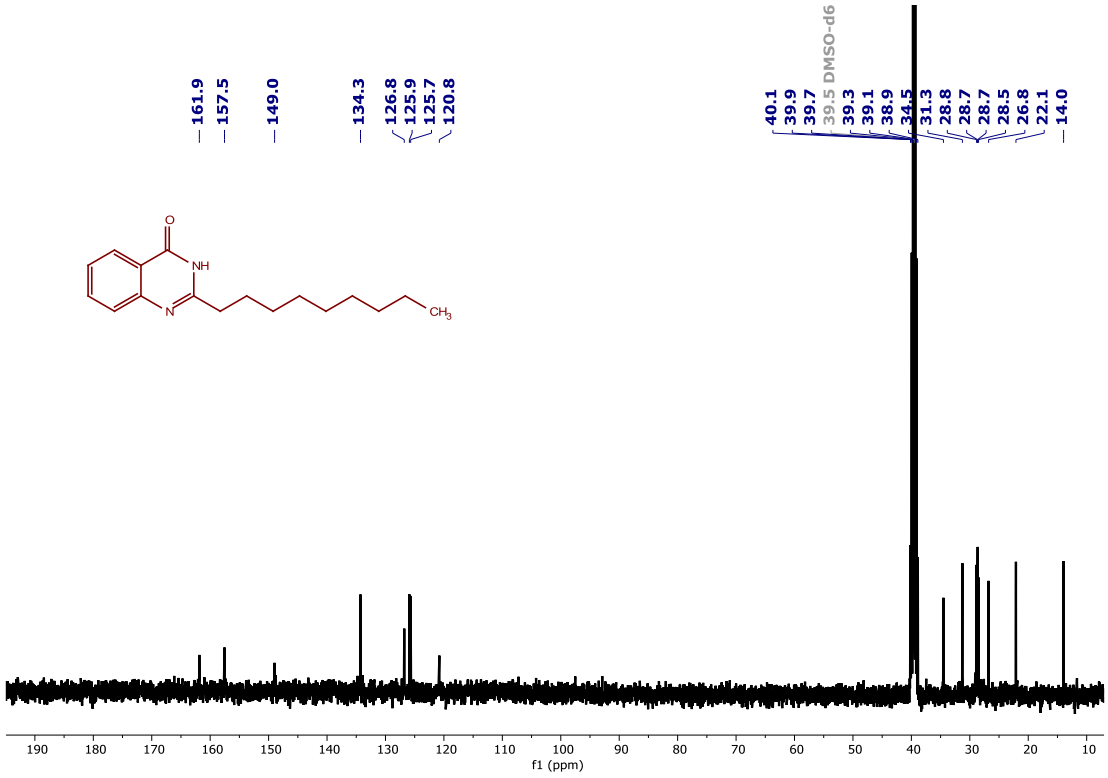
*[1]H NMR of 4-(4-oxo-3,4-dihydroquinazolin-2-yl)butanenitrile (Compound-**8c**) in DMSO-d6. # indicates the solvent impurity of H_2O in DMSO-d_6*



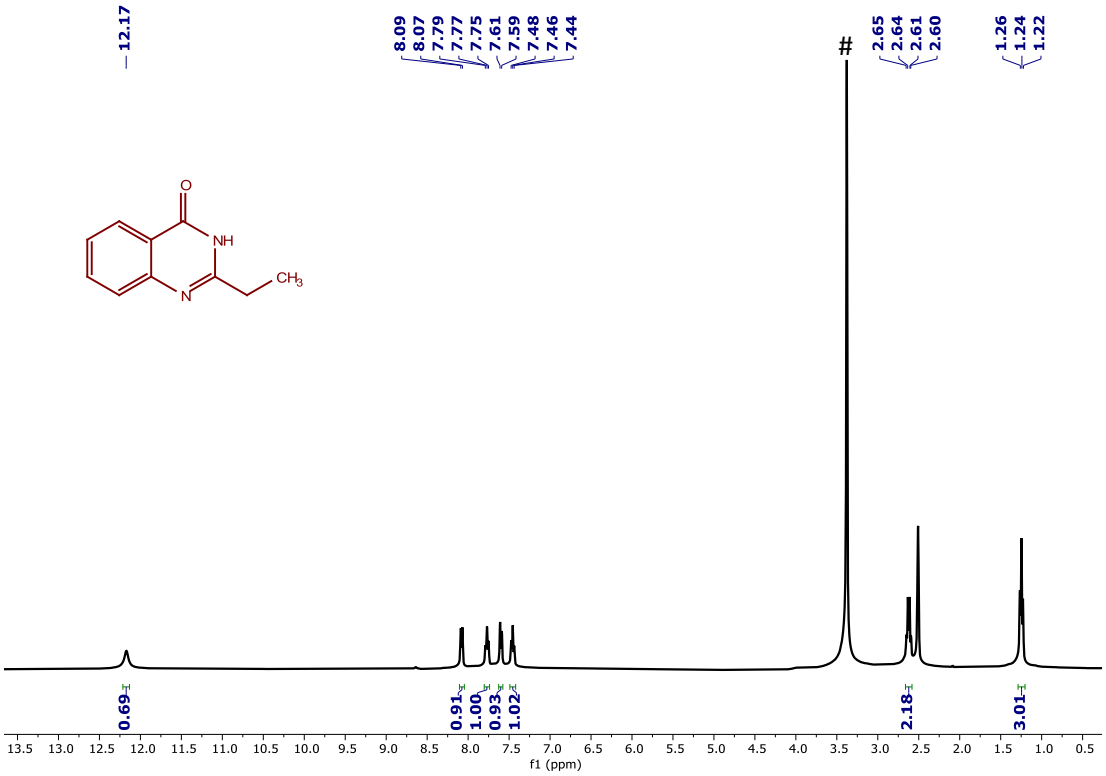
*[13]C{[1]H} NMR of 4-(4-oxo-3,4-dihydroquinazolin-2-yl)butanenitrile (Compound-**8c**) in DMSO-d6*



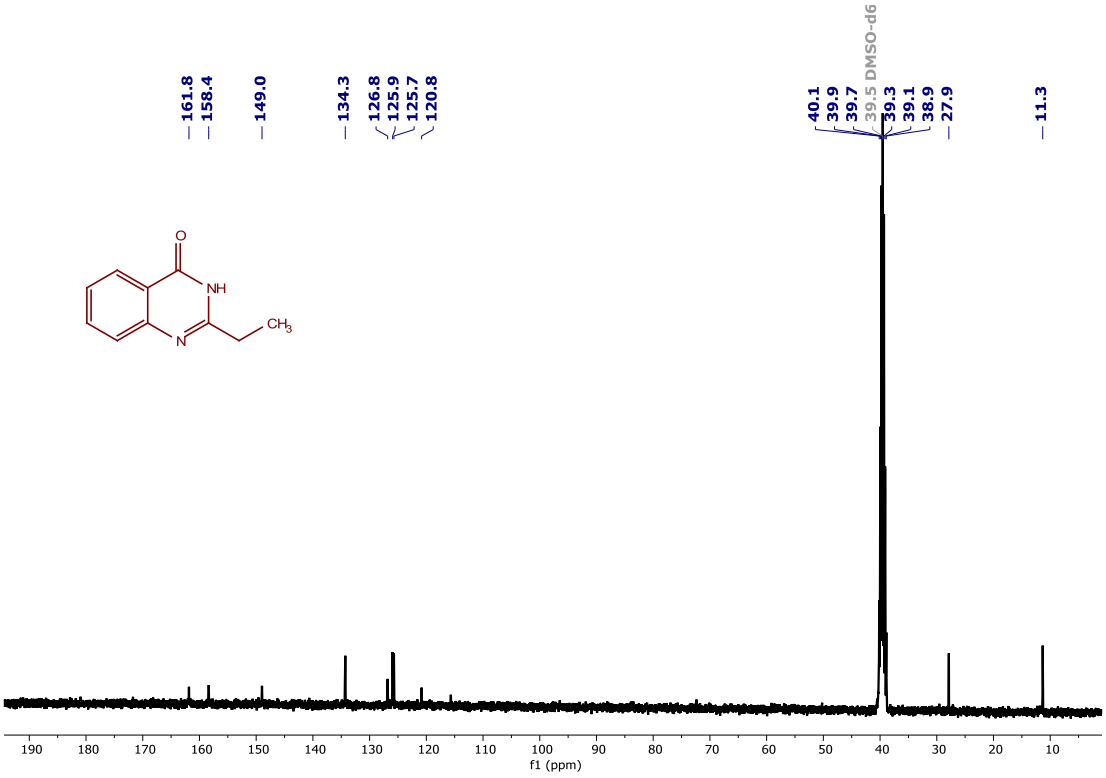
*[1]H NMR of 2-nonylquinazolin-4(3H)-one (Compound-**8d**) in DMSO-d6. # indicates the solvent impurity of H_2O in DMSO-d6*



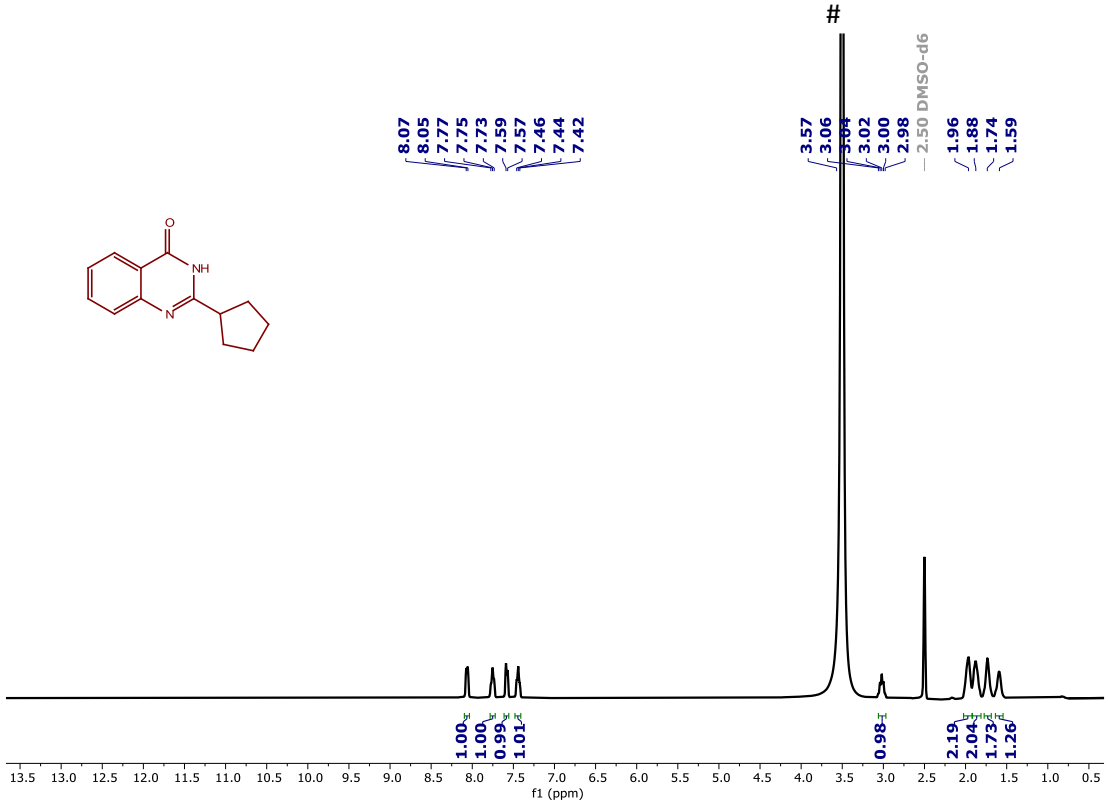
*[13]C{[1]H} NMR of 2-nonylquinazolin-4(3H)-one (Compound-**8d**) in DMSO-d6*



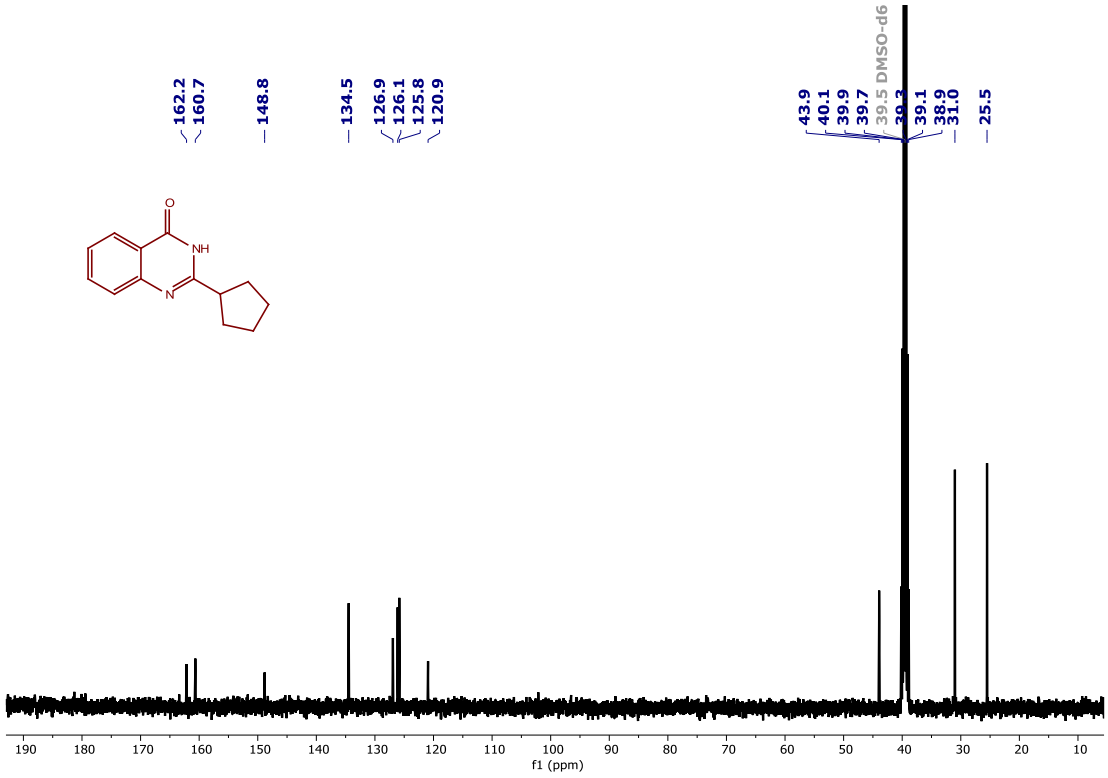
*[1]H NMR of 2-ethylquinazolin-4(3H)-one (Compound-**8e**) in DMSO-d6. # indicates the solvent impurity of H_2O in DMSO-d6*



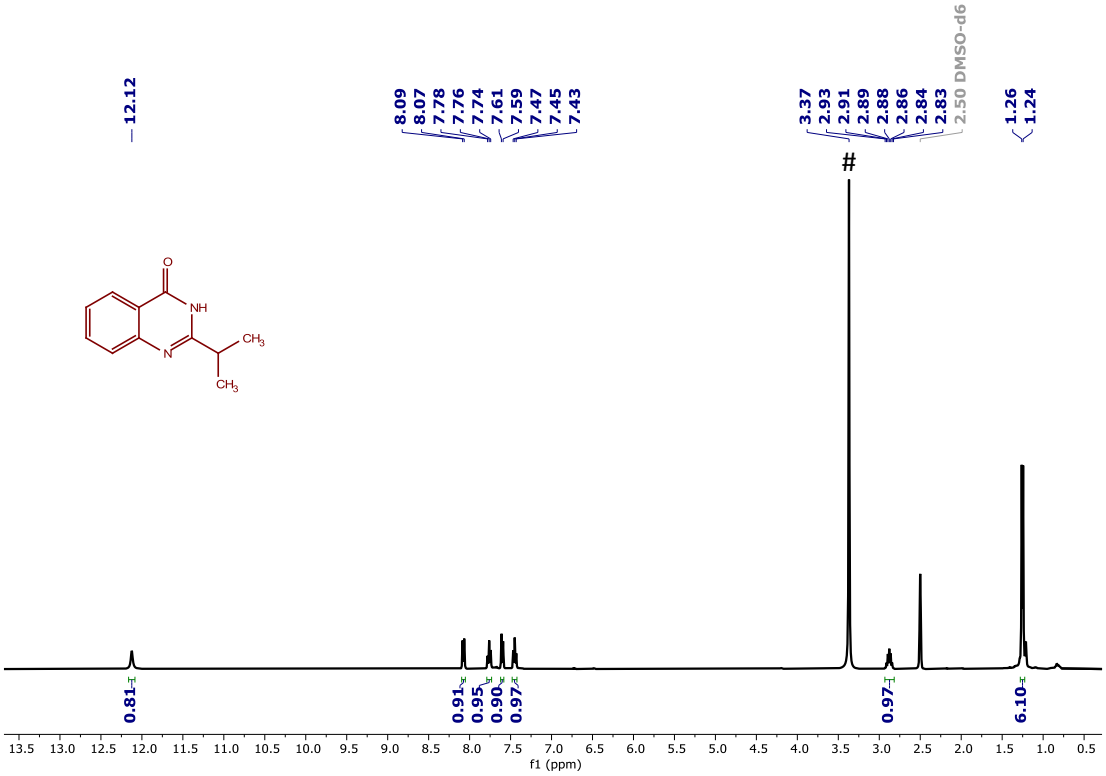
*[13]C{[1]H} NMR of 2-ethylquinazolin-4(3H)-one (Compound-**8e**) in DMSO-d6*



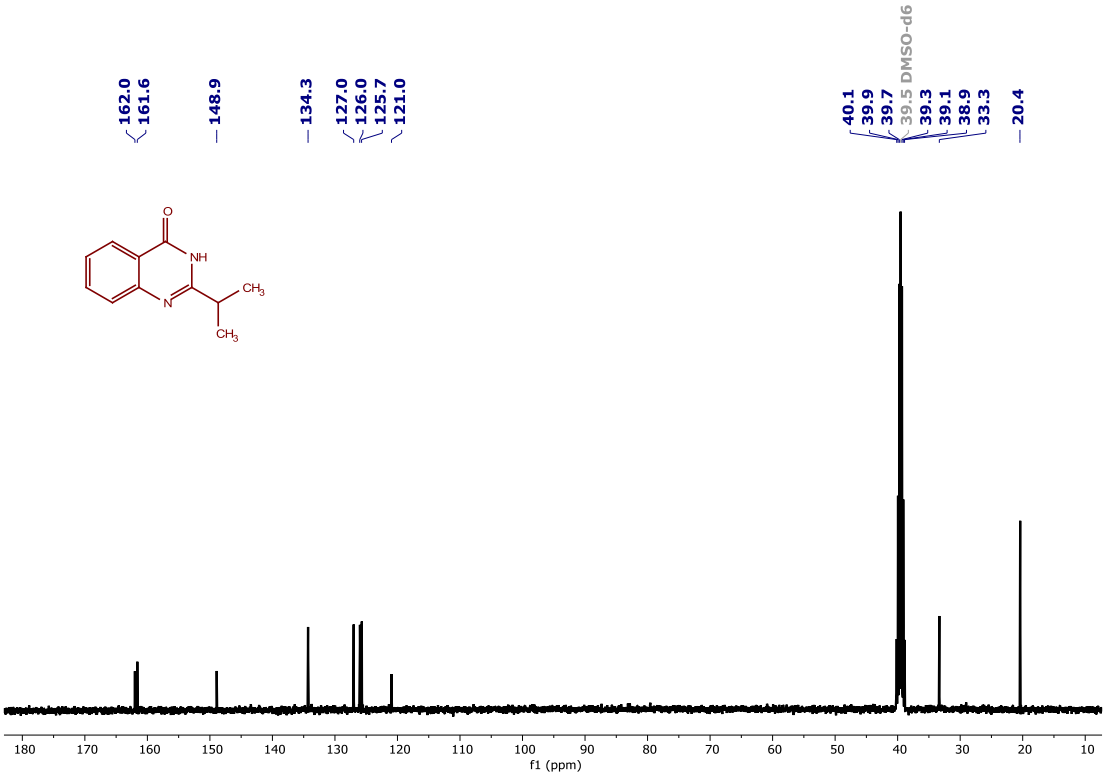
*[1]H NMR of 2-cyclopentylquinazolin-4(3H)-one (Compound-**8f**) in DMSO-d6. # indicates the solvent impurity of H_2O in DMSO-d_6*



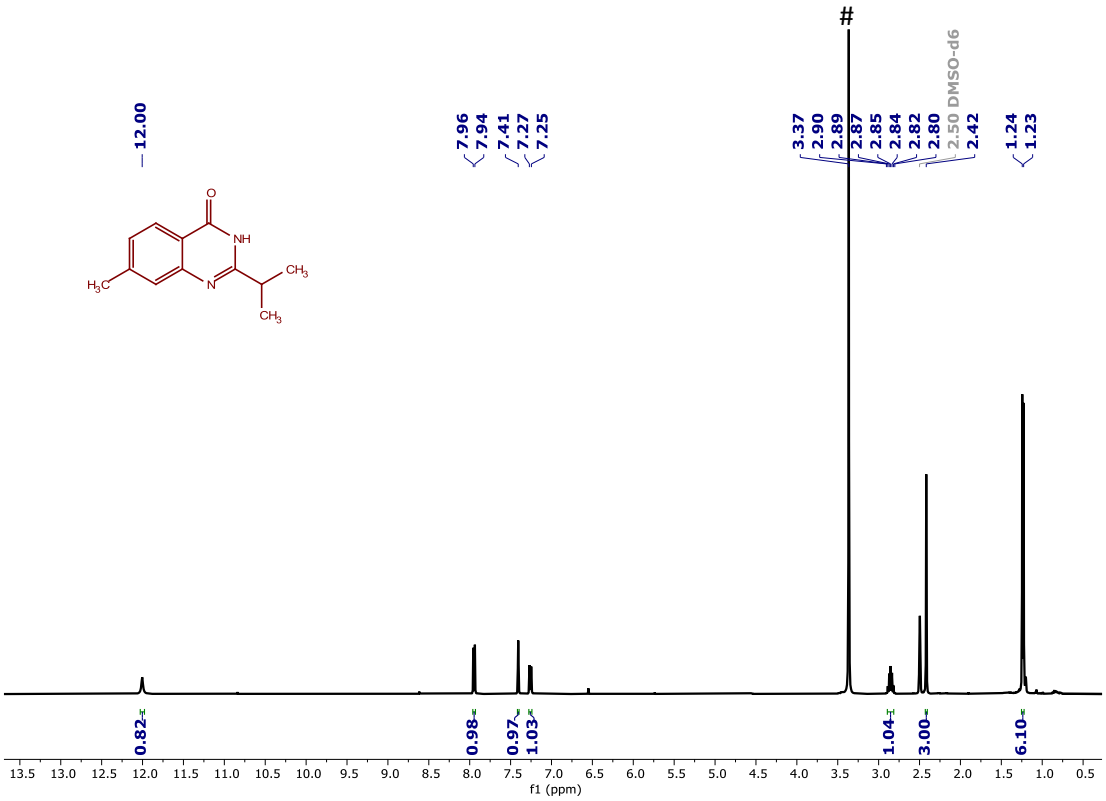
*[13]C{[1]H} NMR of 2-cyclopentylquinazolin-4(3H)-one (Compound-**8f**) in DMSO-d_6*



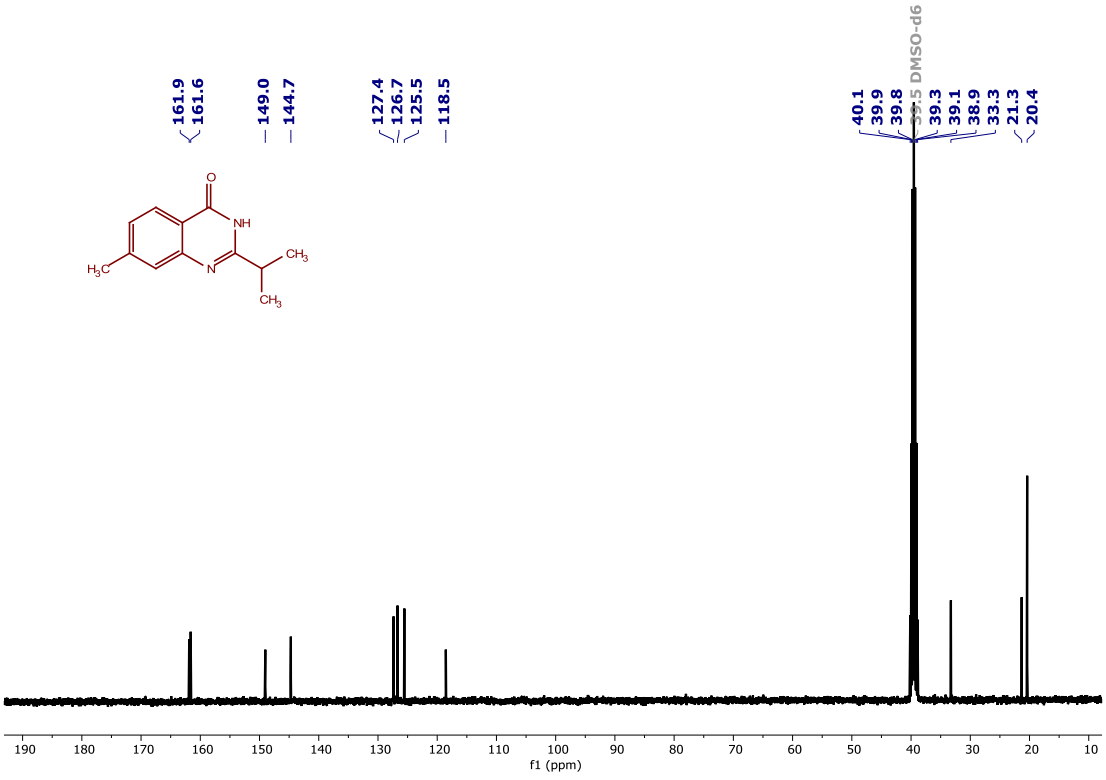
*[1]H NMR of 2-isopropylquinazolin-4(3H)-one (Compound-**8g**) in DMSO-d6. # indicates the solvent impurity of H_2O in DMSO-d6*



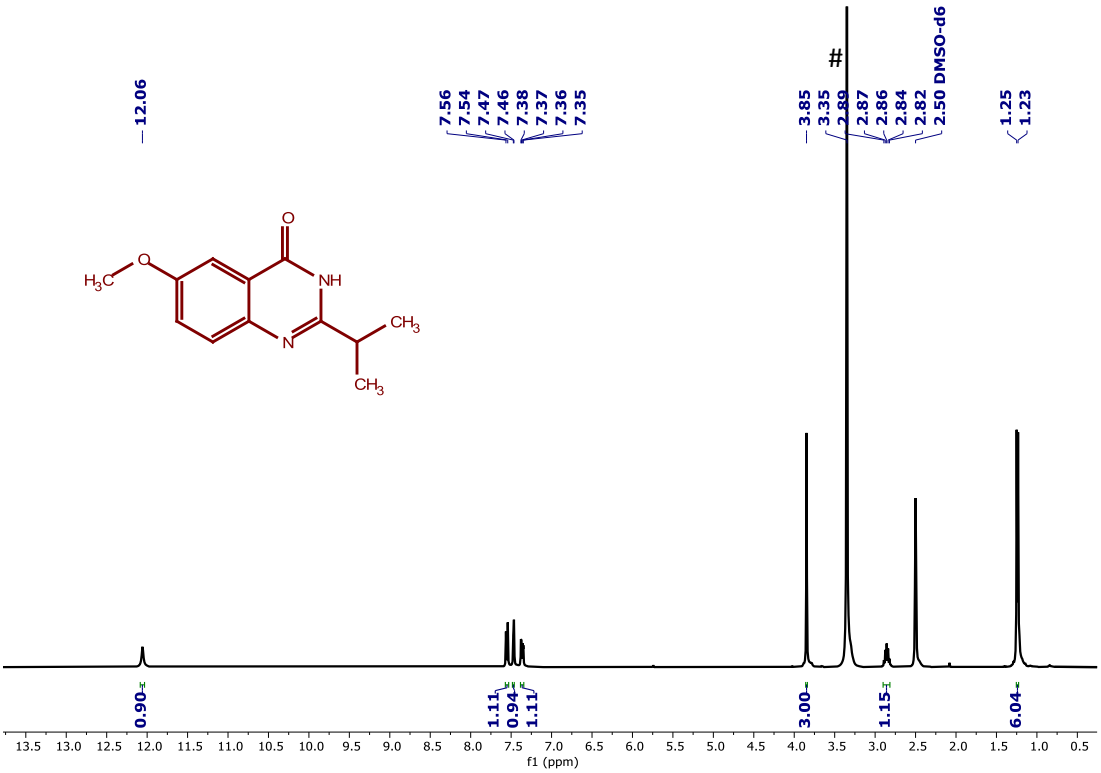
*[13]C{[1]H} NMR of 2-isopropylquinazolin-4(3H)-one (Compound-**8g**) in DMSO-d6*



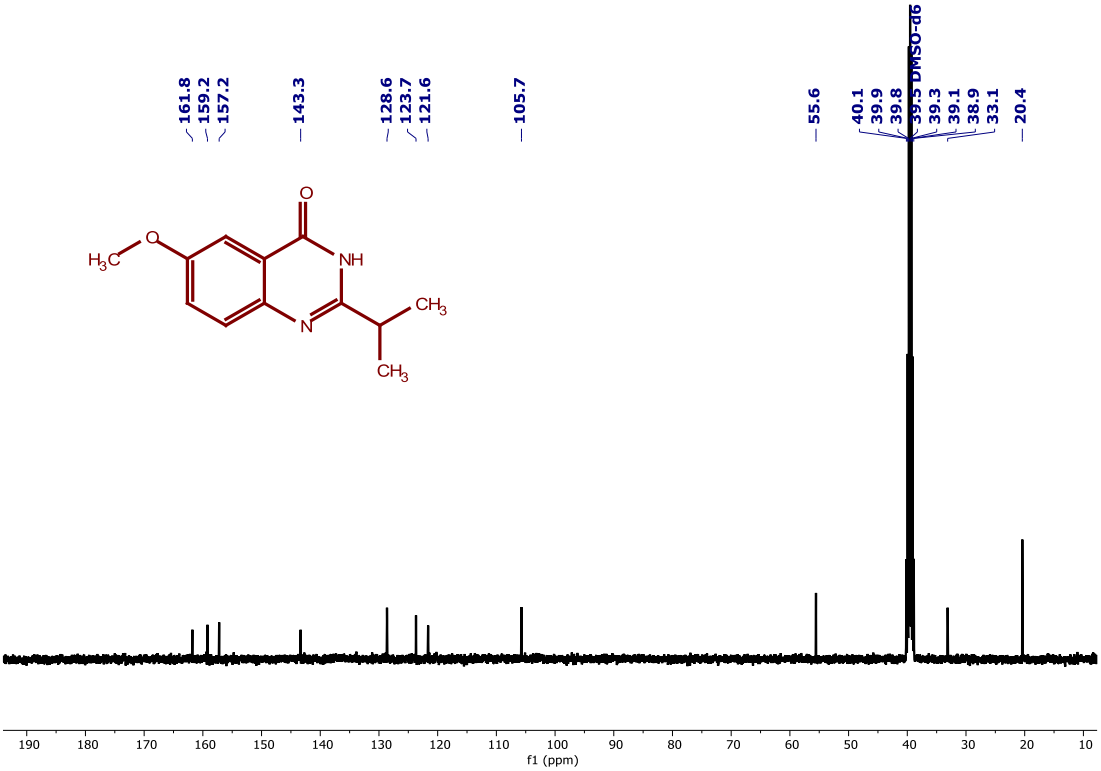
*[1]H NMR of 2-isopropyl-7-methylquinazolin-4(3H)-one (Compound-**8h**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



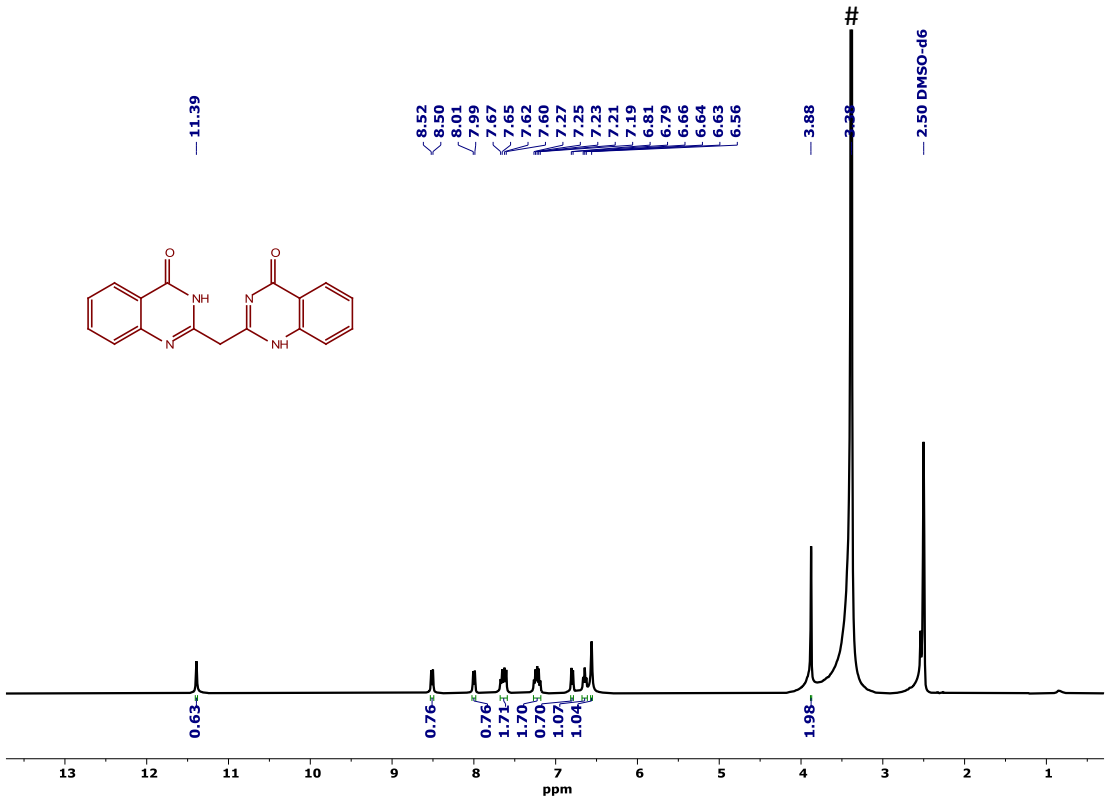
*[13]C{[1]H} NMR of 2-isopropyl-7-methylquinazolin-4(3H)-one (Compound-**8h**) in DMSO-d_6*



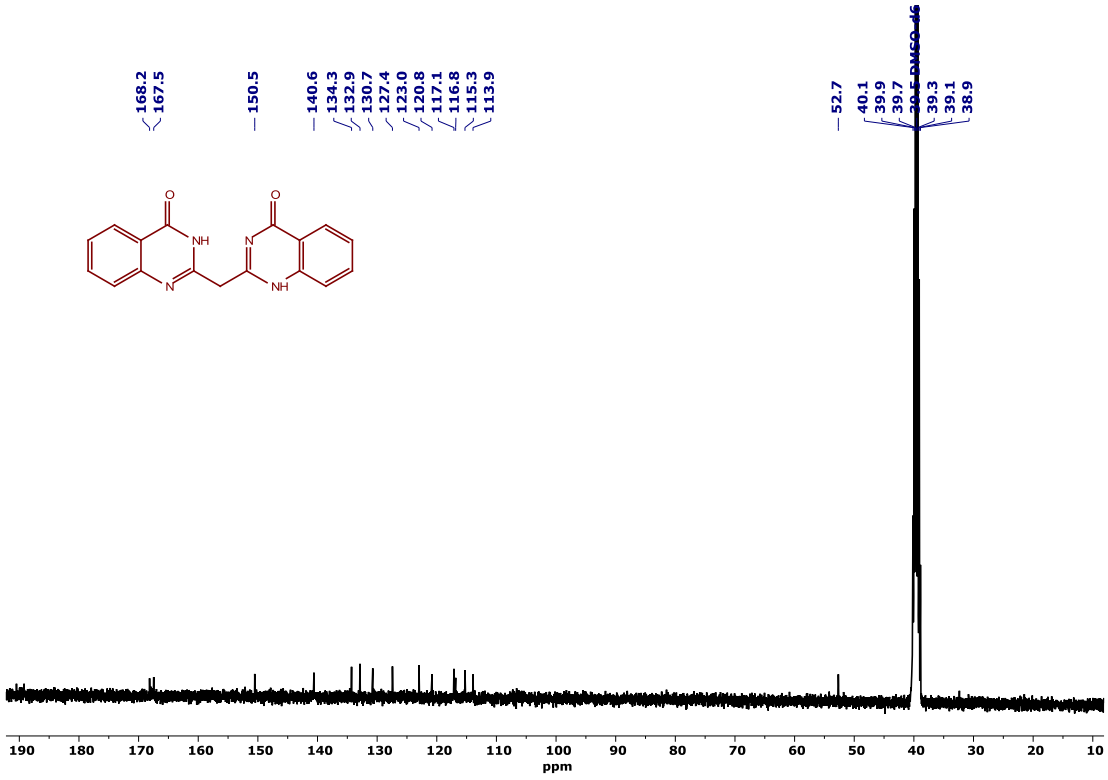
*[1]H NMR of 2-isopropyl-6-methoxyquinazolin-4(3H)-one (Compound-**8i**) in DMSO-d6. # indicates the solvent impurity of H2O in DMSO-d6*



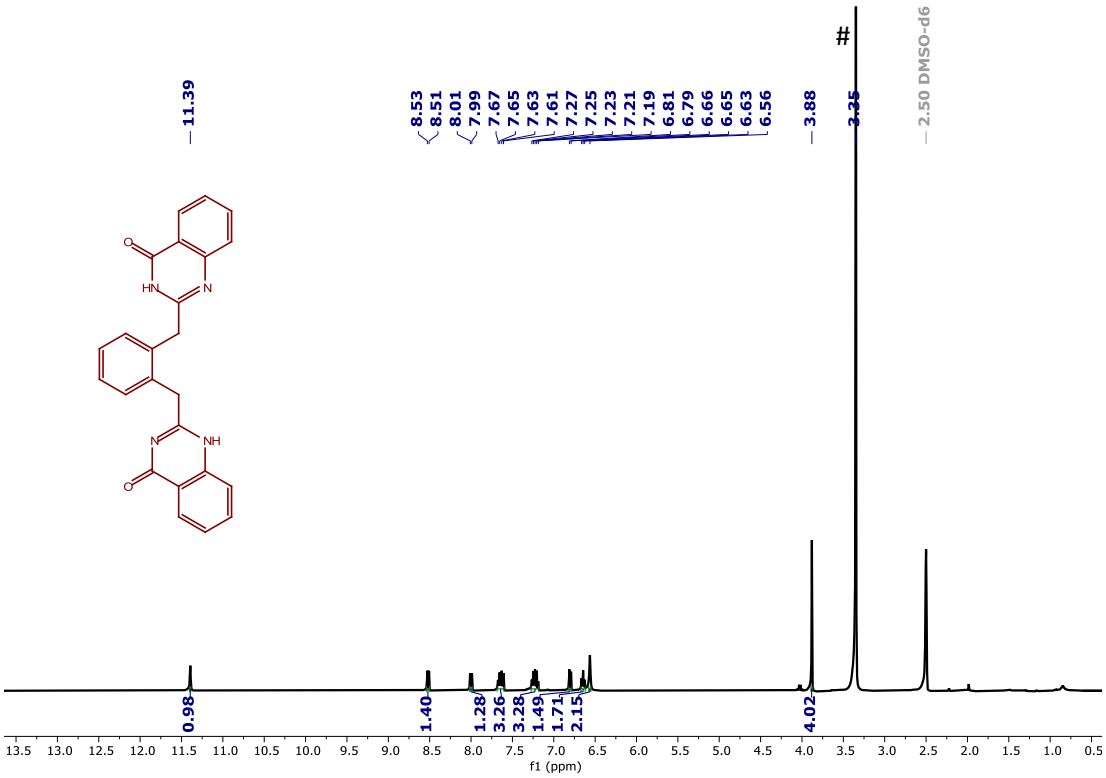
*[13]C{[1]H} NMR of 2-isopropyl-6-methoxyquinazolin-4(3H)-one (Compound-**8i**) in DMSO-d6*



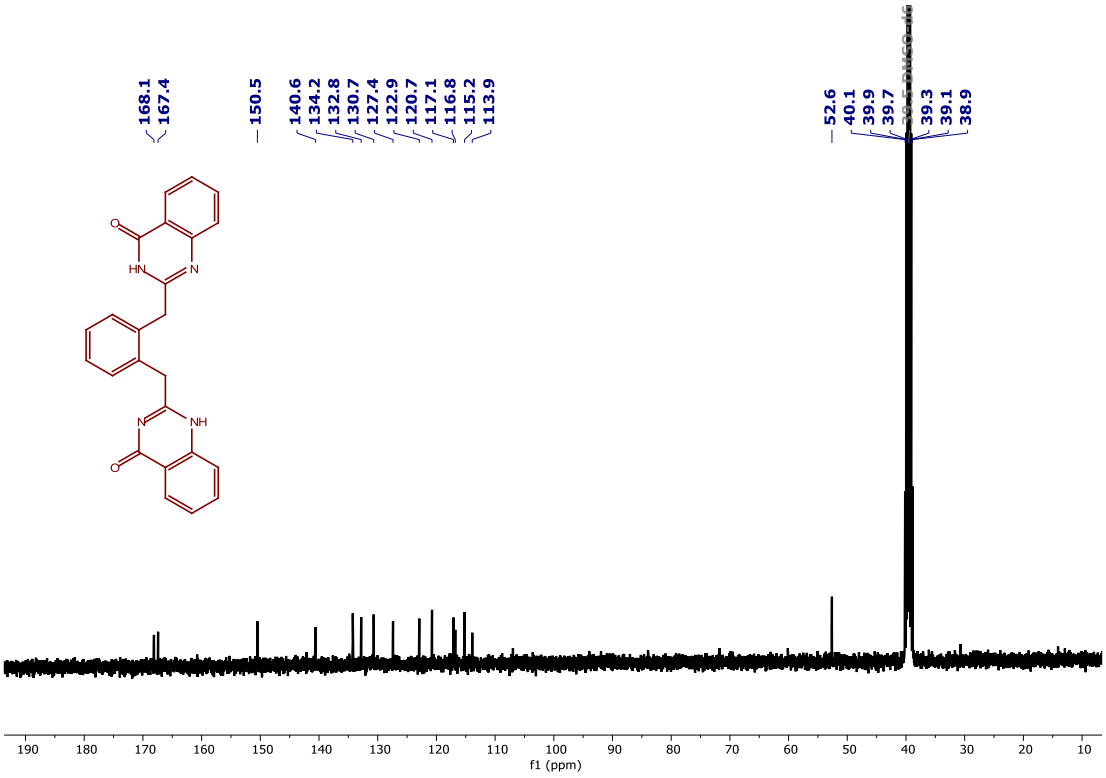
*[1]H NMR of 2-((4-oxo-1,4-dihydroquinazolin-2-yl)methyl)quinazolin-4(3H)-one (Compound-**8j**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



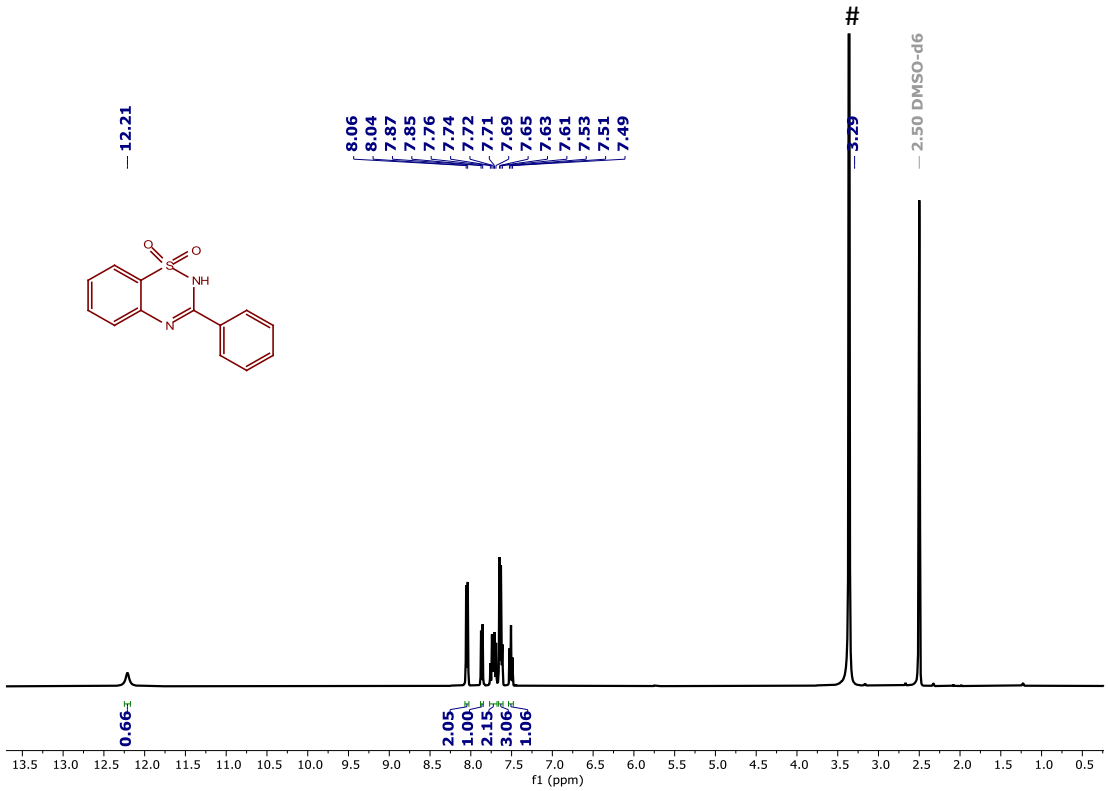
*[13]C{[1]H} NMR of 2-((4-oxo-1,4-dihydroquinazolin-2-yl)methyl)quinazolin-4(3H)-one (Compound-**8j**) in DMSO-d_6*



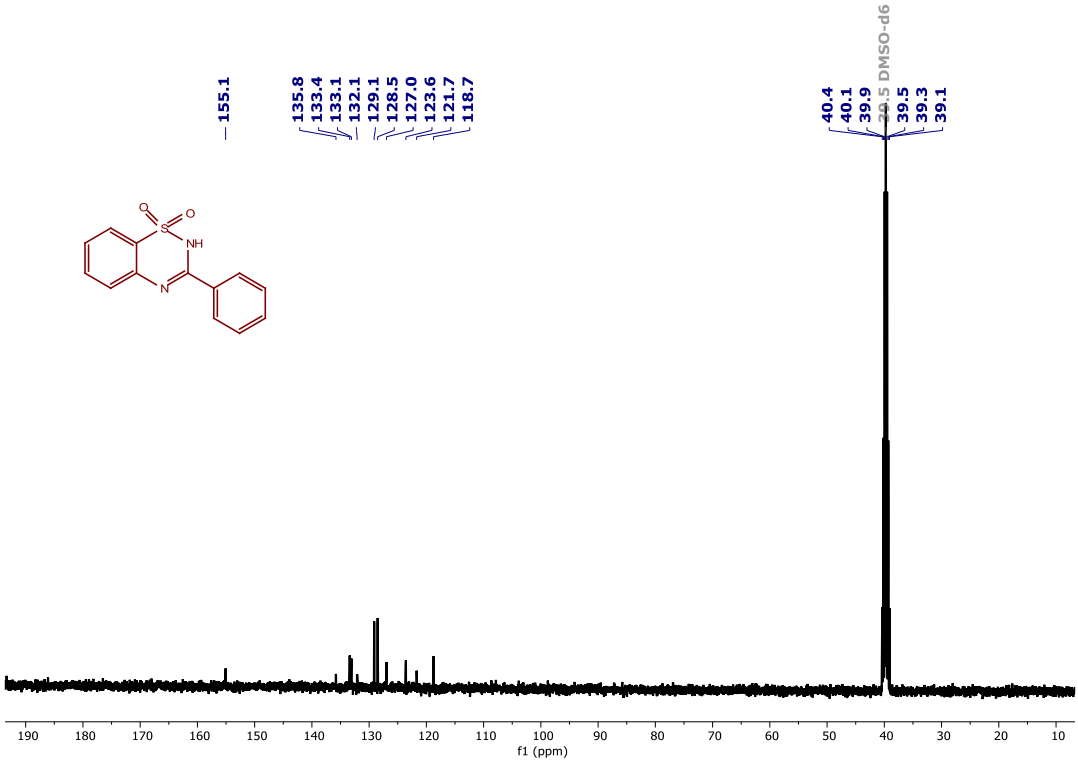
*^{1}H NMR of 2-(2-((4-oxo-1,4,4a,8a-tetrahydroquinazolin-2-yl)methyl)benzyl)quinazolin-4(3H)-one (Compound-**8k**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



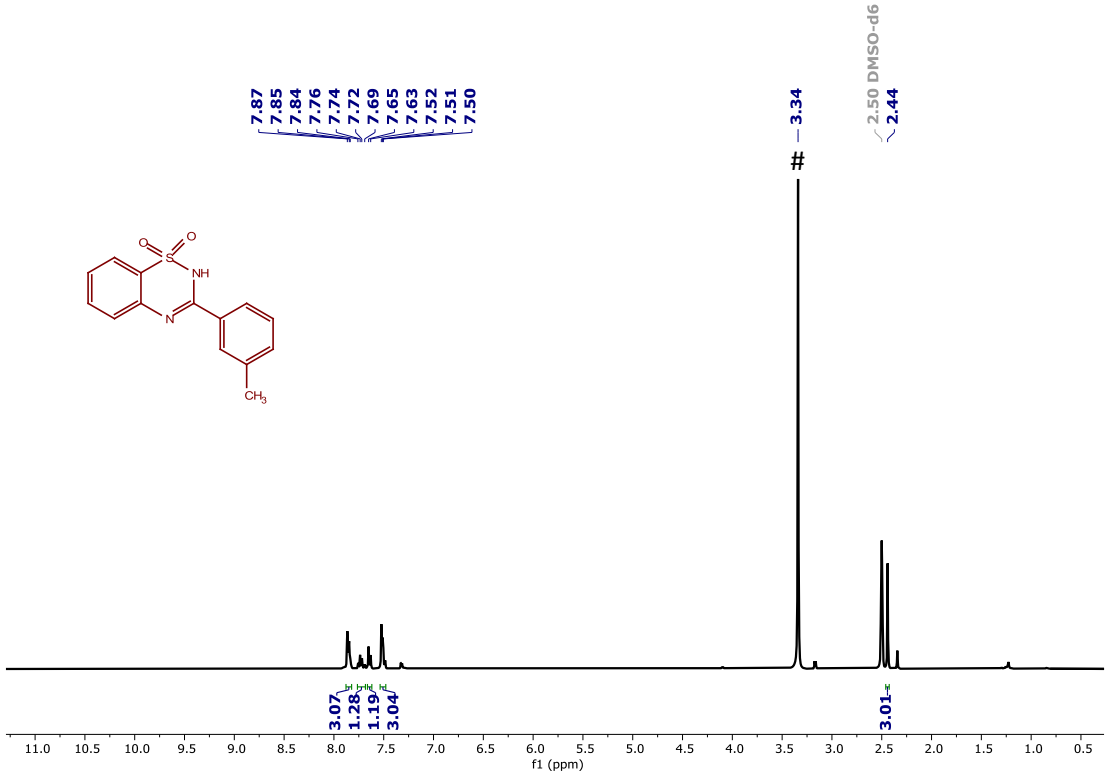
*$^{13}C\{^{1}H\}$ NMR of 2-(2-((4-oxo-1,4,4a,8a-tetrahydroquinazolin-2-yl)methyl)benzyl)quinazolin-4(3H)-one (Compound-**8k**) in DMSO-d_6*



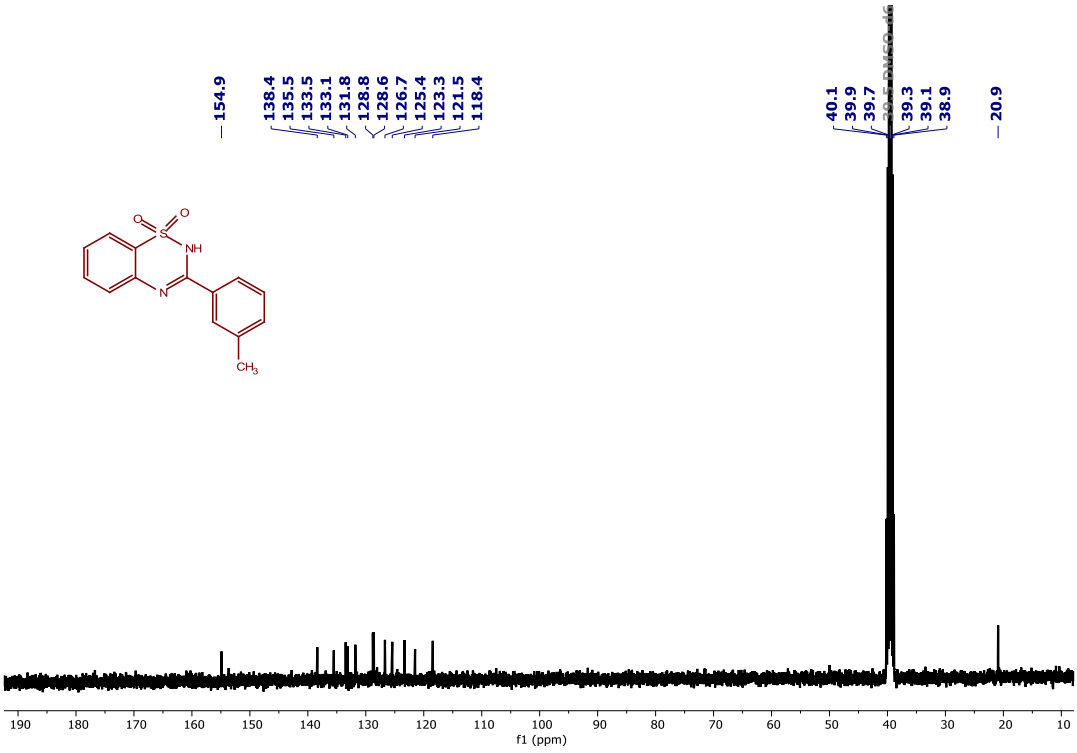
*[1]H NMR of 3-phenyl-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (Compound-**9a**) in DMSO-d6. # indicates the solvent impurity of H_2O in DMSO-d6*



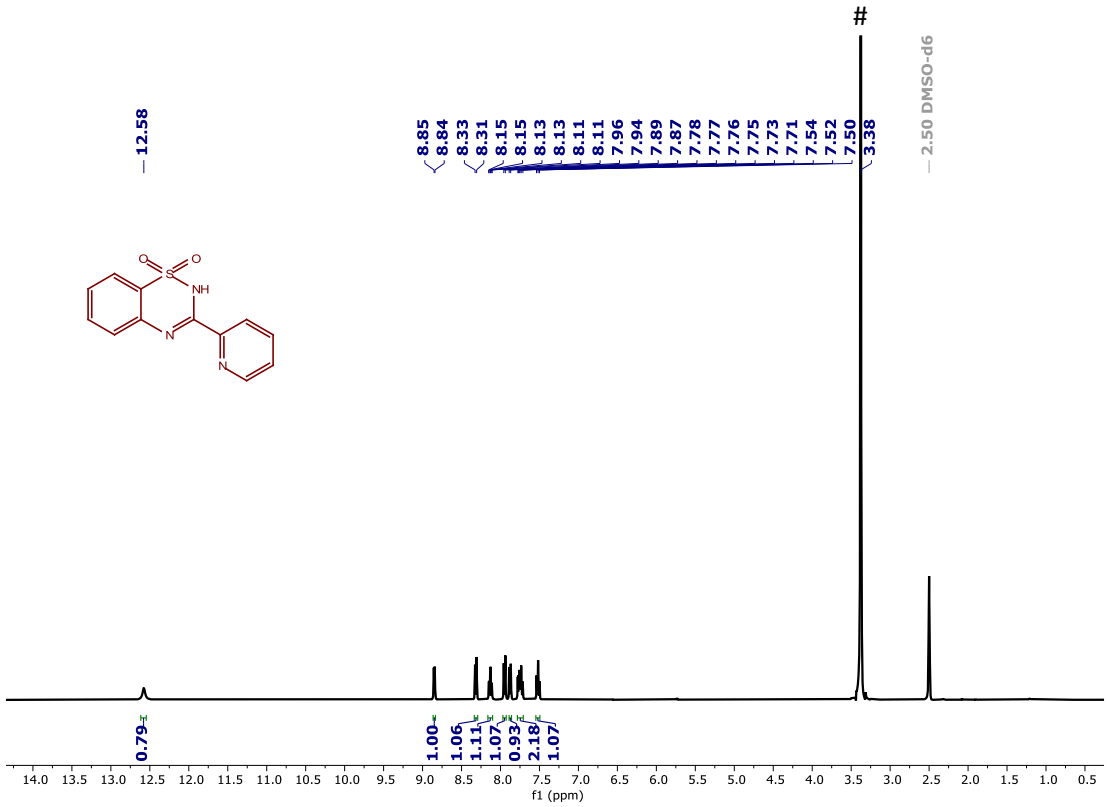
*[13]C{[1]H} NMR of 3-phenyl-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (Compound-**9a**)in DMSO-d6*



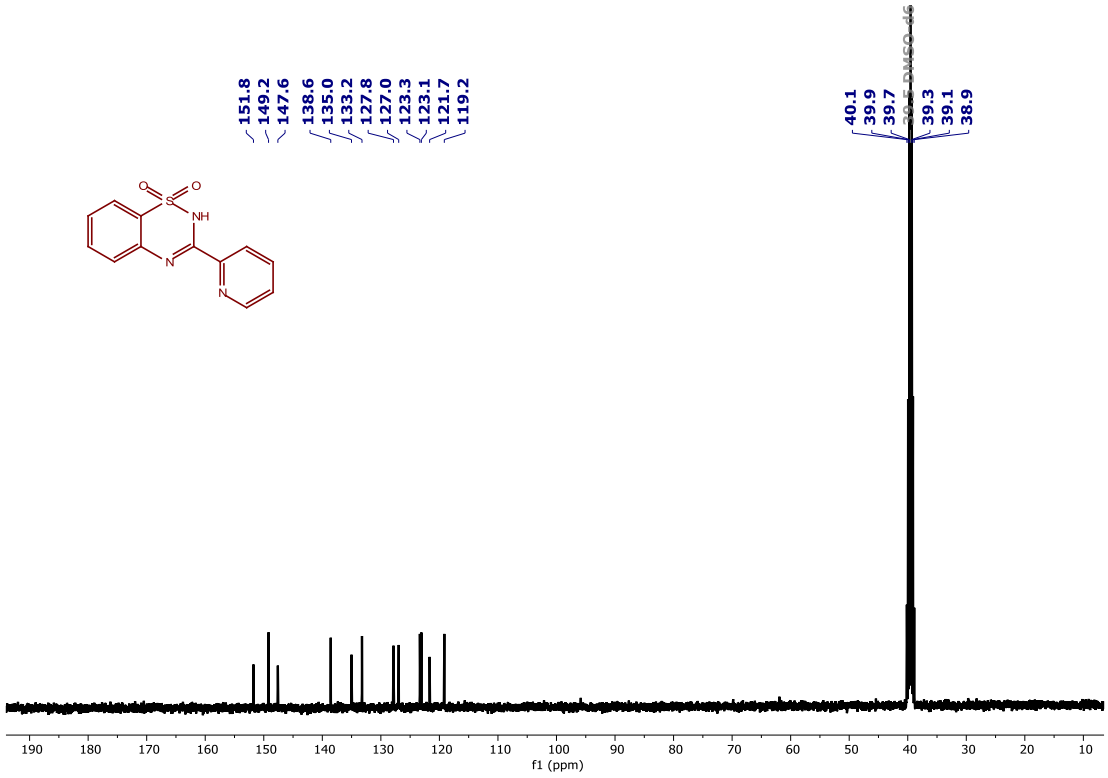
*[1]H NMR of 3-(m-tolyl)-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (Compound-**9b**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



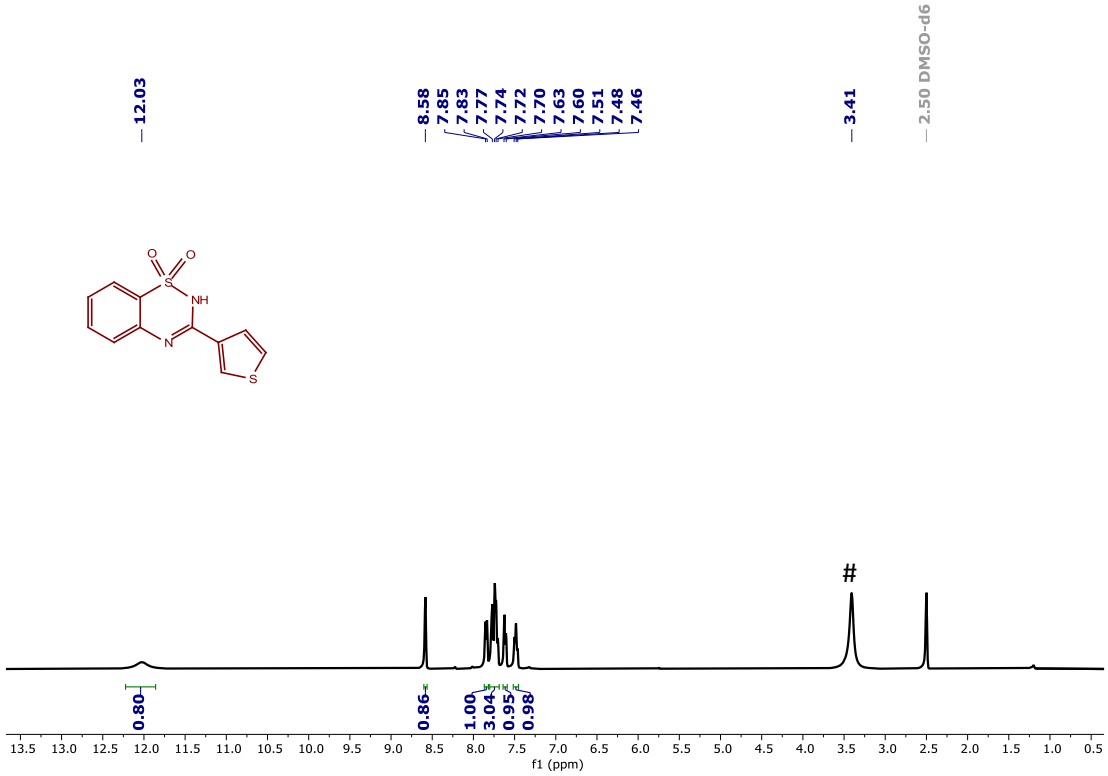
*[13]C{[1]H} NMR of 3-(m-tolyl)-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (Compound-**9b**) in DMSO-d_6*



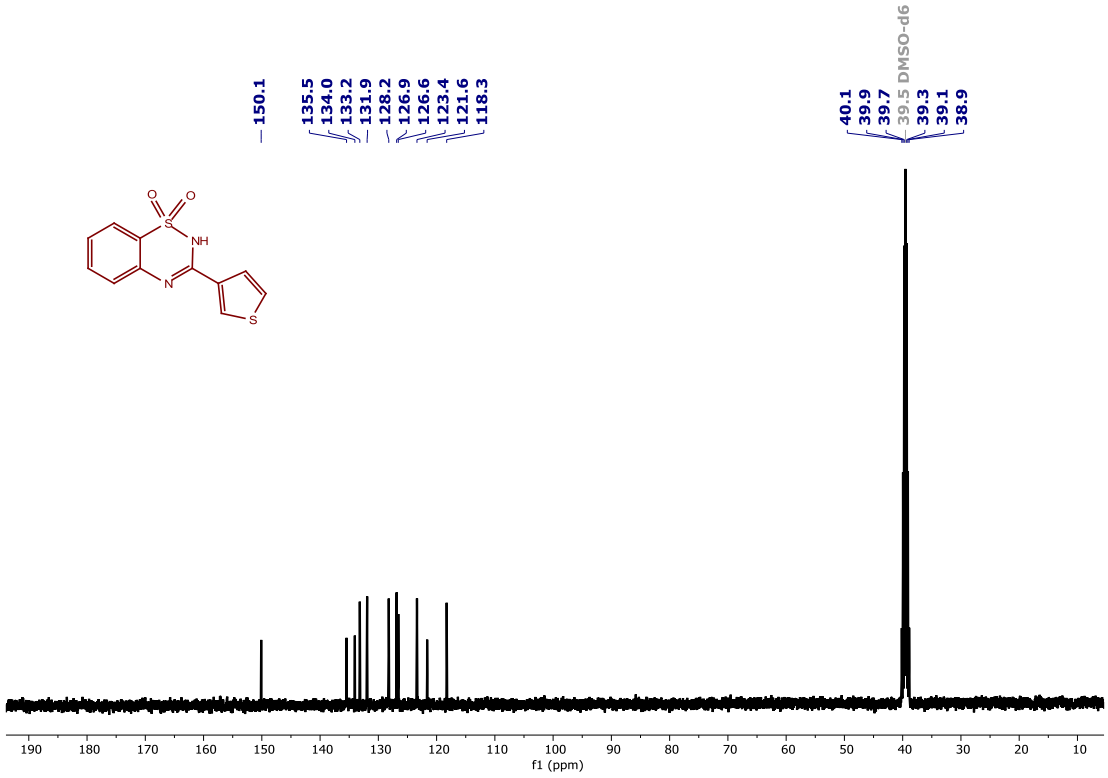
*^{1}H NMR of 3-(pyridin-2-yl)-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (Compound-**9c**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



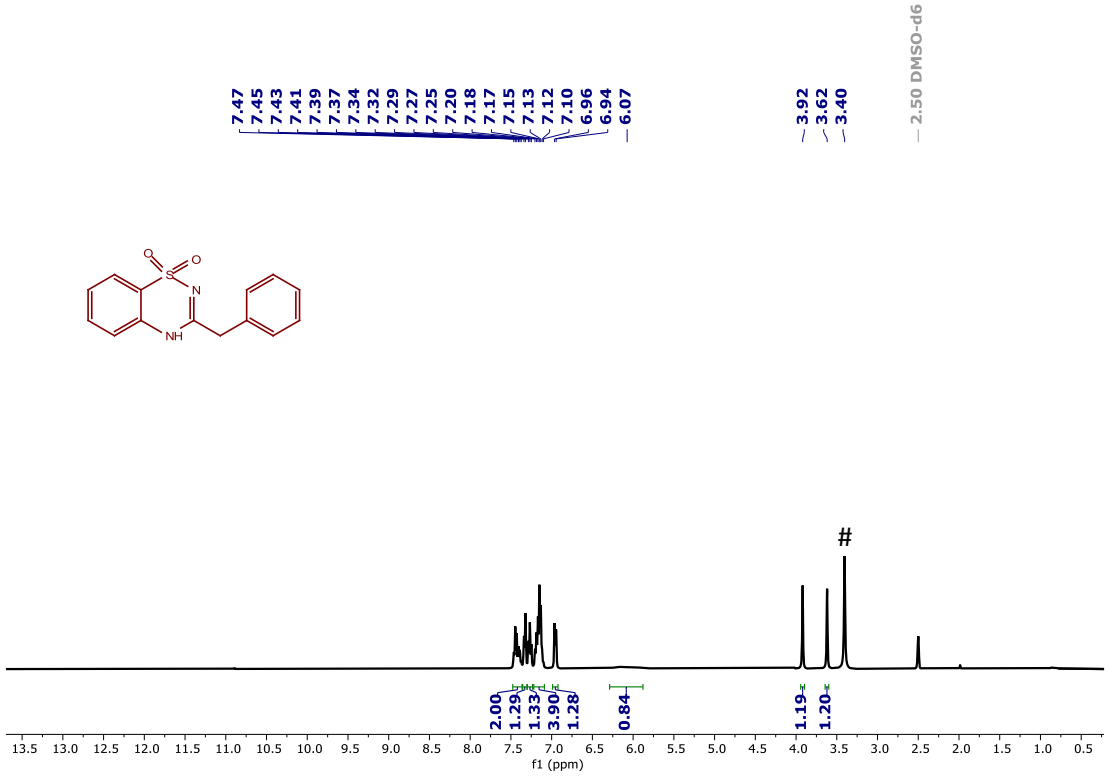
*$^{13}C\{^{1}H\}$ NMR of 3-(pyridin-2-yl)-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (Compound-**9c**) in DMSO-d_6*



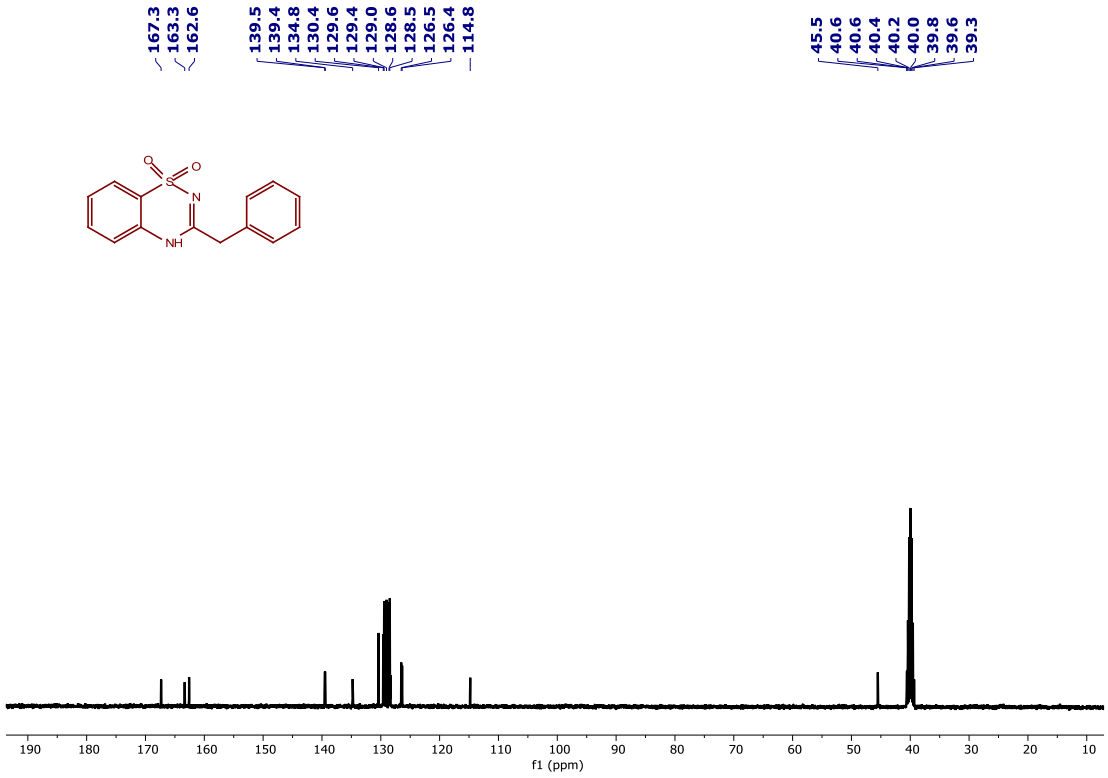
*[1]H NMR of 3-(thiophen-3-yl)-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (Compound-**9d**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



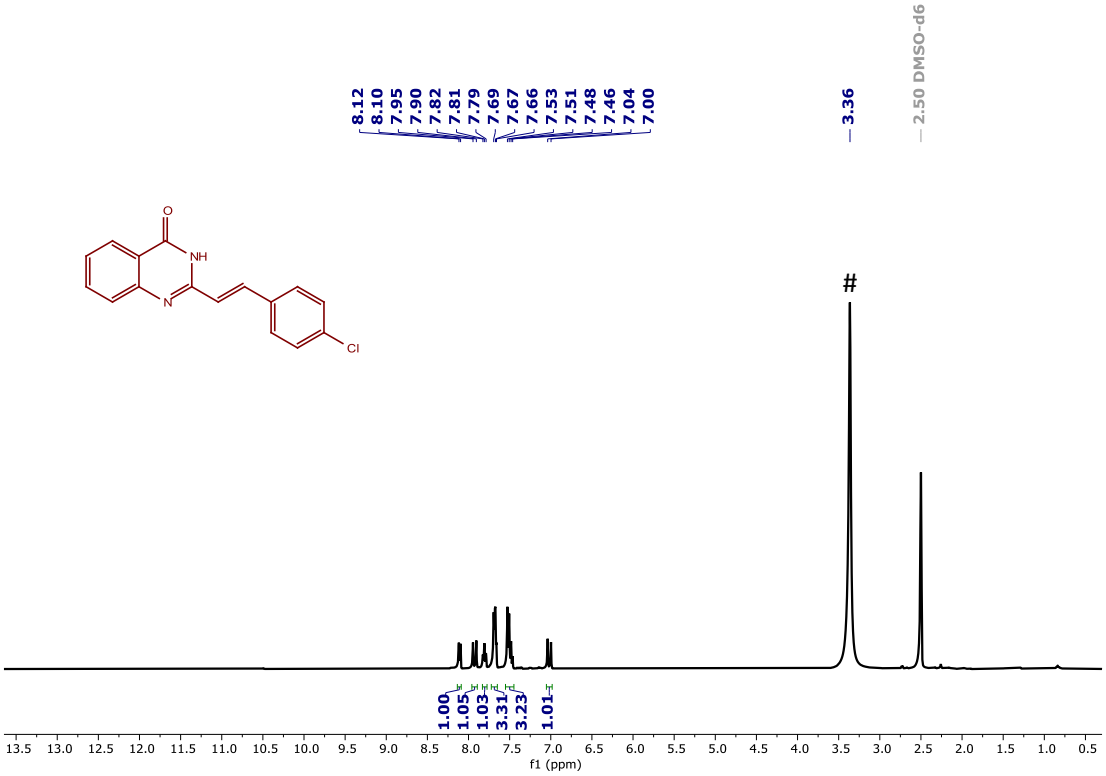
*[13]C{[1]H} NMR of 3-(thiophen-3-yl)-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (Compound-**9d**) in DMSO-d_6*



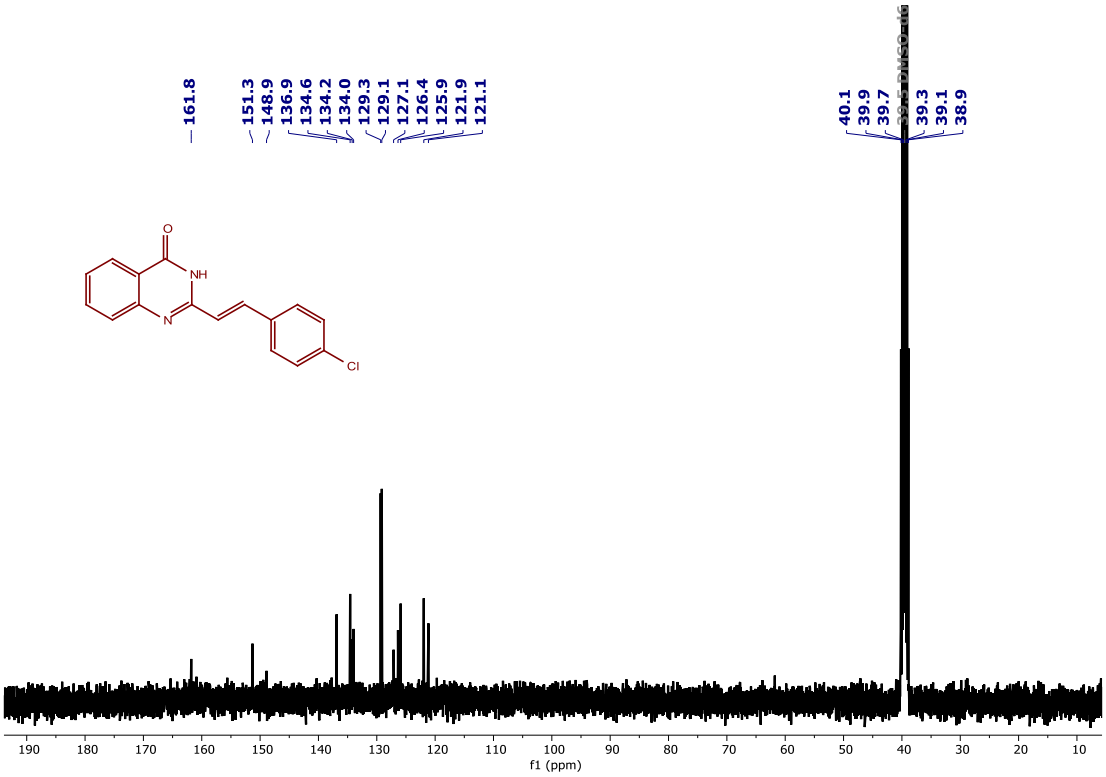
*[1]H NMR of 3-benzyl-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (Compound-**9e**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



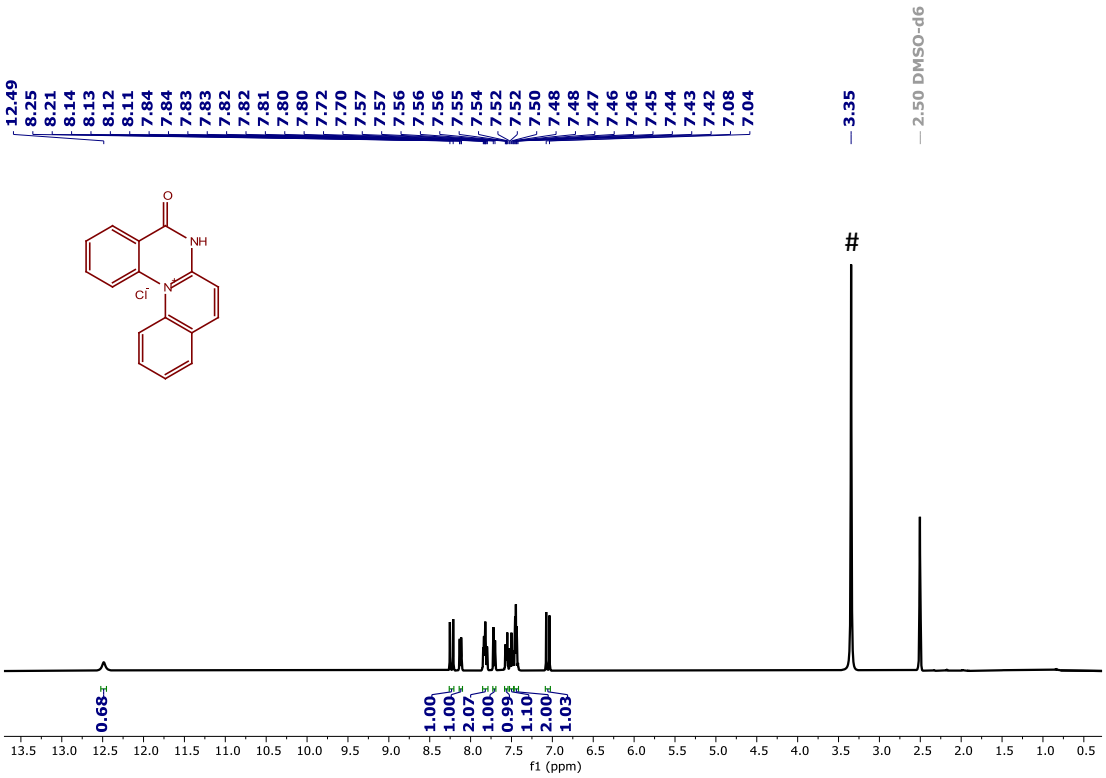
*[13]C{[1]H} NMR of 3-benzyl-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (Compound-**9e**) in DMSO-d_6*



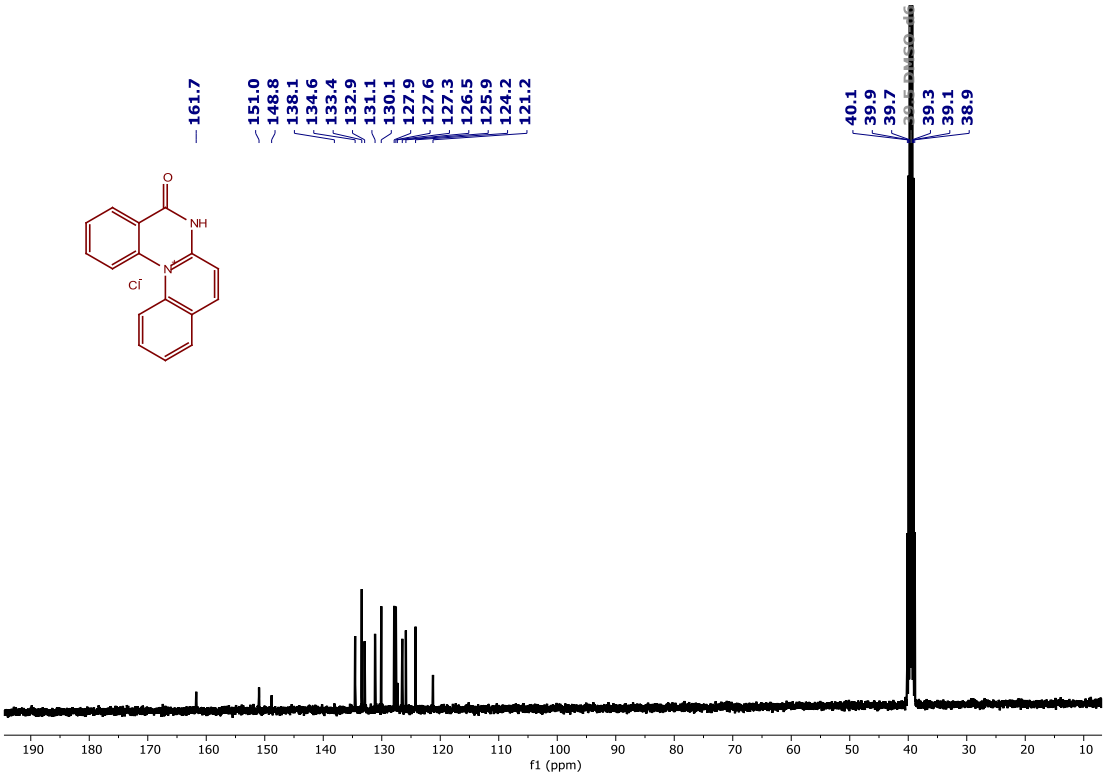
*[1]H NMR of (E)-2-(4-chlorostyryl)quinazolin-4(3H)-one (Compound-**11a**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



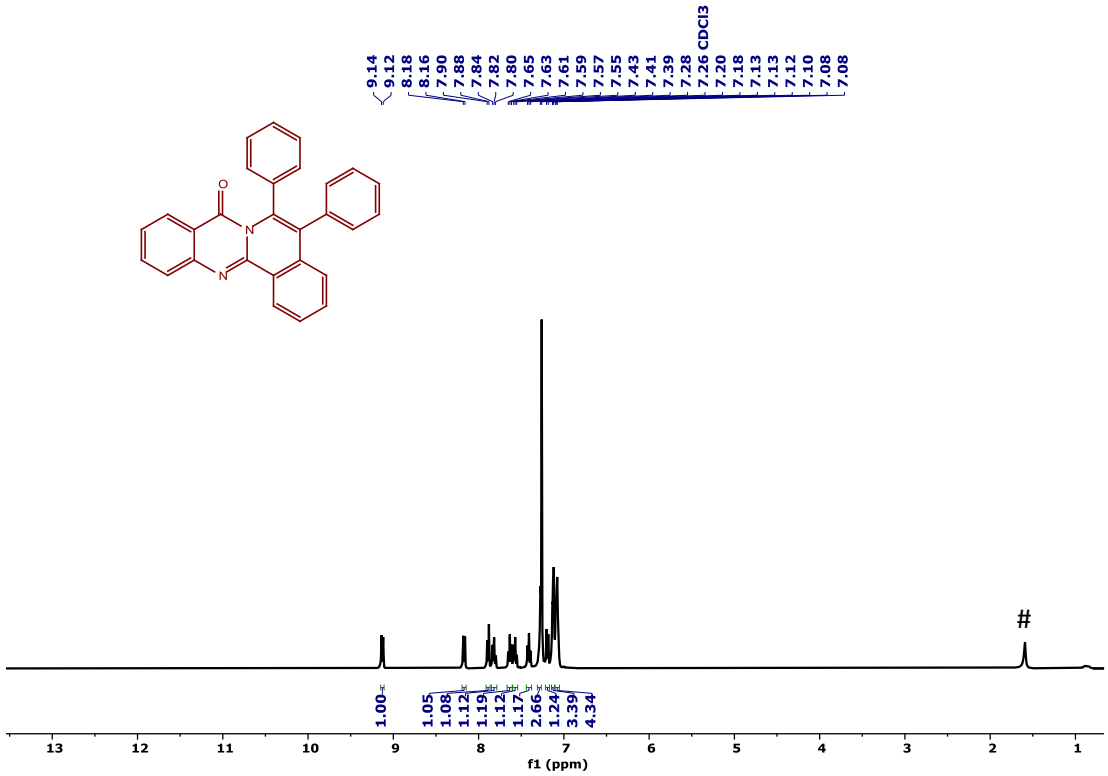
*[13]C{[1]H} NMR of (E)-2-(4-chlorostyryl)quinazolin-4(3H)-one (Compound-**11a**) in DMSO-d_6*



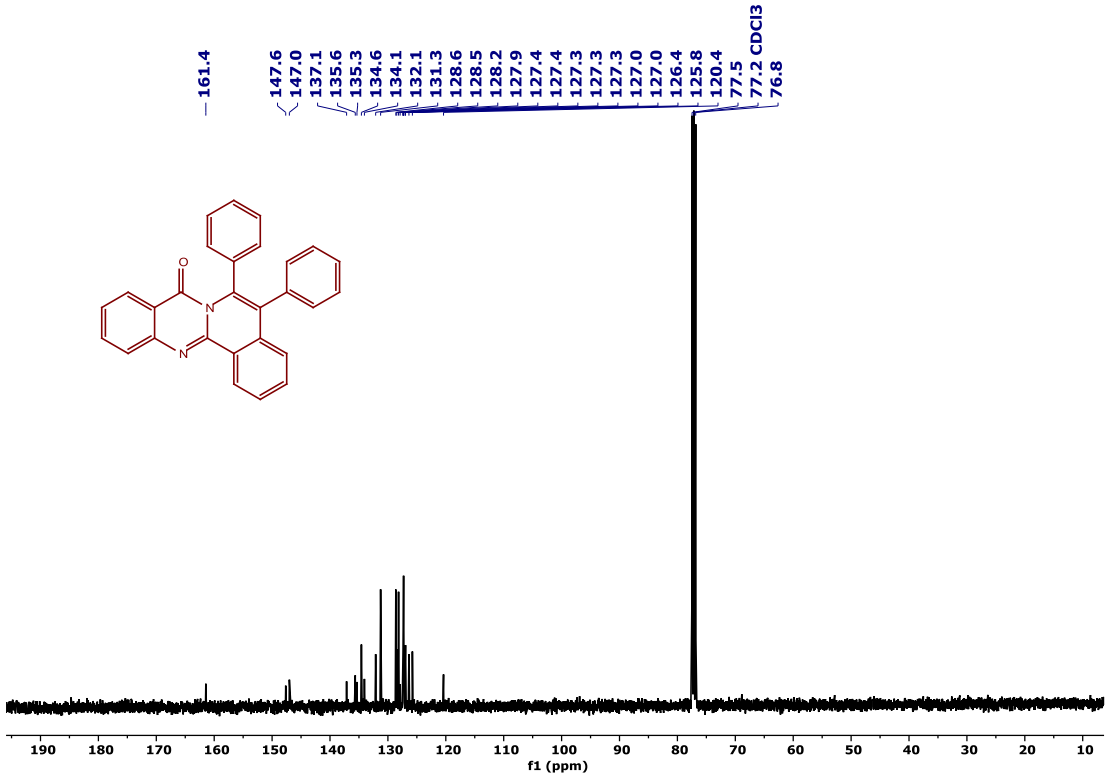
*^{1}H NMR of 5-oxo-5,6-dihydroquinolino[1,2-a]quinazolin-13-ium chloride (Compound-**11b**) in DMSO-d_6. # indicates the solvent impurity of H_2O in DMSO-d_6*



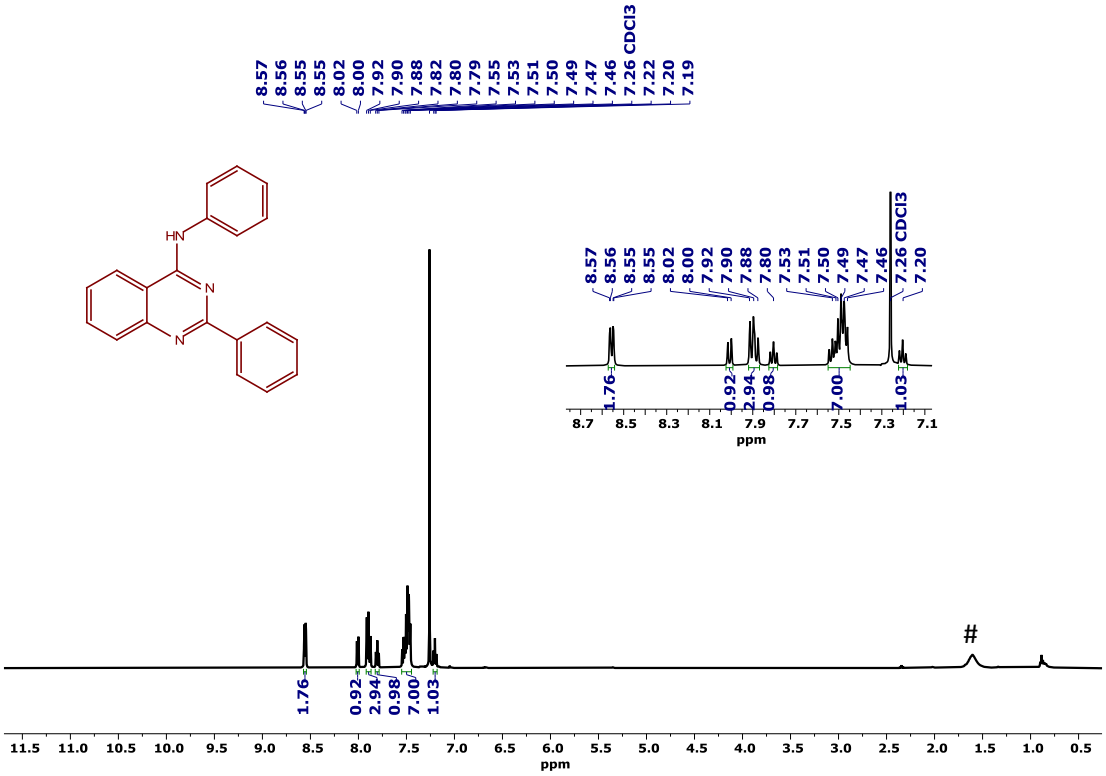
*$^{13}C\{^{1}H\}$ NMR of 5-oxo-5,6-dihydroquinolino[1,2-a]quinazolin-13-ium chloride (Compound-**11b**) in DMSO-d_6*



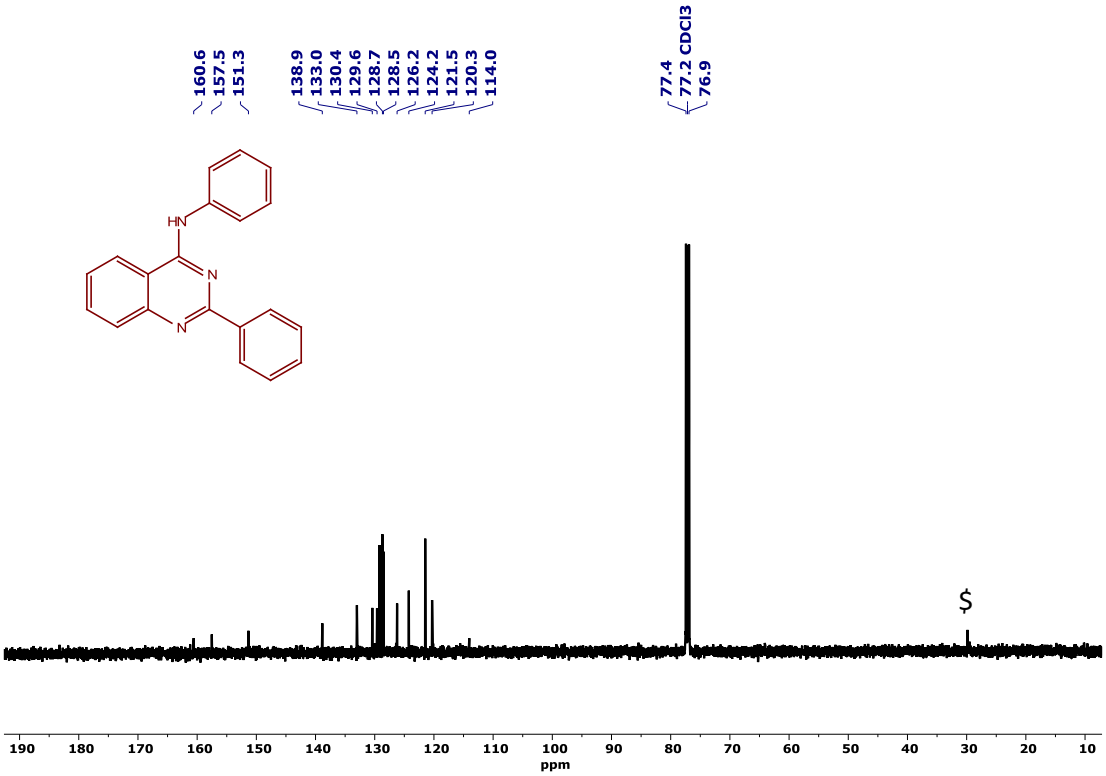
*[1]H NMR of 5,6-diphenyl-8H-isoquinolino[1,2-b]quinazolin-8-one (Compound-**11c**) in $CDCl_3$. # indicates the solvent impurity of H_2O in $CDCl_3$*



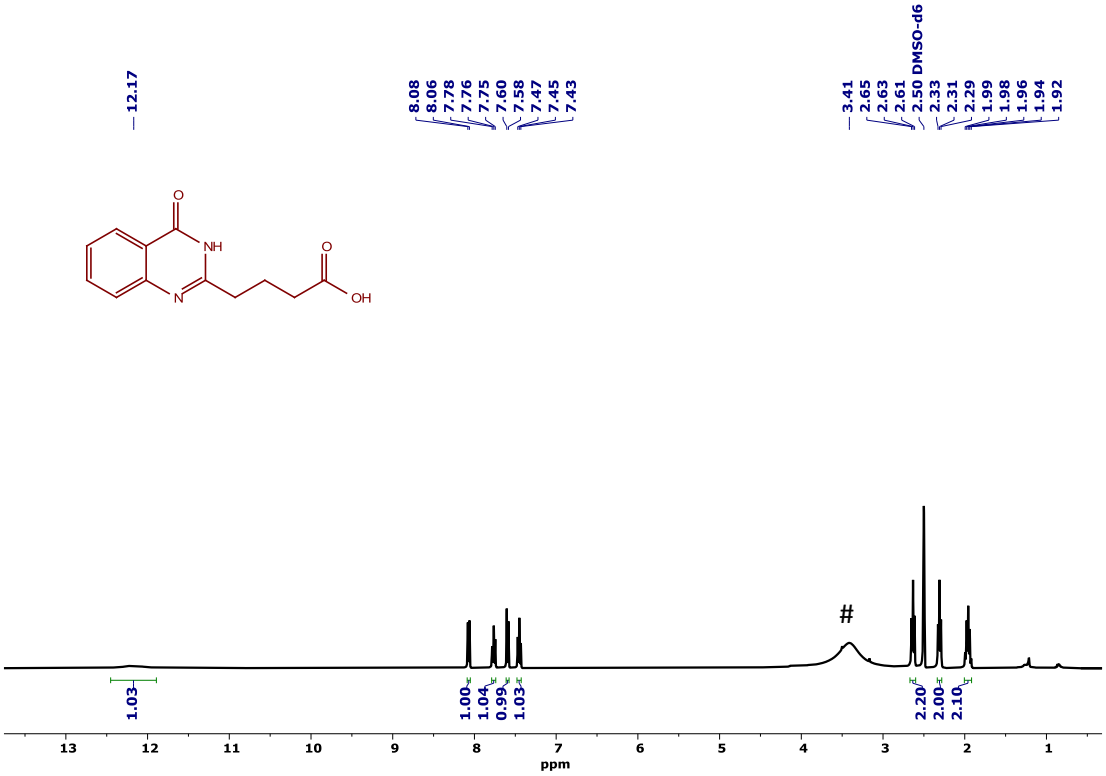
*[13]C{[1]H} NMR of 5,6-diphenyl-8H-isoquinolino[1,2-b]quinazolin-8-one (Compound-**11c**) in $CDCl_3$*



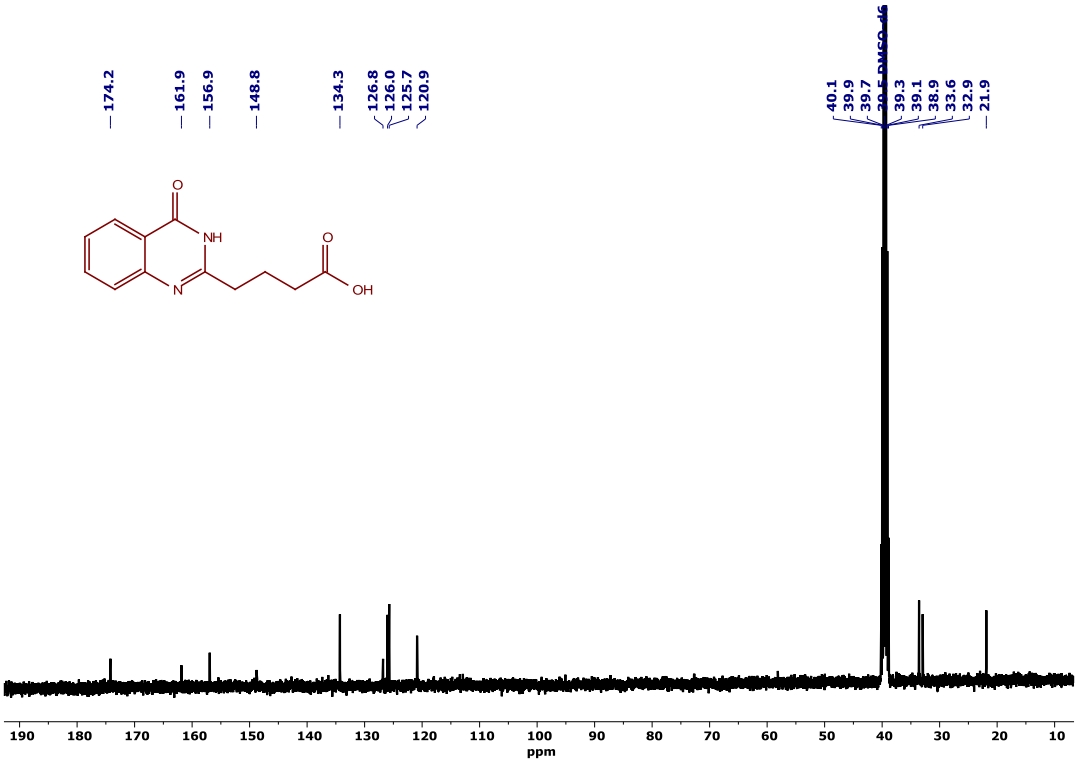
*[1]H NMR of N,2-diphenylquinazolin-4-amine (Compound-**11d**) in $CDCl_3$. # indicates the solvent impurity of H_2O in $CDCl_3$*



*[13]C{[1]H} NMR of N,2-diphenylquinazolin-4-amine (Compound-**11d**) in $CDCl_3$. $ indicates the grease in $CDCl_3$*



*[1]H NMR of 4-(4-oxo-3,4-dihydroquinazolin-2-yl)butanoic acid (Compound-**11e**) in DMSO-d6. # indicates the solvent impurity of H_2O in DMSO-d6*



*[13]C{[1]H} NMR of 4-(4-oxo-3,4-dihydroquinazolin-2-yl)butanoic acid (Compound-**11e**) in DMSO-d6*

16. Mechanistic study

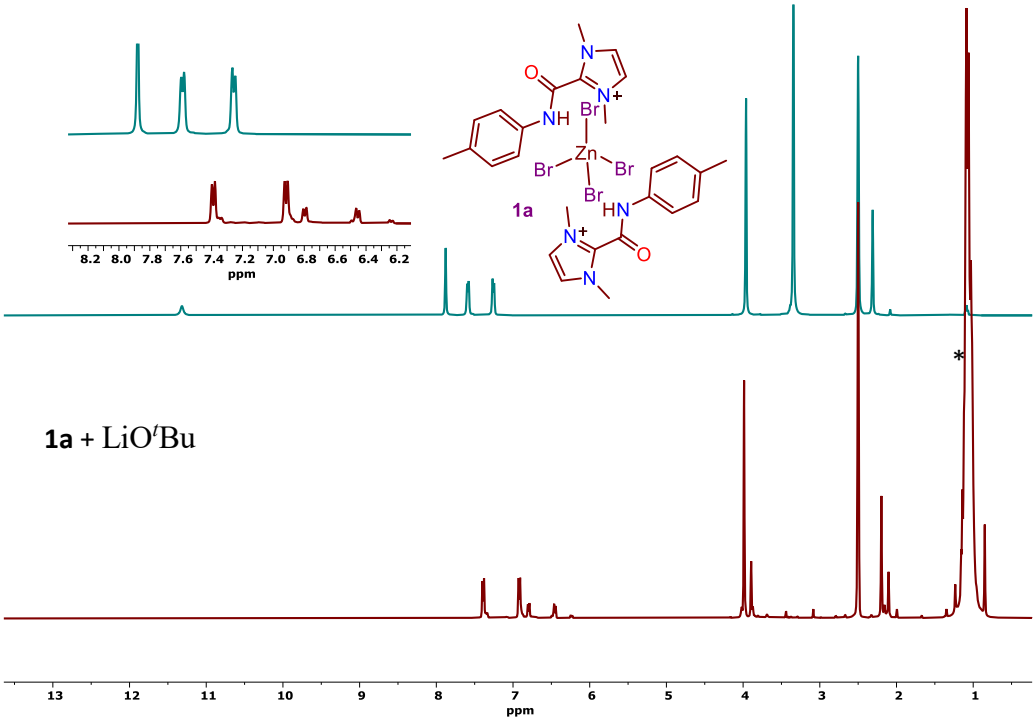


Figure S21. *Stacking of ^{1}H spectra between **1a** and **I** in DMSO-d_6.* * indicates the byproduct ^{t}BuOH

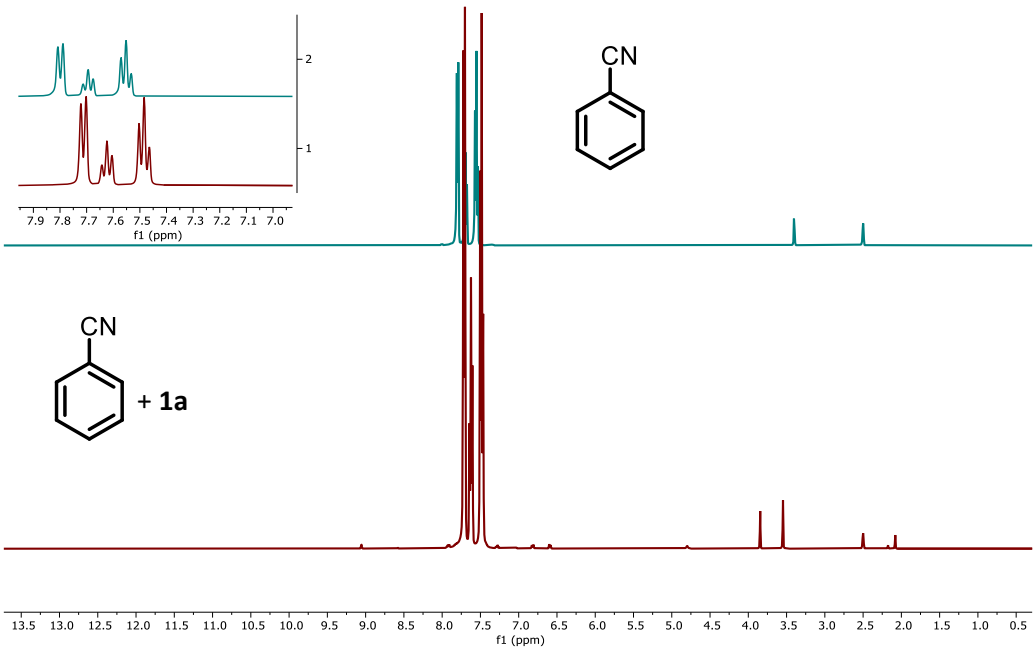


Figure S22. *Stacking of ^{1}H spectra between benzonitrile and the reaction mixture containing **1a** and benzonitrile indicating interaction between compound **1a** and benzonitrile.*

Single crystal X-ray Crystallography:

Single crystal X-ray diffraction data were collected on a Bruker AXS Kappa Apex II equipped with a CCD detector (for **1a**). The compound was measured using MoKα radiation (λ = 0.71073 Å). Crystals were selected using a polarizing optical microscope and then mounted in a crystalmounting loop using Paraton oil. The mounted crystal was then placed on a goniometer head and the crystal was centered with the help of a video microscope. The automatic cell determination routine, with 24/36 frames (10 sec exposure time per frame) at two/three different orientations of the detector, respectively was employed to collect reflections for unit cell determination. The collected reflections were indexed using inbuilt APEX software[21a] to obtain unit cell parameters. Further, intensity data for structure determination were collected through an optimized strategy, which gave an average 4-fold redundancy for the reflections. The program Bruker-SAINT[21b] was used for integrating the frames and multi-scan absorption correction was applied using the program SADABS.[21c] The structure was solved by SHELXS97[21d] and refined by full-matrix least squares techniques on F^2 using SHELXL[21e] computer program incorporated in WinGX[21f] system. The non-hydrogen atoms were refined anisotropically. All hydrogen atoms were fixed at chemically meaningful positions and riding model refinement was applied. The graphical representations were performed using the program Mercury.[21g] The crystal data (CCDC No. 2335188) and refinement details are summarized in Table S4. Halide scrambling during crystallization leads to slight redistribution of halide ions in compound **1a**.

Table S4. Crystallographic data for the compound **1a**

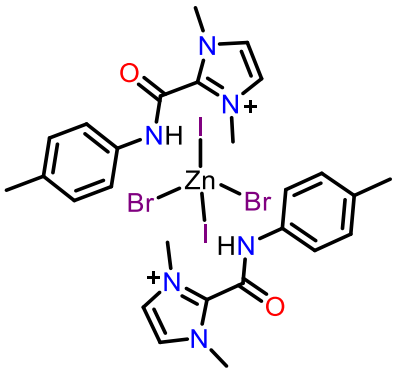
Compound	**1a**
CCDC No	2335188
Empirical formula	$C_{26}H_{32}Br_{2.31}I_{1.69}N_6O_2Zn$
Formula weight	925.23
Crystal system	Triclinic
Space group	*P*-1
a (Å)	8.6011(3)
b (Å)	12.1473(4)
c (Å)	17.1881(6)
α (°)	71.2360(10)
β (°)	80.4740(10)
γ (°)	79.4660(10)
V (Å^3)	1660.70(10)

Z	2
D calc (Mg/m^3)	1.850
F (000)	893
μ (mm^{-1})	5.120
θ Range (°)	1.788 to 24.994
Crystal size (mm^3)	0.120 x 0.100 x 0.070
No. of total reflns collected	18171
No. of unique reflns [I > 2σ(I)]	5838
Data/restraints/ parameters	5838 / 20 / 396
Goodness-of-fit on F^2	1.025
Final R indices [I > 2σ(I)]	0.0258, 0.0483
R indices (all data)	0.0419, 0.0525

17. Computational data

All the calculations were performed using the Gaussian 16, Revision B.01 program.[22] All structures were optimized with B3LYP[23] functional. Metals (Zn) and I were treated with LANL2DZ basis set with an effective core potential, while the other atoms were treated using using 6-31G**, a double-ζ Pople type basis set.

Cartesian Coordinates of all the optimized geometries:



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53	-2.199288000	0.440525000	-2.377590000
6	-0.953766000	3.899994000	0.272464000
1	0.080911000	4.100412000	0.492639000
6	-1.730016000	4.265590000	-0.785231000
1	-1.508931000	4.874122000	-1.646467000
6	-2.927945000	2.927311000	0.512416000

6	-4.076368000	2.186367000	1.162021000
6	-5.555167000	0.224624000	0.778485000
6	-6.447529000	0.436674000	1.836736000
1	-6.339698000	1.306073000	2.470123000
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1	-8.153390000	-0.318368000	2.886689000
6	-7.620103000	-1.631161000	1.267359000
6	-6.713674000	-1.820162000	0.213567000
1	-6.805124000	-2.695383000	-0.424454000
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1	-4.994584000	-1.077107000	-0.849865000
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1	-8.308398000	-3.528938000	2.047401000
1	-9.182864000	-2.982467000	0.617788000
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1	-1.992654000	2.720788000	3.119962000
1	-0.290459000	2.828386000	2.564245000
1	-1.246453000	1.370163000	2.197116000
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6	1.702316000	-3.062432000	2.083078000
1	0.741616000	-3.062197000	2.570793000
6	3.606183000	-2.193013000	1.343724000
6	4.842539000	-1.344260000	1.184623000

6	5.600371000	0.949303000	0.616879000
6	5.167706000	2.154241000	0.042318000
1	4.125554000	2.269246000	-0.239730000
6	6.071424000	3.190508000	-0.163172000
1	5.717330000	4.115665000	-0.611153000
6	7.422162000	3.065241000	0.190974000
6	7.831304000	1.857210000	0.766473000
1	8.871721000	1.730135000	1.055367000
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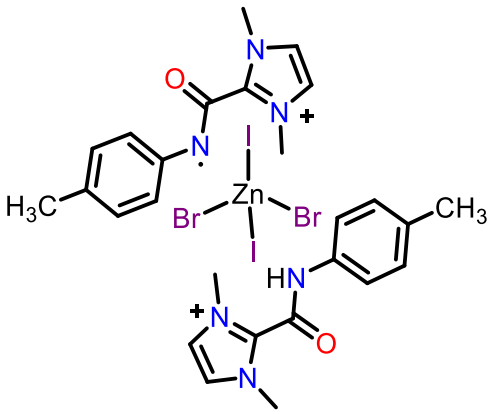

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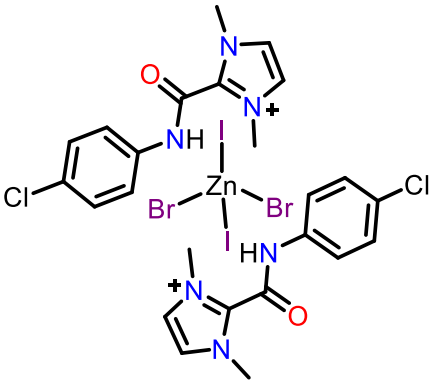

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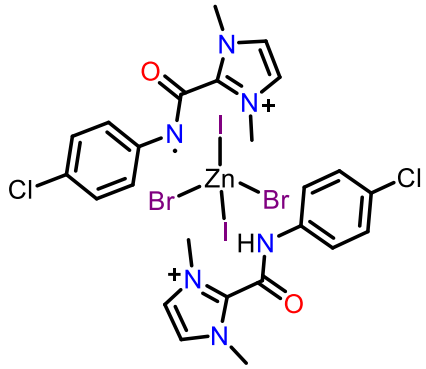

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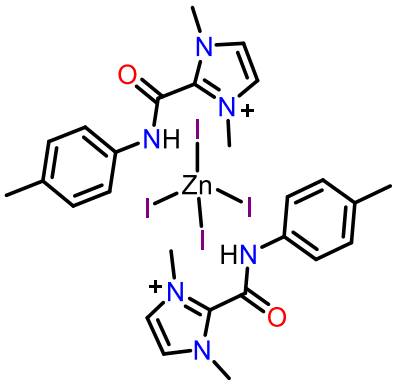

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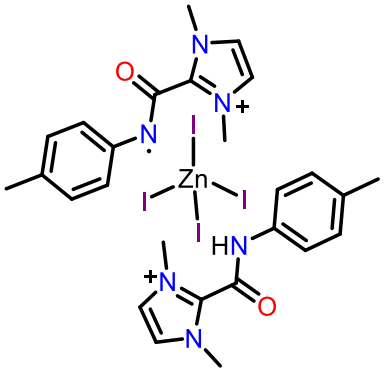

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7	2.656228000	2.877102000	-1.665580000
7	3.597469000	3.499887000	0.195261000
8	5.442756000	1.704277000	-2.040913000
7	4.775644000	0.597448000	-0.110607000
1	3.998228000	0.576257000	0.559057000
6	2.359015000	2.122226000	-2.892003000
1	3.287902000	1.975394000	-3.442783000
1	1.653995000	2.706252000	-3.481466000
1	1.911792000	1.158617000	-2.630676000
6	-2.555723000	-4.450954000	-0.994624000
1	-2.131579000	-5.396727000	-0.700463000
6	-2.112810000	-3.518609000	-1.887439000
1	-1.216607000	-3.484127000	-2.485290000
6	-3.972533000	-2.746372000	-0.956514000
6	-5.119741000	-1.888500000	-0.523888000
6	-5.570247000	0.444035000	-0.605763000
6	-5.958924000	1.534200000	-1.449697000
1	-5.996030000	1.356577000	-2.519153000
6	-6.277975000	2.760631000	-0.911492000
1	-6.573916000	3.576903000	-1.564454000
6	-6.211270000	2.983082000	0.482853000
6	-5.823691000	1.913354000	1.321151000

1	-5.755460000	2.079879000	2.392431000
6	-5.508655000	0.673775000	0.810468000
1	-5.185162000	-0.127310000	1.463532000
6	-6.496513000	4.340908000	1.060365000
1	-6.965155000	4.267601000	2.046297000
1	-7.145110000	4.931079000	0.407060000
1	-5.560665000	4.900911000	1.188762000
6	-4.418680000	-4.633611000	0.666796000
1	-4.289760000	-4.044534000	1.576239000
1	-3.968970000	-5.618872000	0.791552000
1	-5.478280000	-4.717511000	0.438470000
6	-2.824150000	-1.249820000	-2.659489000
1	-3.703047000	-1.085145000	-3.280903000
1	-1.931153000	-1.391044000	-3.266489000
1	-2.669379000	-0.392104000	-2.002725000
7	-3.002845000	-2.474911000	-1.861894000
7	-3.711468000	-3.968523000	-0.435575000
8	-5.918944000	-2.329138000	0.300677000
7	-5.227204000	-0.707028000	-1.200006000
53	-2.031589000	-1.470281000	1.896233000

References:

1. S. Bauri, A. Ramachandran and A. Rit, *Chem Asian J*., 2023, **18**, e2022013.
2. A. Y. H. Helali, M. T. M. Sarg, M. M. S. Koraa and M. S. F. El-Zoghbi, *Open J. Med. Chem.,* 2014, **4**, 12-37.
3. H. Lu, Q. Yang, Y. Zhou, Y. Guo, Z. Deng, Q. Ding and Y. Peng, *Org. Biomol. Chem.,* 2014*,* **12***,* 758-764.
4. Z. Niu, S. Ma, L. Zhang, Q. Liu and S. Zhang, *Molecules,* 2022, **27**, 3906.
5. D. Šakić and H. Zipse, *Adv. Synth. Catal.*, 2016, **358**, 3983-3991.
6. S. Halder, S. Mandal, A. Biswas and D. Adhikari, *Green Chem.,* 2023, **25**, 2840-2845.
7. X. X. Qi, Z. Z. Song, J. L. Gong, Z. Y. Fang and X. F. Wu, *Chinese Chemical Letters,* 2016, **27**, 21-24.
8. K. Wang, H. Chen, X. Dai, X. Huang and Z. Feng, *RSC Adv.,* 2021*,* **11**, 13119-13123.
9. W. Wu, S. Fan, X. Wu, L. Fang and J. Zhu, *J. Org. Chem*., 2023, **88**, 1945-1962.

10. H. Hou, X. Ma, Y. Lin, J. Lin, W. Sun, L. Wang, X. Xu and F. Ke, *RSC Adv*., 2021, **11**, 17721-17726.
11. S. Huang, L. Jin, Y. Liu, G. Yang, A. Wang, Z. Le, G. Jiang, Z. Xie, *Org. Biomol. Chem*. 2024, **22**, 784-789.
12. N. Baltaş, *J. Chem. Res*., 2022, **46**, 174751982210965.
13. X. Wang, S. Shang, Q. Tian, Y. Wang, H. Wu, Z. Li, S. Zhou, H. Liu, Z. Dai, W. Luo, D. Li, X. Xiao and S. Wang, Yuan, J. *Tetrahedron,* 2020, **76**, 131480.
14. Y. Shen, C. Han, S. Cai, P. Lu and Y. Wang, *Tetrahedron Lett*., 2012, **53**, 5671-5673.
15. D. Pal, A. Mondal and D. Srimani, *Catal. Sci. Technol*., 2022, **12**, 3202-3208.
16. T. Abe, K. Kida and K. Yamada, *Chem. Commun.,* 2017, **53**, 4362-4365.
17. H. Zhao, Y. Wu, D. Zhang and H. Huang, *Tetrahedron,* 2022, **115**, 132811.
18. M. Sharif, J. Opalach, P. Langer, M. Beller and X. Wu, *RSC Adv.,* 2014, **4**, 8-17.
19. J. Kim, S. Y. Lee, J. Lee and Y. Do and S. Chang, *J. Org. Chem.* 2008, **73**, 9454-9457.
20. G. Fan, S. Chen, L. Liang, H. Zhang and R. Yu, *Int. J. Mol. Sci.,* 2022, **23**, 15996.
21. a) Bruker AXS APEX Inc., 5465 east Cheryl Parkway, Madison, WI53711; b) Bruker-SAINT V8.40B, 2016; c) SADABS-2016/2 - Bruker AXS area detector scaling and absorption correction. Krause, L.; Herbst-Irmer, R.; Sheldrick, G. M.; Stalke, D. *J. Appl. Cryst.,* 2015, **48**, 3-10; d) G. M. Sheldrick (2015) SHELXT-Integrated space-group and crystal structure determination, *Acta Cryst.* A71, 3-8; e) Sheldrick, G. M. "SHELXS-97 and SHELXL-97, Program for Crystal Structure Solution and Refinement," University of Gottingen, Gottingen, 1997; f) Sheldrick, G. M. (2015) Crystal structure refinement with SHELXL, *Acta Cryst.,* C71, 3-8; g) WingX, An integrated system of windows programs for the solution, Refinement and Analysis of Single crystal diffraction data, L. J. Farrugia, *J. appl. Cryst.,* 2012, **45**, 849-854.
22. Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
23. A. D. Becke, *J. Chem. Phys*., 1993, **98**, 5648-5652; b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B: Condens. Matter Mater. Phys.,* 1988, **37**, 785-789.