Electronic Supplementary Information

Well-defined Manganese Complex Catalyzed Dehydrogenative Synthesis of Quinazolin-4(3H)-ones and 3,4-Dihydro-2*H*-1,2,4-benzothiadiazine 1,1-Dioxides

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List of Content

1. General considerations:

Unless otherwise mentioned, all chemicals were purchased from common commercial sources and used as received. All solvents were dried by using standard procedure. The preparation of catalyst was carried out under argon atmosphere with freshly distilled dry THF. All catalytic reactions were carried out under argon atmosphere using dried glassware and standard syringe/septa techniques. DRX-400 Varian spectrometer and Bruker Avance III 600, 500 and 400 spectrometers were used to record ^{1}H, ^{19}F and ^{13}C NMR spectra using $CDCl_3$, DMSO-d_6 as solvent and TMS as an internal standard. Chemical shifts (δ) are reported in ppm and spin-spin coupling constant (*J*) are expressed in Hz, and other data are reported as follows: s = singlet, d = doublet, t = triplet, m = multiplet, q = quartet, dt = doublet of triplet, td = triplet of doublet and brs = broad singlet. FTIR were collected on PerkinElmer IR spectrometer. Q-TOF ESI-MS instrument (model HAB 273) was used for recording mass spectra. SRL silica gel (100-200 mesh) was used for column chromatography.

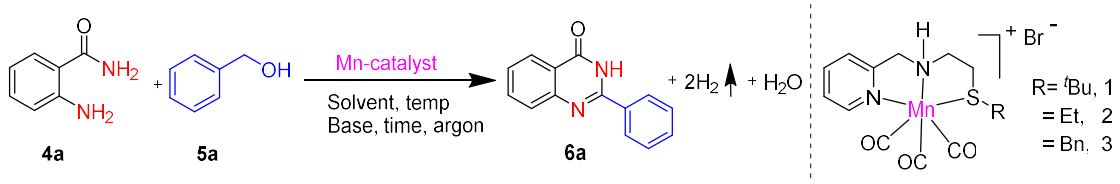
2. Ligands synthesis:

All three ligands were prepared according to previous reported literature methods.[1] Pyridine-2-carboxaldehyde (10 mmol) and amino-thiol compound (10 mmol,) were dissolved in dry CH_2Cl_2 (30 ml) and then Na_2SO_4 (40 mmol) was added to it. The resulting suspension was stirred for 20 h at room temperature. Then, it was filtered and the residue was washed thoroughly with CH_2Cl_2 and the combined solvent was removed under reduced pressure. The residue obtained was directly used for the next step without further purification. The residue was dissolved in methanol (30 ml) and $NaBH_4$ (30 mmol) was added portion wise in stirring condition at 0 °C and the stirring was continued for overnight at room temperature. Then the solvent was evaporated and 30 ml of water was added. After that, it was extracted by CH_2Cl_2 and the organic portion was collected and passed through Na_2SO_4. Then the solvent was evaporated to get the crude product, which was purified further by silica gel (100-200 mess) column chromatography using 20-40 % ethyl acetate in hexane.

3. Complex preparation:

All three complexes were prepared according to previous reported literature methods.[1] Ligand [($PyCH_2$)HN(CH_2CH_2SR), R= Et, ^{t}Bu, Bn] (2.0 mmol) was taken in 5 ml dry THF and was added dropwise to the orange-yellow suspension of [$MnBr(CO)_5$] (2.0 mmol) in 5 ml degassed dry THF. Afterward, the suspension was refluxed for overnight under argon atmosphere. After the completion of the reaction, the reaction mixture was cooled down to the room temperature, then the solvent was evaporated to obtain the residue, which was further washed with hexane and dried under vacuum to get yellow solid of Mn-complex.

4. Optimization of the reaction conditions for the synthesis of Quinazolin-4(3H)-ones[a]

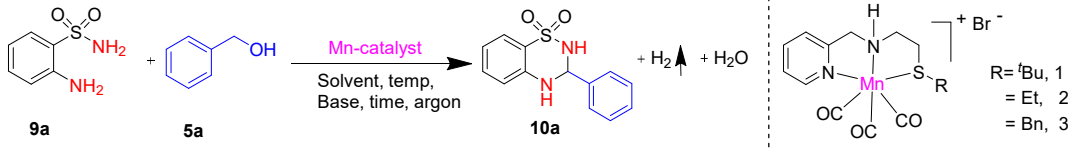


4a **5a** **6a**

Entry	Cat.	Solvent	Base (equiv.)	4a:5a	Temp (^oC)	Time (h)	Yield[b] (%)
1	**Cat-1**	1,4-dioxane	NaO^{t}Bu(0.5)	1:1	100	36	80
2	**Cat-1**	1,4-dioxane	NaO^{t}Bu(0.5)	1:1.5	100	36	80
3	**Cat-1**	1,4-dioxane	NaO^{t}Bu(0.5)	1:1	100	24	68
4	**Cat-1**	1,4-dioxane	NaO^{t}Bu(0.3)	1:1	100	36	70
5	**Cat-1**	1,4-dioxane	KO^{t}Bu(0.5)	1:1	100	36	62
6	**Cat-1**	1,4-dioxane	NaOH(0.5)	1:1	100	36	70
7	**Cat-1**	1,4-dioxane	KOH(0.5)	1:1	100	36	60
8	**Cat-1**	1,4-dioxane	Na_2CO_3(0.5)	1:1	100	36	30
9	**Cat-1**	Xylene	NaO^{t}Bu(0.5)	1:1	100	36	80
10	**Cat-1**	**Xylene**	**NaO^{t}Bu(0.5)**	**1:1**	**140**	**36**	**86**
11	**Cat-1**	Toluene	NaO^{t}Bu(0.5)	1:1	140	36	76
12	**Cat-1**	^{t}AmOH	NaO^{t}Bu(0.5)	1:1	140	36	---
13[c]	**Cat-1**	Xylene	NaO^{t}Bu(0.5)	1:1	140	36	68
14	**Cat-2**	Xylene	NaO^{t}Bu(0.5)	1:1	140	36	82
15	**Cat-3**	Xylene	NaO^{t}Bu(0.5)	1:1	140	36	72
16	-	Xylene	NaO^{t}Bu(0.5)	1:1	140	36	Trace
17	**Cat-1**	Xylene	-	1:1	140	36	Trace
18	**$MnBr(CO)_5$**	Xylene	NaO^{t}Bu(0.5)	1:1	140	36	24

[a]**Conditions**: **4a** (0.5 mmol), **5a** (0.5 – 0.75 mmol), Base (0.15 – 0.25 mmol), Mn-catalyst (5 mol%), Under argon. [b]Isolated yield, [c]Catalyst loading 2 mol%.

5. Optimization of the reaction conditions for the synthesis of 3,4-dihydro-2*H*-1,2,4-benzothiadiazine 1,1-oxide[a]

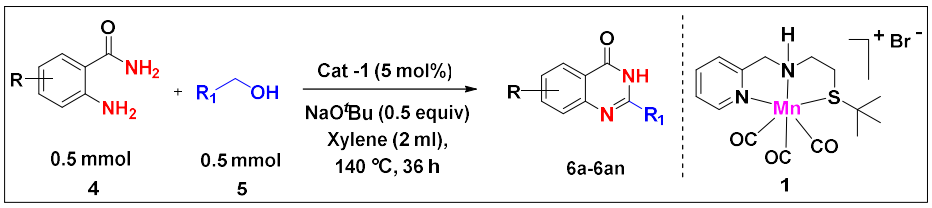


9a 5a 10a

Entry	Cat.	Solvent	Base (equiv.)	9a:5a	Temp (°C)	Time (h)	Yield[b] (%)
1	**Cat-1**	1,4-dioxane	NaO^{t}Bu(1)	1:1	100	36	45
2	**Cat-1**	**1,4-dioxane**	**NaO^{t}Bu(1)**	**1:1.5**	**100**	**36**	**62**
3	**Cat-1**	1,4-dioxane	NaO^{t}Bu(1)	1:2	100	36	62
4	**Cat-1**	1,4-dioxane	NaO^{t}Bu(1)	1:1.5	100	48	62
5	**Cat-1**	1,4-dioxane	NaO^{t}Bu(0.75)	1:1.5	100	36	52
6	**Cat-1**	1,4-dioxane	KO^{t}Bu(1)	1:1.5	100	36	42
7	**Cat-1**	1,4-dioxane	NaOH(1)	1:1.5	100	36	50
8	**Cat-1**	1,4-dioxane	KOH(1)	1:1.5	100	36	40
9	**Cat-1**	1,4-dioxane	Na_2CO_3(1)	1:1.5	100	36	28
10	**Cat-1**	Xylene	NaO^{t}Bu(1)	1:1.5	100	36	30
11	**Cat-1**	Xylene	NaO^{t}Bu(1)	1:1.5	140	36	30
12	**Cat-1**	Toluene	NaO^{t}Bu(1)	1:1.5	100	36	25
13	**Cat-1**	-	NaO^{t}Bu(1)	1:1.5	100	36	45
14[c]	**Cat-1**	1,4-dioxane	NaO^{t}Bu(1)	1:1.5	100	36	48
15	**Cat-2**	1,4-dioxane	NaO^{t}Bu(1)	1:1.5	100	36	60
16	**Cat-3**	1,4-dioxane	NaO^{t}Bu(1)	1:1.5	100	36	51
17	-	1,4-dioxane	NaO^{t}Bu(1)	1:1.5	100	36	Trace
18	**Cat-1**	1,4-dioxane	-	1:1.5	100	36	Trace

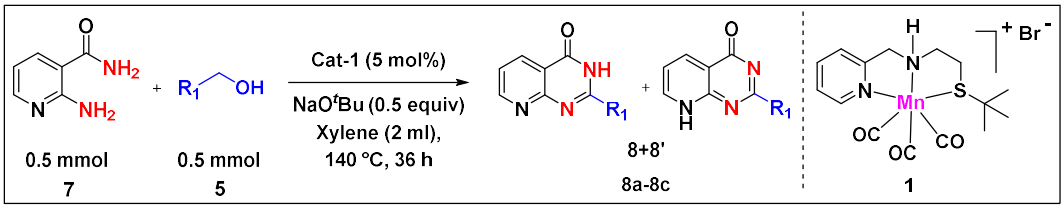
[a]**Conditions**: **9a** (0.5 mmol), **5a** (0.5 – 1.0 mmol), Base (0.375 – 0.5 mmol), Mn-catalyst (8 mol%), Under argon. [b]Isolated yield. [c]Catalyst loading 5 mol%.

6. General experimental procedure for the synthesis of Quinazolin-4(3H)-ones:



To an oven dried 10 ml round bottomed flask, 2-aminobenzamide **4** (0.5 mmol), alcohol **5** (0.5 mmol), NaO^{t}Bu (0.25 mmol) and Cat-**1** (5 mol%) were taken under argon atmosphere, after that 2 ml of xylene was added to the reaction mixture. The resulting mixture was heated in an oil bath at 140 °C for 36 h. After the completion of the reaction, the reaction mixture was subjected to cool at room temperature and ethyl acetate and methanol were added to dilute the mixture and filtered through celite. The filtrate was concentrated under reduced pressure and the residue was purified by silica gel (100-200 mess) column chromatography using 20% ethyl acetate in hexane to obtain pure compound.

7. General experimental procedure for the synthesis of Pyridopyrimidin-4(3H)-one:

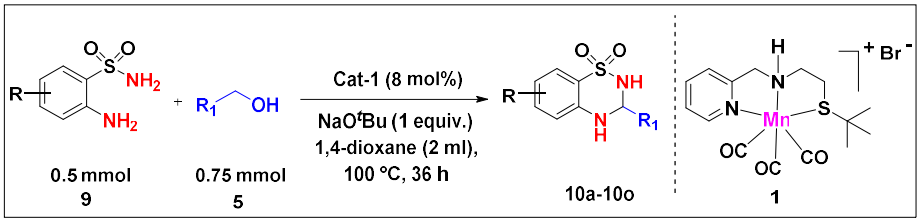


A mixture of 2-aminonicotinamide **7** (0.5 mmol), aromatic primary alcohol **5** (0.5 mmol), NaO^{t}Bu (0.25 mmol) and Cat-**1** (5 mol%) were stirred in xylene (2 ml) under argon atmosphere at 140 °C for 36 h. After the reaction was completed, it was cooled to room temperature and methanol was added to dilute the mixture and filtered through celite. The filtrate was concentrated under reduced pressure and the residue was purified by silica gel (100-200 mess) column chromatography using 50% ethyl acetate in hexane to get pure compound.

8. General experimental procedure for the synthesis of 3,4-dihydro-2*H*-1,2,4-benzothiadiazine 1,1-oxide:

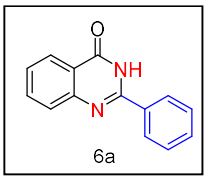
To an oven dried 10 ml round bottom flask, 2-aminobenzenesulfonamide **9** (0.5 mmol), alcohol **5** (0.75 mmol), Cat-**1** (8 mol%), NaO^{t}Bu (0.5 mmol) and 1, 4-dioxane (2 ml) were added under argon atmosphere. The reaction mixture was kept for refluxing in a preheated oil bath at 100 °C for 36 h. Then, the reaction was subjected to cool at room temperature and ethyl acetate and methanol were added to dilute the mixture and filtered through celite. The filtrate was concentrated under reduced pressure

and the residue was purified by silica gel (100-200 mess) column chromatography using 20% ethyl acetate in hexane as an eluent to obtain pure compound.



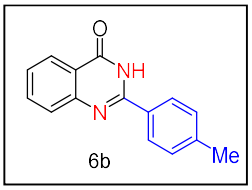
9. Characterization data:

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



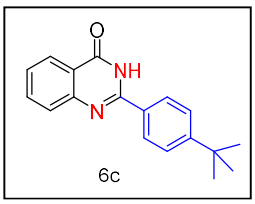
White solid, 86% Yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 11.71 (brs, 1H, NH), 8.34 (dd, *J* = 7.9, 1.7 Hz, 1H), 8.28 – 8.25 (m, 2H), 7.85 – 7.80 (m, 2H), 7.62 – 7.59 (m, 3H), 7.53 – 7.50 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.8, 151.8, 149.6, 135.1, 132.9, 131.8, 129.2, 128.1, 127.4, 127.0, 126.5, 121.0.

2-(p-tolyl)quinazolin-4(3H)-one (6b):[2]



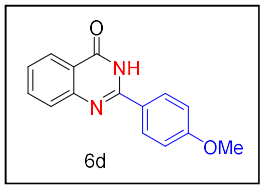
White solid, 80% Yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.49 (brs, 1H, NH), 8.14 (d, *J* = 7.9, 1H), 8.10 (d, *J* = 8.2 Hz, 2H), 7.84 –7.81 (m, 1H), 7.72 (d, *J* = 8.1 Hz, 1H), 7.52 – 7.49 (m, 1H), 7.35 (d, *J* = 7.9 Hz, 2H), 2.39 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 162.3, 152.3, 148.9, 141.5, 134.6, 129.9, 129.2, 127.7, 127.5, 126.5, 125.9, 120.9, 21.0.

2-(4-(tert-butyl)phenyl)quinazolin-4(3H)-one (6c):[3]



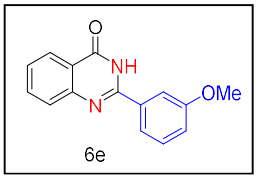
White solid, 80% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.31 (brs, 1H, NH), 8.16 – 8.12 (m, 3H), 7.82 (t, *J* = 7.6 Hz, 1H), 7.72 (d, *J* = 8.1 Hz, 1H), 7.56 (d, *J* = 8.1 Hz, 2H), 7.51 (t, *J* = 7.5 Hz, 1H), 1.32 (s, 9H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 162.3, 154.3, 152.3, 148.8, 134.6, 129.9, 127.6, 127.3, 126.4, 125.8, 125.4, 120.9, 34.7, 30.9.

2-(4-methoxyphenyl)quinazolin-4(3H)-one (6d):[2]



White solid, 75% Yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.43 (brs, 1H, NH), 8.19 (d, *J* = 8.9 Hz, 2H), 8.13 (d, *J* = 8.3 Hz, 1H), 7.83 –7.80 (m, 1H), 7.70 (d, *J* = 8.2 Hz, 1H), 7.48 (t, *J* = 7.1 Hz, 1H), 7.09 (d, *J* = 8.6 Hz, 2H), 3.84 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 162.4, 161.9, 151.9, 149.0, 134.7, 129.5, 127.4, 126.2, 125.9, 124.8, 120.7, 114.1, 55.5.

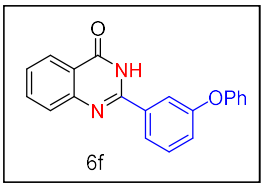
2-(3-methoxyphenyl)quinazolin-4(3H)-one (6e):[2]



6e

White solid, 60% Yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.55 (brs, 1H, NH), 8.15 (d, J = 7.7 Hz 1H), 7.84 (t, J = 7.8 Hz, 1H), 7.79 (d, J = 7.7 Hz, 1H), 7.75 – 7.74 (m, 2H), 7.52 (t, J = 7.8 Hz, 1H), 7.45 (t, J = 8.0 Hz, 1H), 7.14 (dd, J = 8.2, 2.7 Hz, 1H), 3.86 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 162.3, 159.4, 152.1, 148.6, 134.6, 134.1, 129.8, 127.5, 126.7, 125.9, 121.0, 120.2, 117.6, 112.5, 55.4.

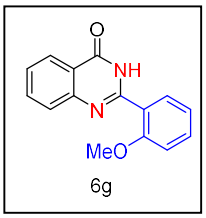
2-(3-phenoxyphenyl)quinazolin-4(3H)-one (6f):[4]



6f

White solid, 73% Yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.60 (brs, 1H, NH), 8.14 (d, J = 7.9 Hz, 1H), 7.97 (d, J = 8.0 Hz, 1H), 7.85 – 7.80 (m, 2H), 7.71 (d, J = 8.2 Hz, 1H), 7.56 (t, J = 8.0 Hz, 1H), 7.52 (t, J = 7.5 Hz, 1H), 7.40 (t, J = 7.4 Hz, 2H), 7.23 (dd, J = 7.9, 1.8 Hz, 1H), 7.19 (t, J = 7.4 Hz, 1H), 7.09 (d, J = 7.8 Hz, 2H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 162.2, 156.9, 156.4, 151.6, 148.6, 134.7, 130.4, 130.2, 127.6, 126.8, 125.9, 123.8, 122.9, 121.7, 121.1, 118.9, 117.9.

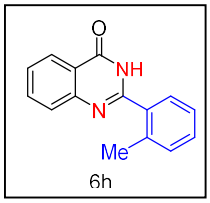
2-(2-methoxyphenyl)quinazolin-4(3H)-one (6g):[5]



6g

White solid, 52% Yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.09 (brs, 1H, NH), 8.15 (d, J = 8.0 Hz, 1H), 7.84 – 7.81 (m, 1H), 7.72 – 7.69 (m, 2H), 7.55 – 7.51 (m, 2H), 7.19 (d, J = 8.4 Hz, 1H), 7.09 (t, J = 7.5 Hz, 1H), 3.86 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 161.2, 157.2, 152.3, 149.0, 134.3, 132.2, 130.4, 127.3, 126.5, 125.7, 122.6, 121.0, 120.4, 111.9, 55.8.

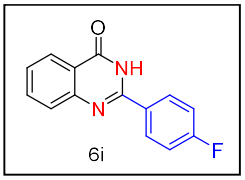
2-(o-tolyl)quinazolin-4(3H)-one (6h):[2]



6h

White solid, 50% Yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.79 (brs, 1H, NH), 8.26 (d, J = 7.9 Hz, 1H), 7.80 – 7.79 (m, 2H), 7.58 – 7.56 (m, 1H), 7.51 – 7.48 (m, 1H), 7.43 – 7.40 (m, 1H), 7.35 – 7.32 (m, 2H), 2.53 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.3, 153.6, 149.3, 137.0, 135.0, 133.8, 131.6, 130.7, 128.9, 128.0, 127.1, 126.53, 126.4, 120.9, 20.2.

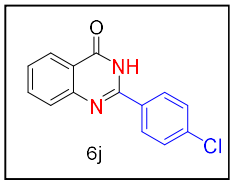
2-(4-fluorophenyl)quinazolin-4(3H)-one (6i):[2]



6i

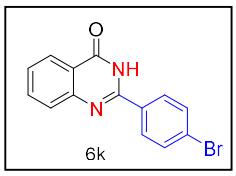
White solid, 75% Yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.57 (brs, 1H, NH), 8.27 – 8.24 (m, 2H), 8.15 (d, J = 8.5 Hz, 1H), 7.85 – 7.81 (m, 1H), 7.73 (d, J = 8.1 Hz, 1H), 7.52 (t, J = 7.3 Hz, 1H), 7.39 (t, J = 8.8 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 164.0 (d, J = 247.9 Hz), 162.2, 151.4, 148.6, 134.6, 130.4 (d, J = 8.8 Hz), 129.2 (d, J = 3.0 Hz), 127.4, 126.6, 125.8, 120.9, 115.6 (d, J = 21.8 Hz). ^{19}F NMR (376 MHz, DMSO-d_6) δ -109.07.

2-(4-chlorophenyl)quinazolin-4(3H)-one (6j):[2]



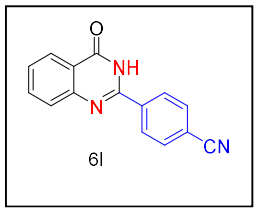
White solid, 72% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.60 (brs, 1H, NH), 8.20 (d, J = 8.3 Hz, 2H), 8.15 (d, J = 8.0 Hz, 1H), 7.84 (t, J = 7.7 Hz, 1H), 7.74 (d, J = 8.1 Hz, 1H), 7.62 (d, J = 8.2 Hz, 2H), 7.53 (t, J = 7.6 Hz, 1H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 162.1, 151.3, 148.6, 136.3, 134.6, 131.5, 129.6, 128.6, 127.5, 126.74, 125.8, 121.0.

2-(4-bromophenyl)quinazolin-4(3H)-one (6k):[2]



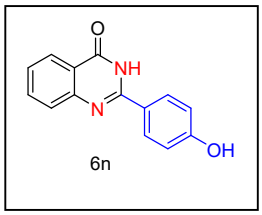
White solid, 68% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.59 (brs, 1H, NH), 8.16 – 8.11 (m, 3H), 7.86 – 7.75 (m, 4H), 7.55 – 7.52 (m, 1H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 162.1, 151.4, 148.6, 134.6, 131.9, 131.6, 129.8, 127.5, 126.8, 125.9, 125.2, 121.0.

4-(4-oxo-3,4-dihydroquinazolin-2-yl)benzonitrile (6l):[6]



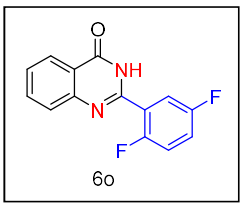
White solid, 34% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.73 (brs, 1H, NH), 8.33 (d, J = 8.2 Hz, 2H), 8.17 (d, J = 7.7 Hz, 1H), 8.03 (d, J = 8.2 Hz, 2H), 7.86 (t, J = 7.7 Hz, 1H), 7.77 (d, J = 8.2 Hz, 1H), 7.56 (t, J = 7.5 Hz, 1H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 162.1, 150.9, 148.4, 136.9, 134.8, 132.5, 128.6, 127.7, 127.2, 125.9, 121.2, 118.3, 113.6.

2-(4-hydroxyphenyl)quinazolin-4(3H)-one (6n):[7]



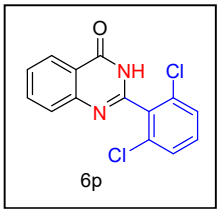
White solid, 52% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.29 (brs, 1H, NH), 10.16 (s, 1H), 8.12 (d, J = 7.9 Hz, 1H), 8.09 (d, J = 8.8 Hz, 2H) 7.78 (t, J = 7.2 Hz, 1H), 7.67 (d, J = 8.2 Hz, 1H), 7.45 (t, J = 7.5 Hz, 1H), 6.90 (d, J = 8.5 Hz, 2H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 162.3, 160.6, 152.1, 149.1, 134.5, 129.6, 127.2, 125.9, 125.8, 123.3, 120.6, 115.4.

2-(2,5-difluorophenyl)quinazolin-4(3H)-one (6o):[8]



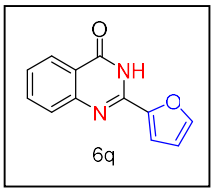
White solid, 65% Yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.62 (brs, 1H, NH), 8.17 (d, J = 8.4 Hz, 1H), 7.86 (t, J = 7.7 Hz, 1H), 7.74 (d, J = 8.1 Hz, 1H), 7.66 – 7.62 (m, 1H), 7.58 (t, J = 7.5 Hz, 1H), 7.50 – 7.44 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.5, 157.8 (dd, J = 239.8 Hz, 2.2 Hz), 155.8 (dd, J = 245.4 Hz, 2.4 Hz), 148.8, 148.4, 134.7, 129.2, 127.3, 125.9, 123.5 (dd, J = 15.7 Hz, 8.5 Hz), 121.2, 119.3 (dd, J = 24.0 Hz, 9.0 Hz), 118.0 (dd, J = 24.4 Hz, 8.7 Hz), 117.4 (dd, J = 25.9, 2.9 Hz).

2-(2,6-dichlorophenyl)quinazolin-4(3H)-one (6p):[2]



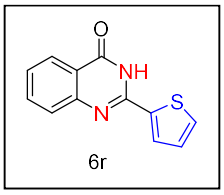
White solid, 48% Yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 11.52 (brs, 1H, NH), 8.16 (d, J = 8.0 Hz, 1H), 7.83 – 7.82 (m, 2H), 7.55 – 7.52 (m, 1H), 7.44 – 7.42 (m, 2H), 7.41 – 7.38 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.3, 149.2, 148.9, 135.0, 134.7, 132.8, 131.8, 128.4, 128.2, 127.7, 126.6, 121.4.

2-(furan-2-yl)quinazolin-4(3H)-one (6q):[2]



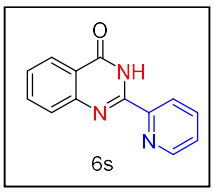
Yellow solid, 76% Yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.97 (brs, 1H, NH), 8.28 (d, J = 7.9 Hz, 1H), 7.79 – 7.77 (m, 1H), 7.76 – 7.72 (m, 1H), 7.67 – 7.66 (m, 2H), 7.46 – 7.42 (m, 1H), 6.63 – 6.62 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.4, 149.5, 146.4, 145.8, 143.8, 135.0, 127.8, 126.7, 126.5, 121.0, 114.3, 112.8.

2-(thiophen-2-yl)quinazolin-4(3H)-one (6r):[3]



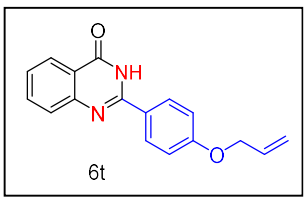
White solid, 80% Yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.66 (brs, 1H, NH), 8.23 (d, J = 3.7 Hz, 1H), 8.12 (d, J = 7.8 Hz, 1H), 7.87 (d, J = 5.2 Hz, 1H), 7.81 – 7.78 (m, 1H), 7.65 (d, J = 8.1 Hz, 1H), 7.48 (t, J = 7.8 Hz, 1H), 7.23 (t, J = 5.0 Hz, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 161.8, 148.6, 147.9, 137.4, 134.7, 132.2, 129.4, 128.5, 127.0, 126.4, 126.0, 120.9.

2-(pyridin-2-yl)quinazolin-4(3H)-one (6s):[2]



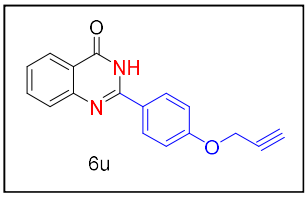
White solid, 78% Yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 11.85 (brs, 1H, NH), 8.75 (d, J = 4.5 Hz, 1H), 8.44 (d, J = 8.2 Hz, 1H), 8.18 (d, J = 8.2 Hz, 1H), 8.07 (t, J = 7.7 Hz, 1H), 7.86 (t, J = 7.8 Hz, 1H), 7.79 (d, J = 8.2 Hz, 1H), 7.66 – 7.63 (m, 1H), 7.56 (t, J = 7.5 Hz, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 160.8, 150.0, 149.0, 148.7, 148.4, 138.0, 134.7, 127.7, 127.3, 126.6, 126.1, 122.2, 122.0.

2-(4-(allyloxy)phenyl)quinazolin-4(3H)-one (6t):



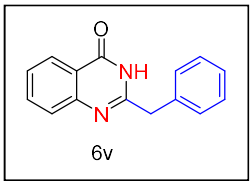
White solid, 60% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.36 (brs, 1H, NH), 8.19 – 8.16 (m, 2H), 8.13 (dd, J = 7.8 Hz, 1.0 Hz, 1H), 7.81 – 7.78 (m, 1H), 7.69 (d, J = 8.1 Hz, 1H), 7.48 (t, J = 7.4 Hz, 1H), 7.10 – 7.08 (m, 2H), 6.09 – 6.02 (m, 1H), 5.42 (dd, J = 17.3, 1.8 Hz, 1H), 5.29 (dd, J = 10.5, 1.8 Hz, 1H), 4.67 – 4.65 (m, 1H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 162.3, 160.8, 151.8, 148.9, 134.5, 133.3, 131.3, 129.4, 127.3, 126.1, 125.8, 124.9, 120.7, 117.7, 114.7, 114.4, 68.4. HRMS (ESI) m/z (M+H): 279.1134, found: 279.1164.

2-(4-(prop-2-yn-1-yloxy)phenyl)quinazolin-4(3H)-one (6u):



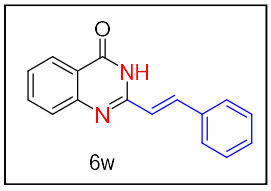
White solid, 58% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.39 (brs, 1H, NH), 8.19 (d, J = 8.5 Hz, 2H), 8.13 (d, J = 7.8 Hz, 1H), 7.81 (t, J = 7.6 Hz, 1H), 7.70 (d, J = 8.2 Hz, 1H), 7.49 (t, J = 7.5 Hz, 1H), 7.14 (d, J = 8.7 Hz, 2H), 4.91 (s, 2H), 3.60 (s, 1H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 162.3, 159.7, 151.8, 148.9, 134.5, 129.4, 128.3, 127.3, 126.2, 125.8, 125.6, 120.7, 114.9, 78.9, 78.6, 55.7. HRMS (ESI) m/z (M+H): 277.0977, found: 277.0976.

2-benzylquinazolin-4(3H)-one (6v):[9]



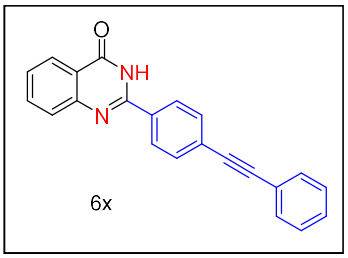
White solid, 72% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.38 (brs, 1H, NH), 8.10 – 8.07 (m, 1H), 8.03 (d, J = 8.3 Hz, 1H), 7.96 (s, 1H), 7.91 (d, J = 7.4 Hz, 1H), 7.78 – 7.74 (m, 1H), 7.67 (t, J = 8.8 Hz, 1H), 7.47 – 7.42 (m, 1H), 7.38 – 7.32 (m, 1H), 7.29 (d, J = 8.0 Hz, 1H), 2.34 (s, 2H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 162.2, 141.4, 137.9, 134.6, 132.6, 132.0, 129.9, 129.2, 128.5, 128.3, 127.7, 126.5, 126.4, 125.8, 124.9, 120.9, 20.9.

(E)-2-styrylquinazolin-4(3H)-one (6w):[10]



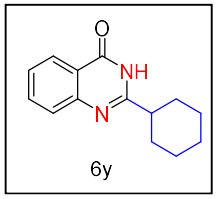
White solid, 58% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.30 (brs, 1H, NH), 8.11 (d, J = 7.9 Hz, 1H), 7.95 (d, J = 16.2 Hz, 1H), 7.80 (t, J = 8.1 Hz, 1H), 7.66 (t, J = 8.8 Hz, 3H), 7.48 – 7.44 (m, 3H), 7.42 –7.39 (m, 1H), 7.01 (d, J = 16.2 Hz, 1H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 161.7, 151.4, 149.0, 138.2, 135.0, 134.4, 129.7, 129.0, 127.6, 127.1, 126.2, 125.8, 121.1.

2-(4-(phenylethynyl)phenyl)quinazolin-4(3H)-one (6x):



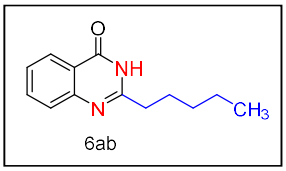
White solid, 54% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.65 (brs, 1H, NH), 8.30 (d, J = 8.2 Hz, 2H), 8.22 (d, J = 7.8 Hz, 1H), 7.90 (t, J = 7.6 Hz, 1H), 7.81 (d, J = 8.2 Hz, 1H), 7.78 (d, J = 8.1 Hz, 2H), 7.67 – 7.65 (m, 2H), 7.59 (t, J = 7.4 Hz, 1H), 7.52 – 7.50 (m, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 162.1, 151.5, 148.6, 134.6, 132.5, 131.5, 131.4, 129.2, 128.8, 128.0, 127.5, 126.7, 125.9, 125.1, 121.9, 121.0, 91.7, 88.7. HRMS (ESI) m/z (M+H): 323.1184, found: 323.1214.

2-cyclohexylquinazolin-4(3H)-one (6y):[11]



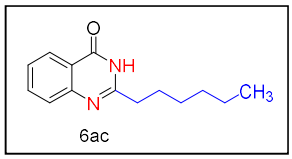
White solid, 60% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.04 (brs, 1H, NH), 8.07 (dd, J = 7.9 Hz, 1.4 Hz, 1H), 7.76 – 7.72 (m, 1H), 7.58 (d, J = 8.2 Hz, 1H), 7.43 (t, J = 7.3 Hz, 1H), 2.59 – 2.53 (m, 1H), 1.90 (d, J = 11.4 Hz, 2H), 1.78 (d, J = 13.0 Hz, 2H), 1.67 (d, J = 12.1 Hz, 1H), 1.61 – 1.53 (m, 2H), 1.37 – 1.11 (m, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 161.8, 160.7, 148.9, 134.1, 126.9, 125.8, 125.6, 120.9, 42.8, 30.1, 25.5, 25.3.

2-pentylquinazolin-4(3H)-one (6ab):[12]



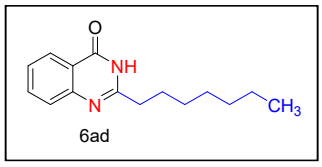
White solid, 50% Yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.82 (brs, 1H, NH), 8.29 (d, J = 8.0 Hz, 1H), 7.77 (t, J = 7.6 Hz, 1H), 7.71 (d, J = 8.2 Hz, 1H), 7.47 (t, J = 7.5 Hz, 1H), 2.79 (t, J = 7.5 Hz, 2H), 1.92 – 1.86 (m, 2H), 1.48 – 1.38 (m, 4H), 0.93 (t, J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.4, 157.1, 149.6, 134.9, 127.4, 126.5, 126.4, 120.7, 36.1, 31.5, 27.4, 22.5, 14.1.

2-hexylquinazolin-4(3H)-one (6ac):



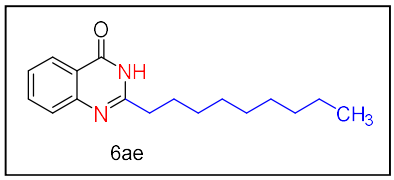
White solid, 53% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.12 (brs, 1H, NH), 8.07 (d, J = 7.9 Hz, 1H), 7.74 (t, J = 7.7 Hz, 1H), 7.58 (d, J = 8.2 Hz, 1H), 7.43 (t, J = 7.5 Hz, 1H), 2.58 (t, J = 7.6 Hz, 2H), 1.73 – 1.67 (m, 2H), 1.31 – 1.23 (m, 6H), 0.83 (t, J = 7.0 Hz, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 161.8, 157.4, 148.9, 134.1, 126.7, 125.8, 125.6, 120.7, 34.4, 30.9, 28.1, 26.7, 21.9, 13.8. HRMS (ESI) m/z (M+H): 231.1497, found: 231.1519.

2-heptylquinazolin-4(3H)-one (6ad):[13]



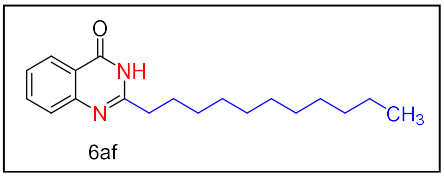
White solid, 56% Yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.14 (brs, 1H, NH), 8.20 (d, J = 7.9 Hz, 1H), 7.68 – 7.61 (m, 2H), 7.37 (t, J = 7.5 Hz, 1H), 2.72 (t, J = 7.9 Hz, 2H), 1.83 – 1.77 (m, 2H), 1.41 – 1.20 (m, 8H), 0.78 (t, J = 6.2 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.6, 157.3, 149.7, 134.8, 127.3, 126.4, 126.3, 120.6, 36.0, 31.8, 29.3, 29.0, 27.7, 22.7, 14.1.

2-nonylquinazolin-4(3H)-one (6ae):[14]



White solid, 60% Yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.28 (brs, 1H, NH), 8.18 (d, J = 7.9 Hz, 1H), 7.67 – 7.61 (m, 2H), 7.37 – 7.33 (m, 1H), 2.71 (t, J = 7.9 Hz, 2H), 1.83 – 1.77 (m, 2H), 1.40 – 1.34 (m, 2H), 1.26 – 1.15 (m, 10H), 0.77 (t, J = 6.9 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.7, 157.4, 149.6, 134.8, 127.2, 126.3, 126.2, 120.5, 36.0, 31.9, 29.5, 29.4, 27.7, 22.7.

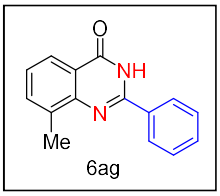
2-undecylquinazolin-4(3H)-one (6af):[15]



6af

White solid, 62% Yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.11 (brs, 1H, NH), 8.27 (d, J = 7.9 Hz, 1H), 7.75 (t, J = 7.6 Hz, 1H), 7.70 (d, J = 8.1 Hz, 1H), 7.45 (t, J = 7.4 Hz, 1H), 2.79 (t, J = 7.9 Hz , 2H), 1.90 – 1.84 (m, 2H), 1.47 – 1.42 (m, 2H), 1.28 – 1.23 (m, 14H), 0.86 (t, J = 6.6 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.6, 157.2, 149.7, 134.9, 127.3, 126.4, 126.3, 120.6, 36.0, 32.0, 29.8, 29.7, 29.6, 29.5, 29.4, 29.3, 27.7, 22.8, 14.2.

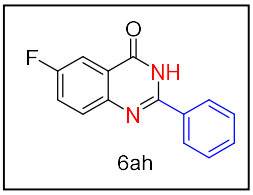
8-methyl-2-phenylquinazolin-4(3H)-one (6ag):[3]



6ag

White solid, 74% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.50 (brs, 1H, NH), 8.23 (d, J = 7.7 Hz, 2H), 7.99 (d, J = 7.8 Hz, 1H), 7.68 (d, J = 7.2 Hz, 1H), 7.58 – 7.53 (m, 3H), 7.39 (t, J = 7.6 Hz, 1H), 2.62 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 162.5, 151.0, 147.1, 135.6, 134.9, 133.0, 131.3, 128.6, 127.7, 126.0, 123.5, 120.9, 17.1.

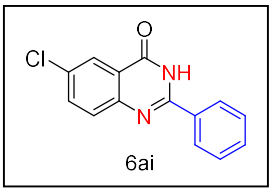
6-fluoro-2-phenylquinazolin-4(3H)-one (6ah):[16]



6ah

White solid, 72% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.63 (brs, 1H, NH), 8.16 (d, J = 7.4 Hz, 2H), 7.83 – 7.80 (m, 2H), 7.72 (t, J = 8.7 Hz, 1H), 7.60 – 7.53 (m, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 161.7, 160.1 (d, J = 244.0 Hz), 151.9, 145.6, 132.5, 131.4, 130.3, 128.6, 127.7, 123.0 (d, J = 24.1 Hz), 122.2 (d, J = 8.4 Hz), 110.5 (d, J = 23.2 Hz).

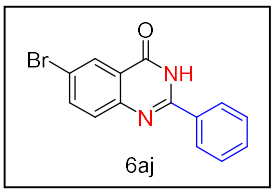
6-chloro-2-phenylquinazolin-4(3H)-one (6ai):[16]



6ai

White solid, 68% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.68 (brs, 1H, NH), 8.18 (d, J = 7.2 Hz, 2H), 8.09 (d, J = 2.5 Hz, 1H), 7.86 (dd, J = 8.7, 2.6 Hz, 1H), 7.77 (d, J = 8.8 Hz, 1H), 7.62 – 7.54 (m, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 161.2, 152.8, 147.5, 134.6, 132.4, 131.5, 130.7, 129.7, 128.6, 127.8, 124.8, 122.2.

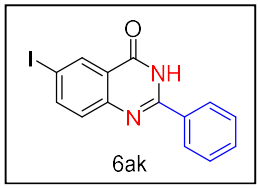
6-bromo-2-phenylquinazolin-4(3H)-one (6aj):[2]



6aj

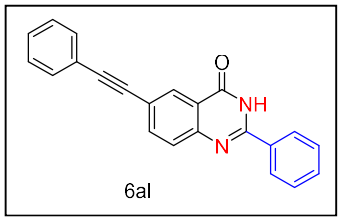
White solid, 62% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.68 (brs, 1H, NH), 8.22 (s, 1H), 8.17 (d, J = 7.8 Hz, 2H), 7.96 (d, J = 6.8 Hz, 1H), 7.68 (d, J = 8.7 Hz, 1H), 7.61 – 7.53 (m, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 161.1, 152.8, 147.7, 137.3, 132.4, 131.5, 129.8, 128.5, 127.9, 127.8, 122.6, 118.8.

6-iodo-2-phenylquinazolin-4(3H)-one (6ak):[2]



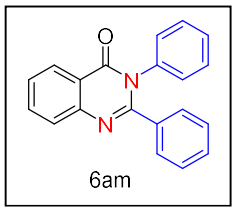
White solid, 56% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.50 (brs, 1H, NH), 8.19 – 8.14 (m, 3H), 7.82 (t, J = 7.2 Hz, 1H), 7.74 (d, J = 8.2 Hz, 1H), 7.58 – 7.49 (m, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 162.2, 152.3, 148.7, 134.5, 132.7, 131.3, 128.6, 127.7, 127.5, 126.5, 125.8, 121.0.

2-phenyl-6-(phenylethynyl)quinazolin-4(3H)-one (6al):



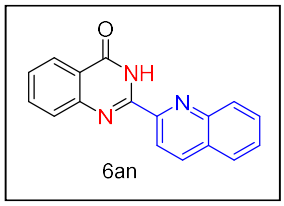
White solid, 58% Yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.68 (brs, 1H, NH), 8.25 (s, 1H), 8.19 (d, J = 7.6 Hz, 2H), 7.93 (d, J = 8.3 Hz, 1H), 7.75 (d, J = 8.3 Hz, 1H), 7.61 – 7.54 (m, 5H), 7.45 – 7.44 (m, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 161.4, 153.1, 148.5, 136.7, 132.4, 131.5, 131.4, 129.0, 128.8, 128.7, 128.6, 128.1, 127.8, 122.0, 121.2, 120.1, 90.5, 88.5. HRMS (ESI) m/z (M+H): 323.1184, found: 323.1177.

2,3-diphenylquinazolin-4(3H)-one (6am):[17]



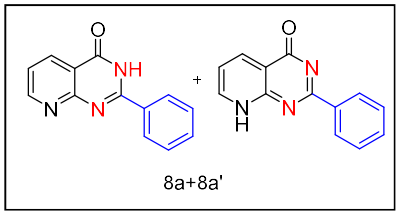
White solid, 52% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.21 (dd, J = 7.9, 1.0 Hz, 1H), 7.92 – 7.88 (m, 1H), 7.77 (d, J = 7.9 Hz, 1H), 7.61 (t, J = 7.6 Hz, 1H), 7.38 – 7.36 (m, 2H), 7.33 – 7.28 (m, 4H), 7.27 – 7.19 (m, 4H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 161.3, 155.1, 147.2, 137.8, 135.6, 134.7, 129.5, 128.9, 128.8, 128.5, 128.1, 127.4, 127.4, 127.1, 126.4, 120.7.

2-(quinolin-2-yl)quinazolin-4(3H)-one (6an):[2]



White solid, 82% Yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.13 (brs, 1H, NH), 8.57 (d, J = 8.6 Hz, 1H), 8.33 (d, J = 7.9 Hz, 1H), 8.28 (d, J = 8.5 Hz, 1H), 8.09 (d, J = 8.5 Hz, 1H), 7.83 – 7.81 (m, 2H), 7.75 (q, J = 8.0 Hz, 2H), 7.58 (t, J = 7.5 Hz, 1H), 7.49 (t, J = 7.5 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.4, 149.2, 149.0, 148.1, 146.8, 137.6, 134.6, 130.5, 129.7, 129.3, 128.3, 128.2, 127.8, 127.6, 126.8, 122.7, 118.5.

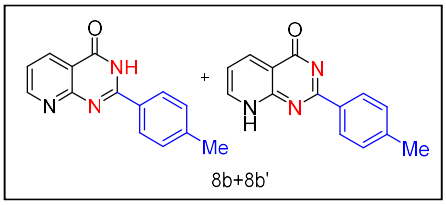
2-phenylpyrido[2,3-d]pyrimidin-4(3H)-one and 2-phenylpyrido[2,3-d]pyrimidin-4(8H)-one (8a+8a'):[18]



White solid, 74% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.79 (brs, 1H, NH), 8.97 – 8.96 (m, 1H), 8.55 – 8.51 (m, 2H), 8.22 (d, J = 7.6 Hz, 2H), 8.14 – 8.13 (m, 1H), 7.96 (s, 1H), 7.91 (d, J = 7.5 Hz, 1H), 7.63 – 7.61 (m, 1H), 7.58 – 7.55 (m, 2H), 7.54 – 7.51 (m, 1H), 7.44 (d, J = 8.2 Hz, 1H), 7.38 – 7.35 (m, 1H), 7.32

– 7.29 (m, 1H), 6.70 – 6.68 (m, 1H), 5.83 (brs, 1H, NH). ^{13}C NMR (125 MHz, DMSO-d_6) δ 162.7, 157.4, 156.0, 155.4, 152.8, 142.2, 135.7, 135.5, 132.4, 131.9, 128.6, 128.4, 128.3, 128.0, 126.2, 122.2, 116.1, 113.7, 109.5, 65.1.

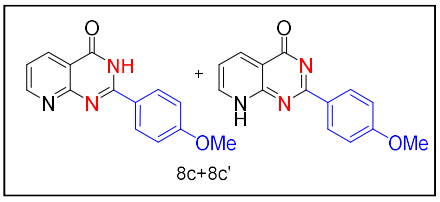
2-(p-tolyl)pyrido[2,3-d]pyrimidin-4(3H)-one and 2-(p-tolyl)pyrido[2,3-d]pyrimidin-4(8H)-one (8b+8b'):



8b+8b'

White solid, 72% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.68 (brs, 1H, NH), 8.95 (s, 1H), 8.52 (s, 2H), 8.13 (s, 3H), 7.93 – 7.83 (m, 2H), 7.51 (s, 1H), 7.37 – 7.30 (m, 3H), 7.16 (s, 1H), 6.69 (s, 1H), 5.79 (brs, 1H, NH), 2.39 (s, 3H), 2.26 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 163.0, 162.7, 159.0, 157.4, 156.0, 155.3, 152.6, 142.1, 139.2, 137.5, 135.7, 135.5, 129.6, 129.2, 128.8, 128.0, 126.1, 122.0, 116.0, 113.6, 109.6, 65.0, 21.0, 20.6. HRMS (ESI) m/z (M+H): 238.0980, found: 238.0974.

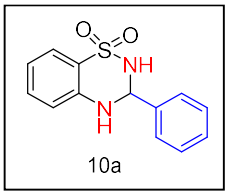
2-(4-methoxyphenyl)pyrido[2,3-d]pyrimidin-4(3H)-one and 2-(4-methoxyphenyl)pyrido[2,3-d]pyrimidin-4(8H)-one (8c+8c'):



8c+8c'

White solid, 70% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.65 (brs, 1H, NH), 8.94 (s, 1H), 8.49 (d, J = 7.8 Hz, 1H), 8.24 (d, J = 8.7 Hz, 2H), 7.50 – 7.47 (m, 1H), 7.36 – 7.34 (m, 1H), 7.11 (d, J = 8.7 Hz, 1H), 3.86 (s, 3H), 3.73 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 162.8, 162.4, 159.3, 158.7, 157.5, 156.0, 155.0, 152.7, 135.7, 135.5, 134.1, 129.9, 128.3, 127.6, 124.4, 121.8, 115.8, 114.1, 113.7, 109.5, 64.9, 55.5, 55.1. HRMS (ESI) m/z (M+H): 254.0930, found: 254.0923.

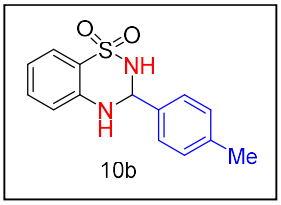
3-phenyl-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide (10a):[19]



10a

White solid, 62% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.89 (d, J = 12.1 Hz, 1H), 7.69 (d, J = 7.2 Hz, 2H), 7.55 (d, J = 7.4 Hz, 1H), 7.49 – 7.43 (m, 3H), 7.38 (s, 1H), 7.35 – 7.31 (m, 1H), 6.95 (d, J = 8.4 Hz, 1H), 6.79 (t, J = 7.6 Hz, 1H), 5.81 (d, J = 12.1 Hz, 1H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 143.9, 137.3, 132.8, 129.1, 128.5, 127.5, 123.7, 121.7, 116.7, 116.4, 68.4.

3-(p-tolyl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide (10b):[19]

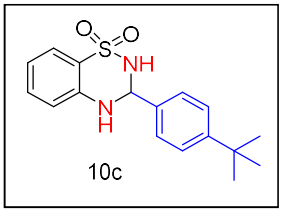


10b

White solid, 60% Yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.84 (d, J = 12.1 Hz, 1H), 7.55 (d, J = 8.0 Hz, 2H), 7.53 (d, J = 7.8 Hz, 1H), 7.33 – 7.29 (m, 2H), 7.27 (d, J = 8.2 Hz, 2H), 6.91 (d, J = 8.4 Hz, 1H), 6.76 (t, J = 7.6 Hz, 1H), 5.74 (d, J = 12.1 Hz, 1H), 2.35 (s, 3H). ^{13}C NMR (150 MHz, DMSO-

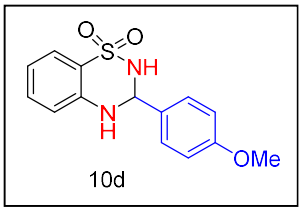
d_6) δ 143.9, 138.5, 134.4, 132.8, 129.0, 127.4, 123.7, 121.6, 116.6, 116.4, 68.2, 20.8.

3-(4-(tert-butyl)phenyl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide (10c):



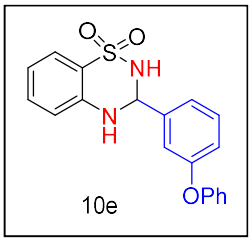
White solid, 65% Yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.84 (d, J = 12.0 Hz, 1H), 7.60 (d, J = 8.1 Hz, 2H), 7.52 (d, J = 7.7 Hz, 1H), 7.48 (d, J = 8.5 Hz, 2H), 7.36 (s, 1H), 7.33 – 7.28 (m, 1H), 6.90 (d, J = 8.4 Hz, 1H), 6.76 (t, J = 7.5 Hz, 1H), 5.75 (d, J = 12.0 Hz, 1H), 1.31 (s, 9H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 151.7, 143.9, 134.4, 132.7, 127.2, 125.2, 123.6, 121.6, 116.6, 116.3, 68.1, 34.4, 31.0. HRMS (ESI) m/z (M+H): 317.1324, found: 317.1349.

3-(4-methoxyphenyl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide (10d):[20]



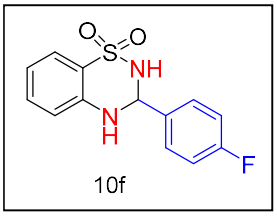
White solid, 56% Yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.83 (d, J = 12.1 Hz, 1H), 7.60 (d, J = 8.3 Hz, 2H), 7.54 (d, J = 7.9 Hz, 1H), 7.33 – 7.30 (m, 2H), 7.02 (d, J = 8.3 Hz, 2H), 6.92 (d, J = 8.4 Hz, 1H), 6.77 (t, J = 7.6 Hz, 1H), 5.74 (d, J = 12.0 Hz, 1H), 3.79 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 159.8, 143.9, 132.8, 129.5, 128.9, 123.7, 121.6, 116.6, 116.4, 113.8, 68.0, 55.3.

3-(3-phenoxyphenyl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide (10e):[21]



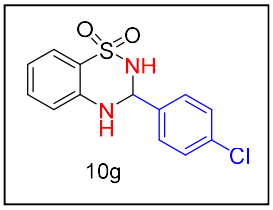
White solid, 58% Yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.96 (d, J = 11.8 Hz, 1H), 7.52 (d, J = 7.6 Hz, 1H), 7.47 – 7.40 (m, 6H), 7.31 (t, J = 8.0 Hz, 1H), 7.16 (t, J = 7.4 Hz, 1H), 7.07 – 7.05 (m, 3H), 6.91 (d, J = 8.0 Hz, 1H), 6.77 (t, J = 7.4 Hz, 1H), 5.80 (d, J = 11.8 Hz, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 156.7, 156.4, 143.8, 139.3, 132.9, 130.2, 130.1, 123.8, 123.7, 122.8, 121.7, 119.3, 118.7, 117.8, 116.9, 116.4, 68.0.

3-(4-fluorophenyl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide (10f):[21]



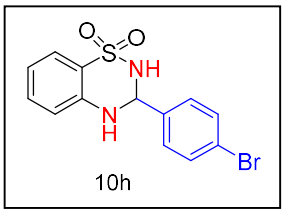
White solid, 60% Yield. ^{1}H NMR (600 MHz, $CDCl_3$ + DMSO-d_6) δ 7.66 – 7.60 (m, 3H), 7.32 – 7.27 (m, 1H), 7.14 – 7.10 (m, 2H), 6.86 – 6.78 (m, 2H), 6.52 – 6.49 (m, 1H), 5.95 – 5.91 (m, 1H), 5.51 – 5.49 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$ + DMSO-d_6) δ 163.3 (d, J = 247.9 Hz), 143.0, 133.2, 133.0, 129.0 (d, J = 8.3 Hz), 124.5, 122.8, 118.6, 116.7, 115.9 (d, J = 21.7 Hz), 68.4.

3-(4-chlorophenyl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide (10g):[20]



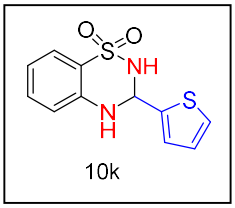
White solid, 63% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.93 (d, J = 12.0 Hz, 1H), 7.70 (d, J = 8.5 Hz, 2H), 7.54 (d, J = 8.5 Hz, 3H), 7.38 (s, 1H), 7.35 – 7.31 (m, 1H), 6.92 (d, J = 8.2 Hz, 1H), 6.78 (t, J = 7.7 Hz, 1H), 5.82 (d, J = 12.0 Hz, 1H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 143.7, 136.2, 133.6, 132.8, 129.4, 128.4, 123.7, 121.7, 116.9, 116.4, 67.6.

3-(4-bromophenyl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide (10h):[21]



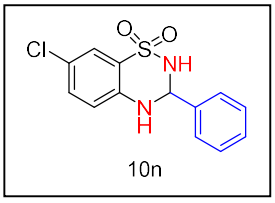
White solid, 65% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.92 (d, J = 12.0 Hz, 1H), 7.68 – 7.62 (m, 4H), 7.54 (d, J = 7.4 Hz, 1H), 7.38 (s, 1H), 7.34 – 7.30 (m, 1H), 6.91 (d, J = 8.3 Hz, 1H), 6.78 (t, J = 7.5 Hz, 1H), 5.80 (d, J = 12.0 Hz, 1H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 143.7, 136.6, 132.8, 131.4, 129.7, 123.7, 122.2, 121.7, 116.9, 116.4, 67.7.

3-(thiophen-2-yl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide (10k):[21]



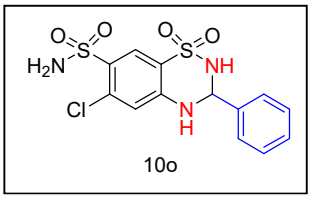
White solid, 60% Yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.08 (d, J = 11.7 Hz, 1H), 7.62 (d, J = 5.0 Hz, 1H), 7.54 – 7.52 (m, 2H), 7.43 (d, J = 3.5 Hz, 1H), 7.34 (t, J = 7.8 Hz, 1H), 7.12 – 7.09 (m, 1H), 6.96 (d, J = 8.3 Hz, 1H), 6.80 (t, J = 7.5 Hz, 1H), 6.08 (d, J = 11.6 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 143.5, 140.1, 132.9, 126.8, 126.7, 126.6, 123.6, 121.8, 117.1, 116.5, 64.2.

7-chloro-3-phenyl-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide (10n):[22]



White solid, 58% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.03 (d, J = 12.0 Hz, 1H), 7.66 (d, J = 7.5 Hz, 2H), 7.60 (s, 1H), 7.55 (d, J = 2.6 Hz, 1H), 7.48 -7.45 (m, 3H), 7.38 (dd, J = 8.9, 2.6 Hz, 1H), 6.96 (d, J = 8.9 Hz, 1H), 5.79 (d, J = 12.0 Hz, 1H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 142.7, 136.8, 132.8, 129.2, 128.5, 127.5, 122.8, 122.2, 120.1, 118.4, 68.3.

6-chloro-3-phenyl-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine-7-sulfonamide 1,1-dioxide (10o):

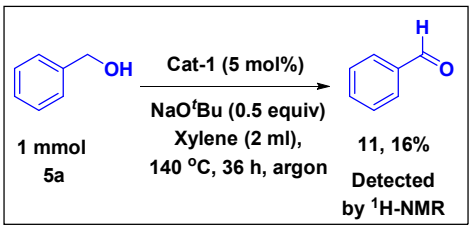


White solid, 60% Yield. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.26 (s, 1H), 8.22 (d, J = 11.9 Hz, 1H), 8.07 (s, 1H), 7.68 – 7.66 (m, 2H), 7.52 – 7.48 (m, 5H), 7.10 (s, 1H), 5.90 (d, J = 11.8 Hz, 1H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 146.6, 136.1, 134.4, 129.5, 128.6, 128.3, 127.5, 125.4, 118.6, 117.4, 68.3. HRMS (ESI) m/z (M+H): 374.0036, found: 374.0043.

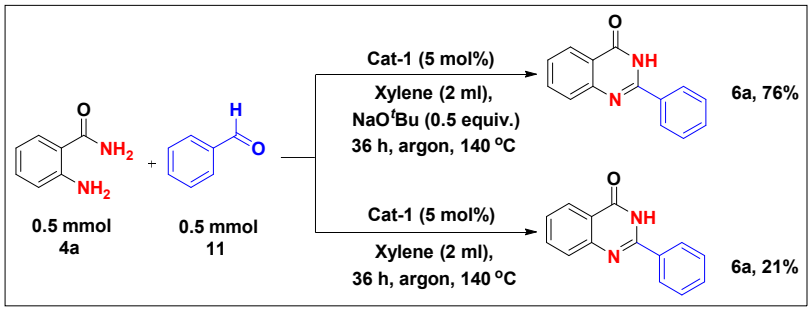
10. Mechanistic investigation:

10.1. Manganese catalyzed dehydrogenation of alcohol:

To an oven-dried 10 ml round bottomed flask, Cat-**1** (5 mol%), benzyl alcohol (1.0 mmol), NaO^{t}Bu (0.5 mmol) and xylene (2 ml) were added under argon. The reaction mixture was kept for refluxing in a preheated oil bath at 140 °C for 36 h. Then, the reaction mixture was subjected to cool, submitted and analysed by ^{1}H-NMR confirming that 16% of benzaldehyde **11** was detected.

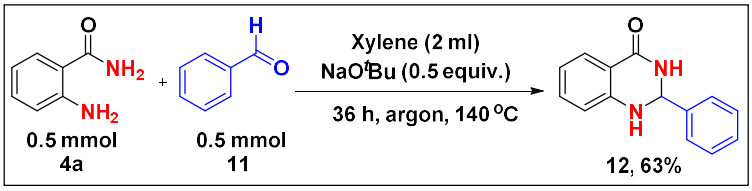


10.2. Manganese catalyzed synthesis of Quinazolin-4(3H)-one (6a) from 2-aminobenzamide (4a) and benzaldehyde (11):



To an oven-dried 10 ml round bottomed flask, 2-aminobenzamide **4a** (0.5 mmol), benzaldehyde **11** (0.5 mmol), Cat-**1** (5 mol%), NaO^{t}Bu (0.25 mmol) and xylene (2 ml) were added under argon atmosphere. The reaction vessel was then placed in a preheated oil bath at 140 °C for refluxing. After 36 h, the crude reaction mixture was diluted by ethyl acetate, methanol and filter through celite. The filtrate was concentrated under vacuum and resultant residue was purified by column chromatography using 100-200 mesh size silica employing 20% ethyl acetate in hexane as an eluent. The 76% of the desired product (**6a**) was isolated under standard reaction conditions. Whereas, only 21% of the product (**6a**) was formed in the absence of base NaO^{t}Bu.

10.3. Synthesis of the intermediate 2-phenyl-2,3-dihydroquinazolin-4(1H)-one (12)[2] from 2-aminobenzamide (4a) and benzaldehyde (11):



2-aminobenzamide **4a** (0.5 mmol), benzaldehyde **11** (0.5 mmol), NaO^{t}Bu (0.25 mmol) and xylene (2 ml) were added under argon atmosphere in an oven-dried 10 ml round bottomed flask. The reaction vessel was placed in a preheated oil bath at 140 °C for 36 h. Afterwards, the crude reaction mixture was subjected to cool to room temperature, diluted by ethyl acetate, methanol and filter through celite. Then, the filtrate was concentrated under vacuum and resultant residue was purified by column chromatography using 100-200 mesh silica employing 25% ethyl acetate in hexane as an eluent. It was found that 63% of the intermediate product **12** was isolated in absence of Mn-catalyst. White solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.26 (s, 1H), 7.64 (d, J = 7.8 Hz, 1H), 7.51 (d, J = 7.2 Hz, 1H), 7.38 (dt, J = 15.4, 7.0 Hz, 2H), 7.25 (t, J = 6.8 Hz, 1H), 7.09 (s, 1H), 6.77 (d, J = 8.2 Hz, 1H), 6.68 (t, J = 7.4 Hz, 1H), 5.77 (s, 1H). ^{13}C NMR (125 MHz, DMSO-d_6): δ 163.5, 147.8, 141.6, 133.2, 128.3, 128.2, 127.3, 126.8, 117.1, 114.9, 114.4, 66.5.

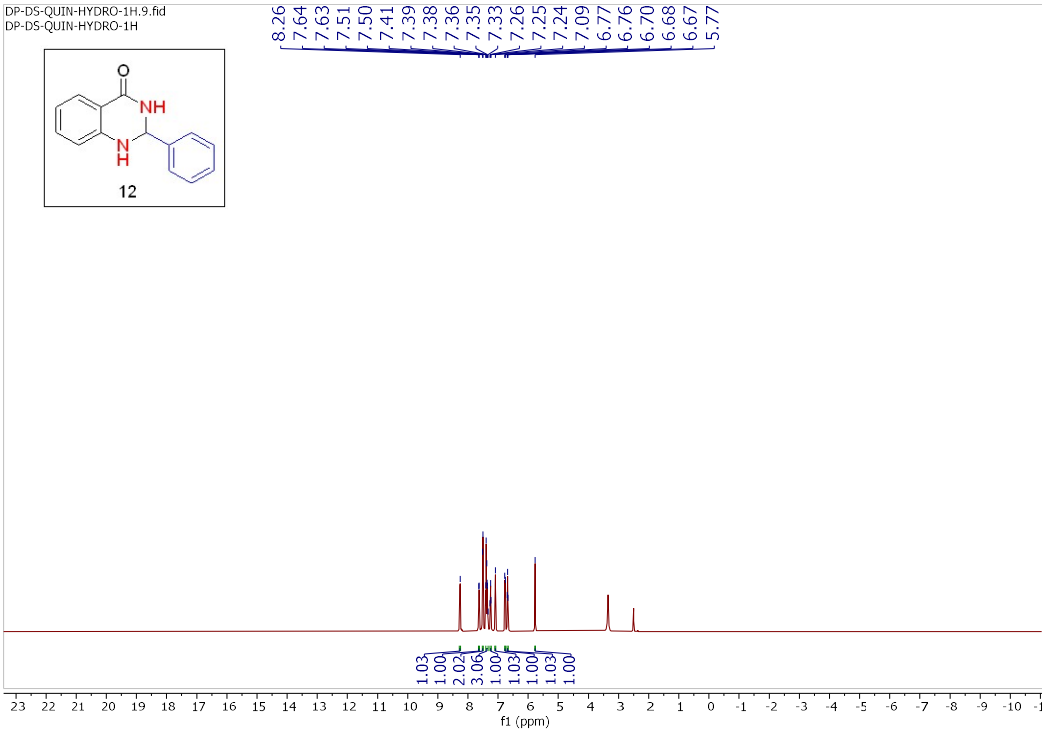


Figure S1. ^{1}H NMR Spectrum of 2-phenyl-2, 3-dihydroquinazolin-4(1H)-one **(12)** in DMSO-d_6.

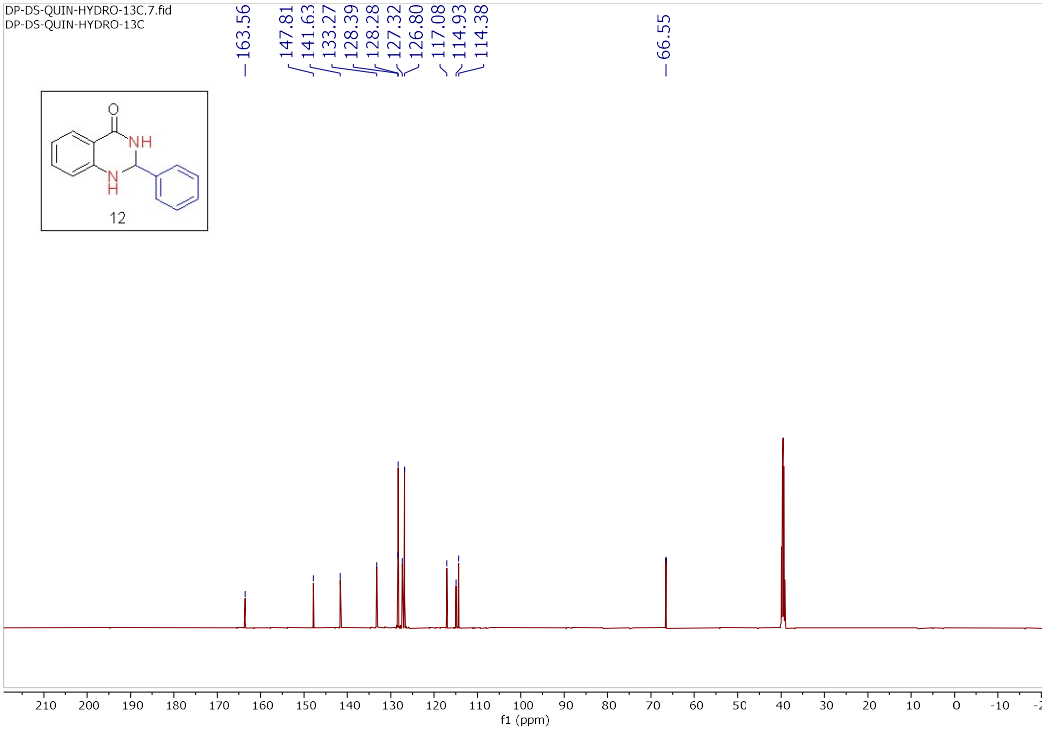
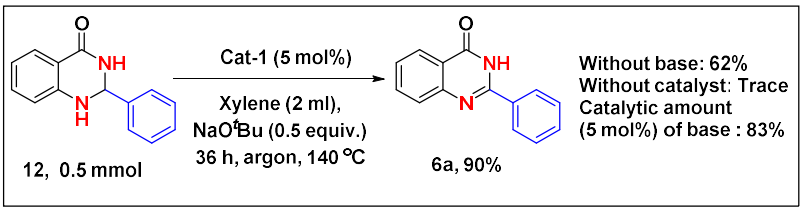


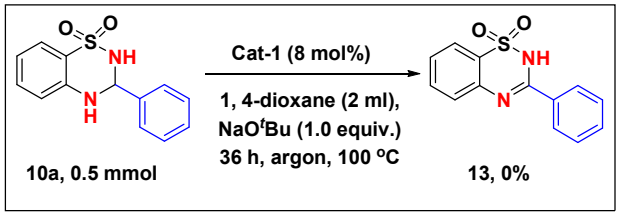
Figure S2. ^{13}C NMR Spectrum of 2-phenyl-2, 3-dihydroquinazolin-4(1H)-one **(12)** in DMSO-d_6.

10.4. Manganese catalyzed dehydrogenation of intermediate 2-phenyl-2, 3-dihydroquinazolin-4(1H)-one (12) to product Quinazolin-4(3H)-one (6a):



To an oven-dried 10 ml round bottomed flask, the intermediate 2-phenyl-2, 3-dihydroquinazolin-4(1H)-one **12** (0.5 mmol), Cat-**1** (5 mol%), NaO^{t}Bu (0.25 mmol) and xylene (2 ml) were taken under argon atmosphere. The reaction vessel was then placed in a preheated oil bath at 140 °C for refluxing. After 36 h, the crude reaction mixture was diluted by ethyl acetate, methanol and filter through celite. The filtrate was concentrated under vacuum, taking an aliquot amount to perform gas chromatography, which showed full conversion and furthermore, resultant residue was purified by column chromatography using 100-200 mesh size silica employing 20% ethyl acetate in hexane as an eluent to get 90% yield of the desired product **6a**. 62% of the product **6a** was formed in absence of base NaO^{t}Bu whilst trace amount of the product detected in absence of catalyst. Albeit, 83% of desired product was isolated in presence of catalytic *i.e.* 5 mol% of base loading instead of 50 mol% of base.

10.5. Manganese catalyzed dehydrogenation of 3-phenyl-3, 4-dihydro-2H-1, 2, 4 benzothiadiazine 1, 1-dioxide (10a) to 3-phenyl-2H-1, 2, 4 benzothiadiazine 1, 1-dioxide (13):



To an oven-dried 10 ml round bottomed flask, 3-phenyl-3, 4-dihydro-2H-1, 2, 4 benzothiadiazine 1, 1-dioxide **10a** (0.5 mmol), Cat-**1** (8 mol%), NaO^{t}Bu (0.5 mmol) and 1, 4-dioxane (2 ml) were taken under argon atmosphere. The reaction vessel was placed in a preheated oil bath at 100 °C for refluxing. After 36 h, the crude reaction mixture was diluted by ethyl acetate, methanol and filter through celite. Then, the filtrate was concentrated under vacuum and subjected to do ^{1}H NMR, upon analysis, which indicates that the reaction was failed to deliver the formation of dehydrogenated product 3-phenyl-2H-1, 2, 4 benzothiadiazine 1, 1-dioxide **13**.

10.6. Preparation of deuterated alcohol:

Deuterated benzyl alcohol was prepared according to previously reported literature method.[23] Initially, Benzyl alcohol (10 mmol), Ru-MACHO (0.020 mmol), KO^{t}Bu (0.06 mmol) were charged in a 60 ml seal tube. The degas D_2O (10 ml) was added using syringe and reaction mixture purged with argon and tube is sealed with cap and heated at 60 °C in an oil bath. The reaction was stopped after 4 h and reaction mixture is extracted with dichloromethane .The removal of solvent under reduced pressure provided pure products for further reaction. The ^{1}H-NMR data reveals that 95% deuterium incorporation occur in benzyl alcohol.

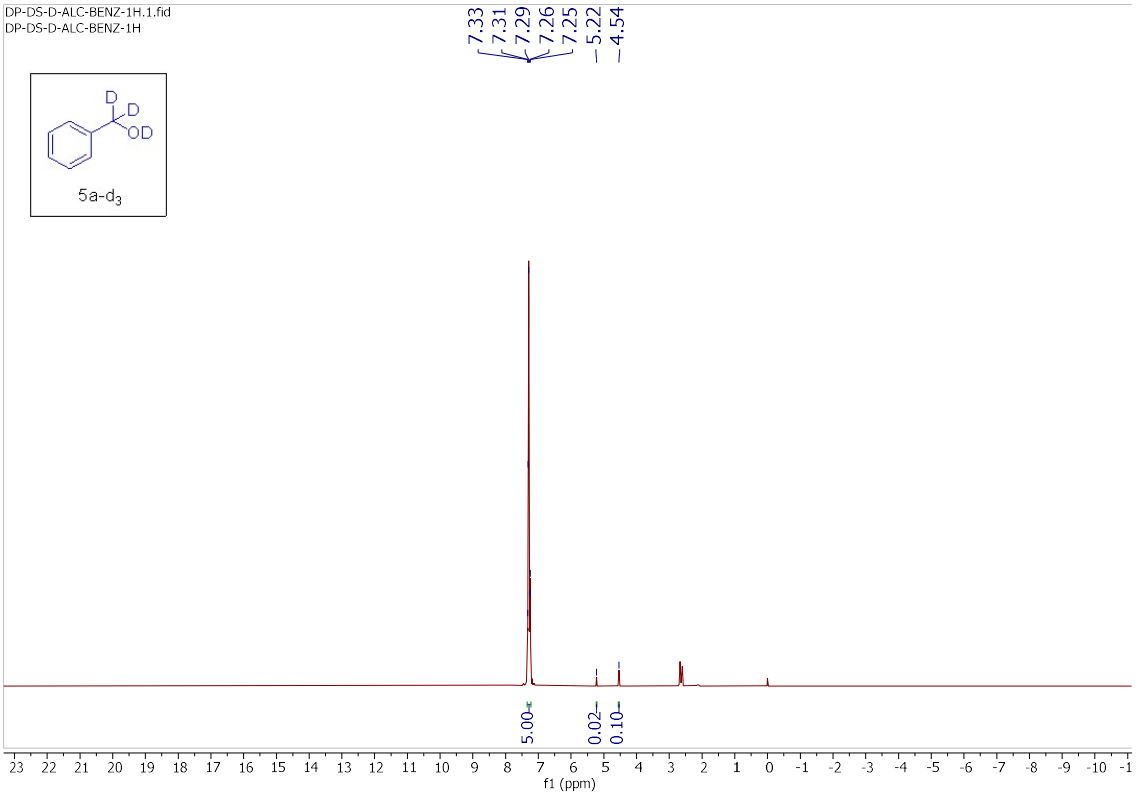
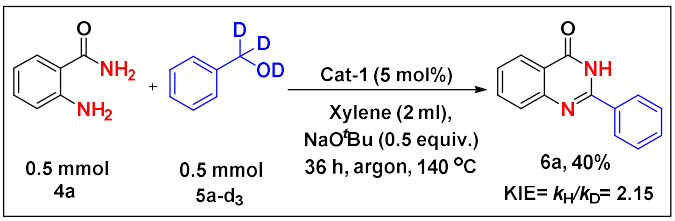


Figure S3. ^{1}H NMR Spectrum of phenylmethan-d$_2$-ol-d **(5a-d$_3$)** in $CDCl_3$.

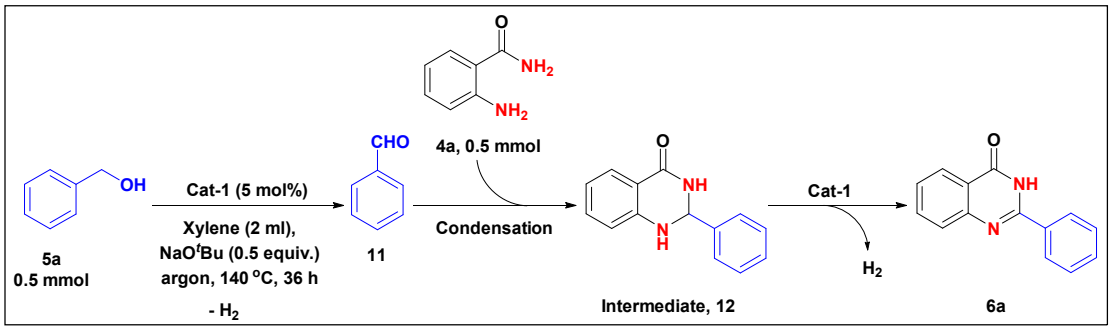
10.7. Determination of the kinetic isotope effect:



In an oven dried 10 ml round bottomed flask 2-aminobenzamide **4a** (0.5 mmol), deuterated benzyl alcohol **5a-d$_3$** (0.5 mmol), Cat-**1** (5 mol%), NaO^{t}Bu (0.25 mmol) were taken and then 2 ml xylene was added under argon atmosphere. The resulting mixture was placed in an oil bath at 140 °C for 36 h. After completion of the reaction, it was cooled to room temperature and ethyl acetate, methanol were poured into the reaction mixture to make it dilute and filtered through celite. The filtrate was concentrated under vacuum and the residue was purified by column chromatography over silica gel (100–200 mesh) employing 20% ethyl acetate/hexane as an eluent obtaining 40% of the desired product **6a**. When the same reaction was performed employing benzyl alcohol **5a** as a coupling partner under the similar reaction conditions 86% of **6a** was isolated which reveals that the value of KIE= k_H/k_D= 2.15.

11. Determination of hydrogen gas formation:

11.1. Hydrogen gas quantification- A volumetric quantitative analysis:



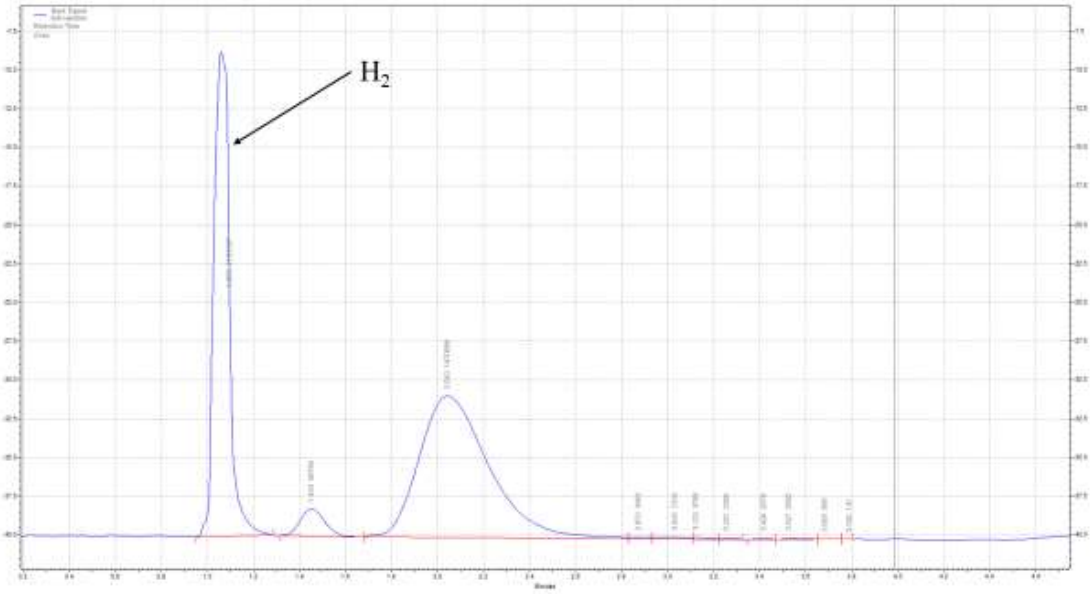
The volumetric quantification of hydrogen gas was accomplished according to the previously reported literature methods.[24] To an oven dried 10 ml round bottomed flask, 2-aminobenzamide **4a** (0.5 mmol, 1equiv.), benzyl alcohol **5a** (0.5 mmol, 1equiv.), NaO^{t}Bu (0.25 mmol, 50 mol%) and Cat-**1** (0.025 mmol, 5 mol%) were taken under argon atmosphere, after that 2 ml of xylene was added to the reaction mixture and joined with an one neck adapter condenser set up. The adapter was connected to the gas collection apparatus (standard water displacement apparatus, using a graduated cylinder to determine the volume) and the entire system was flushed with argon for 5 minutes and allowed to equilibrate for 5 minutes. The reaction vessel was placed in a preheated oil-bath to the appropriate temperature (140 °C). The reaction was stirred vigorously at a constant temperature until gas evolution ceased. The volume of collected gas was noted. After 36 h, the reaction mixture was removed from preheated oil-bath, subjected to cool at room temperature. It was filtered, purified by silica gel (100-200 mess) column chromatography using 20% ethyl acetate in hexane, analysed by ^{1}H-NMR which conformed that 86% isolated yield of the desired 2-phenylquinazolinone (**6a**) was delivered. The collected volume of gas in that experiment was 21 ml. The experiment was repeated twice to obtain consistent readings and the number of moles of hydrogen was evolved was calculated taking into account the vapor pressure of water at 298K = 23.7695 Torr. Volume of water displaced = 21 ml. Atmospheric Pressure = 758.3124 Torr, R = 62.3635 L Torr K^{-1} mol^{-1}

$nH_2 = [(P_{atm} - P_{water}) \times V] / RT = 0.00083$ moles = 0.83 mmoles

The yield of molecular hydrogen 83%.

11.2. Detection of evolved gas by GC-Thermal Detector (GC-TCD):

To an oven dried Ace pressure tube (100 ml), 2-aminobenzamide **4a** (0.5 mmol, 1equiv.), benzyl alcohol **5a** (0.5 mmol, 1equiv.), NaO^{t}Bu (0.25 mmol, 50 mol%) and Cat-**1** (0.025 mmol, 5 mol%) were taken under argon atmosphere, after that 2 ml of xylene was added to the reaction mixture and placed in a preheated oil-bath at 140 °C for 36 h. Afterwards, the crude reaction mixture was subjected to cool at room temperature and the head gas was collected by a 1 ml gas-tight syringe and analysed by GC-TCD with a Carbon plot capillary column gas chromatography which showed the presence of H_2 gas at retention time 1.097 **(Figure S4)**.

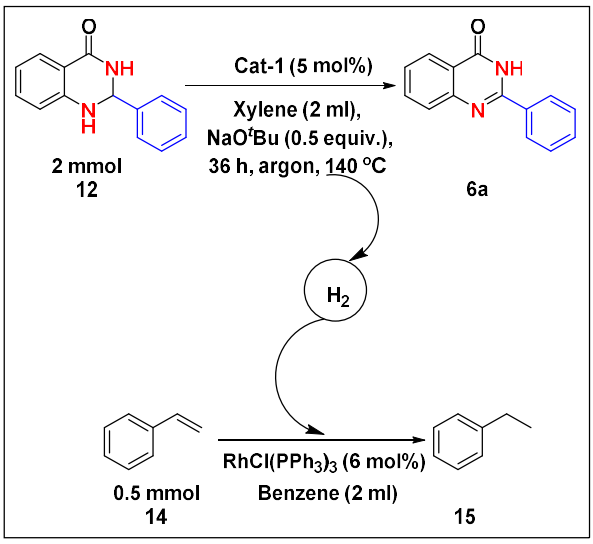


Back Signal
Results

Retention Time	Area	Area %	Height	Height %
1.097	1135597	41.61	119888	57.58
1.453	98789	3.62	13423	6.45
2.043	1470898	53.90	70167	33.70

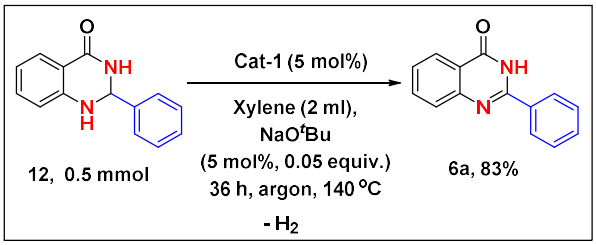
Figure S4. Gas Chromatography Spectrum for evolved gas (TCD mode)

11.3. Detection of hydrogen gas by dual catalysis:



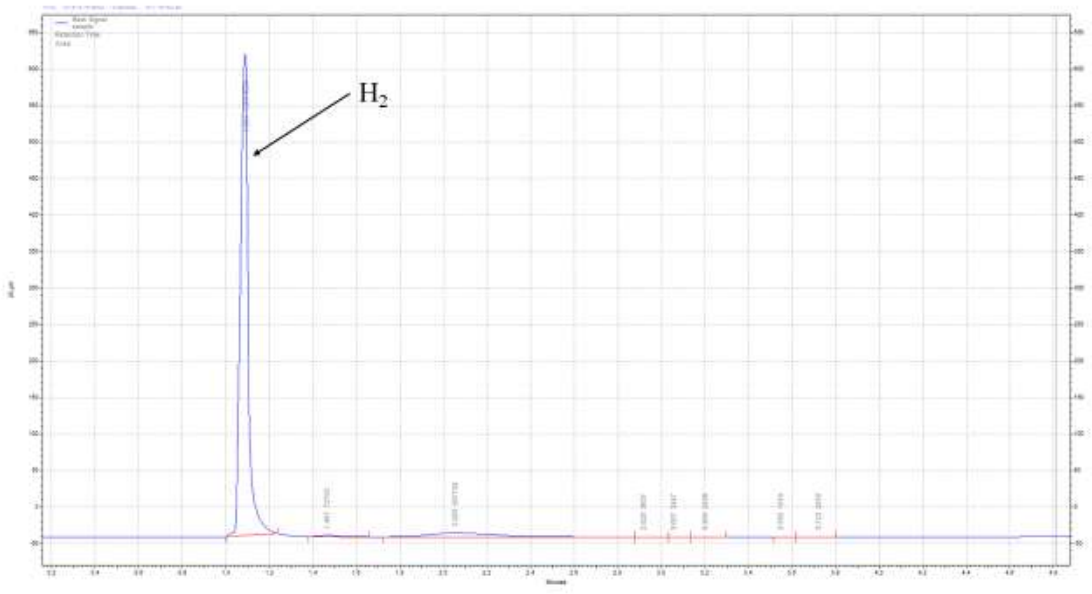
Initially, the intermediate 2-phenyl-2, 3-dihydroquinazolin-4(1H)-one **12** (2 mmol), Cat-**1** (5 mol%) and NaO^{t}Bu (1 mmol, 50 mol%) were taken in an oven dried 10 ml round bottomed flask (**A**). The entire system was degassed, flushed with argon for 5 minutes (three times) and packed with 14 joint rubber septum upon which dry xylene (2 ml) was added. To an another 10 ml round bottomed flask (**B**) Wilkinson's catalyst *i.e.* RhCl(PPh$_3$)$_3$ (6 mol%) catalyst, and styrene **14** (0.5 mmol) were dissolved in benzene (2 ml) and also packed with 14 joint rubber septum. Both the flask (**A** & **B**) were connected through a double headed syringe and allowed to equilibrate for 5 minutes. The mixture in the flask (**A**) was heated at 140 °C (oil-bath temperature), whilst the mixture in the flask (**B**) was stirred at 60 °C (oil-bath temperature).

11.4. Manganese catalyzed dehydrogenation of intermediate 2-phenyl-2, 3-dihydroquinazolin-4(1H)-one (12) to product Quinazolin-4(3H)-one (6a) in presence of catalytic amount (5 mol%) of base:



To an oven dried Ace pressure tube (100 ml), the intermediate 2-phenyl-2, 3-dihydroquinazolin-4(1H)-one **12** (0.5 mmol), Cat-**1** (5 mol%), NaO^{t}Bu (0.025 mmol, 5 mol%) and xylene (2 ml) were taken under argon atmosphere and the pressure tube was then placed in a preheated oil bath at 140 °C for 36 h.

Afterwards, the crude reaction mixture was subjected to cool at room temperature and the head gas was collected by a 1 ml gas-tight syringe and analysed by GC-TCD with a Carbon plot capillary column gas chromatography which showed the presence of H_2 gas at retention time 1.097 **(Figure S5)**.

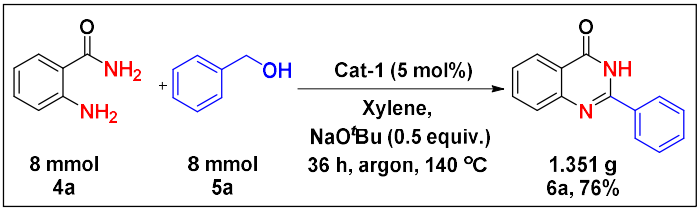


Back Signal
Results

Retention Time	Area	Area %	Height	Height %
1.097	12814534	92.69	4174742	98.59
1.467	72792	0.53	11635	0.27
2.053	907734	6.57	42486	1.00

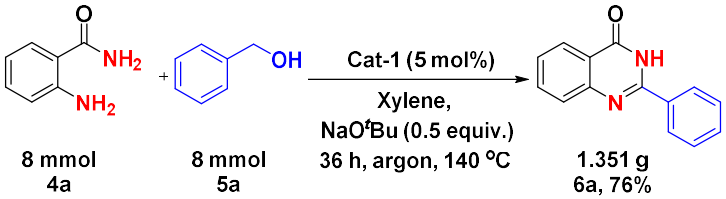
Figure S5. Gas Chromatography Spectrum for evolved gas (TCD mode) for Manganese catalyzed dehydrogenation of intermediate **12** to product **6a** in presence of catalytic amount (5 mol%) of base

12. Gram scale synthesis:



To an oven dried 50 ml round bottomed flask 2-aminobenzamide **4a** (8 mmol), benzyl alcohol **5a** (8 mmol), NaO^{t}Bu (4 mmol, 50 mol%) and Cat-**1** (5 mol%) were taken under argon atmosphere, then xylene was added to the reaction mixture. The resulting mixture was then placed into a preheated oil bath at 140 °C for 36 h. Upon completion, the reaction was cooled to room temperature, ethyl acetate and methanol was added to it to make it dilute and filtered through celite. The filtrate was concentrated under vacuum, the residue was purified by column chromatography over silica gel (100-200 mesh) with hexane/ethyl acetate mixture (20%) as eluent. 76% of the desired product 2-phenyl quinazolin-4(3H)-one **6a** was obtained. Yield 76% (1.351 g).

13. Calculation of green chemistry metrics:



2-aminobenzamide	Benzyl alcohol	2-phenyl quinazolin-4(3H)-one
Chemical formula: $C_7H_8N_2O$	Chemical formula: C_7H_8O	Chemical formula: $C_{14}H_{10}N_2O$
Molecular weight = 136.15	Molecular weight = 108.14	Molecular weight = 222.25
Exact mass = 136. 0637	Exact mass = 108.0575	Exact mass = 222.0793

Total molecular weight of the reactant = (136. 0637+ 108.0575) = 244.1212

Product yield = 76%

Reactant-1	2-aminobenzamide	1.089 g	FW= 136.15
Reactant-2	Benzyl alcohol	0.865 g	FW= 108.14
Base	NaO^{t}Bu	0.384 g	FW= 96.105
Solvent	Xylene	6.943 g	FW= 106.16
Auxiliary	-	-	-
Product	2-phenyl quinazolin-4(3H)-one	1.351 g	FW= 222.25

Total weight = (1.089+0.865+0.384) g = 2.338 g

1. **E factor** = [(2.338–1.351)/1.351] = 0.987/1.351 = 0.731 *i.e.* 0.731 kg waste per 1 kg of product

2. **Atom economy** = [(Molecular mass of desired product/ Molecular masses of reactants) × 100%]

= [{222.0793/ (136.0637+108.0575)} × 100%]

= [{222.0793/ 244.1212} × 100%] = 91%

3. **Atom efficiency** = [Percentage yield × (Atom economy/ 100)]

= [76 × (91/ 100] = 69.16%

4. **Carbon efficiency** = [(Number of carbon atoms in desire product/ Number of carbon atoms in reactants) × 100%]

Here, number of carbon atoms in desire product = 14 and total number of carbon atoms in reactants = (7+7) = 14

Therefore, **carbon efficiency** = [(14/14) × 100] = 100%

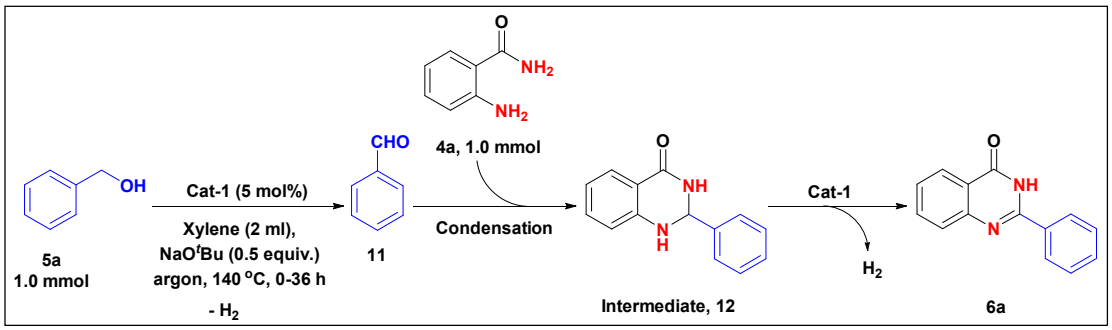
5. **Reaction mass efficiency** = [(Actual mass of desired product/ Actual mass of reactants) × 100%]

= [{1.351/ (1.089+0.865)} × 100]

= [(1.351/1.954) × 100] = 69.14%

14. Kinetic experiments:

14.1. Monitoring the kinetics of the reaction:



Experimental procedure: To an oven dried 10 ml 2-neck round bottomed flask, 2-aminobenzamide **4a** (1.0 mmol, 1equiv.), benzyl alcohol **5a** (1.0 mmol, 1equiv.), NaO^{t}Bu (0.5 mmol, 50 mol%) and Cat-**1** (0.05 mmol, 5 mol%), mesitylene (1.0 mmol, 1 equiv.) as an internal standard and xylene as a solvent were added under argon to make up the total volume of the reaction mixture 2 ml. Afterwards, the reaction mixture was kept in a preheated oil bath for stirring at 140 °C. At regular intervals (1 h, 2 h, 3 h, 4 h, 8 h, 12 h, 16 h, 20 h, 24 h, 28 h, 32 h, 36 h) the reaction mixture was cooled to ambient temperature and an aliquot of mixture was taken in a GC vial. The GC sample was diluted with methanol and subjected to gas chromatographic analysis. The concentration of the product was determined with respect to mesitylene internal standard. The data was accomplished to draw the concentration of the product (mmol) *vs* time (h) plot **(Figure S6)**.

Time (h)	Concentration of benzyl alcohol **5a** (mmol)	Concentration of benzaldehyde **11** (mmol)	Concentration of 2-Aminobenzamide **4a** (mmol)	Concentration of intermediate **12** (mmol)	Concentration of product **6a** (mmol)
0	1	0	1	0	0
1	0.931	0.037	0.93	0.044	0.051
2	0.861	0.038	0.866	0.051	0.101
3	0.785	0.041	0.796	0.054	0.151
4	0.699	0.046	0.739	0.06	0.2
8	0.618	0.048	0.62	0.07	0.28
12	0.54	0.05	0.539	0.042	0.36
16	0.438	0.045	0.44	0.024	0.48
20	0.381	0.04	0.4	0.015	0.6
24	0.261	0.032	0.28	0.009	0.72
28	0.201	0.028	0.22	0.007	0.781
32	0.141	0.021	0.159	0.002	0.841
36	0.06	0.021	0.08	0.001	0.921

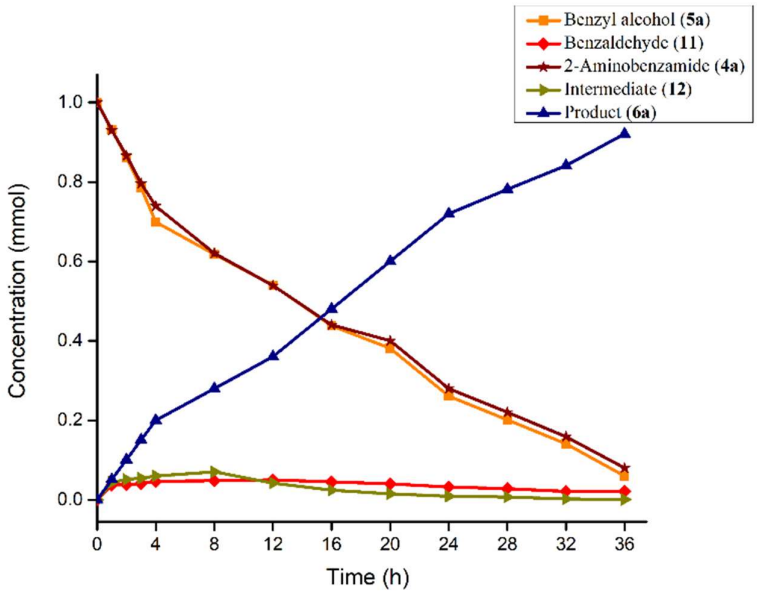
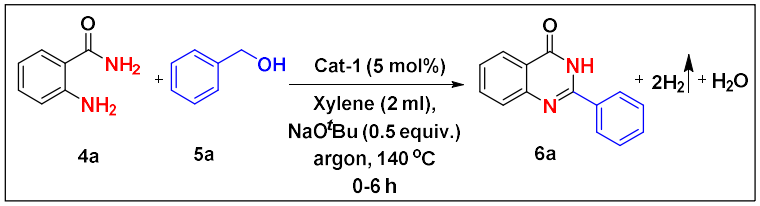


Figure S6. Kinetic monitoring of Manganese (I)-catalyzed acceptorless dehydrogenative coupling (ADC) of 2-aminobenzamide **4a** with benzyl alcohol **5a** towards the synthesis of 2-phenyl quinazolin-4(3H)-one **6a**.

14.2. Rate order determination:

The initial rate method was used to determine the rate order of the 2-phenyl quinazolin-4(3H)-one **6a** synthesis reaction with respect to various components of the reaction. The data of the concentration (mM) *vs* time (h) plot was fitted to linear using origin pro 9. The slope of the linear fitted curve represents the initial rate of the reaction. The order of the reaction was determined by plotting initial rate (mM/h) *vs* concentration (mM) of that particular component.

14.2.1. Rate order determination with respect to benzyl alcohol (5a)



To determine the order of the 2-phenyl quinazolin-4(3H)-one **6a** synthesis reaction, initial rates at different initial concentration of benzyl alcohol **5a** were recorded.

Experimental procedure: To an oven dried 10 ml 2-neck round bottomed flask, 2-aminobenzamide **4a** (0.5 mmol, 1equiv.), NaO^{t}Bu (0.25 mmol, 50 mol%) and Cat-**1** (0.025 mmol, 5 mol%), mesitylene (0.5 mmol, 1 equiv.) as an internal standard, specific amount of benzyl alcohol **5a** and xylene as a solvent were added under argon to make up the total volume of the reaction mixture 2 ml. Afterwards, the reaction mixture was kept in an oil bath of 140 °C for stirring. At regular intervals (1 h, 2 h, 3 h, 4 h, 5 h, 6 h) the reaction mixture was cooled to ambient temperature and an aliquot of mixture was taken in a GC vial. The GC sample was diluted with methanol and subjected to gas chromatographic analysis. The concentration of the product was determined with respect to mesitylene internal standard. The data was accomplished to draw the concentration of the product (mM) *vs* time (h) plot **(Figure S7a)**. The rate of the reaction at different initial concentration of benzyl alcohol **5a** was given below and used to plot the initial rate (mM/h) *vs* concentration of benzyl alcohol **5a** (mM) to determine the order of the reaction with respect to benzyl alcohol **5a (Figure S7b)**.

Time (h)	Concentration of product **6a** formed at initial concentration of benzyl alcohol **5a** 0.2 mM	Concentration of product **6a** formed at initial concentration of benzyl alcohol **5a** 0.25 mM	Concentration of product **6a** formed at initial concentration of benzyl alcohol **5a** 0.3 mM	Concentration of product **6a** formed at initial concentration of benzyl alcohol **5a** 0.35 mM
0	0	0	0	0
1	0.002	0.005	0.011	0.0175
2	0.014	0.02	0.03	0.042
3	0.028	0.0375	0.048	0.063
4	0.038	0.05	0.063	0.084
5	0.05	0.065	0.081	0.1015
6	0.062	0.08	0.102	0.1225

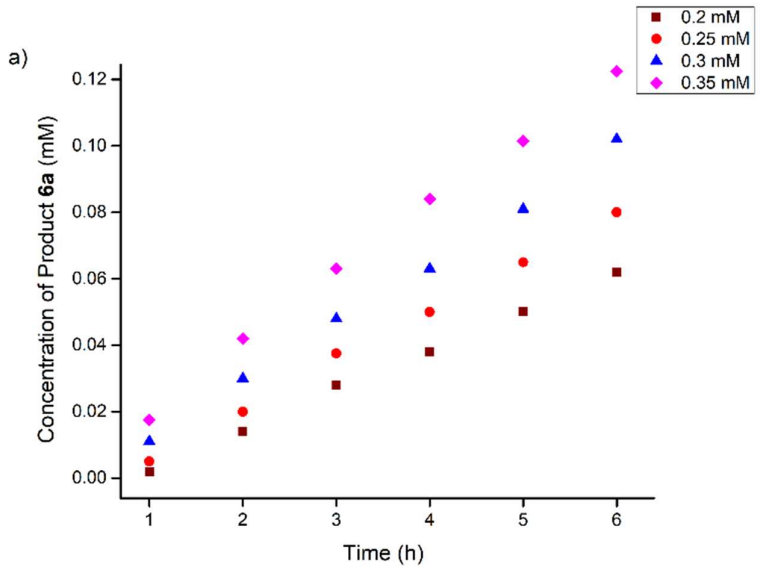


Figure S7a. Concentration versus time plot at various concentration of benzyl alcohol **5a**.

Initial concentration of benzyl alcohol **5a** (mM)	Initial rate of the reaction (mM/h)
0.2	0.01093
0.25	0.01393
0.3	0.01711
0.35	0.02063

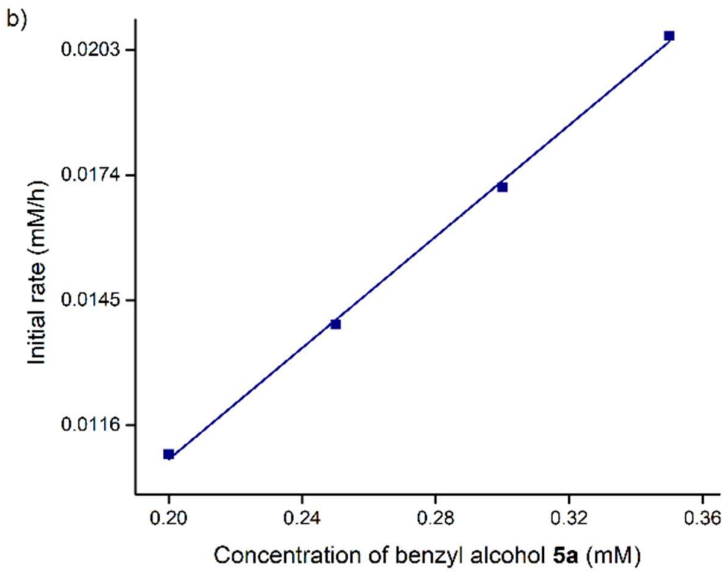


Figure S7b. Plot for determining the order of the reaction with respect to benzyl alcohol **5a**.

For the calculation of order, considering the steady state approximation for benzyl alcohol **5a**,

Slope = $k[5a]^n$ where n = order of the reaction

From 0.2 mM scale reaction, $0.01093 = k[0.2]^n$ ……(1)

From 0.25 mM scale reaction, $0.01393 = k[0.25]^n$ ……(2)

From 0.3 mM scale reaction, $0.01711 = k[0.3]^n$ ……(3)

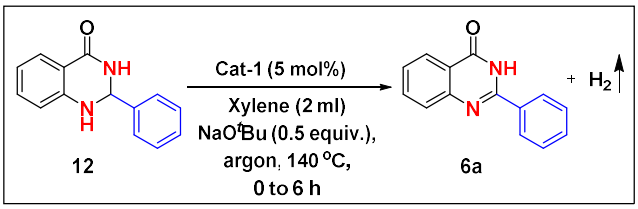
From 0.35 mM scale reaction, $0.02063 = k[0.35]^n$ ……(4)

Herein, for order calculation taking equation (1) and (2),

$$0.01393/0.01093 = [0.25/0.2]^n \Rightarrow 1.2744 = [1.25]^n \Rightarrow \log(1.2744) = n\log(1.25)$$

$\Rightarrow 0.105 = n \times 0.097 \Rightarrow n = 1.09 \approx 1 \Rightarrow$ Rate w.r.t. benzyl alcohol $= k[5a]^1$ and this data is also matched with **Figure S8b.** as the straight line nearly passing through origin. Therefore, the reaction is first order with respect to concentration of benzyl alcohol **5a**.

14.2.2. Rate order determination of third step of the reaction with respect to intermediate 12



Experimental procedure: To an oven dried 10 ml 2-neck round bottomed flask, intermediate **12** (0.2 mmol), NaO^{t}Bu (0.1 mmol, 50 mol%) and Cat-**1** (0.01 mmol, 5 mol%), mesitylene (0.2 mmol, 1 equiv.) as an internal standard and xylene as a solvent were added under argon to make up the total volume of the reaction mixture 2 ml. Afterwards, the reaction mixture was kept in an oil bath of 140 °C for stirring. At regular intervals (1 h, 2 h, 3 h, 4 h, 5 h, 6 h) the reaction mixture was cooled to ambient temperature and an aliquot of mixture was taken in a GC vial. The GC sample was diluted with methanol and subjected to gas chromatographic analysis. The concentration of the consumption of intermediate **12** was determined with respect to mesitylene internal standard. The same analysis was repeated taking 0.3 mmol and 0.4 mmol of the intermediate **12** and with respect to it internal standard, base catalyst were taken. The data was accomplished to draw the concentration of the consumption of intermediate **12** (mM) *vs* time (h) plot **(Figure S8a)**. The rate of the reaction (mM/h) at different initial concentration of intermediate **12** was plotted with respect to concentration of initial concentration of intermediate **12** (mM) to determine the order of the reaction with respect to intermediate **12 (Figure S8b)**.

Time (h)	Concentration of consumption of intermediate **12** when initial concentration 0.1 mM	Concentration of consumption of intermediate **12** when initial concentration 0.15 mM	Concentration of consumption of intermediate **12** when initial concentration 0.2 mM
0	0.1	0.15	0.2
1	0.091	0.137	0.182
2	0.082	0.123	0.164
3	0.074	0.111	0.148
4	0.066	0.099	0.132
5	0.057	0.086	0.114
6	0.048	0.072	0.096

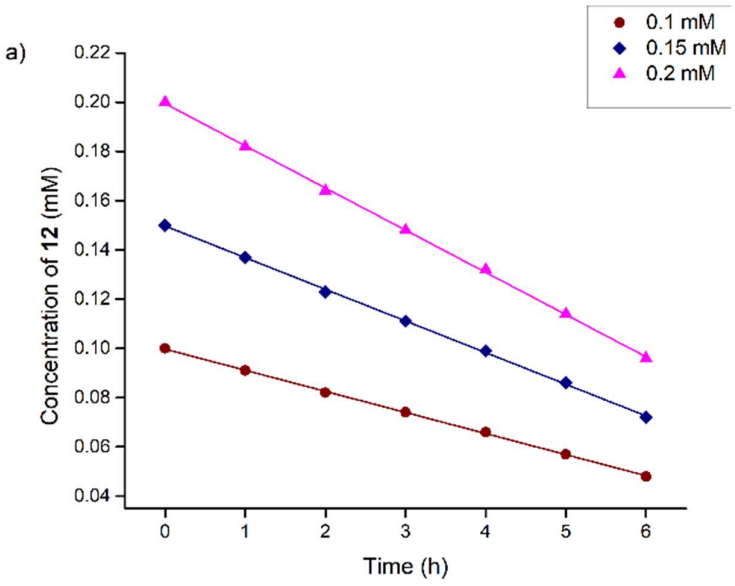


Figure S8a. Concentration versus time plot at various concentration of intermediate **12**

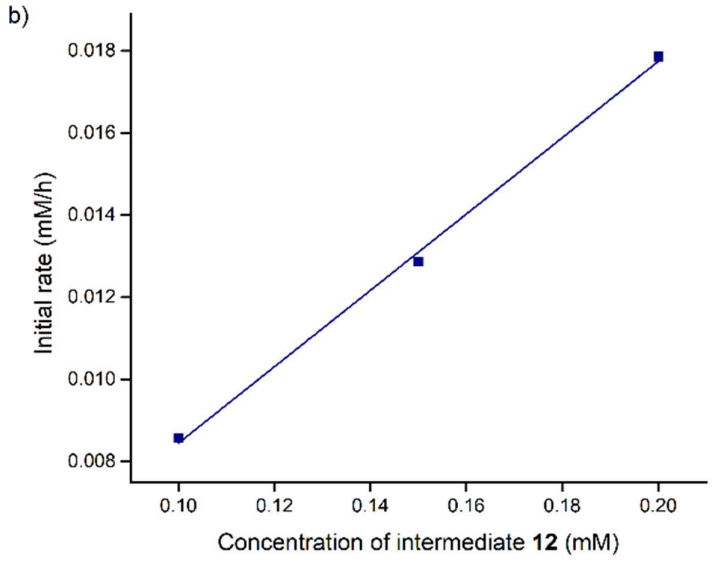


Figure S8b. Plot for determining the order of the reaction with respect to intermediate **12**

When we plotted initial rate of the reaction (mM/h) with respect to concentration of initial concentration of intermediate **12** (mM) we observed that the straight line nearly passing through origin which indicates that the third step of the reaction is first order with respect to concentration of intermediate **12**.

15. Figures reproducing ^{1}H and ^{13}C NMR spectra:

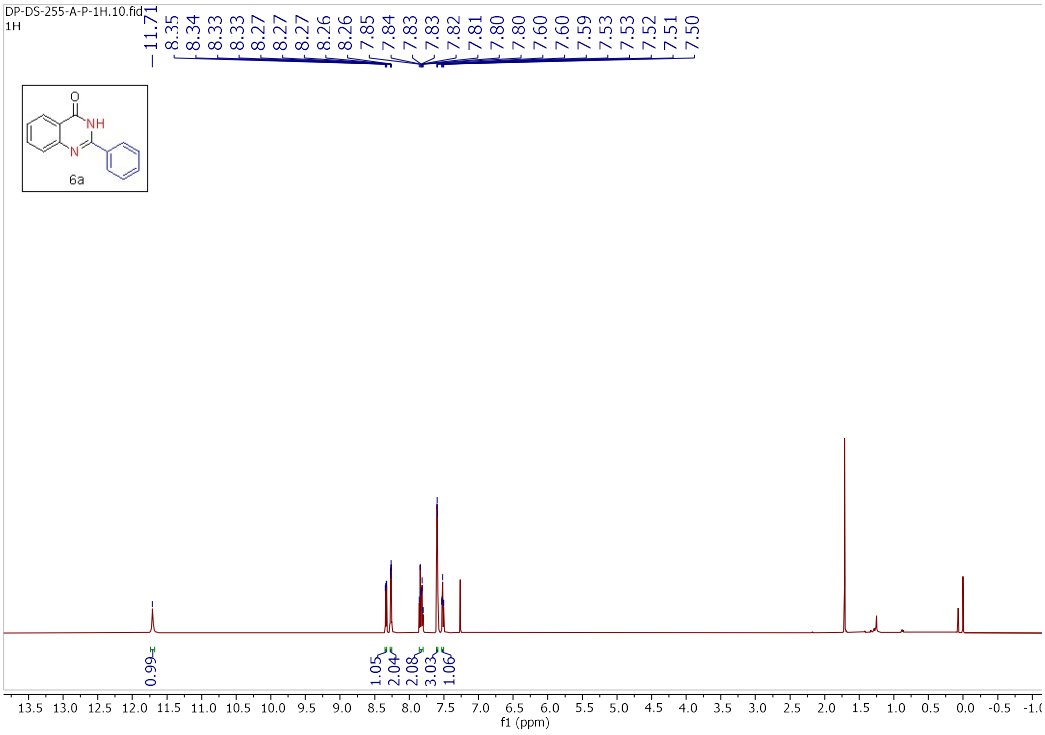


Figure S9. ^{1}H NMR Spectrum of 2-phenylquinazolin-4(3H)-one **(6a)** in $CDCl_3$.

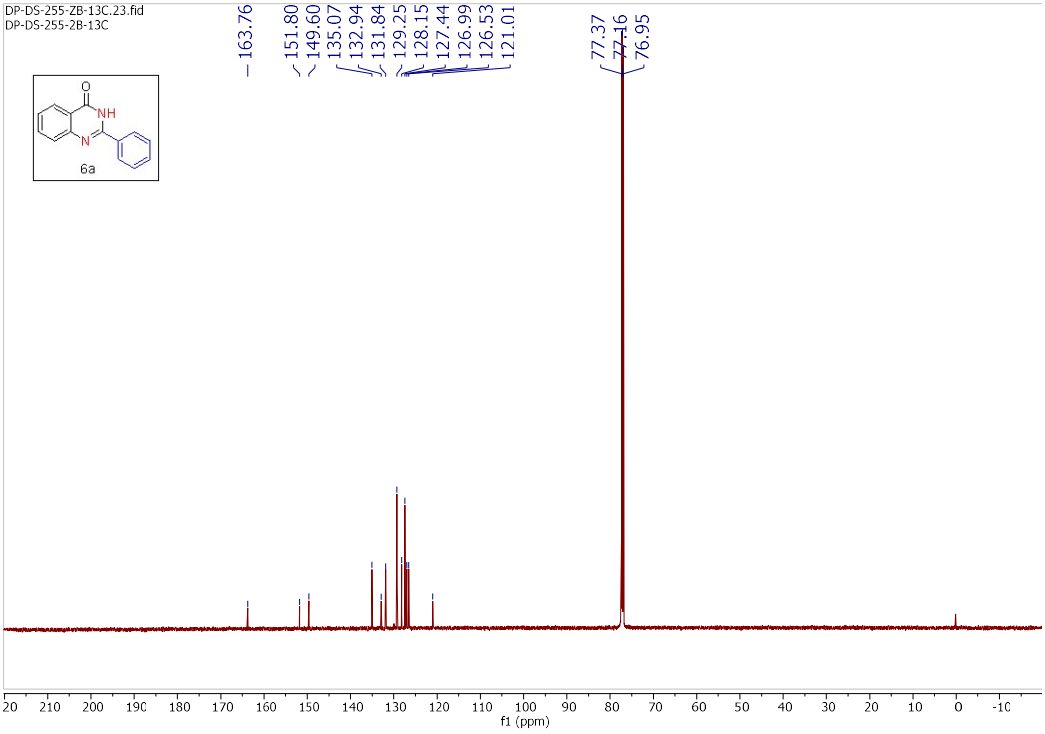


Figure S10. ^{13}C NMR Spectrum of 2-phenylquinazolin-4(3H)-one **(6a)** in $CDCl_3$.

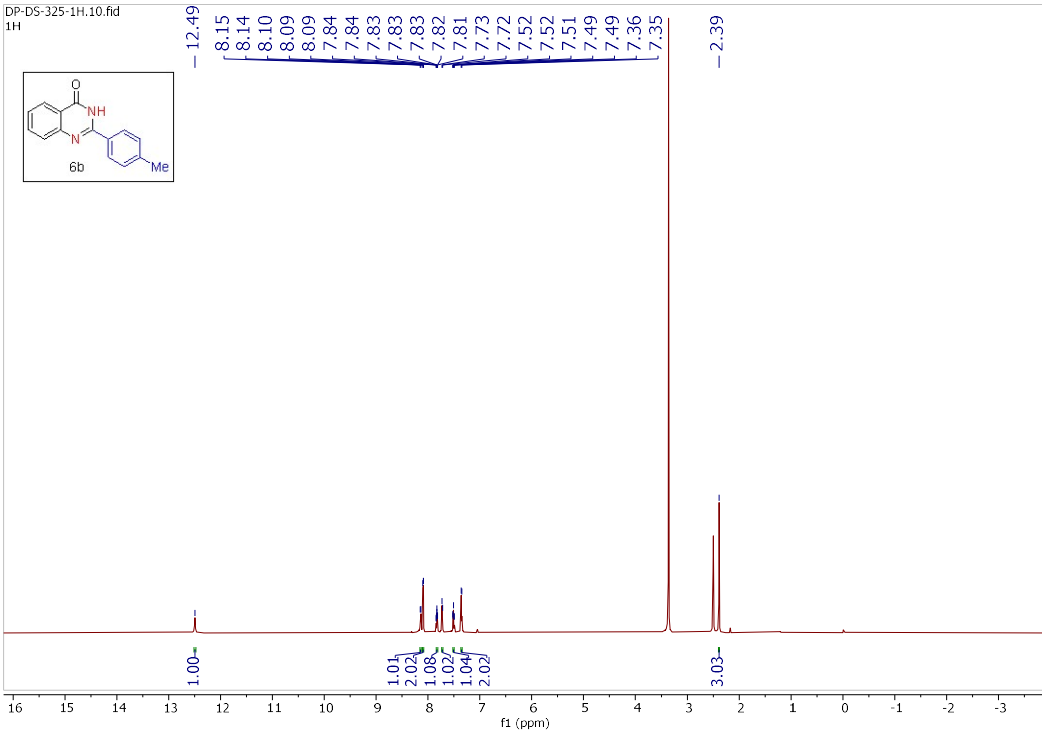


Figure S11. [1]H NMR Spectrum of 2-(p-tolyl)quinazolin-4(3H)-one **(6b)** in DMSO-*d*$_6$.

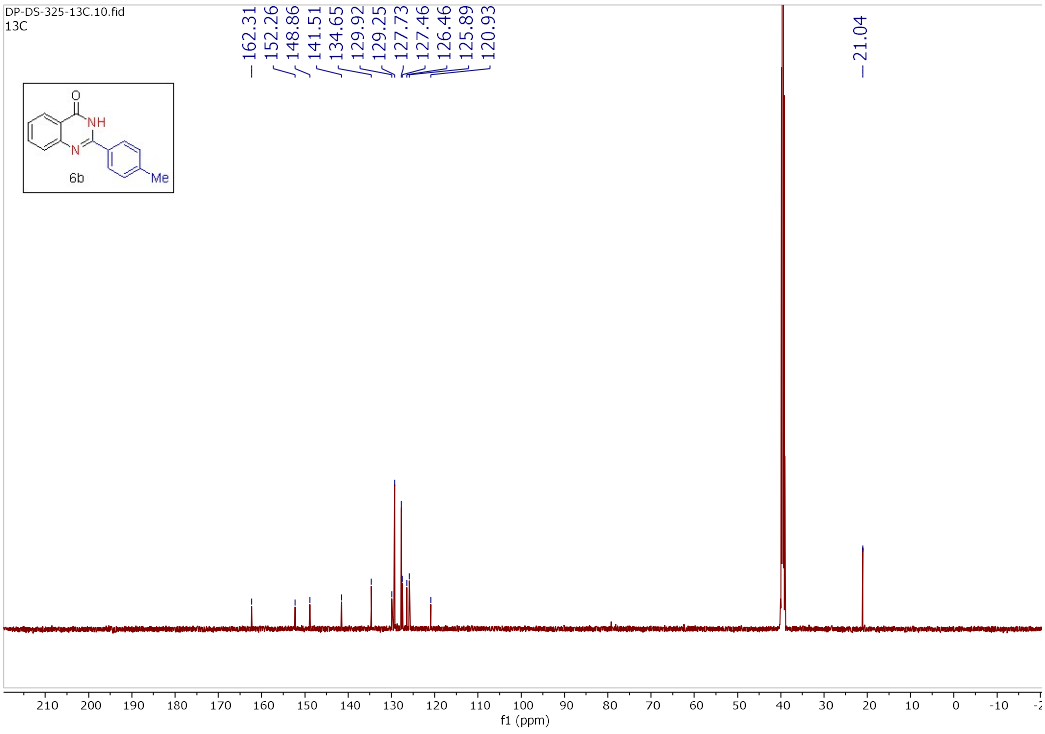


Figure S12. [13]C NMR Spectrum of 2-(p-tolyl)quinazolin-4(3H)-one **(6b)** in DMSO-*d*$_6$.

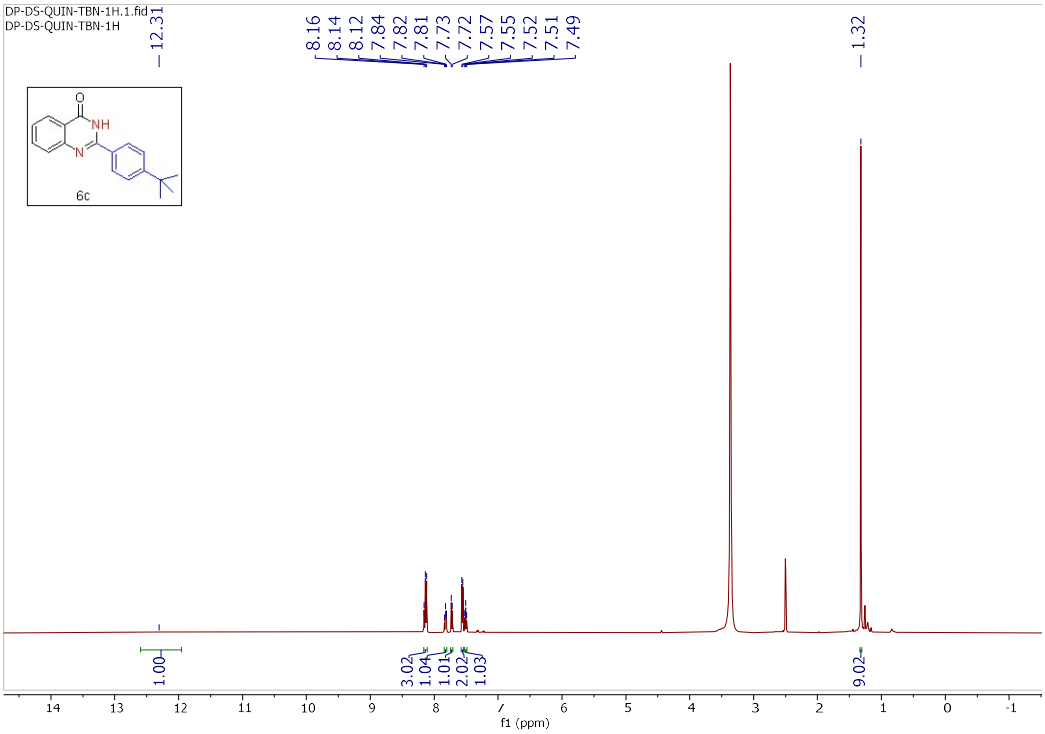


Figure S13. [1]H NMR Spectrum of 2-(4-(tert-butyl)phenyl)quinazolin-4(3H)-one **(6c)** in DMSO-d_6.

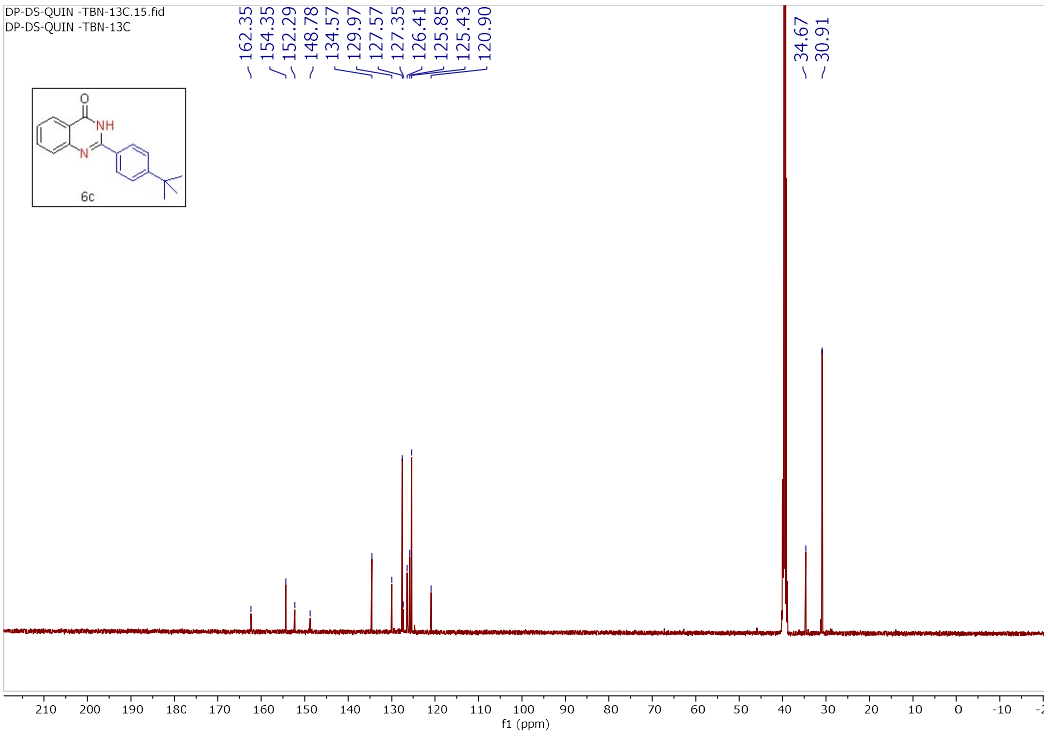


Figure S14. [13]C NMR Spectrum of 2-(4-(tert-butyl)phenyl)quinazolin-4(3H)-one **(6c)** in DMSO-d_6.

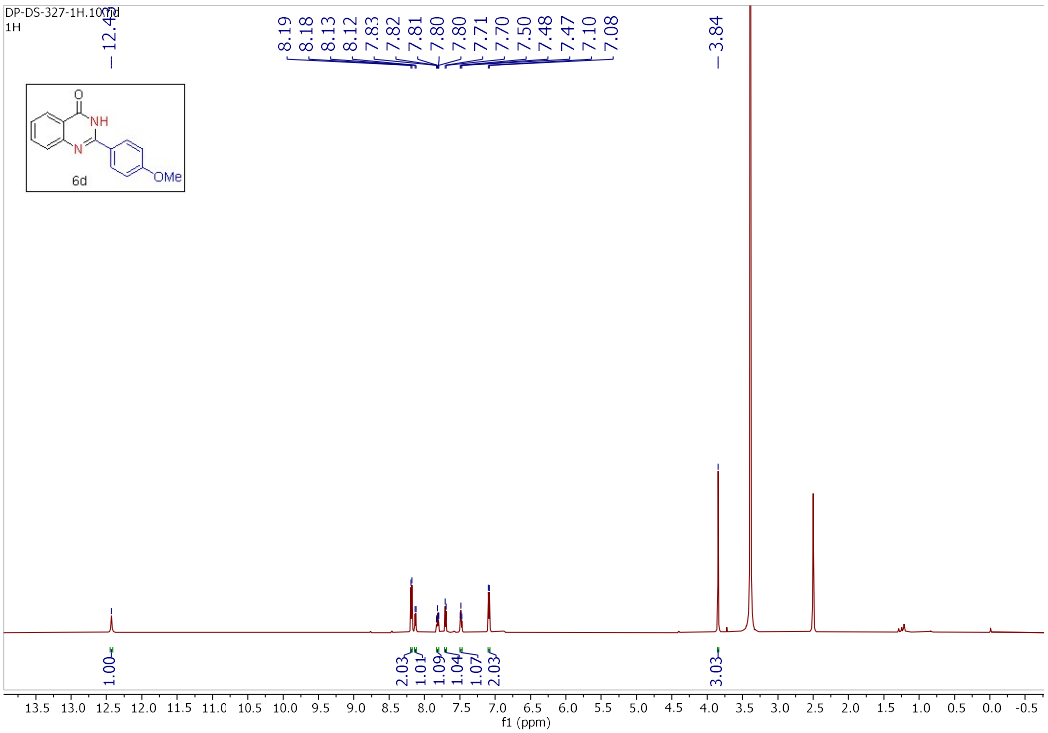


Figure S15. [1]H NMR Spectrum of 2-(4-methoxyphenyl)quinazolin-4(3H)-one **(6d)** in DMSO-d_6.

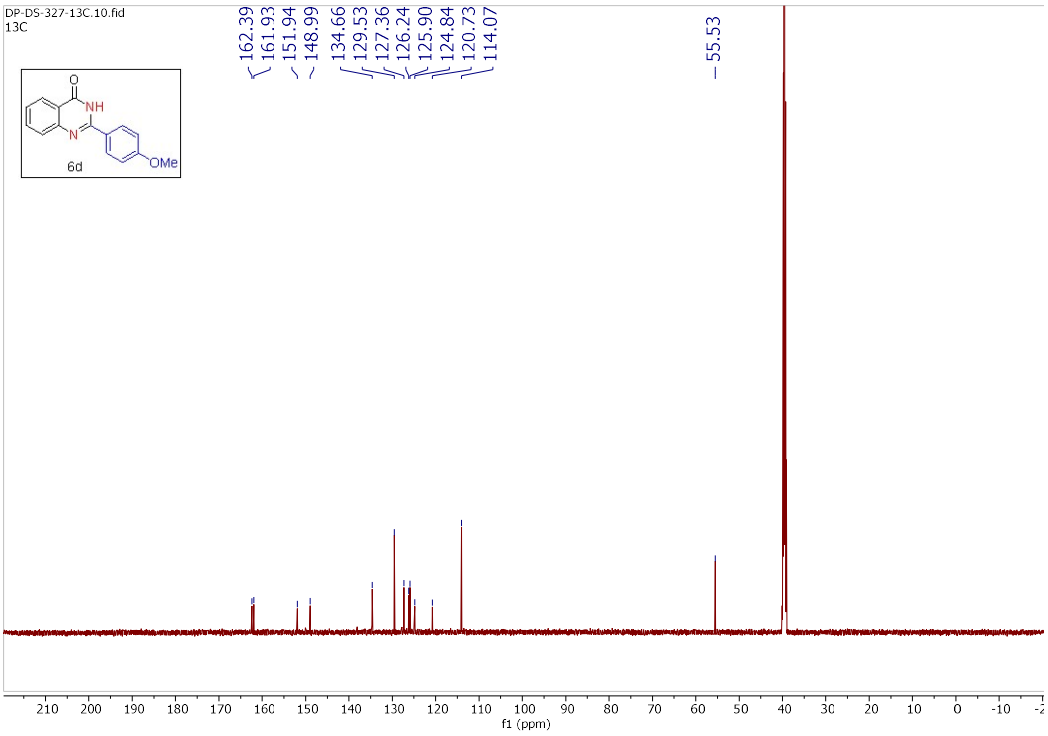


Figure S16. [13]C NMR Spectrum of 2-(4-methoxyphenyl)quinazolin-4(3H)-one **(6d)** in DMSO-d_6.

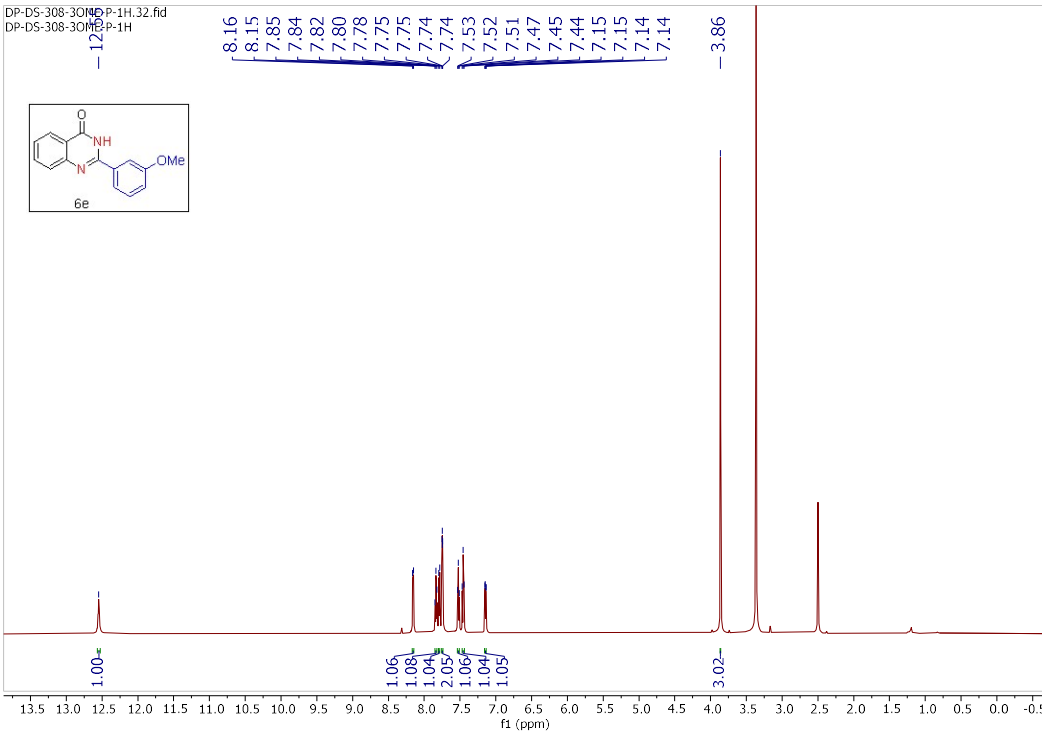


Figure S17. [1]H NMR Spectrum of 2-(3-methoxyphenyl)quinazolin-4(3H)-one **(6e)** in DMSO-d_6.

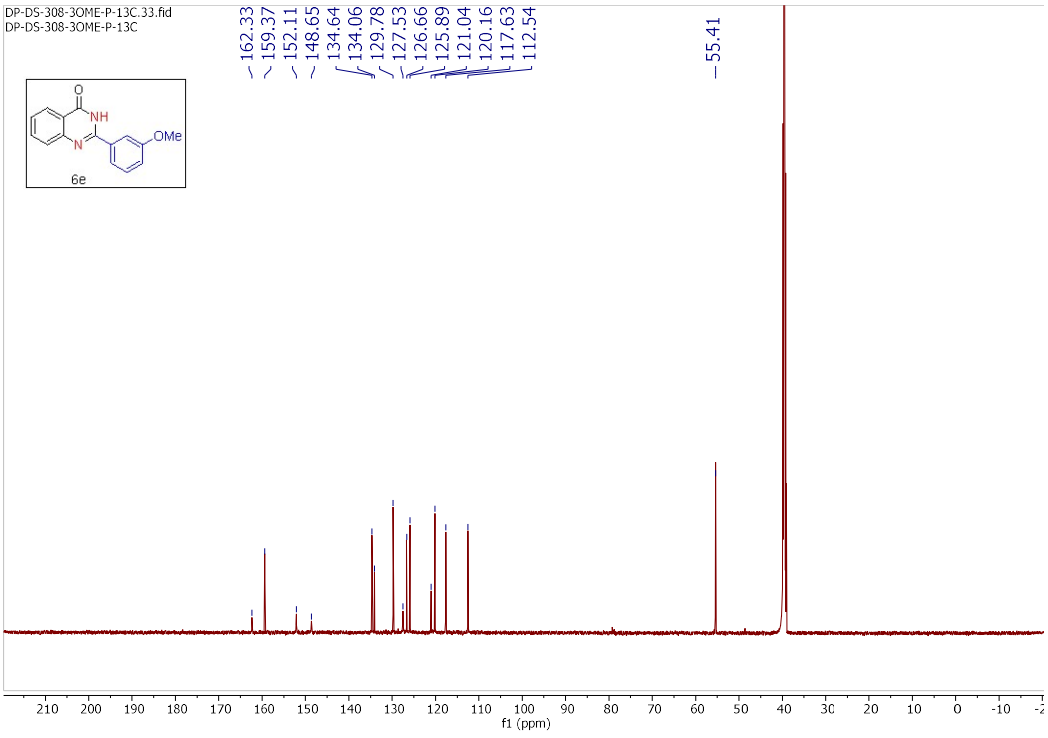


Figure S18. [13]C NMR Spectrum of 2-(3-methoxyphenyl)quinazolin-4(3H)-one **(6e)** in DMSO-d_6.

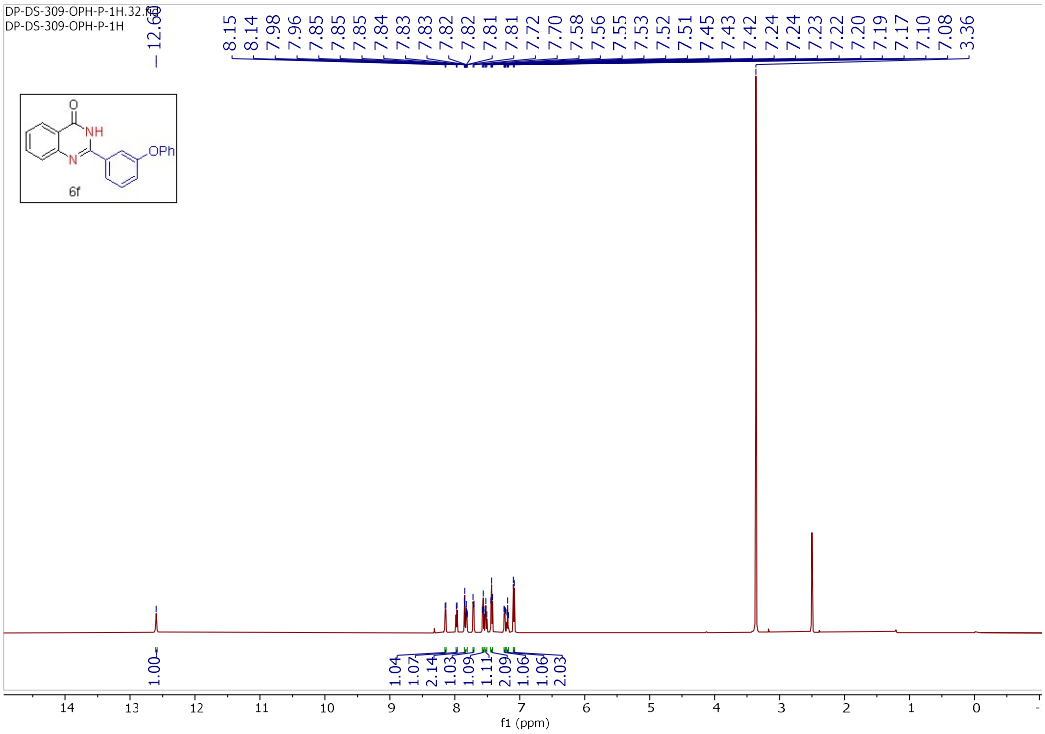


Figure S19. [1]H NMR Spectrum of 2-(3-phenoxyphenyl)quinazolin-4(3H)-one **(6f)** in DMSO-d_6.

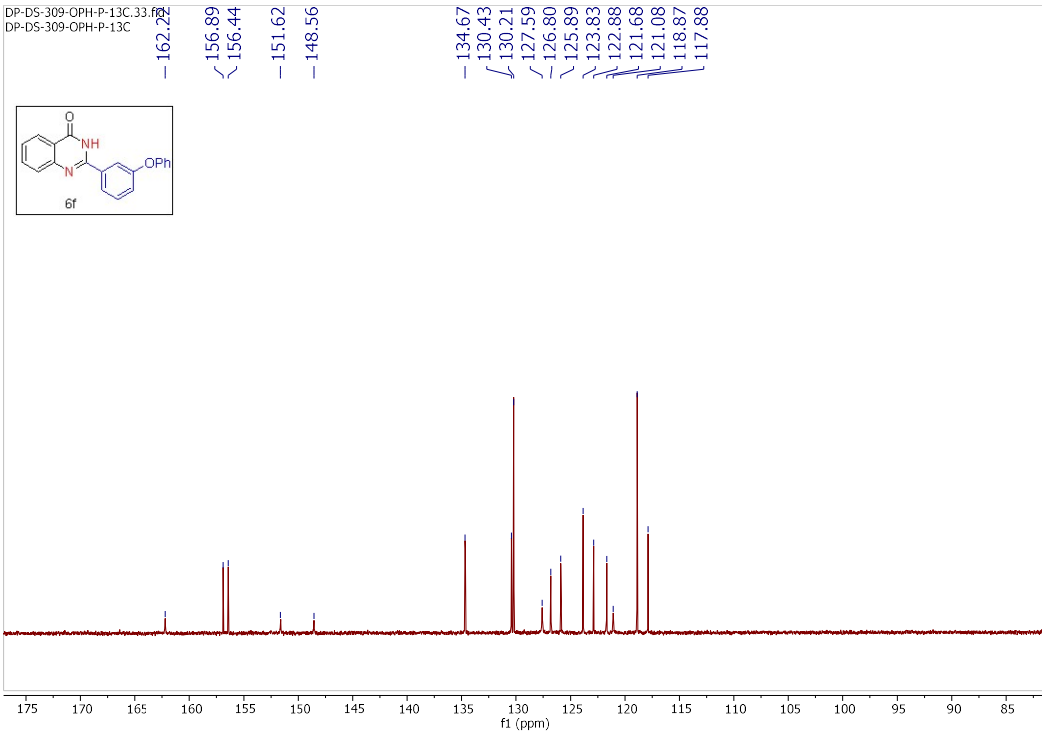


Figure S20. [13]C NMR Spectrum of 2-(3-phenoxyphenyl)quinazolin-4(3H)-one **(6f)** in DMSO-d_6.

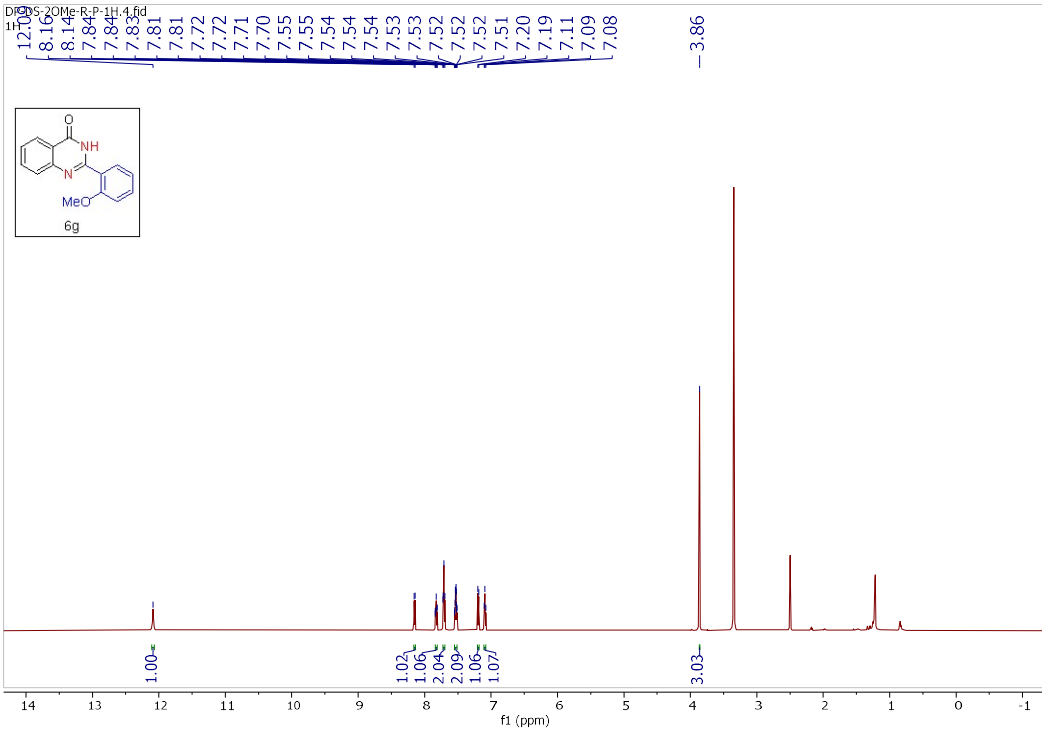


Figure S21. [1]H NMR Spectrum of 2-(2-methoxyphenyl)quinazolin-4(3H)-one **(6g)** in DMSO-d_6.

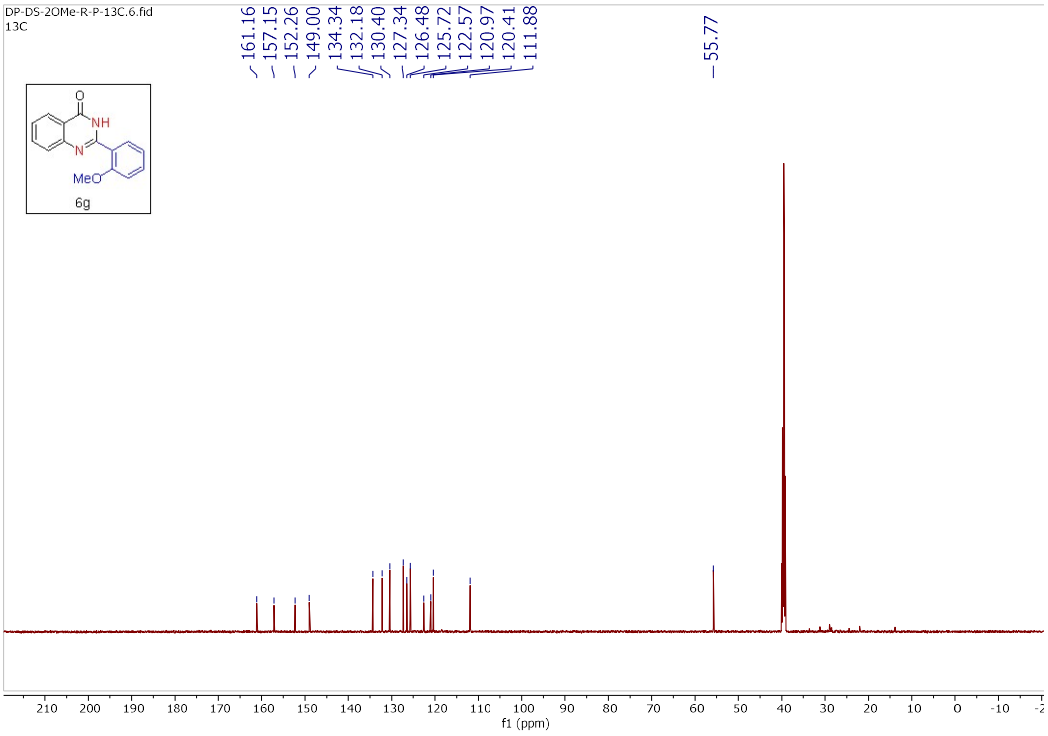


Figure S22. [13]C NMR Spectrum of 2-(2-methoxyphenyl)quinazolin-4(3H)-one **(6g)** in DMSO-d_6.

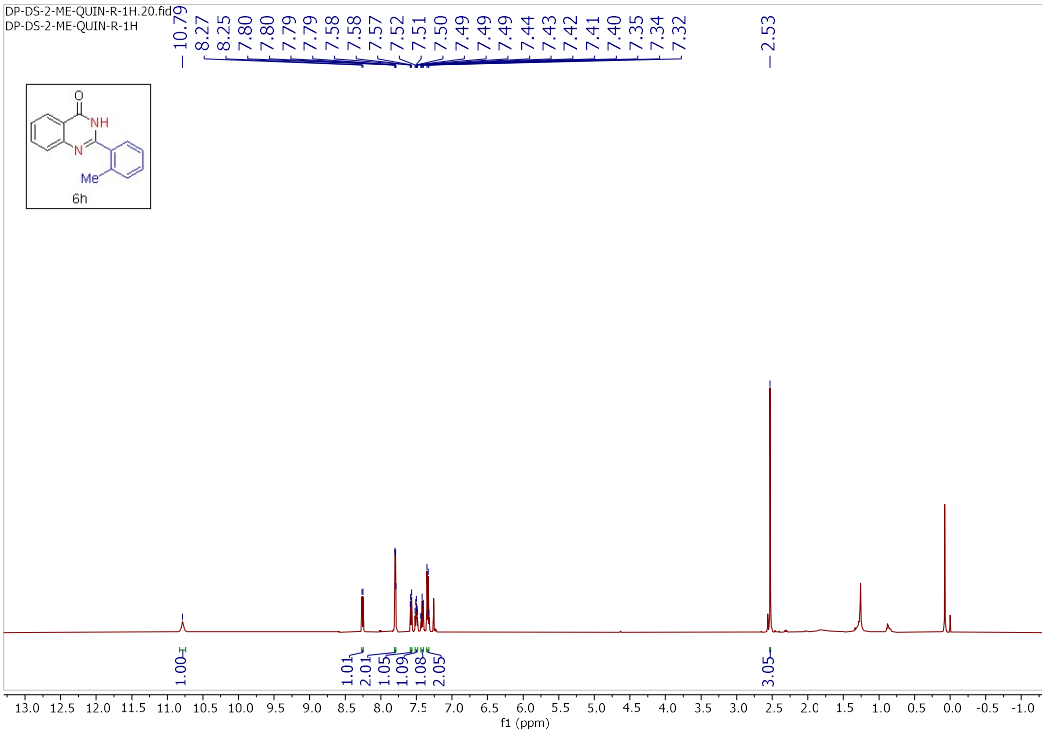


Figure S23. ^{1}H NMR Spectrum of 2-(o-tolyl)quinazolin-4(3H)-one **(6h)** in $CDCl_3$.

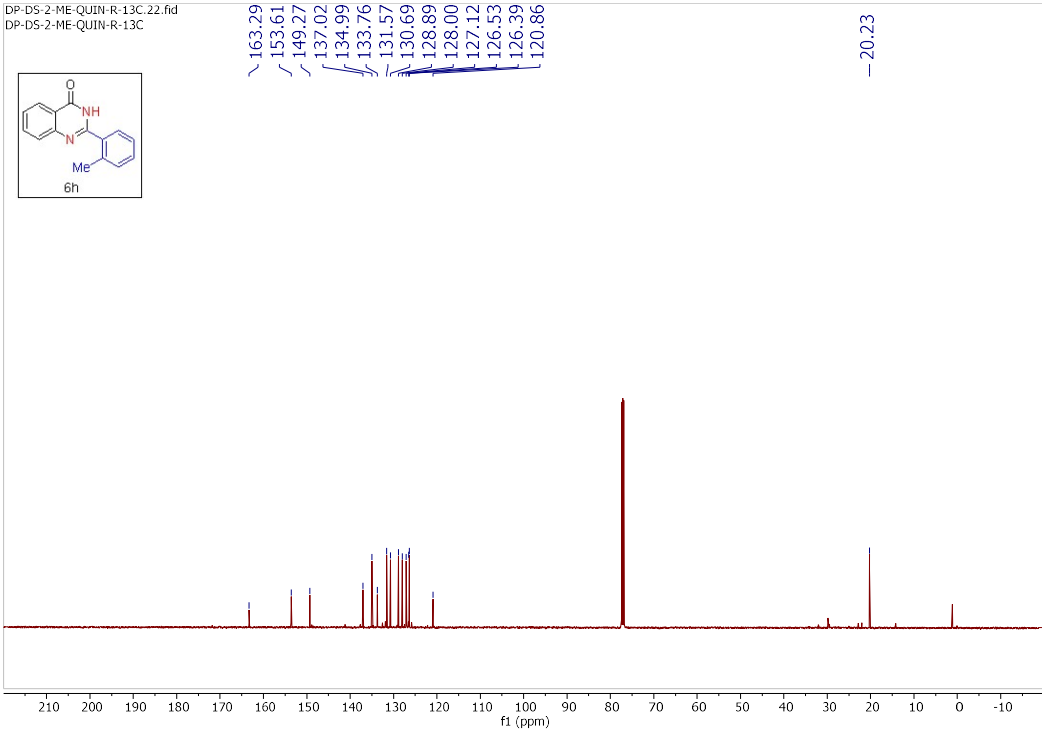


Figure S24. ^{13}C NMR Spectrum of 2-(o-tolyl)quinazolin-4(3H)-one **(6h)** in $CDCl_3$.

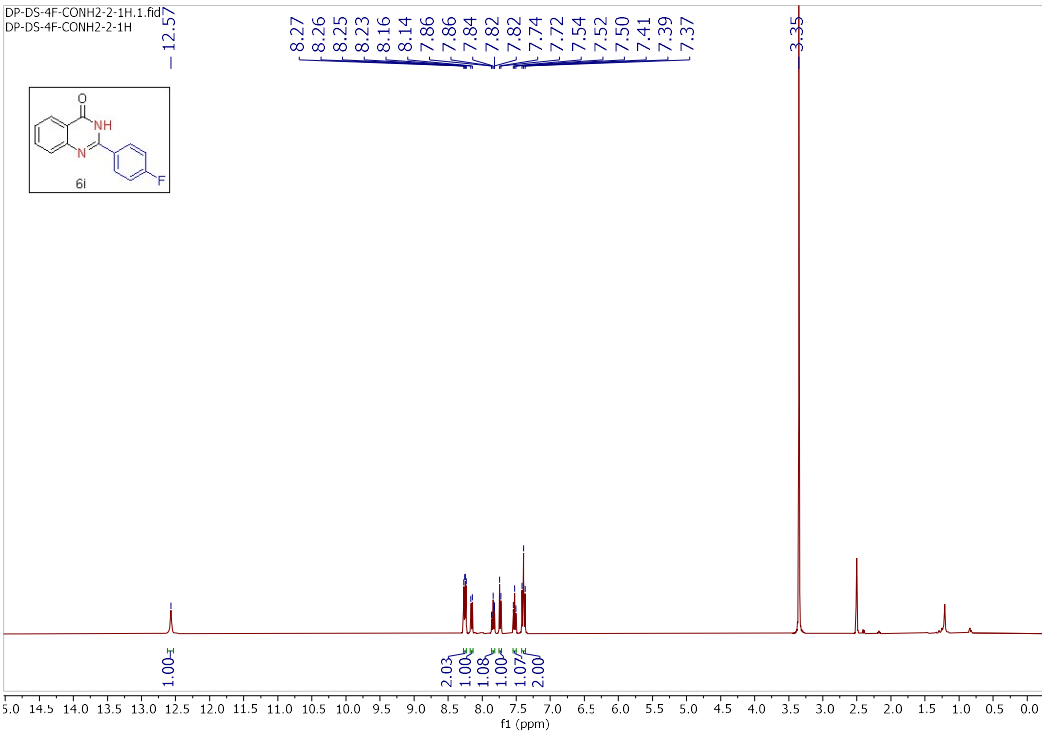


Figure S25. [1]H NMR Spectrum of 2-(4-fluorophenyl)quinazolin-4(3H)-one **(6i)** in DMSO-d_6.

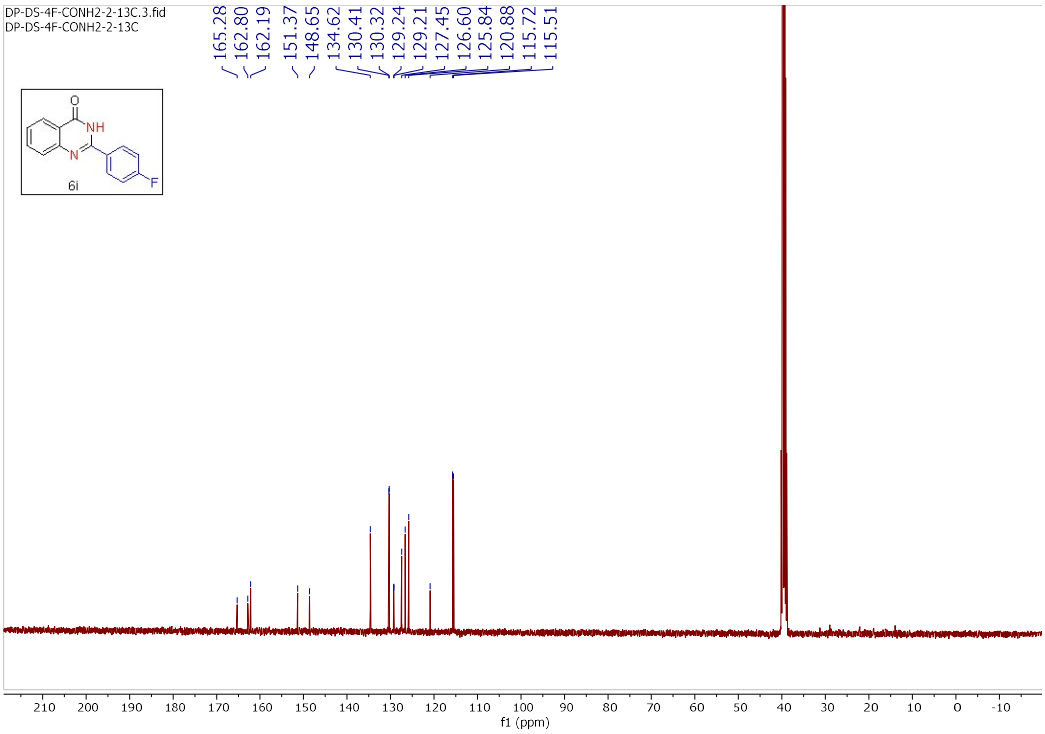


Figure S26. [13]C NMR Spectrum of 2-(4-fluorophenyl)quinazolin-4(3H)-one **(6i)** in DMSO-d_6.

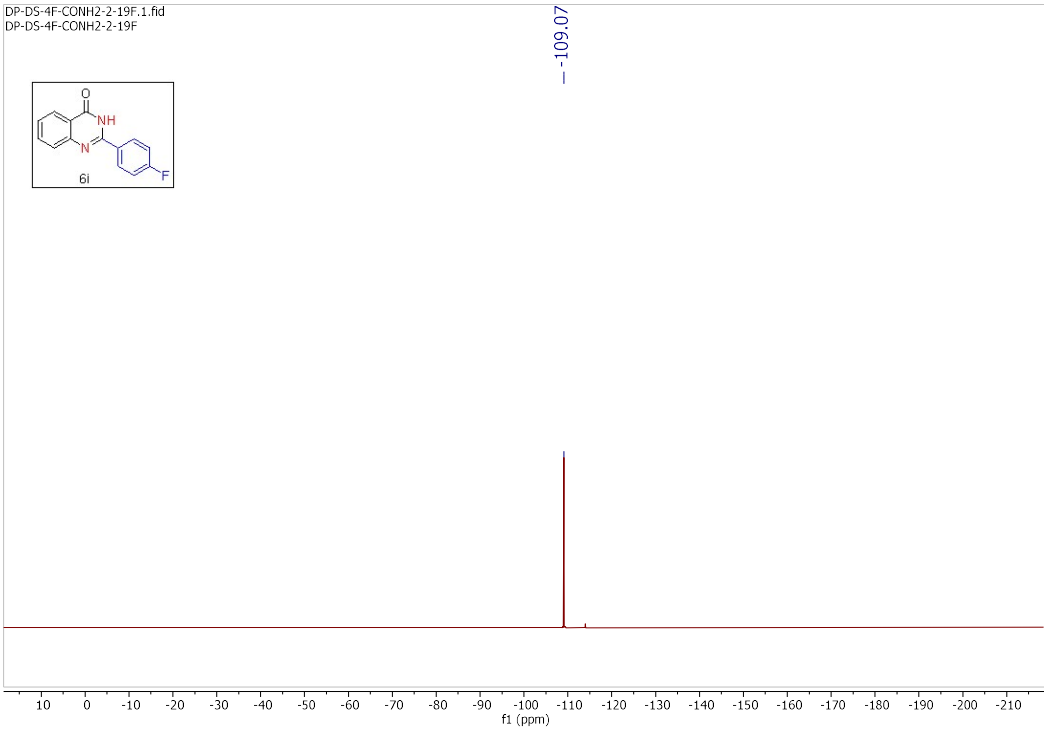


Figure S27. ^{19}F NMR Spectrum of 2-(4-fluorophenyl)quinazolin-4(3H)-one **(6i)** in DMSO-d_6.

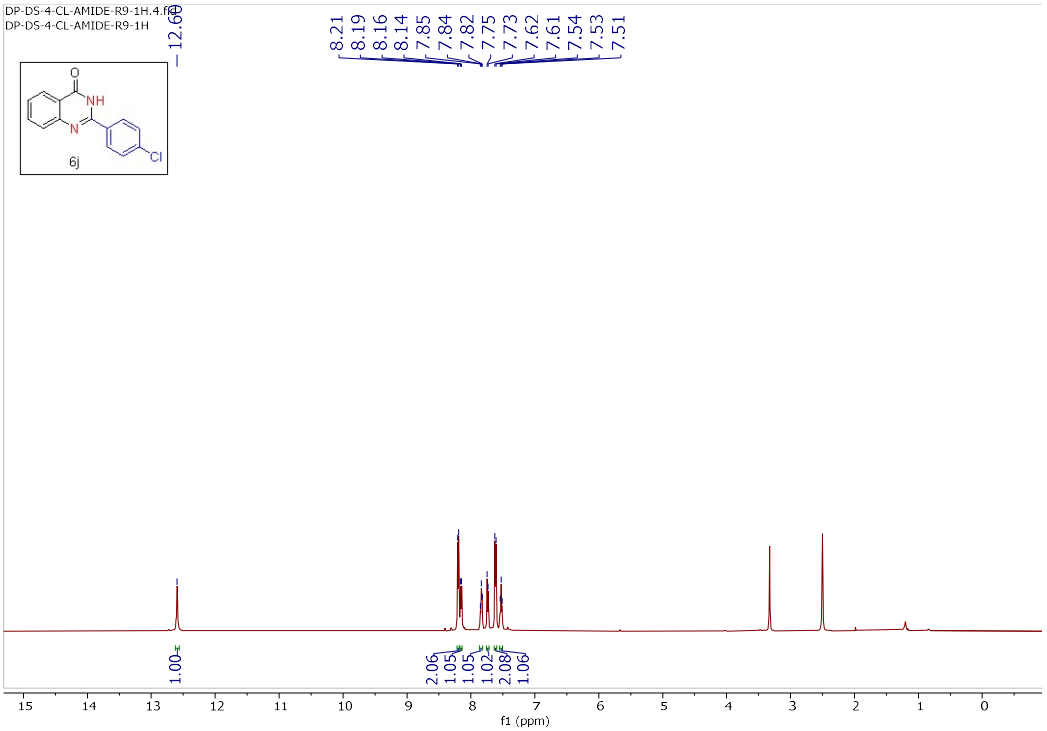


Figure S28. ^{1}H NMR Spectrum of 2-(4-chlorophenyl)quinazolin-4(3H)-one **(6j)** in DMSO-d_6.

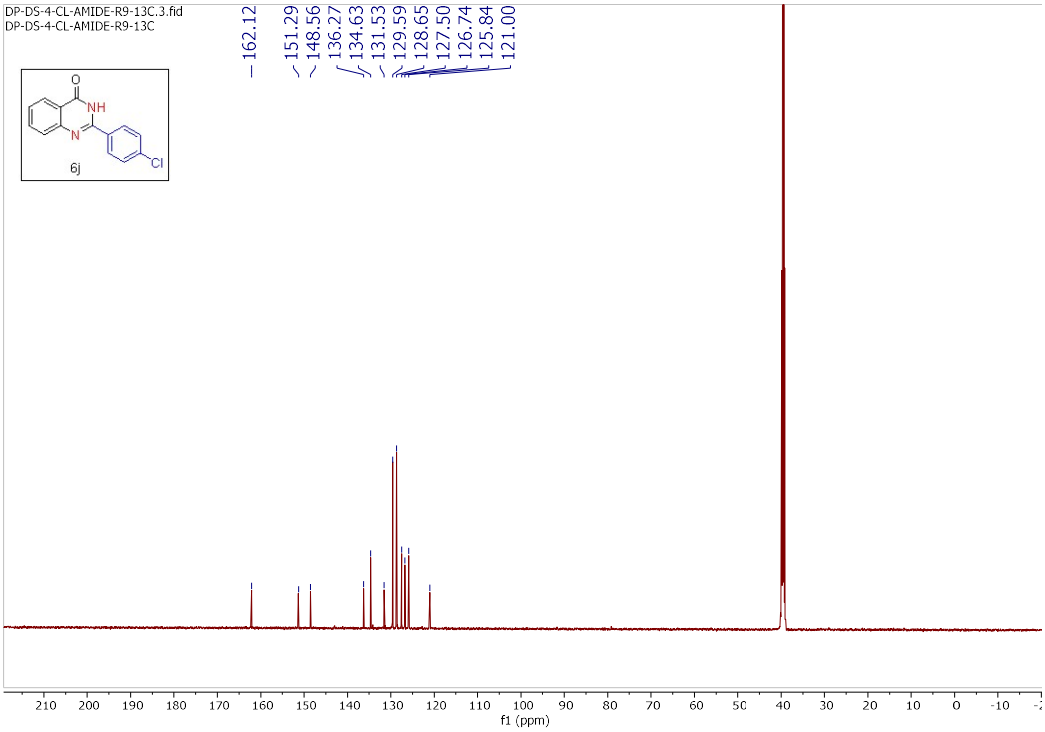


Figure S29. ^{13}C NMR Spectrum of 2-(4-chlorophenyl)quinazolin-4(3H)-one **(6j)** in DMSO-d_6.

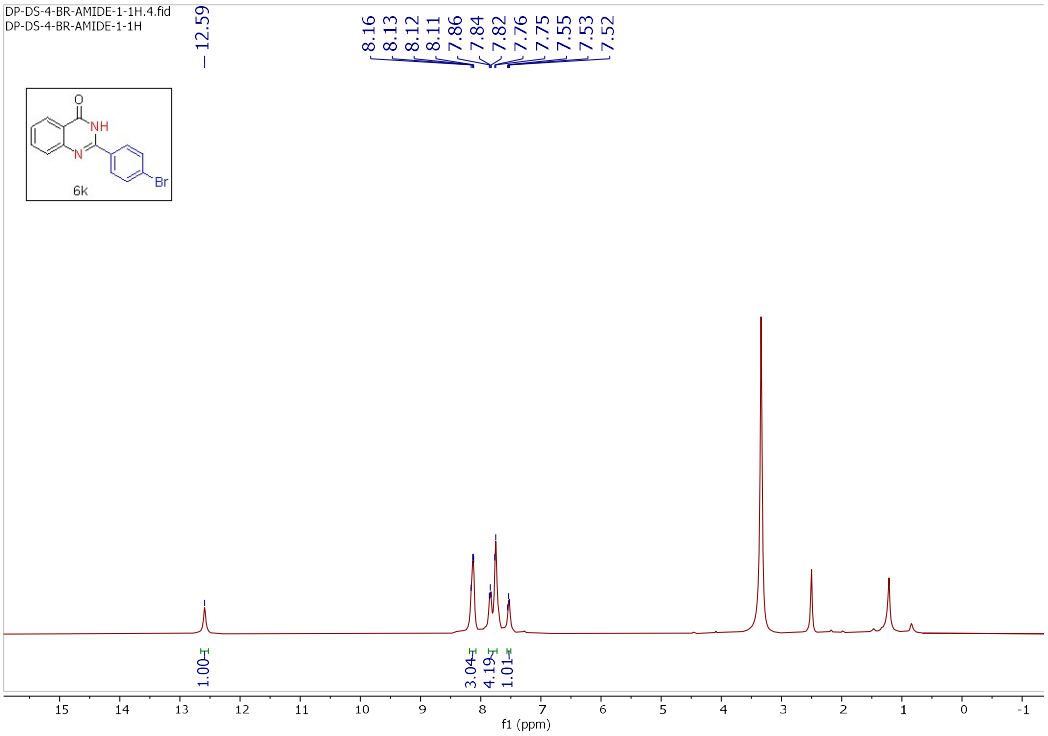


Figure S30. ^{1}H NMR Spectrum of 2-(4-bromophenyl)quinazolin-4(3H)-one **(6k)** in DMSO-d_6.

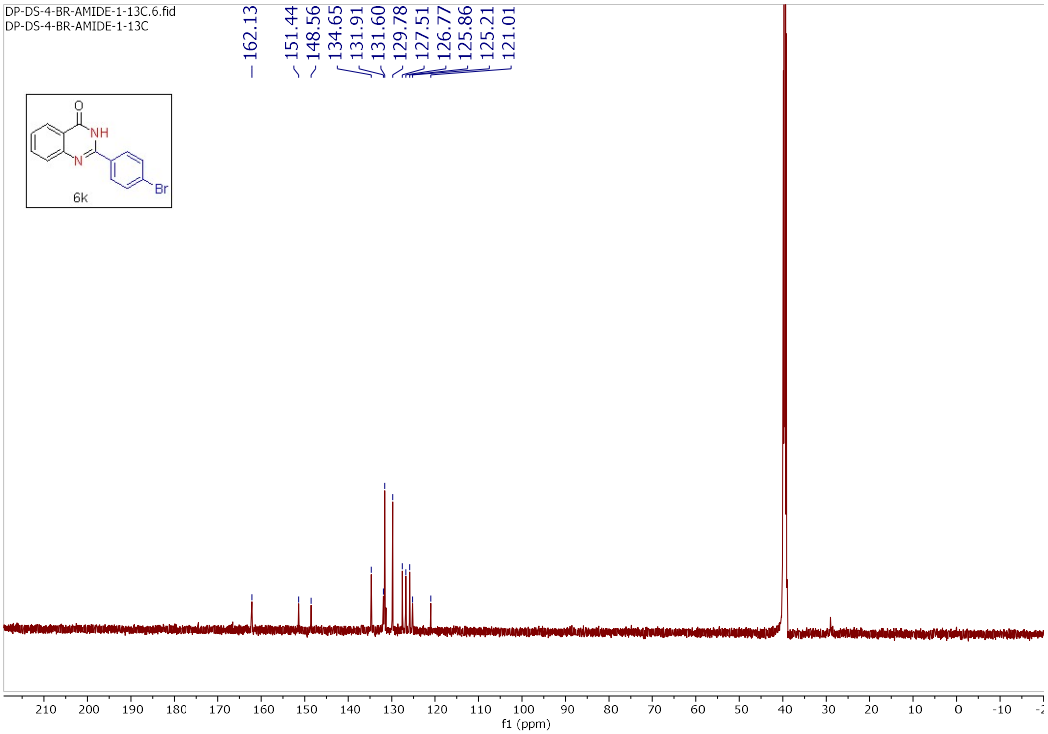


Figure S31. ^{13}C NMR Spectrum of 2-(4-bromophenyl)quinazolin-4(3H)-one **(6k)** in DMSO-*d*$_6$.

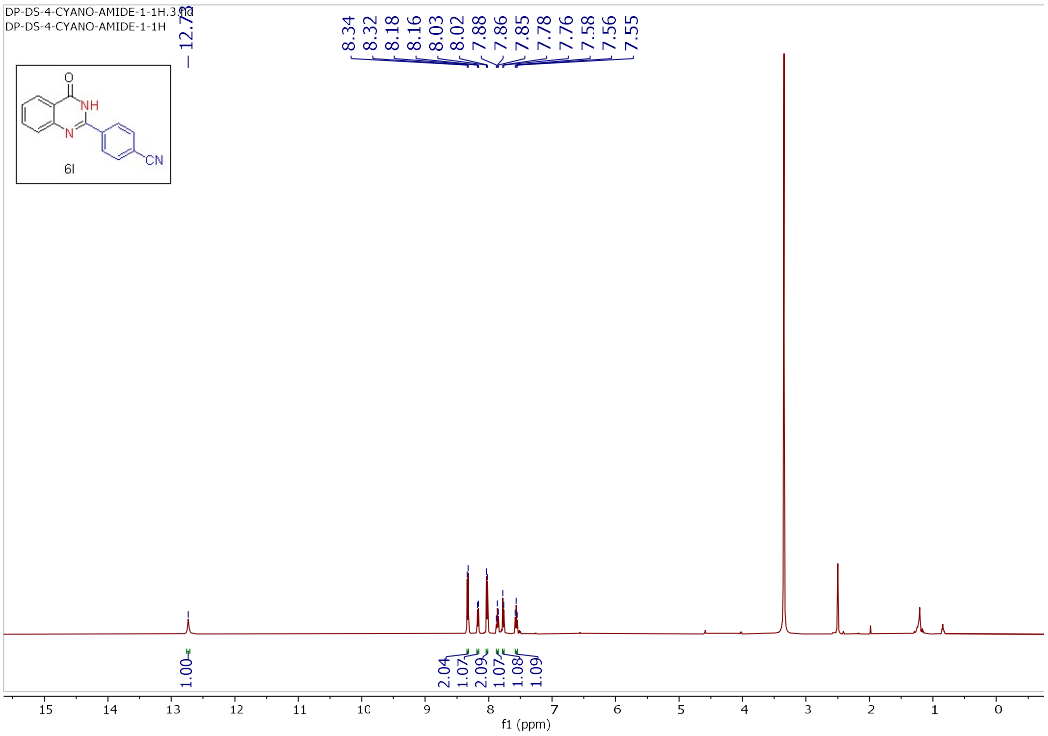


Figure S32. ^{1}H NMR Spectrum of 4-(4-oxo-3,4-dihydroquinazolin-2-yl)benzonitrile **(6l)** in DMSO-*d*$_6$.

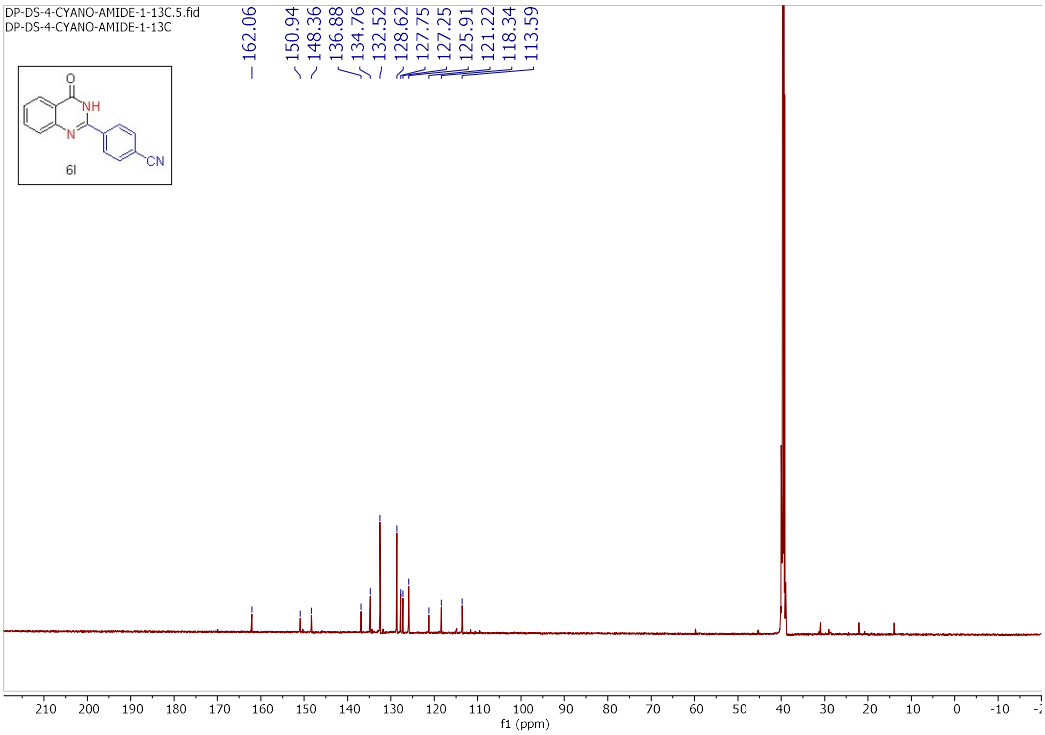


Figure S33. ^{13}C NMR Spectrum of 4-(4-oxo-3,4-dihydroquinazolin-2-yl)benzonitrile **(6l)** in DMSO-*d*$_6$.

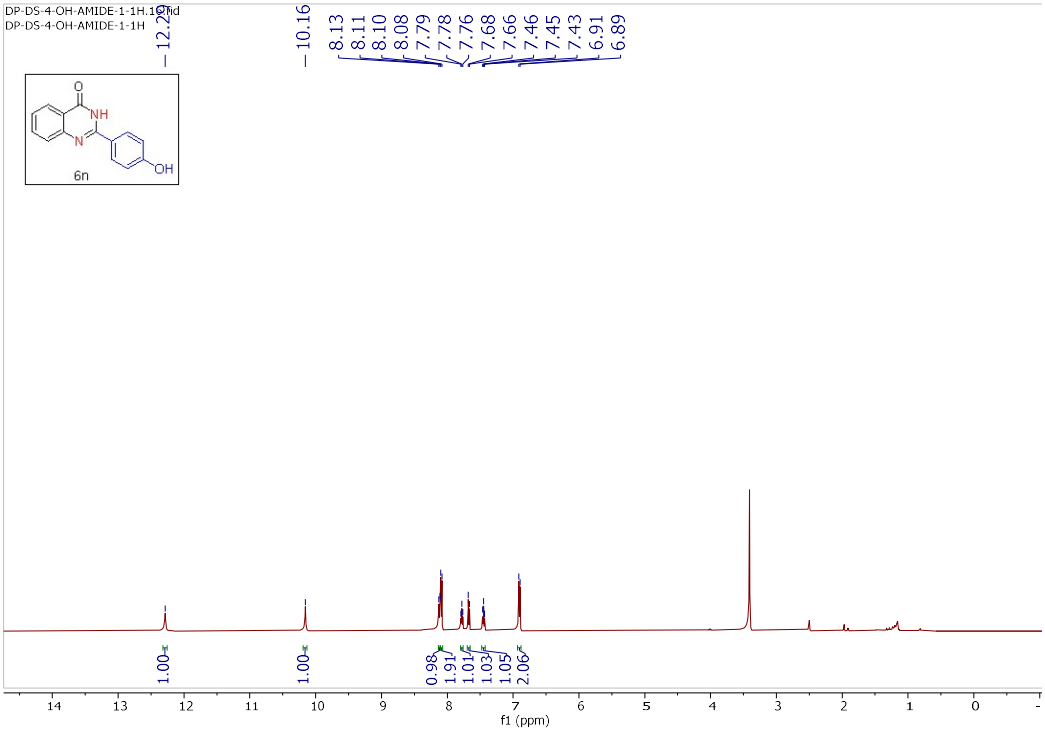


Figure S34. ^{1}H NMR Spectrum of 2-(4-hydroxyphenyl)quinazolin-4(3H)-one **(6n)** in DMSO-*d*$_6$.

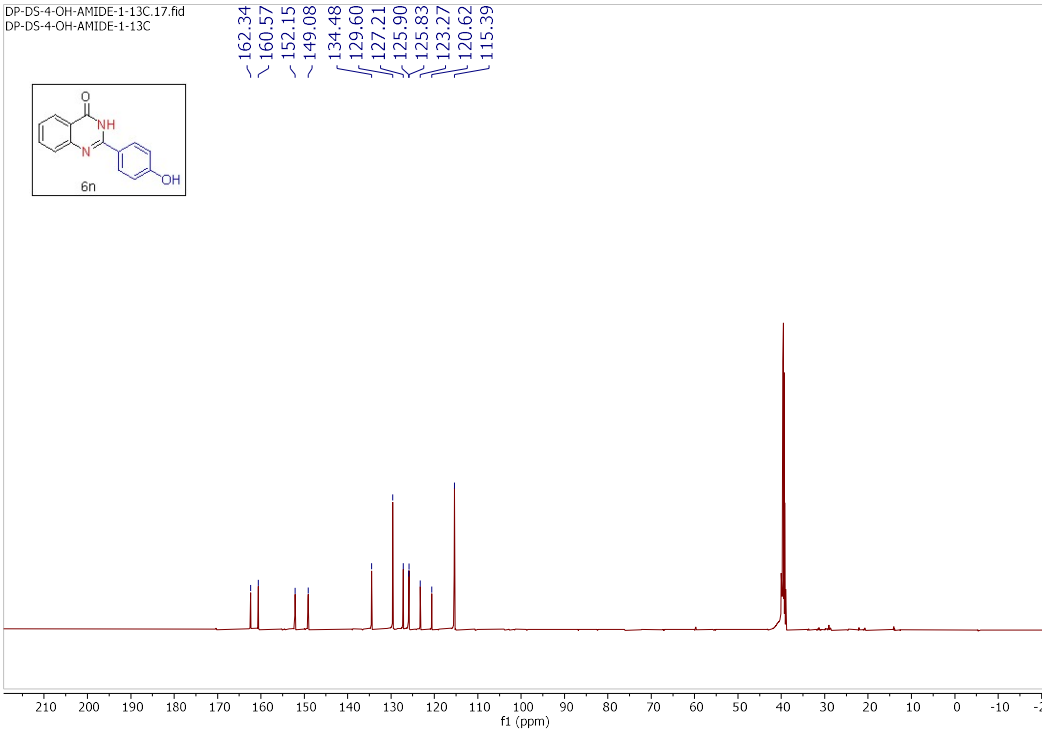


Figure S35. ^{13}C NMR Spectrum of 2-(4-hydroxyphenyl)quinazolin-4(3H)-one **(6n)** in DMSO-d_6.

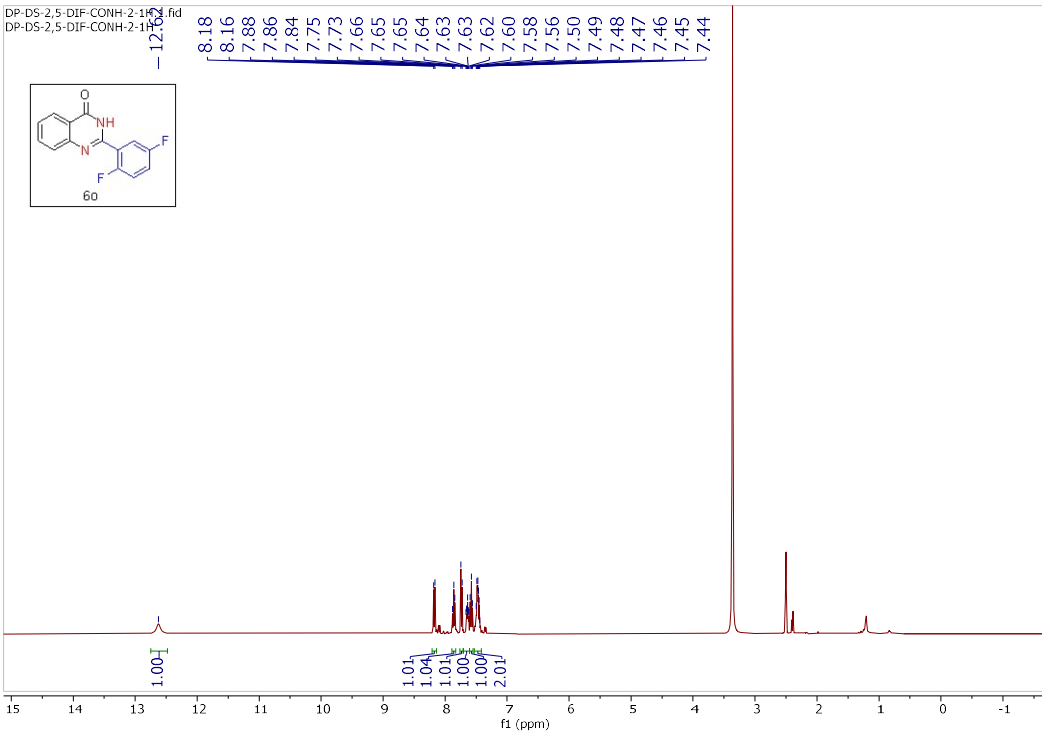


Figure S36. ^{1}H NMR Spectrum of 2-(2,5-difluorophenyl)quinazolin-4(3H)-one **(6o)** in DMSO-d_6.

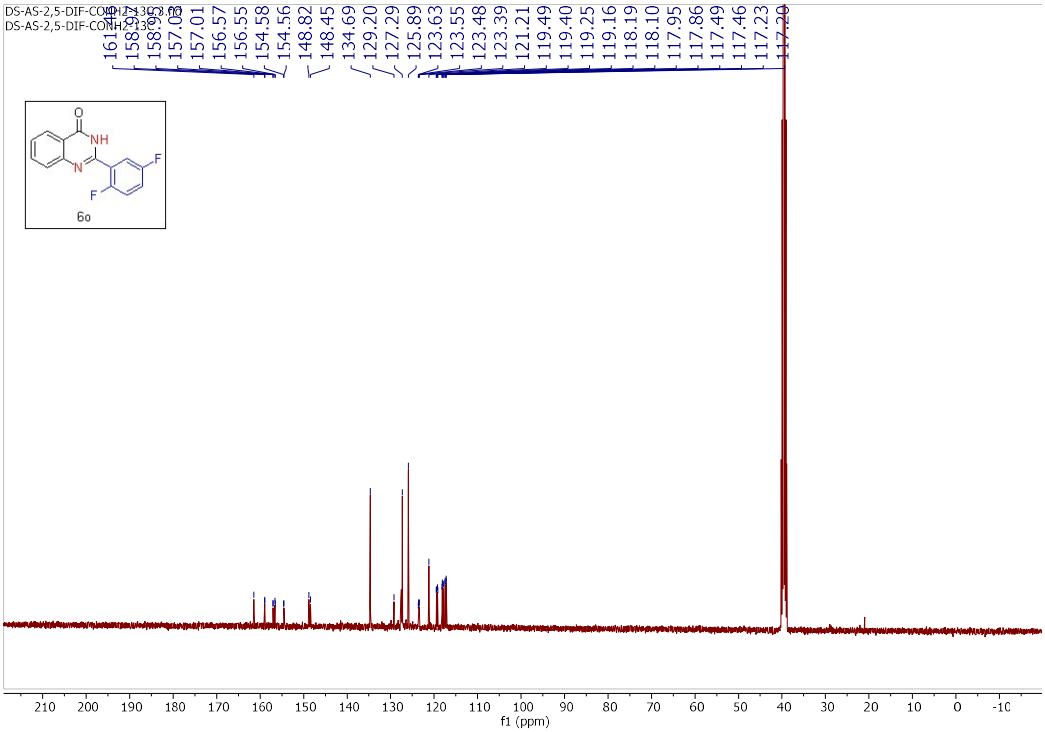


Figure S37. ^{13}C NMR Spectrum of 2-(2,5-difluorophenyl)quinazolin-4(3H)-one **(6o)** in DMSO-d_6.

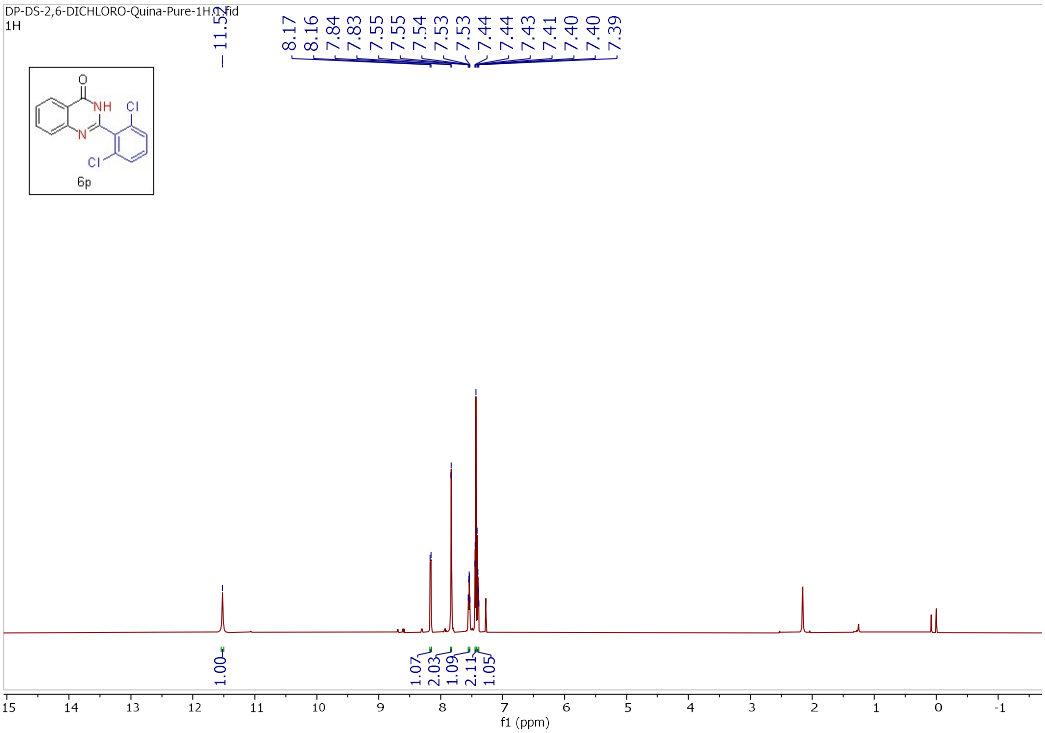


Figure S38. ^{1}H NMR Spectrum of 2-(2,6-dichlorophenyl)quinazolin-4(3H)-one **(6p)** in $CDCl_3$.

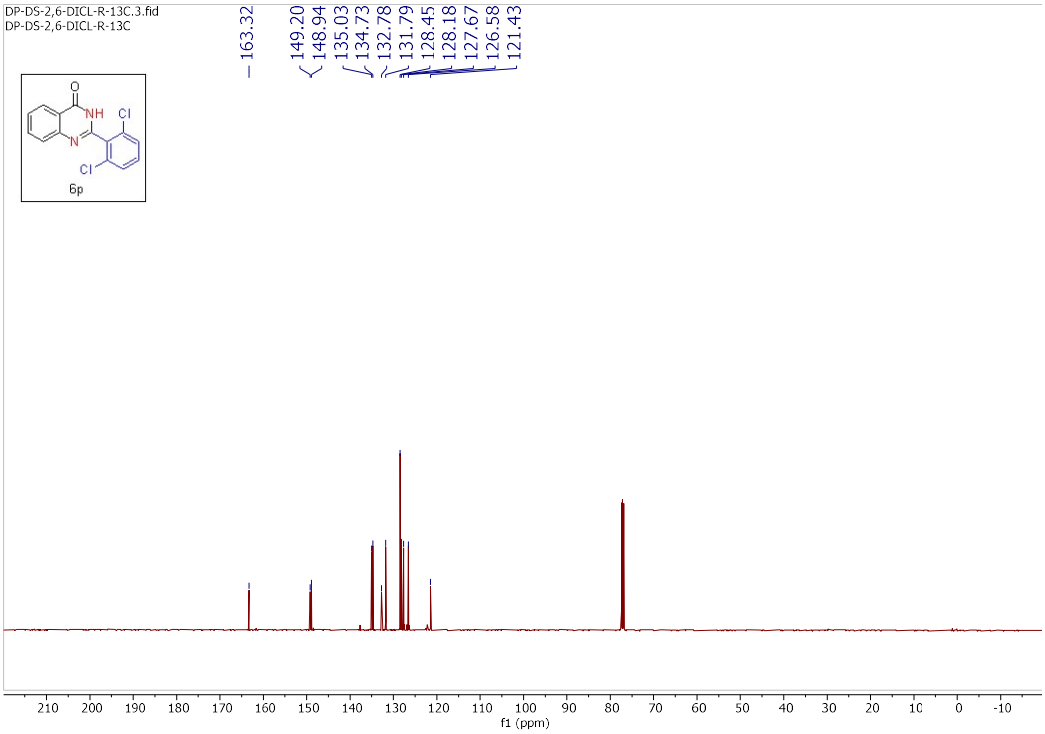


Figure S39. ^{13}C NMR Spectrum of 2-(2,6-dichlorophenyl)quinazolin-4(3H)-one **(6p)** in $CDCl_3$.

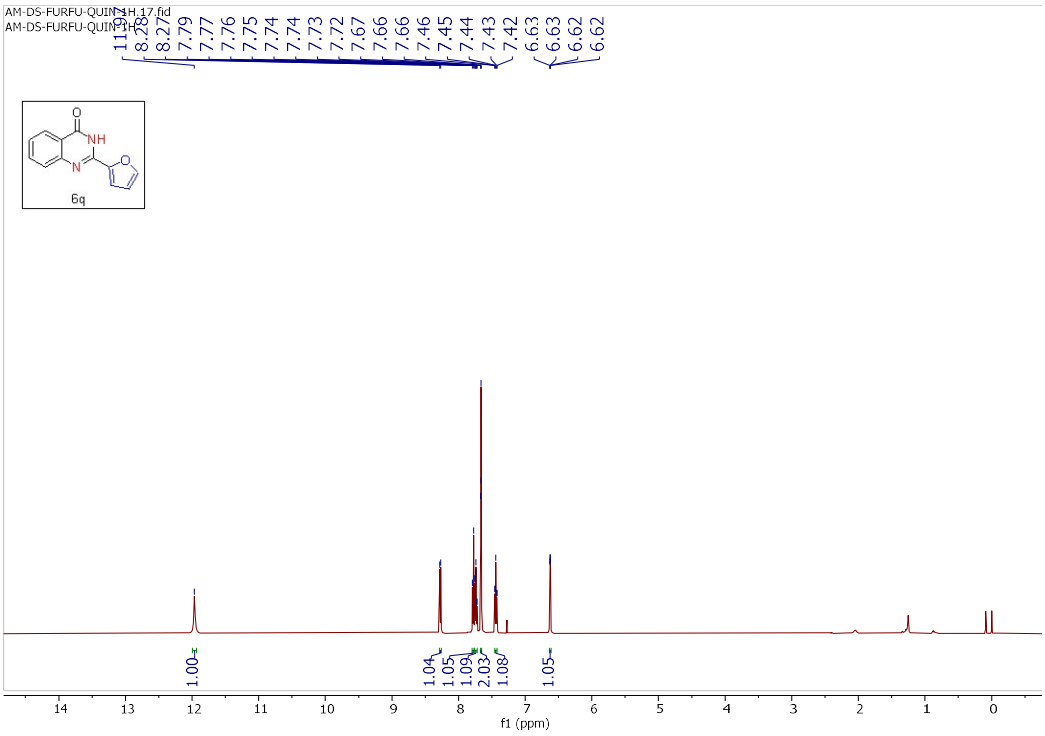


Figure S40. ^{1}H NMR Spectrum of 2-(furan-2-yl)quinazolin-4(3H)-one **(6q)** in $CDCl_3$.

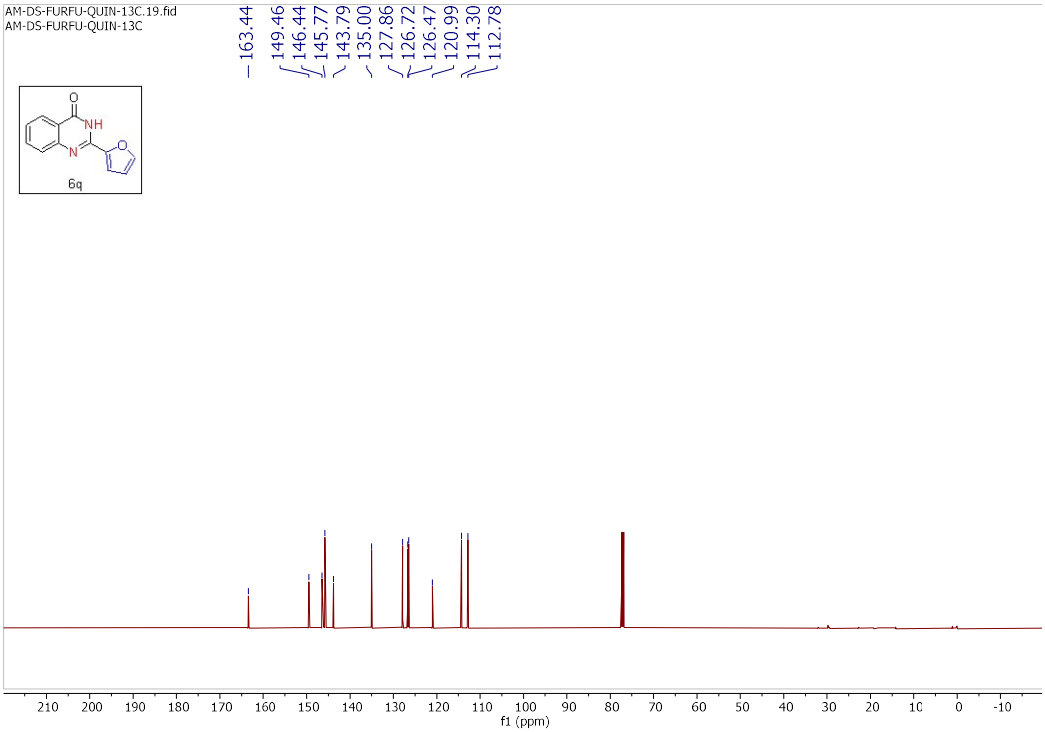


Figure S41. ^{13}C NMR Spectrum of 2-(furan-2-yl)quinazolin-4(3H)-one **(6q)** in $CDCl_3$.

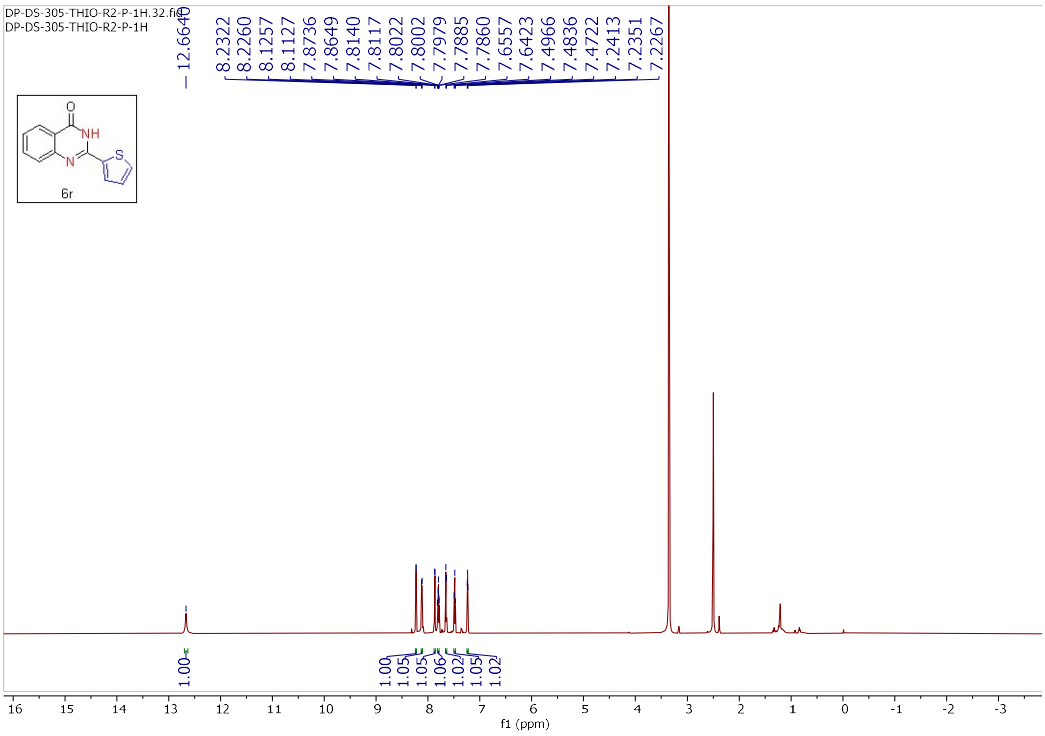


Figure S42. ^{1}H NMR Spectrum of 2-(thiophen-2-yl)quinazolin-4(3H)-one **(6r)** in DMSO-d_6.

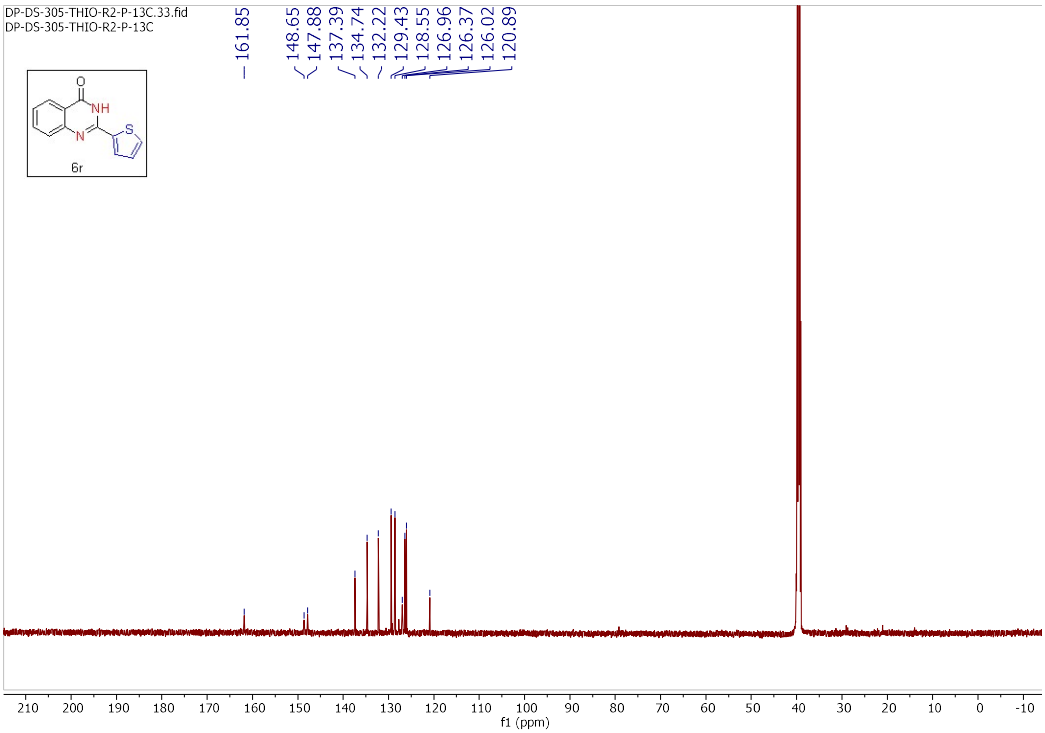


Figure S43. ^{13}C NMR Spectrum of 2-(thiophen-2-yl)quinazolin-4(3H)-one **(6r)** in DMSO-d_6.

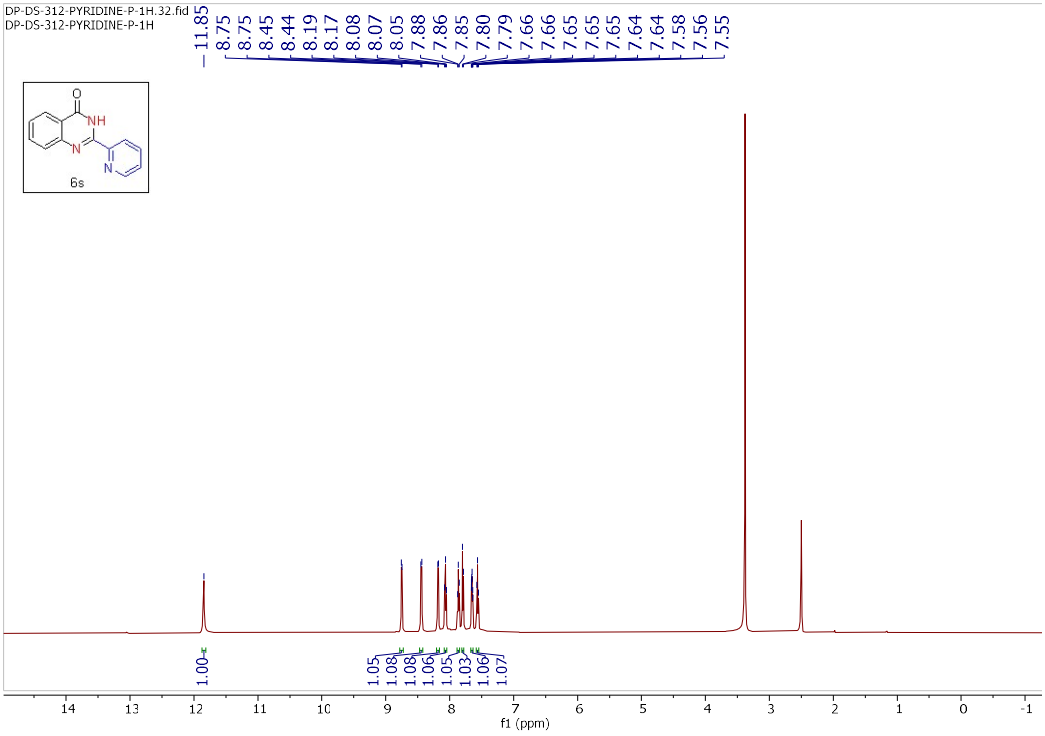


Figure S44. ^{1}H NMR Spectrum of 2-(pyridin-2-yl)quinazolin-4(3H)-one **(6s)** in DMSO-d_6.

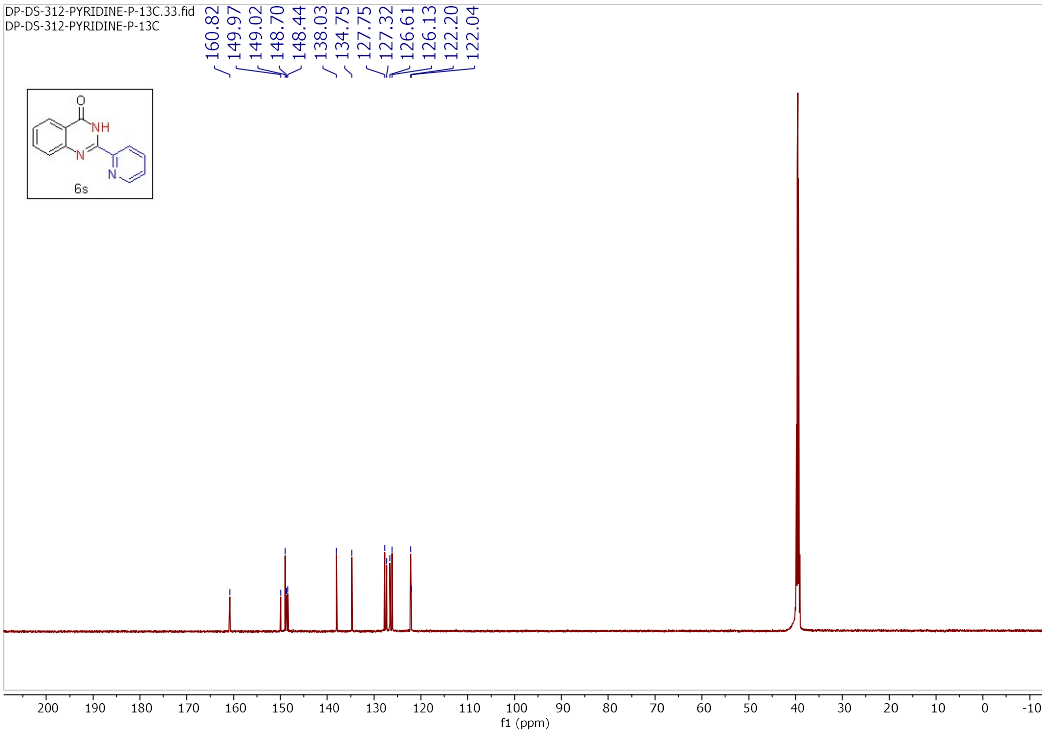


Figure S45. ^{13}C NMR Spectrum of 2-(pyridin-2-yl)quinazolin-4(3H)-one **(6s)** in DMSO-d_6.

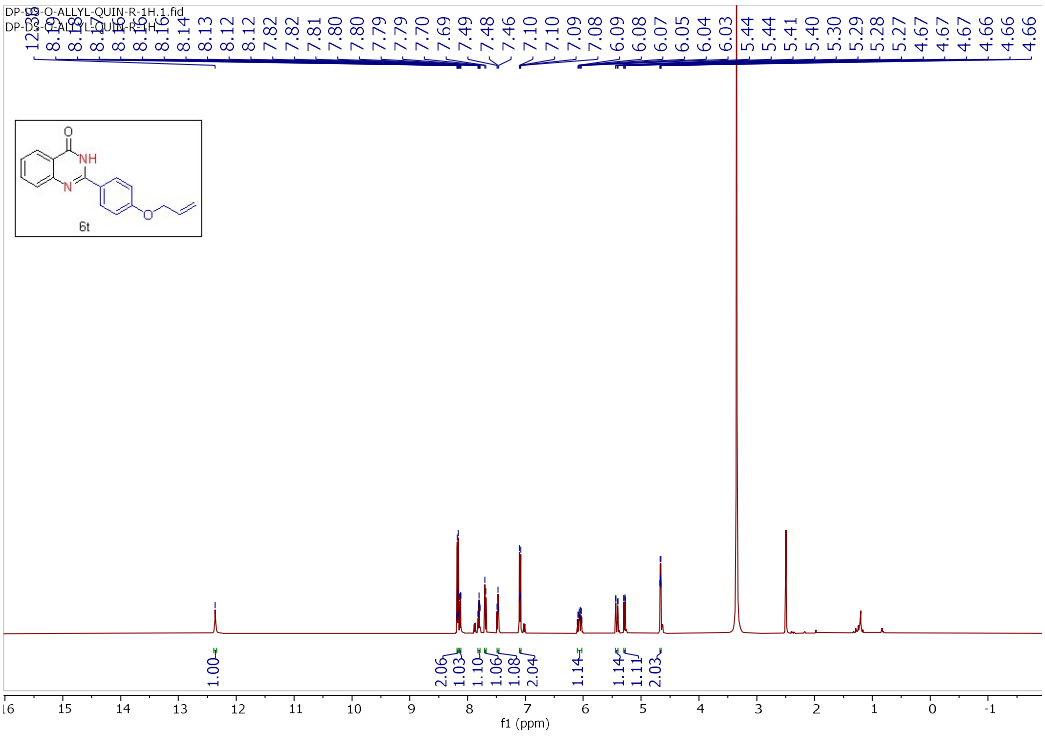


Figure S46. ^{1}H NMR Spectrum of 2-(4-(allyloxy)phenyl)quinazolin-4(3H)-one **(6t)** in DMSO-d_6.

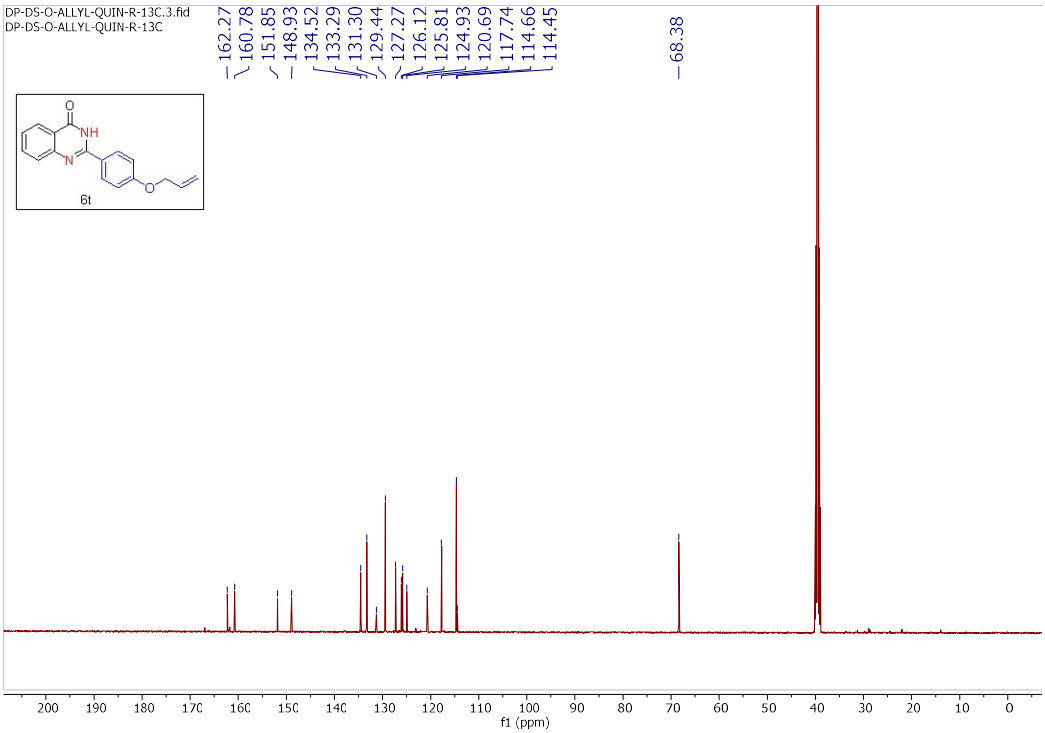


Figure S47. ^{13}C NMR Spectrum of 2-(4-(allyloxy)phenyl)quinazolin-4(3H)-one **(6t)** in DMSO-d_6.

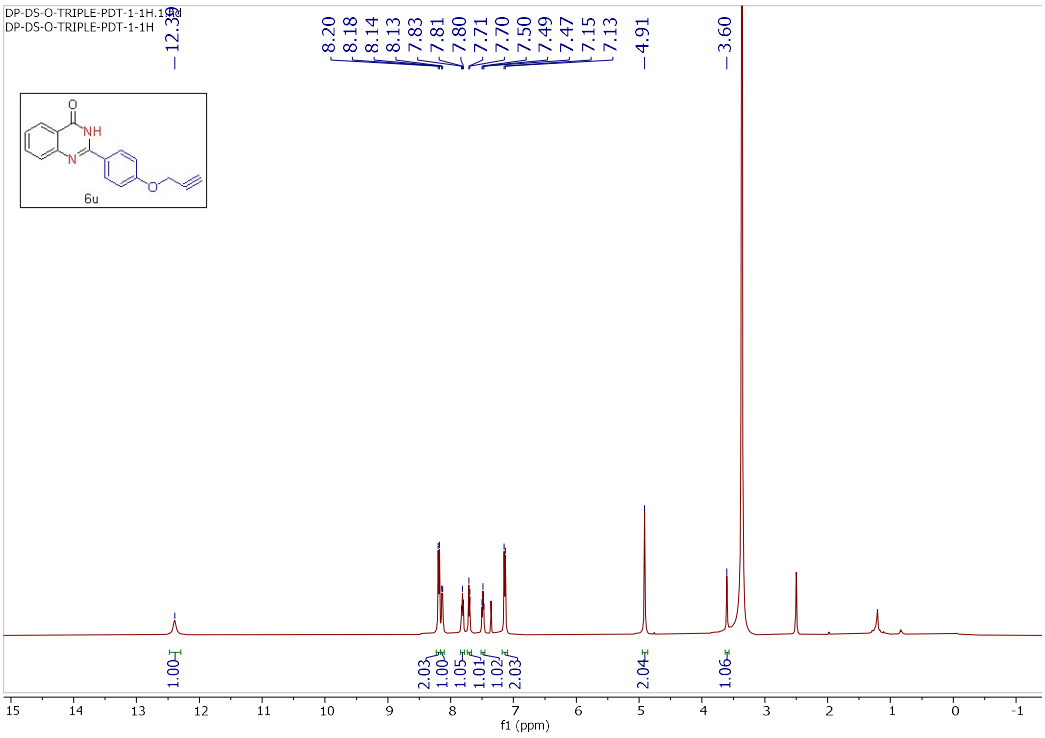


Figure S48. ^{1}H NMR Spectrum of 2-(4-(prop-2-yn-1-yloxy)phenyl)quinazolin-4(3H)-one **(6u)** in DMSO-d_6.

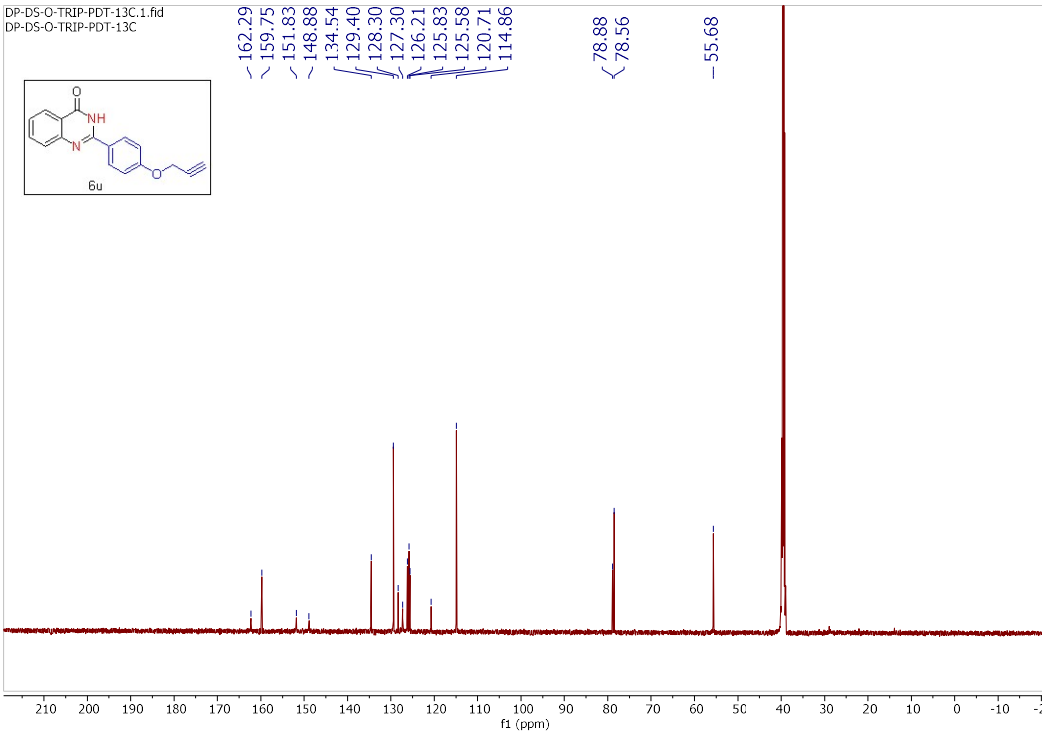


Figure S49. ^{13}C NMR Spectrum of 2-(4-(prop-2-yn-1-yloxy)phenyl)quinazolin-4(3H)-one **(6u)** in DMSO-d_6.

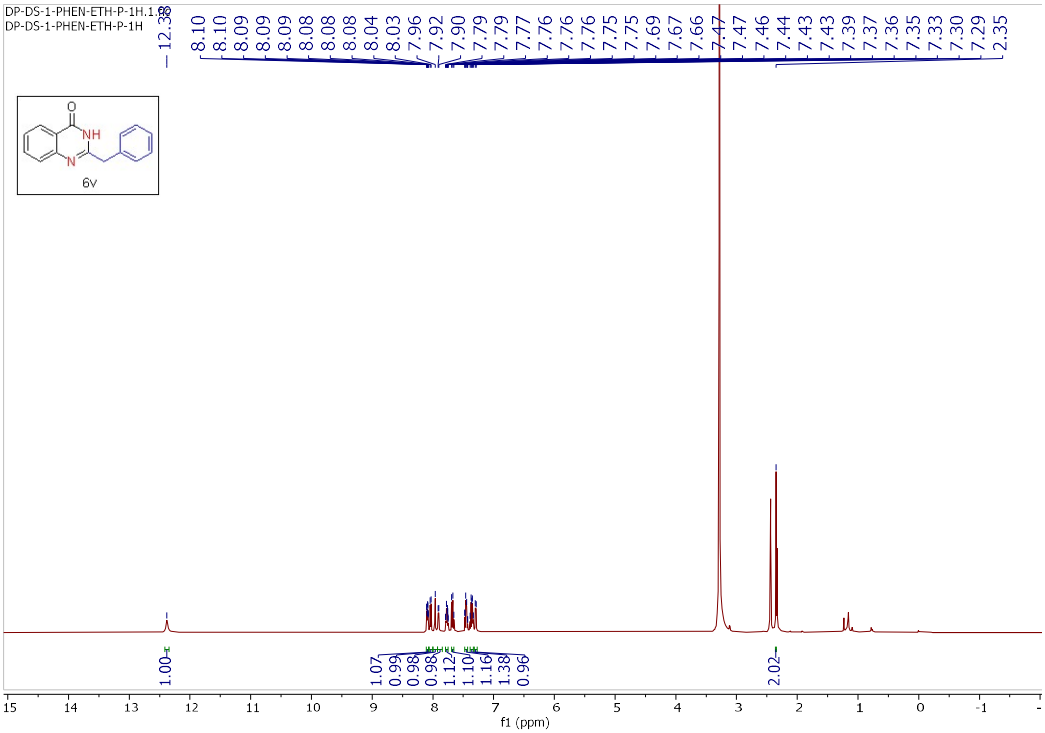


Figure S50. ^{1}H NMR Spectrum of 2-benzylquinazolin-4(3H)-one **(6v)** in DMSO-d_6.

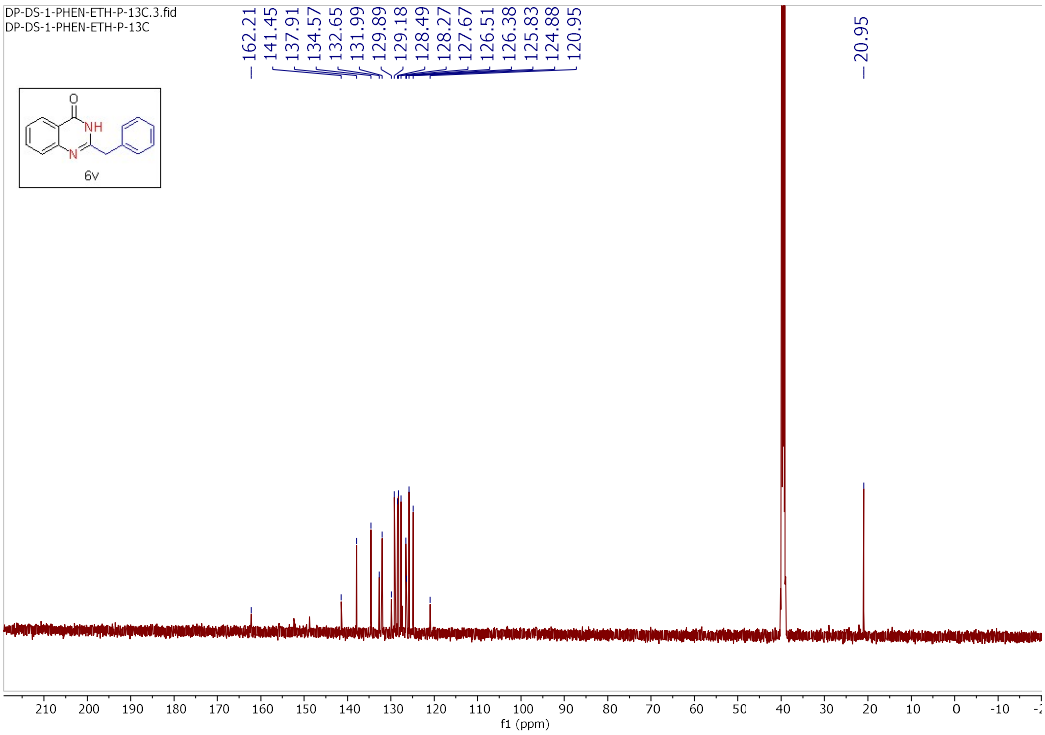


Figure S51. ^{13}C NMR Spectrum of 2-benzylquinazolin-4(3H)-one **(6v)** in DMSO-d_6.

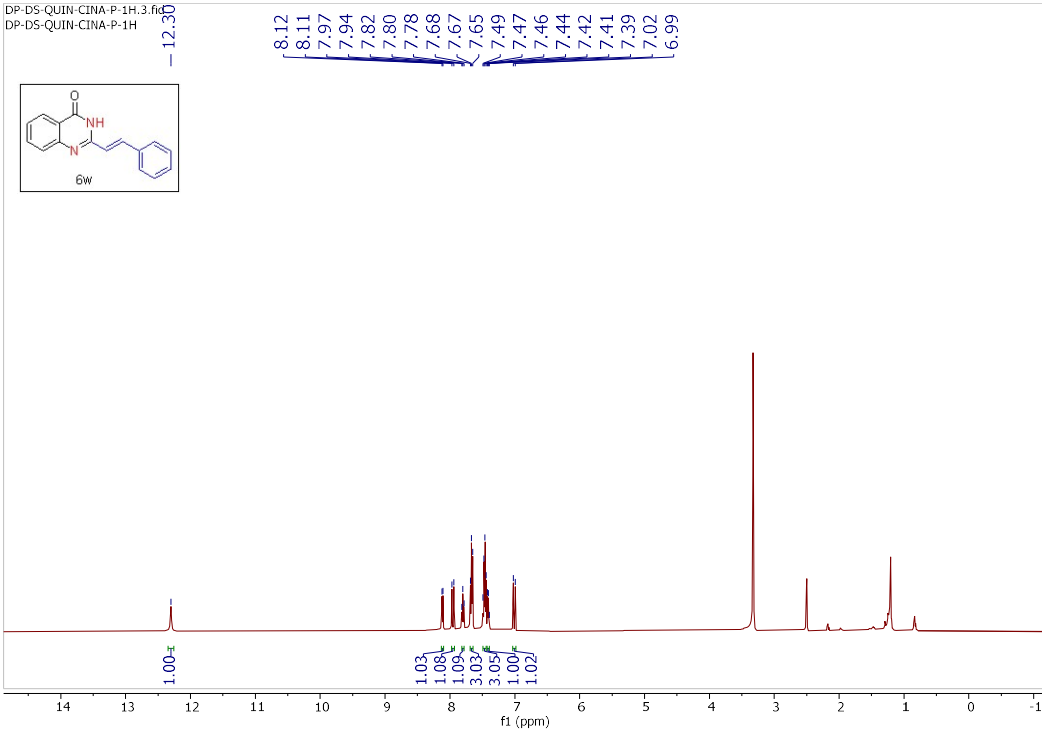


Figure S52. ^{1}H NMR Spectrum of (E)-2-styrylquinazolin-4(3H)-one **(6w)** in DMSO-d_6.

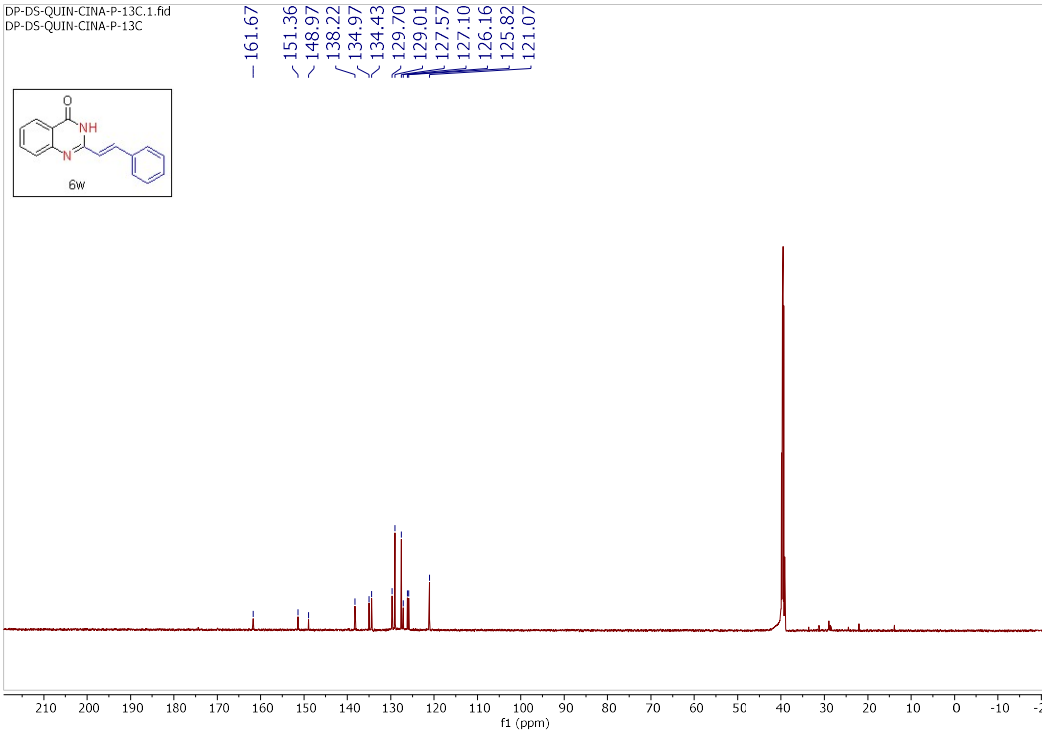


Figure S53. ^{13}C NMR Spectrum of (E)-2-styrylquinazolin-4(3H)-one **(6w)** in DMSO-d_6.

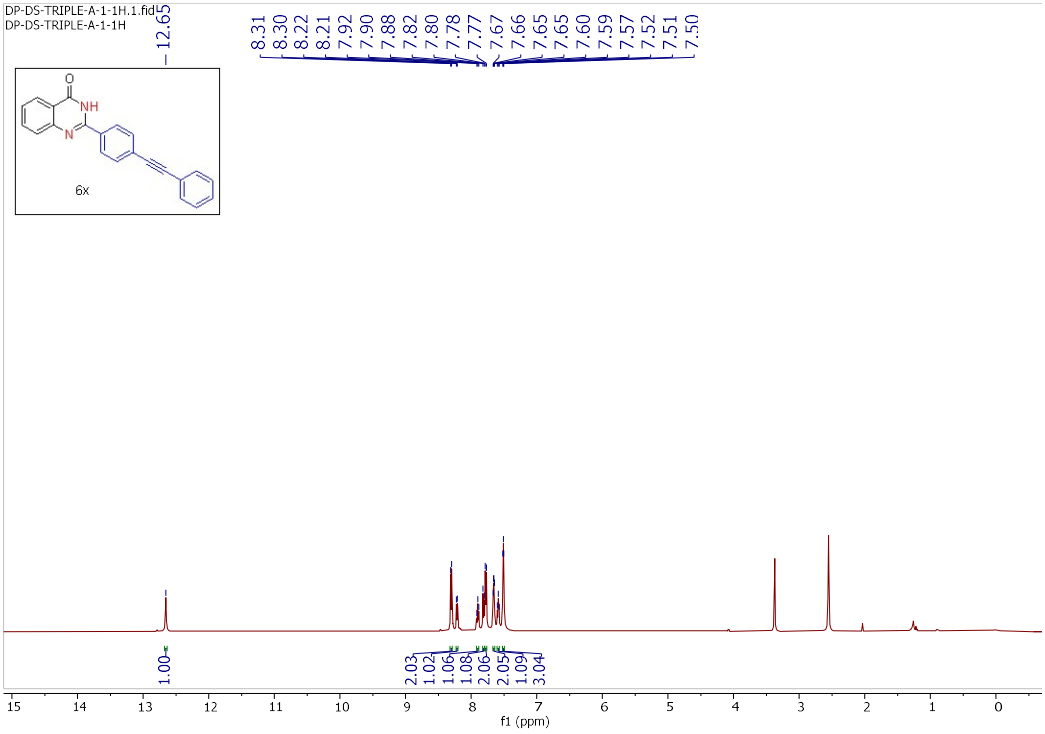


Figure S54. ^{1}H NMR Spectrum of 2-(4-(phenylethynyl)phenyl)quinazolin-4(3H)-one **(6x)** in DMSO-d_6.

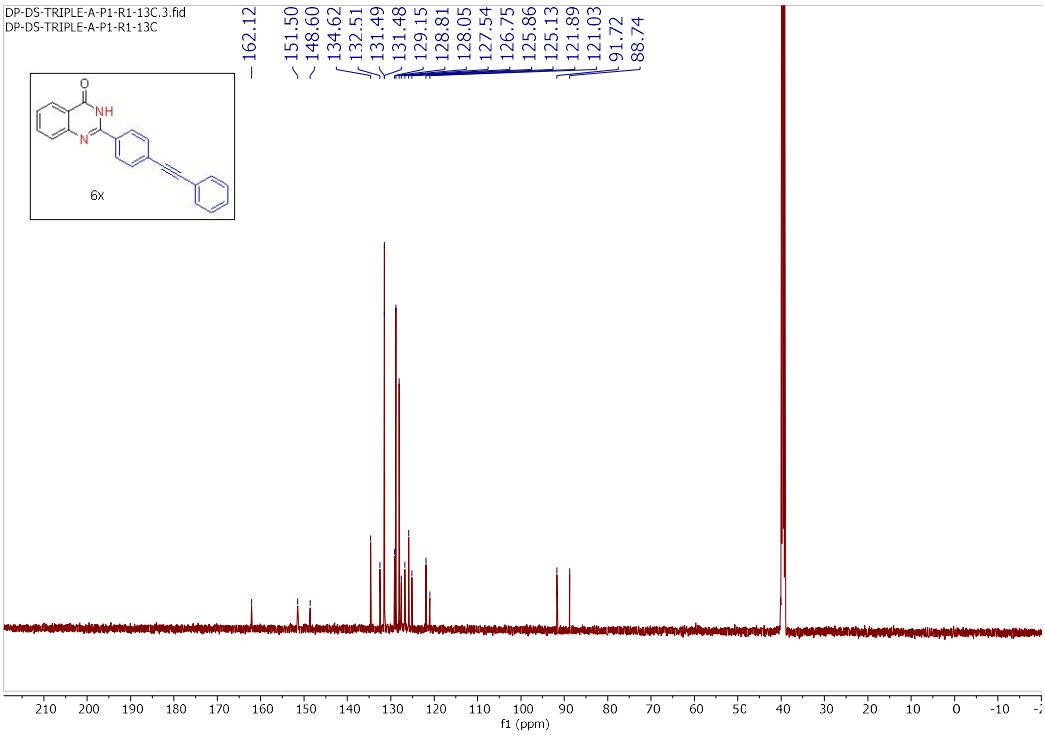


Figure S55. ^{13}C NMR Spectrum of 2-(4-(phenylethynyl)phenyl)quinazolin-4(3H)-one **(6x)** in DMSO-*d*$_6$.

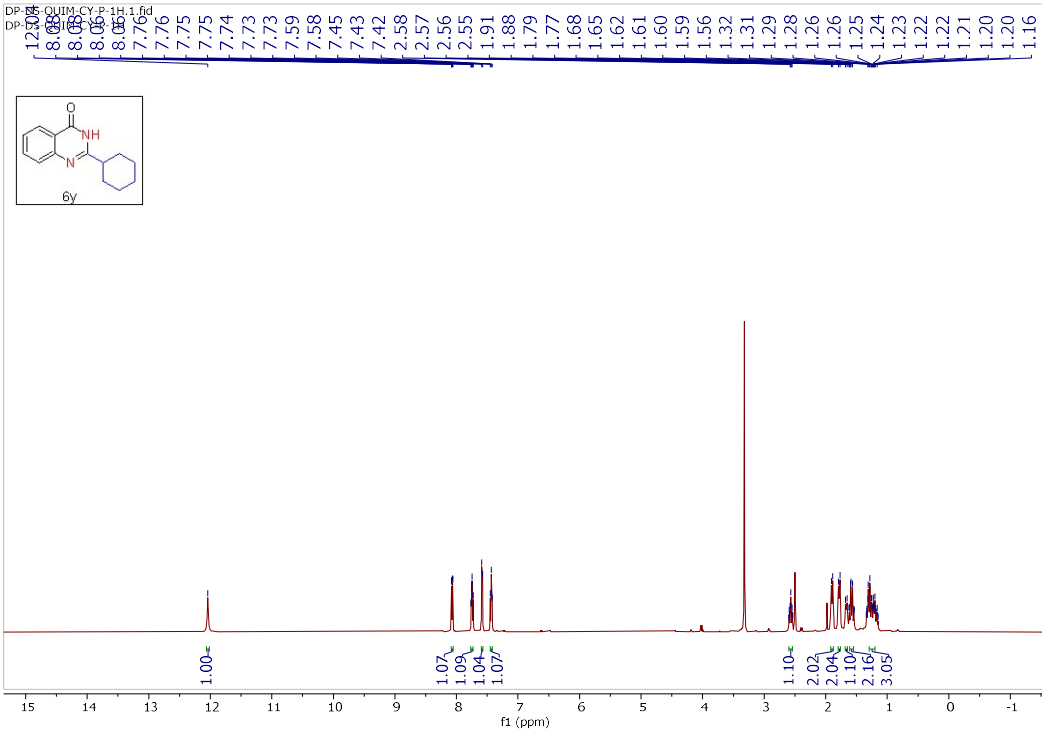


Figure S56. ^{1}H NMR Spectrum of 2-cyclohexylquinazolin-4(3H)-one **(6y)** in DMSO-*d*$_6$.

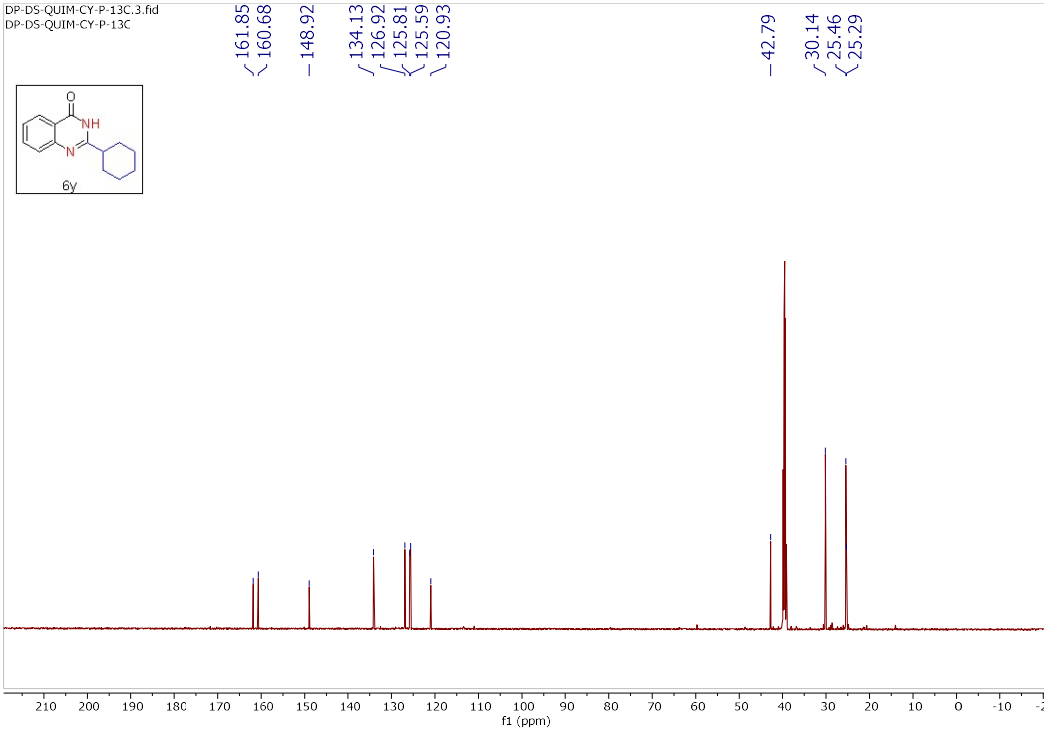


Figure S57. ^{13}C NMR Spectrum of 2-cyclohexylquinazolin-4(3H)-one **(6y)** in DMSO-*d*$_6$.

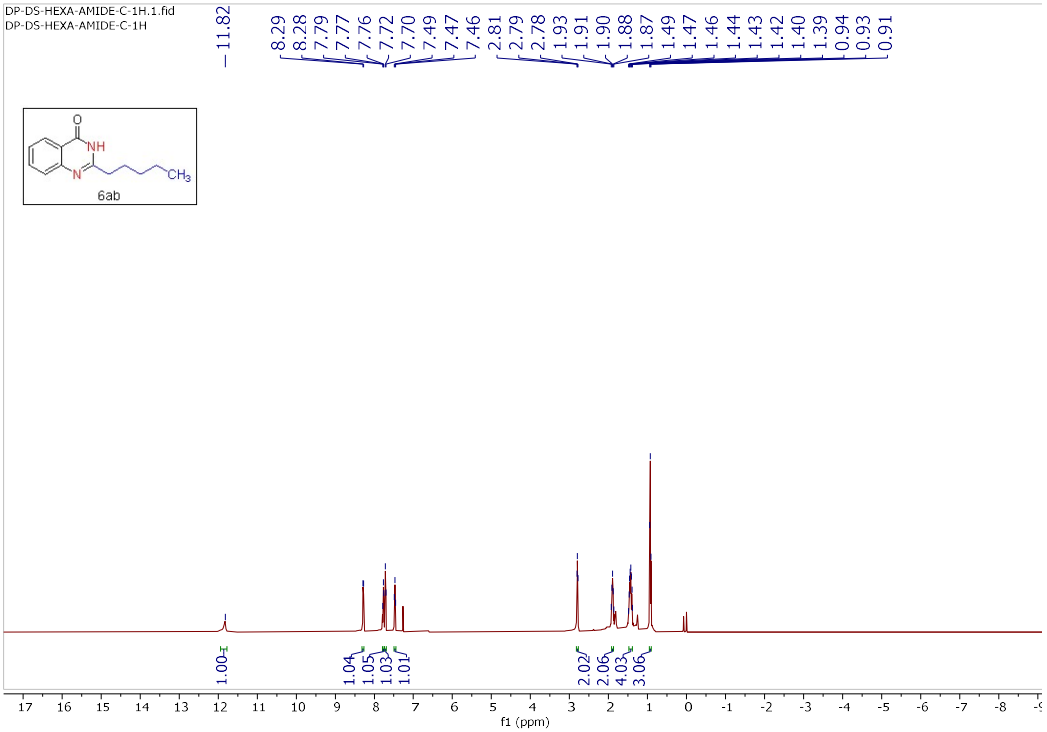


Figure S58. ^{1}H NMR Spectrum of 2-pentylquinazolin-4(3H)-one **(6ab)** in $CDCl_3$.

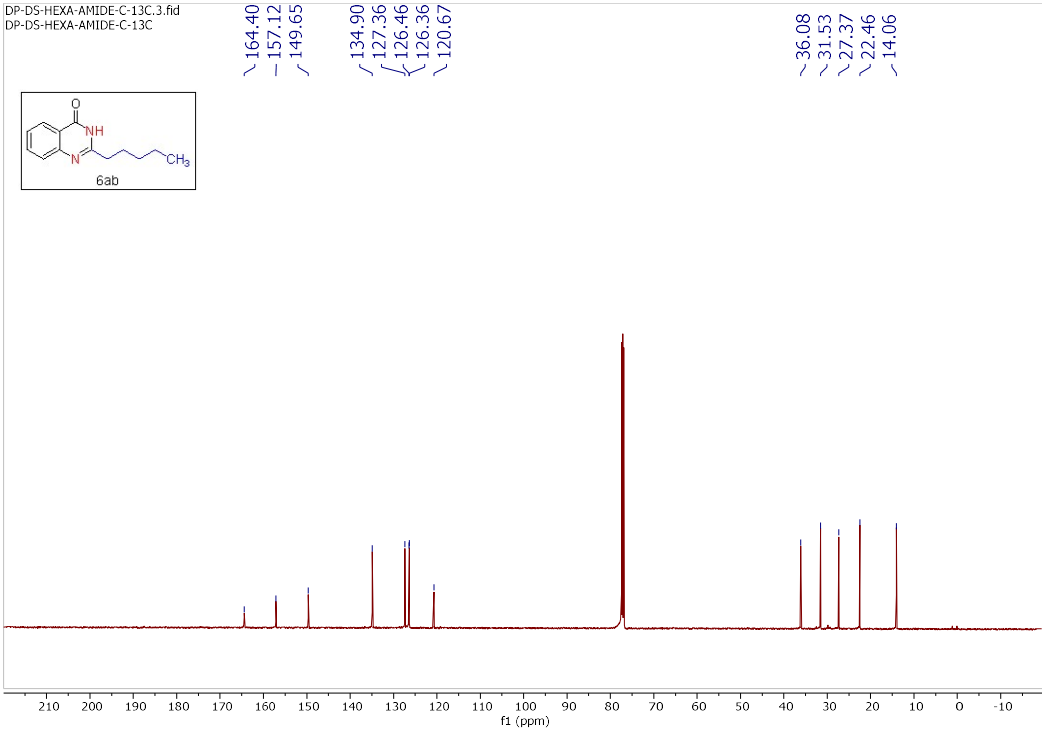


Figure S59. ^{13}C NMR Spectrum of 2-pentylquinazolin-4(3H)-one **(6ab)** in $CDCl_3$.

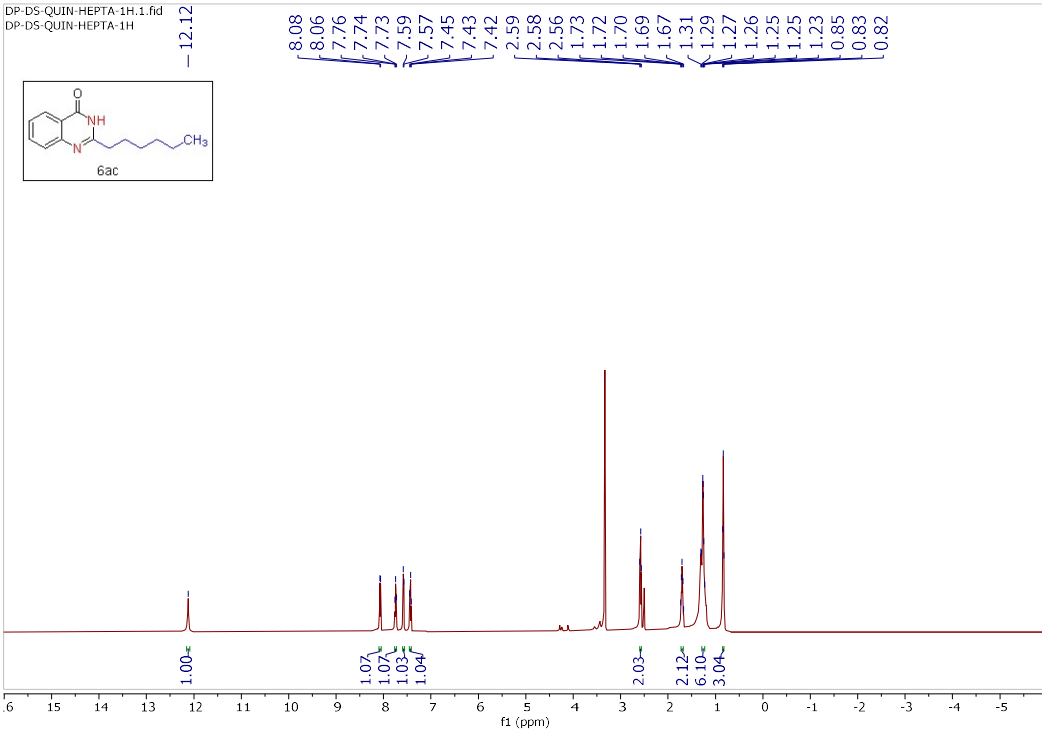


Figure S60. ^{1}H NMR Spectrum of 2-hexylquinazolin-4(3H)-one **(6ac)** in DMSO-d_6.

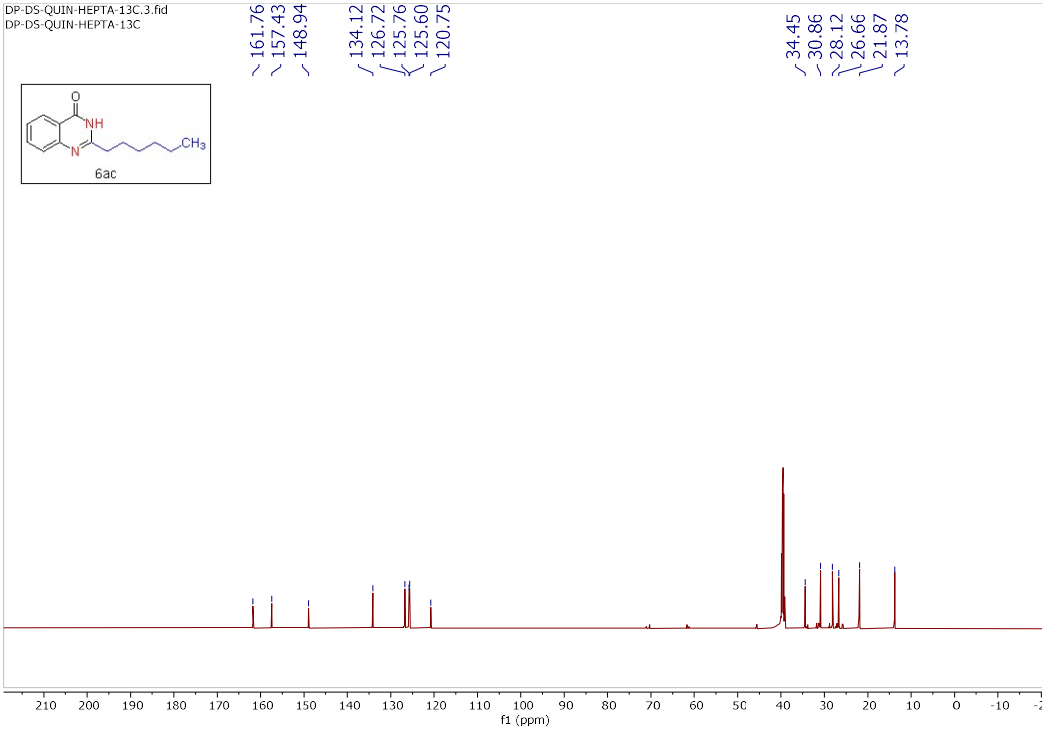


Figure S61. ^{13}C NMR Spectrum of 2-hexylquinazolin-4(3H)-one **(6ac)** in DMSO-d_6.

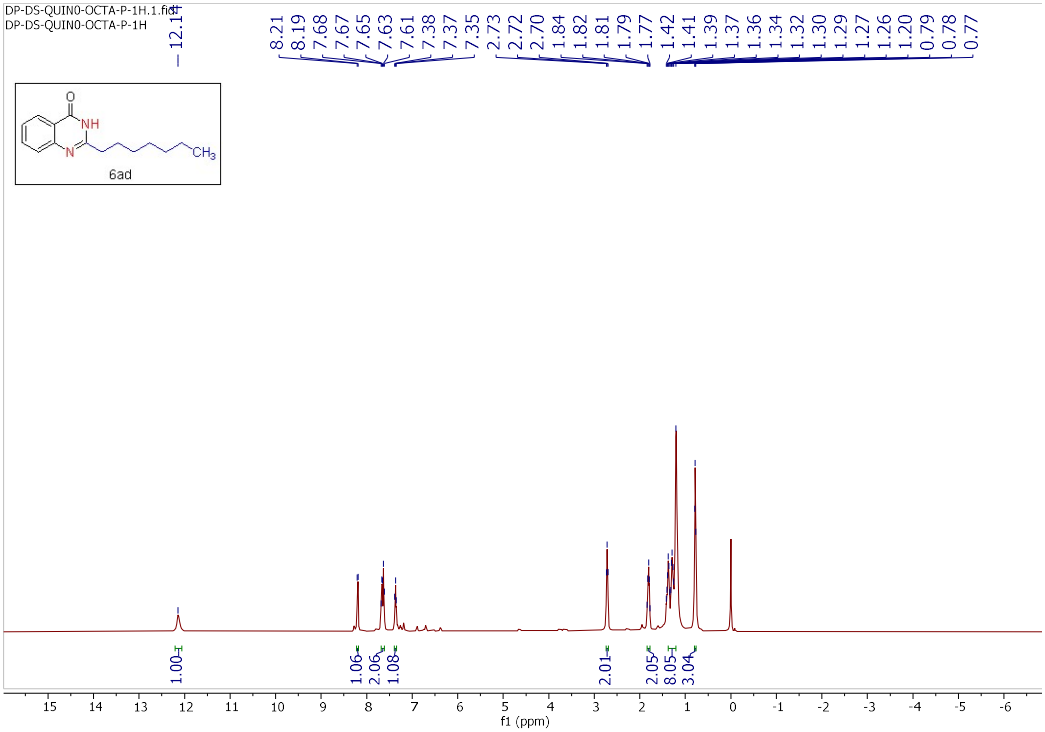


Figure S62. ^{1}H NMR Spectrum of 2-heptylquinazolin-4(3H)-one **(6ad)** in $CDCl_3$.

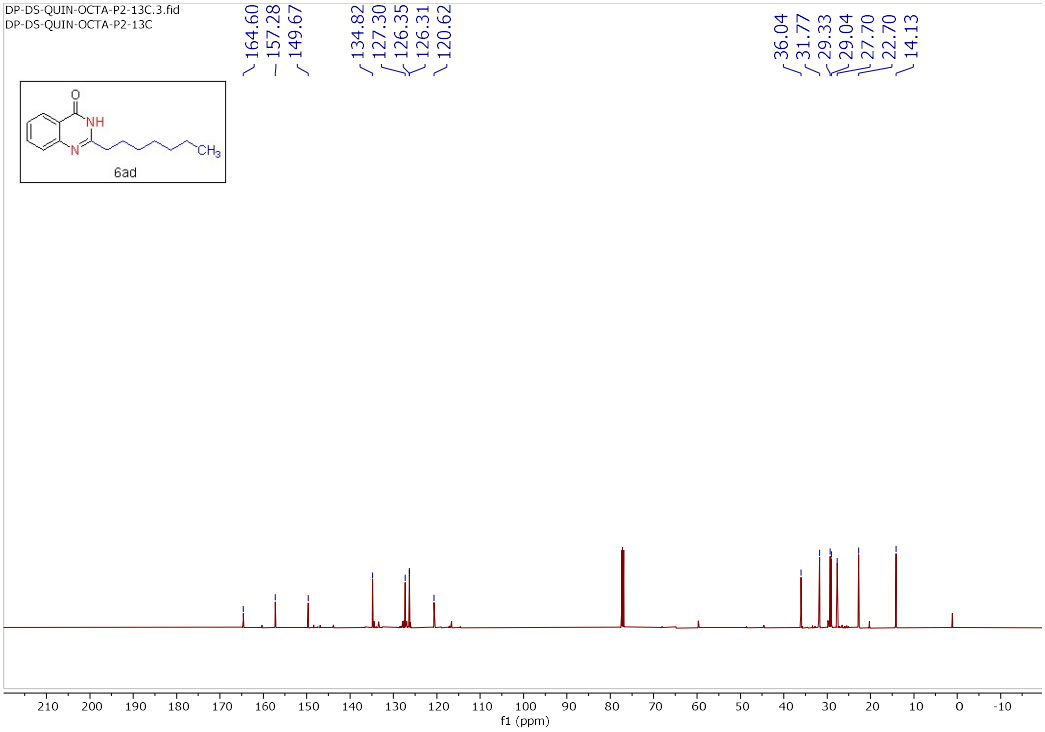


Figure S63. ^{13}C NMR Spectrum of 2-heptylquinazolin-4(3H)-one **(6ad)** in $CDCl_3$.

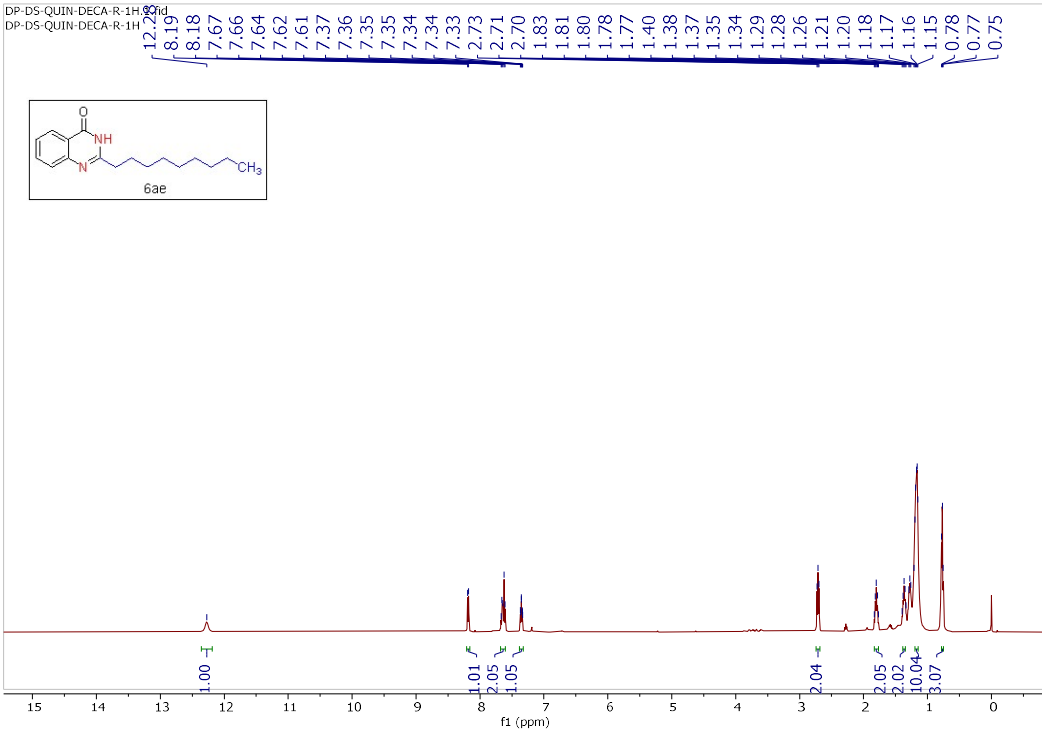


Figure S64. ^{1}H NMR Spectrum of 2-nonylquinazolin-4(3H)-one **(6ae)** in $CDCl_3$.

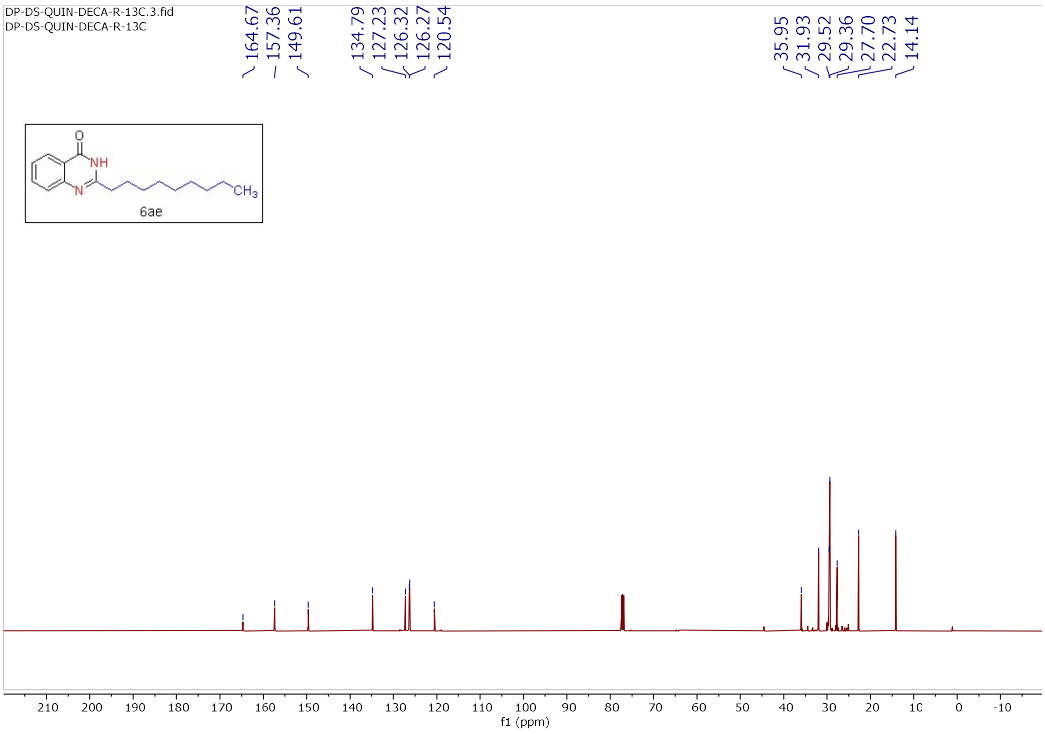


Figure S65. ^{13}C NMR Spectrum of 2-nonylquinazolin-4(3H)-one **(6ae)** in $CDCl_3$.

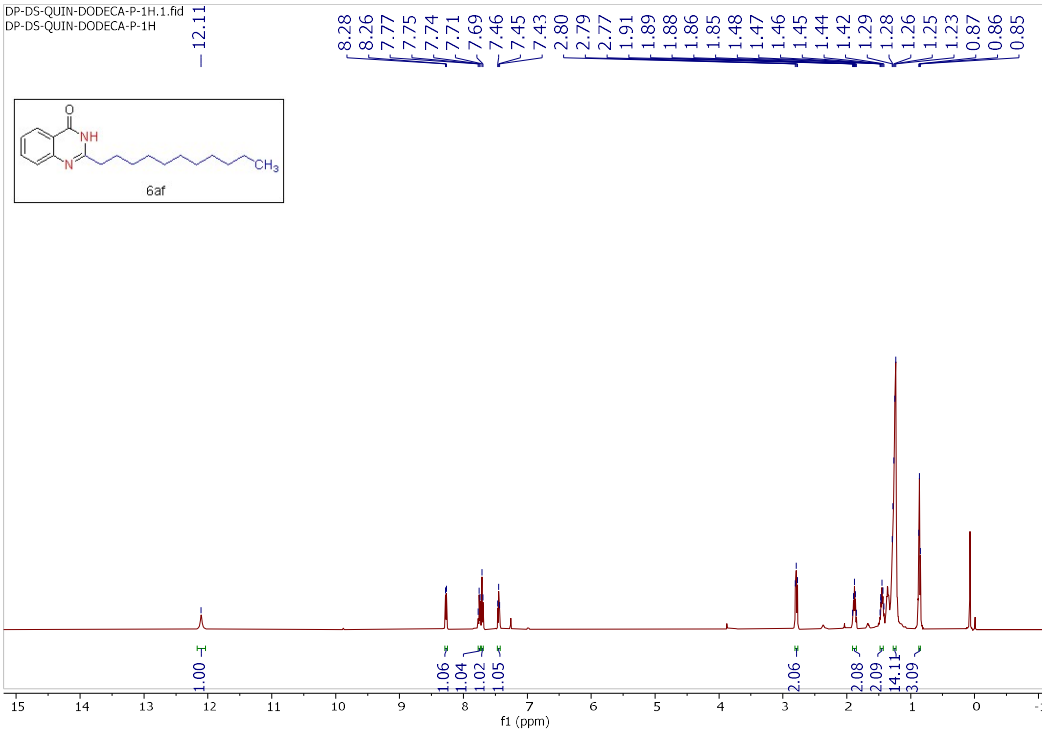


Figure S66. ^{1}H NMR Spectrum of 2-undecylquinazolin-4(3H)-one **(6af)** in $CDCl_3$.

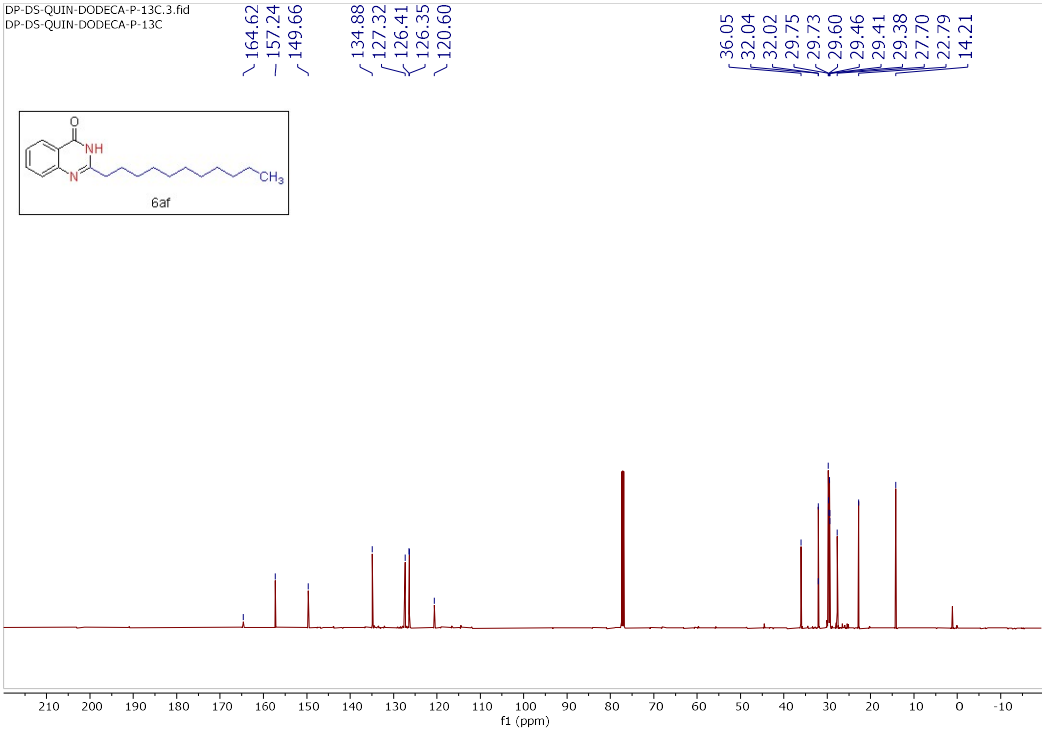


Figure S67. ^{13}C NMR Spectrum of 2-undecylquinazolin-4(3H)-one **(6af)** in $CDCl_3$.

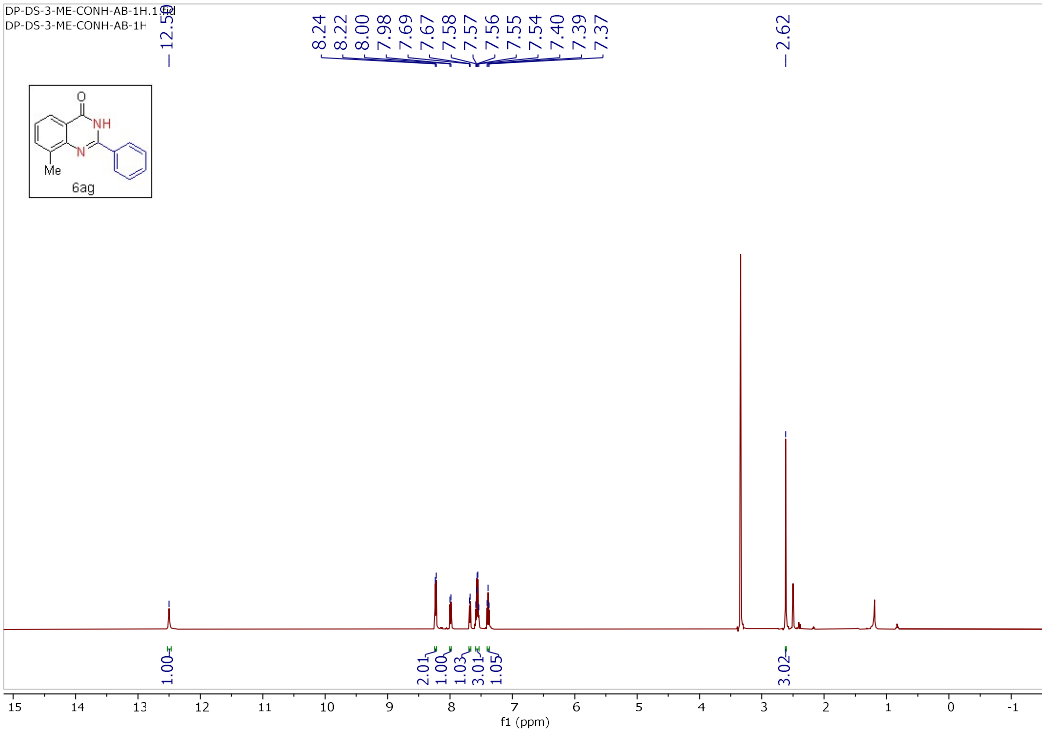


Figure S68. ^{1}H NMR Spectrum of 8-methyl-2-phenylquinazolin-4(3H)-one **(6ag)** in DMSO-d_6.

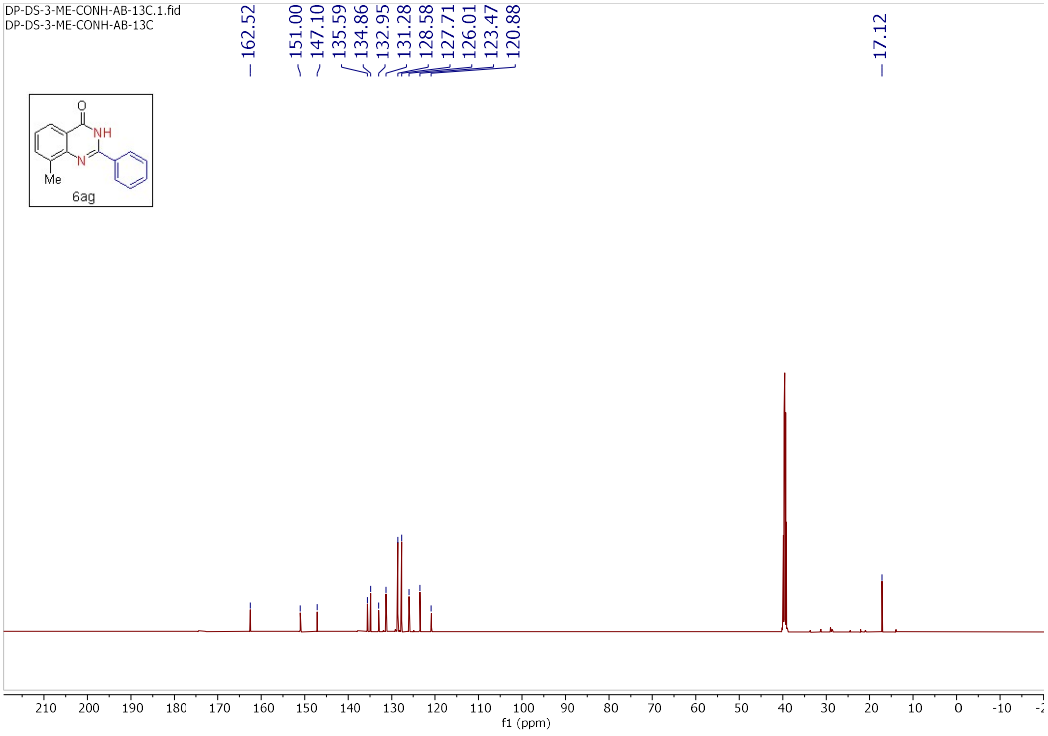


Figure S69. ^{13}C NMR Spectrum of 8-methyl-2-phenylquinazolin-4(3H)-one **(6ag)** in DMSO-d_6.

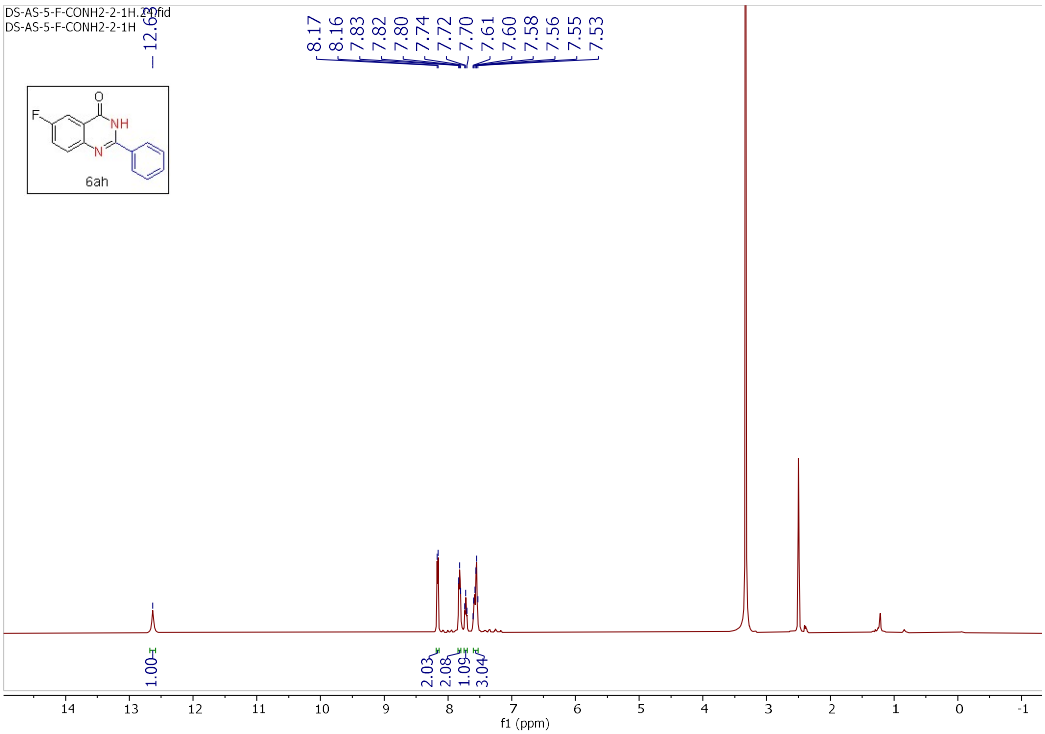


Figure S70. ^{1}H NMR Spectrum of 6-fluoro-2-phenylquinazolin-4(3H)-one **(6ah)** in DMSO-d_6.

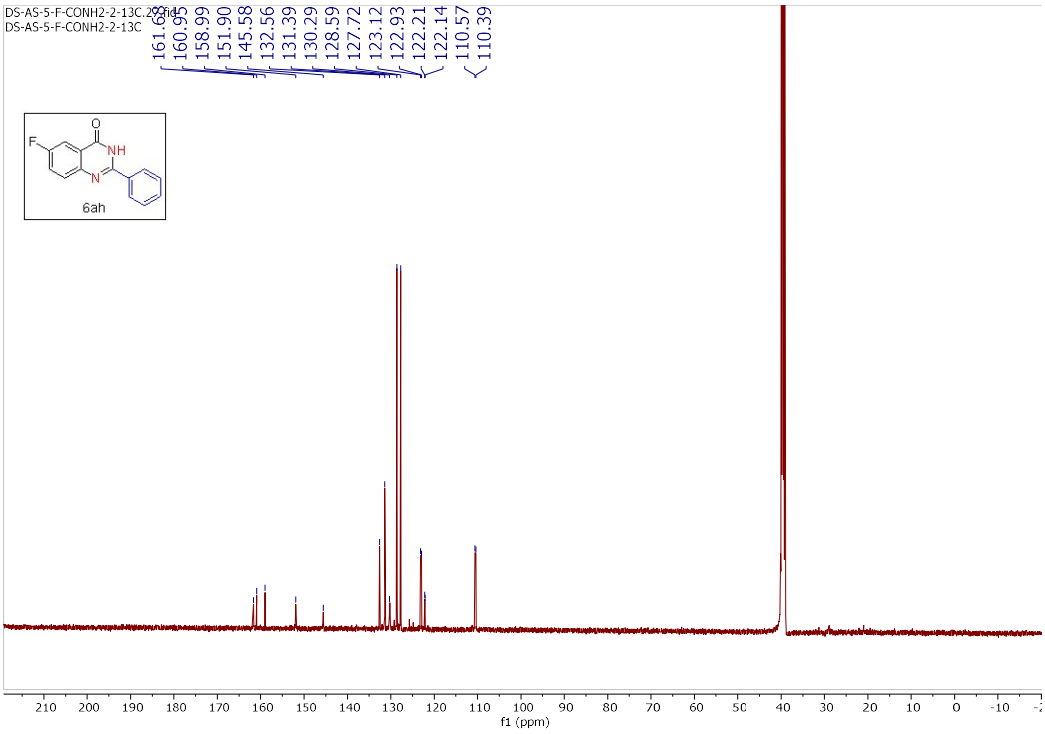


Figure S71. ^{13}C NMR Spectrum of 6-fluoro-2-phenylquinazolin-4(3H)-one **(6ah)** in DMSO-d_6.

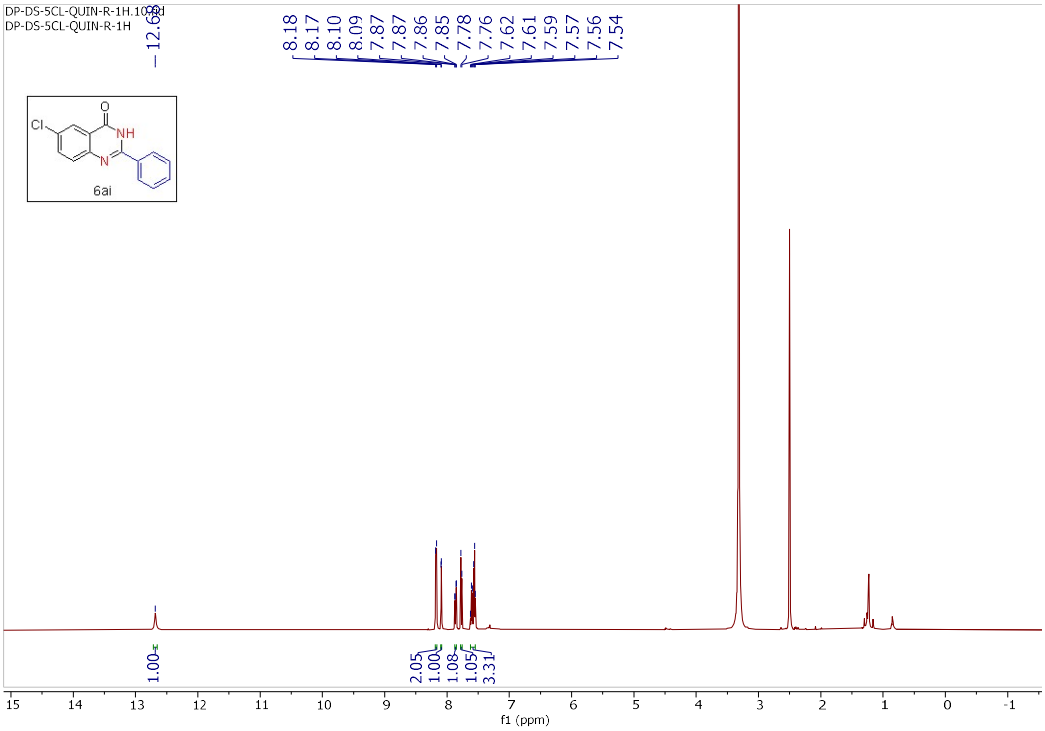


Figure S72. ^{1}H NMR Spectrum of 6-chloro-2-phenylquinazolin-4(3H)-one **(6ai)** in DMSO-d_6.

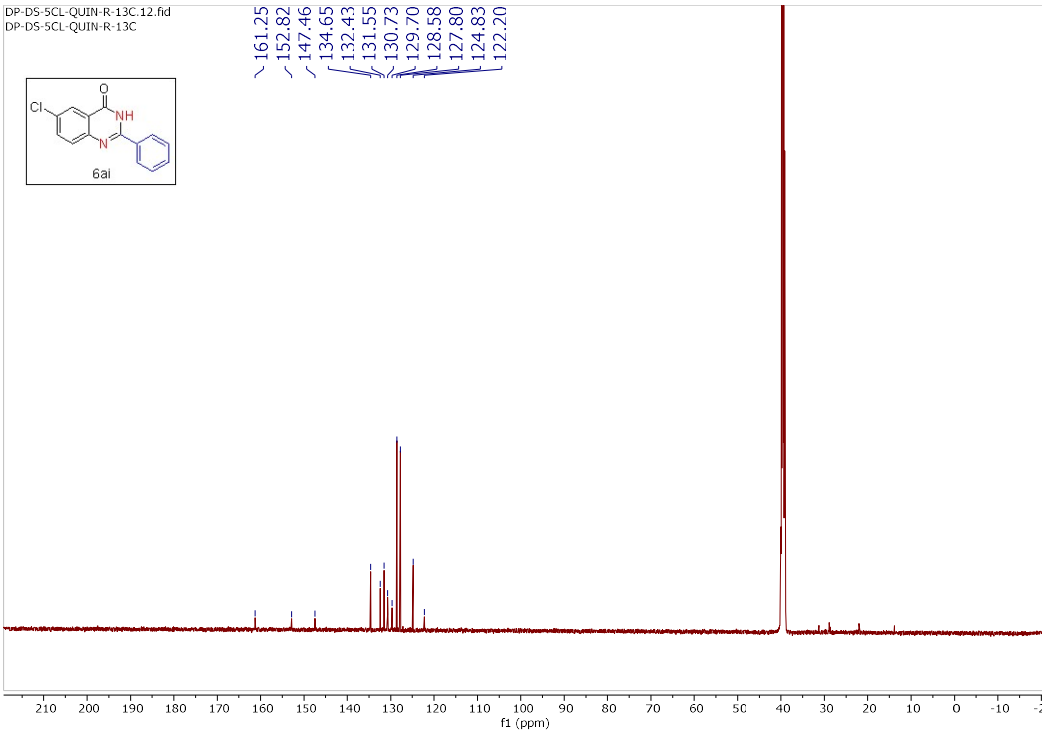


Figure S73. ^{13}C NMR Spectrum of 6-chloro-2-phenylquinazolin-4(3H)-one **(6ai)** in DMSO-d_6.

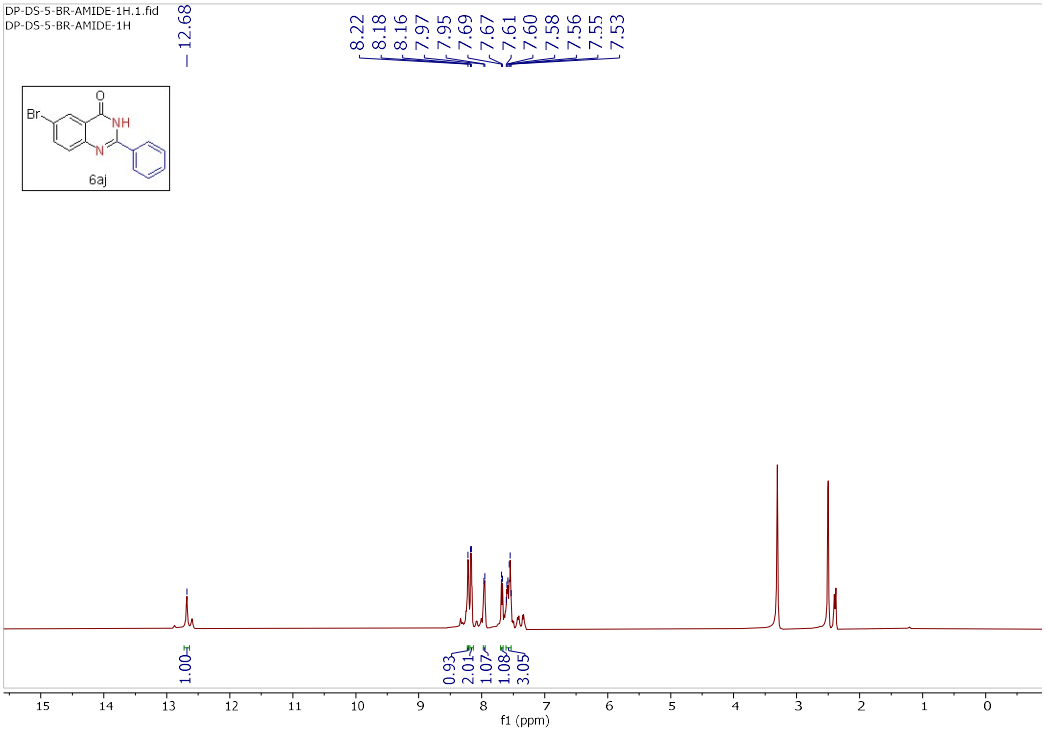


Figure S74. ^{1}H NMR Spectrum of 6-bromo-2-phenylquinazolin-4(3H)-one **(6aj)** in DMSO-d_6.

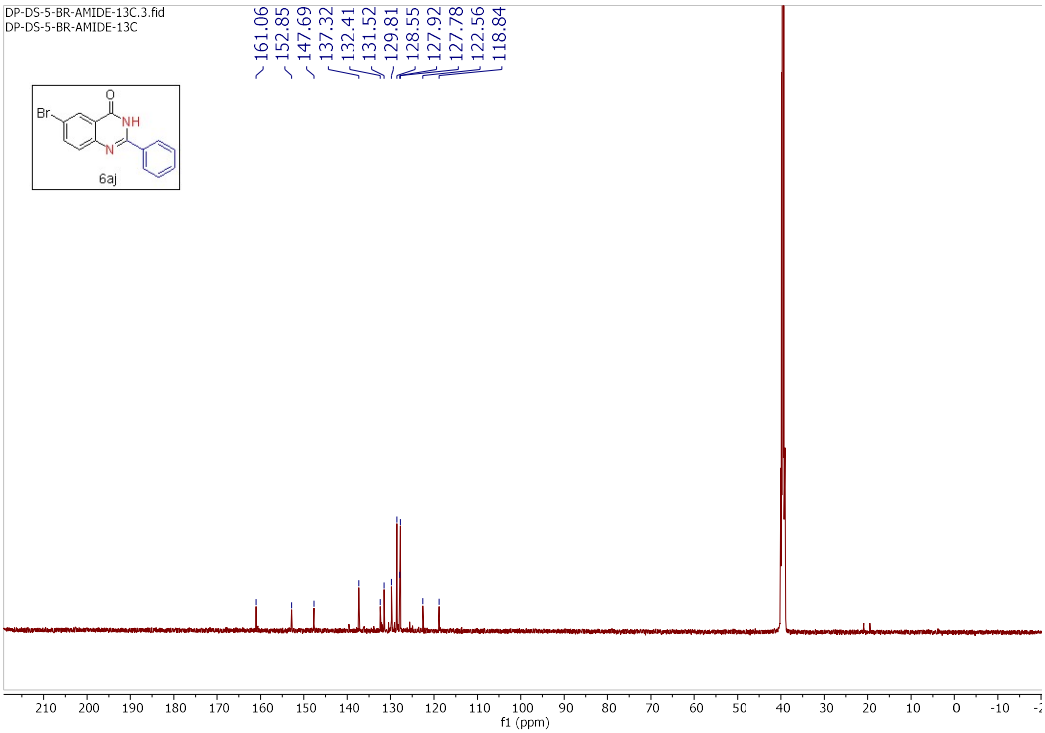


Figure S75. ^{13}C NMR Spectrum of 6-bromo-2-phenylquinazolin-4(3H)-one **(6aj)** in DMSO-d_6.

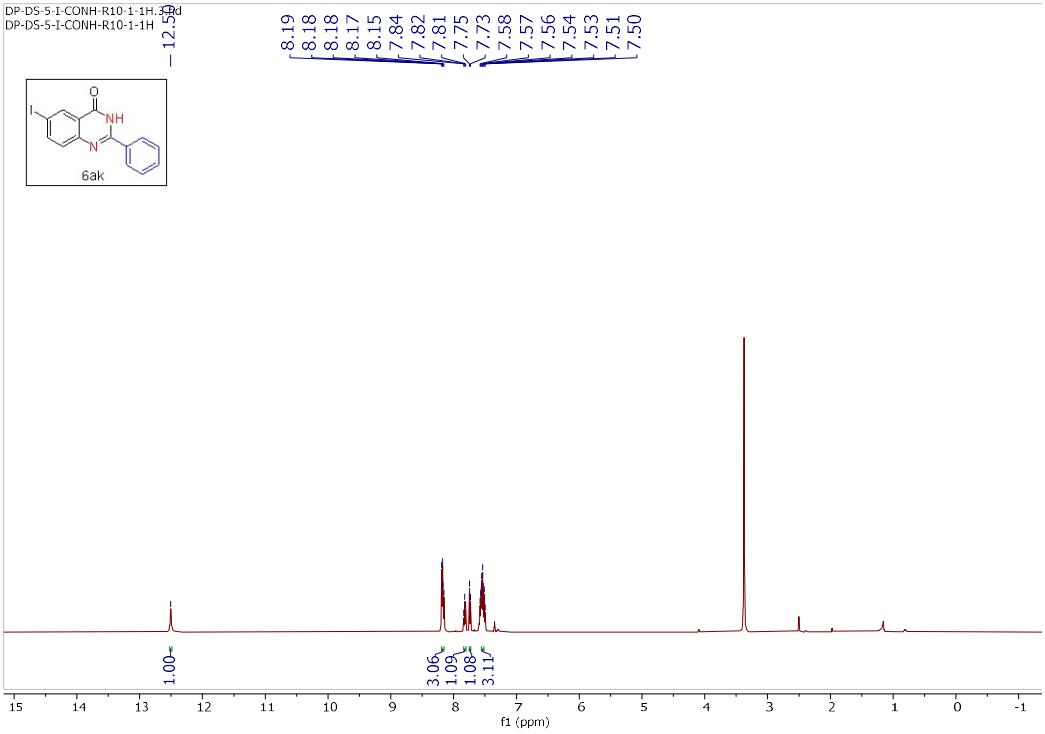


Figure S76. ^{1}H NMR Spectrum of 6-iodo-2-phenylquinazolin-4(3H)-one **(6ak)** in DMSO-d_6.

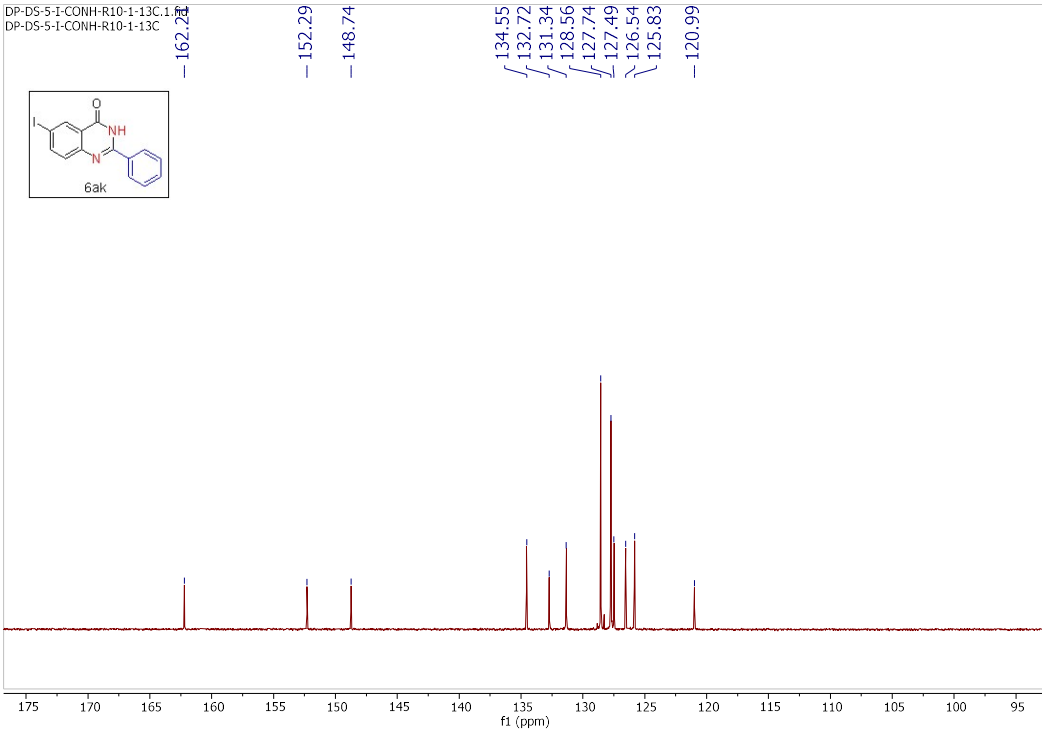


Figure S77. ^{13}C NMR Spectrum of 6-iodo-2-phenylquinazolin-4(3H)-one **(6ak)** in DMSO-d_6.

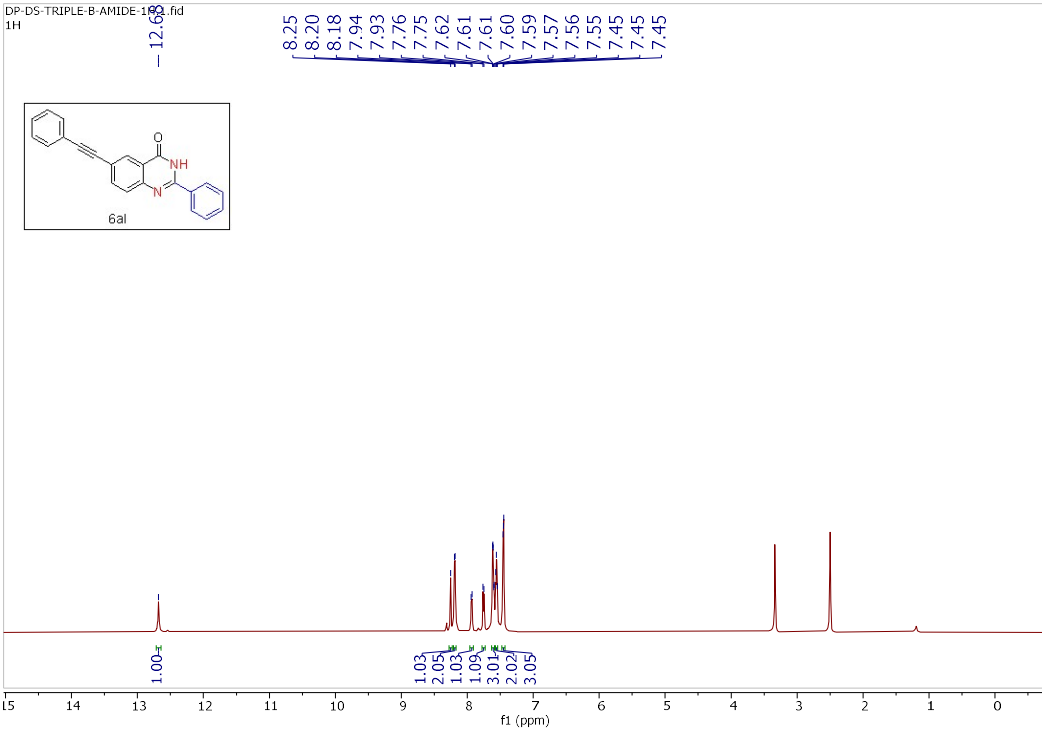


Figure S78. ^{1}H NMR Spectrum of 2-phenyl-6-(phenylethynyl)quinazolin-4(3H)-one **(6al)** in DMSO-d_6.

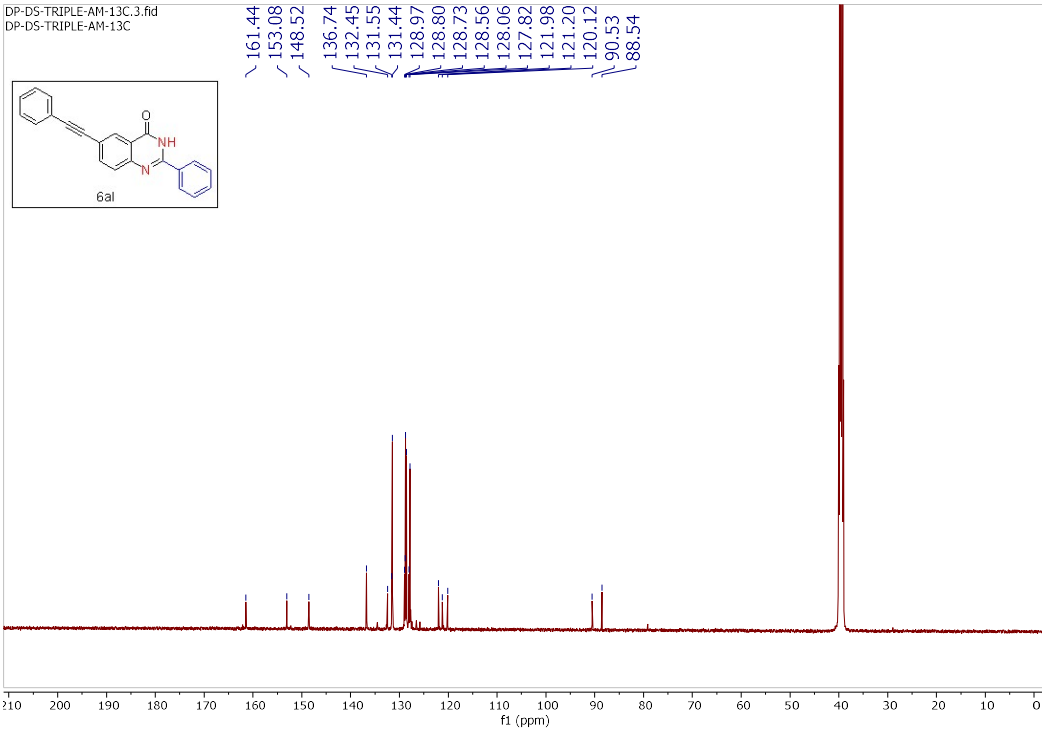


Figure S79. ^{13}C NMR Spectrum of 2-phenyl-6-(phenylethynyl)quinazolin-4(3H)-one **(6al)** in DMSO-d_6.

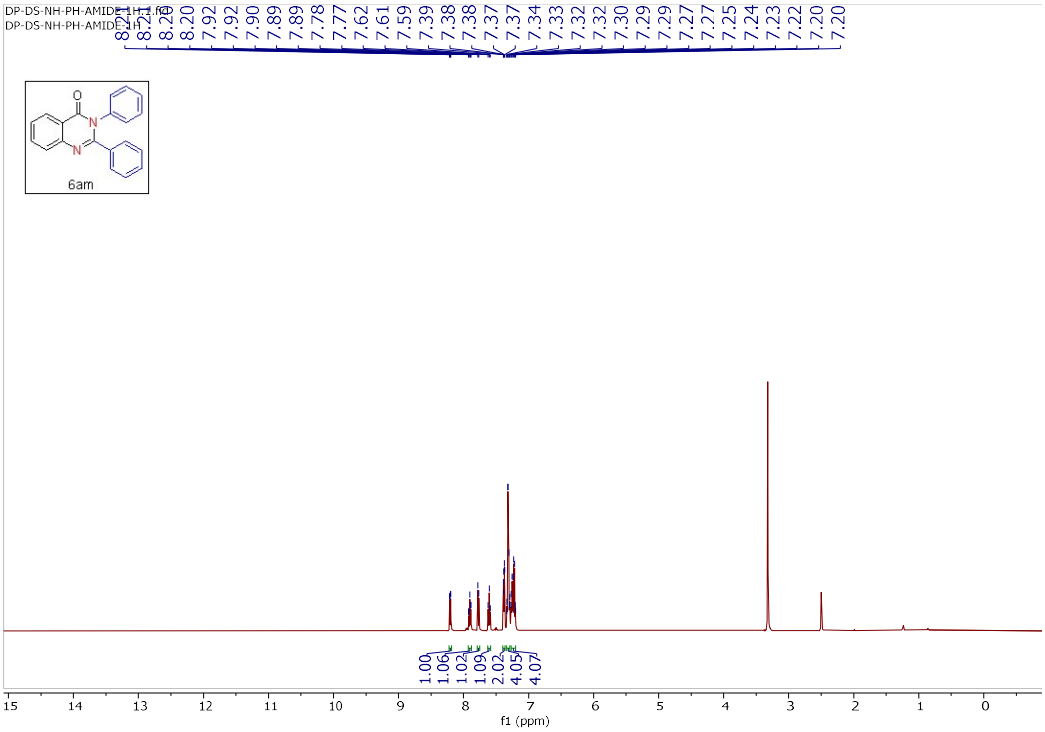


Figure S80. ^{1}H NMR Spectrum of 2,3-diphenylquinazolin-4(3H)-one **(6am)** in DMSO-d_6.

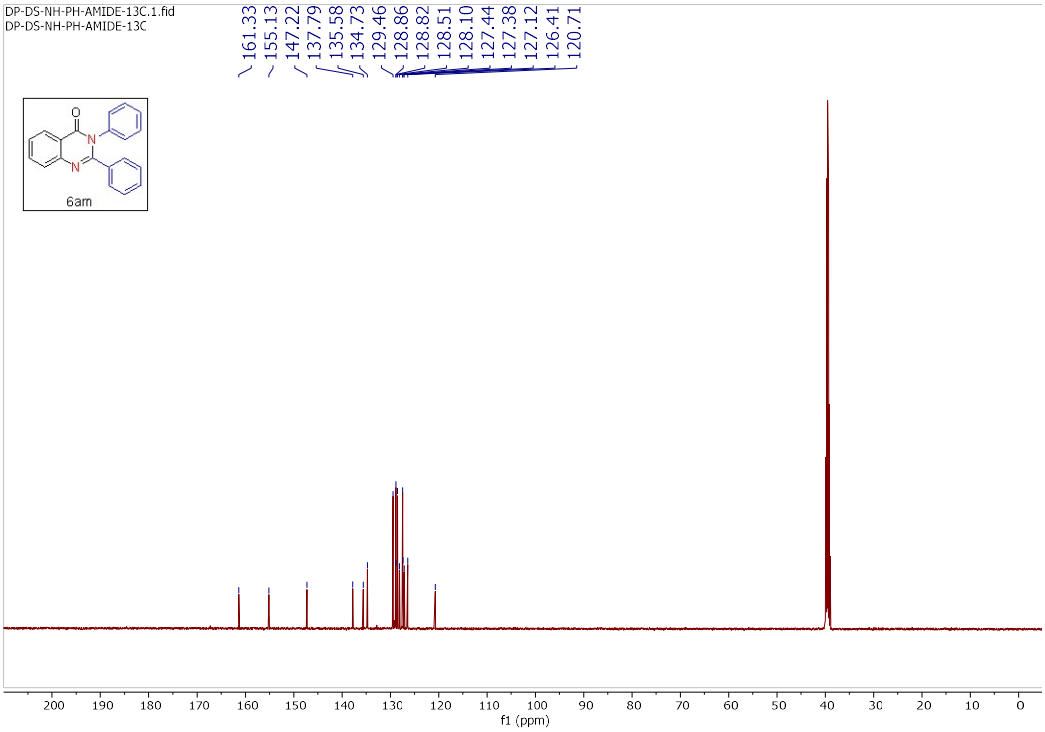


Figure S81. ^{13}C NMR Spectrum of 2,3-diphenylquinazolin-4(3H)-one **(6am)** in DMSO-d_6.

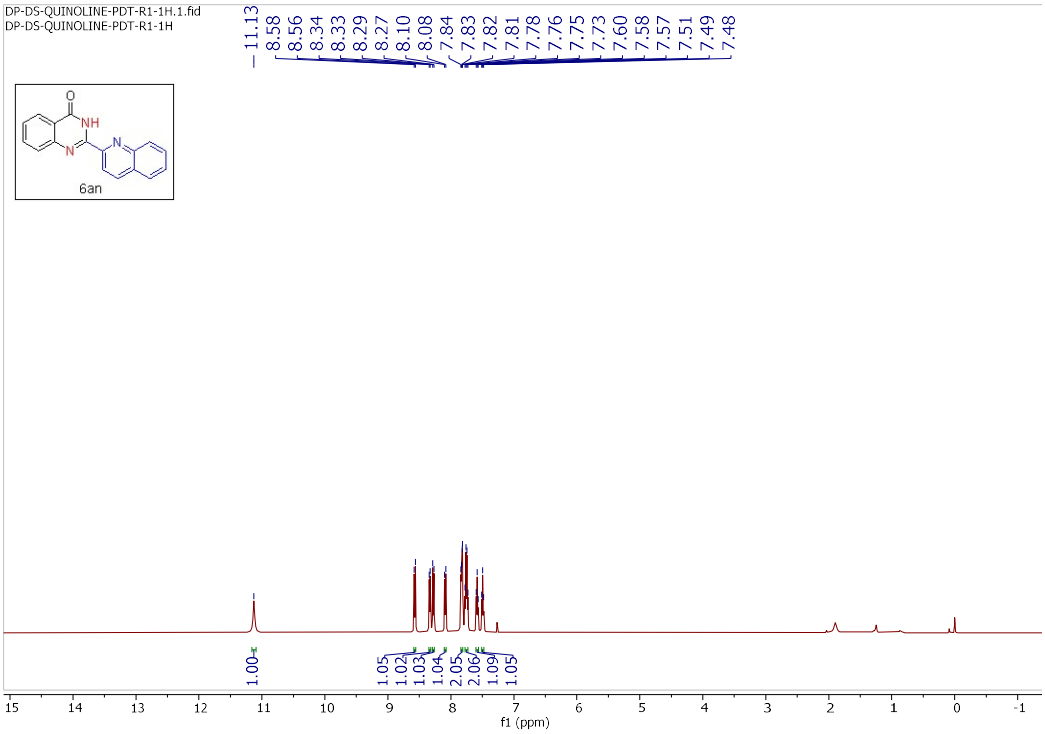


Figure S82. ^{1}H NMR Spectrum of 2-(quinolin-2-yl)quinazolin-4(3H)-one **(6an)** in $CDCl_3$.

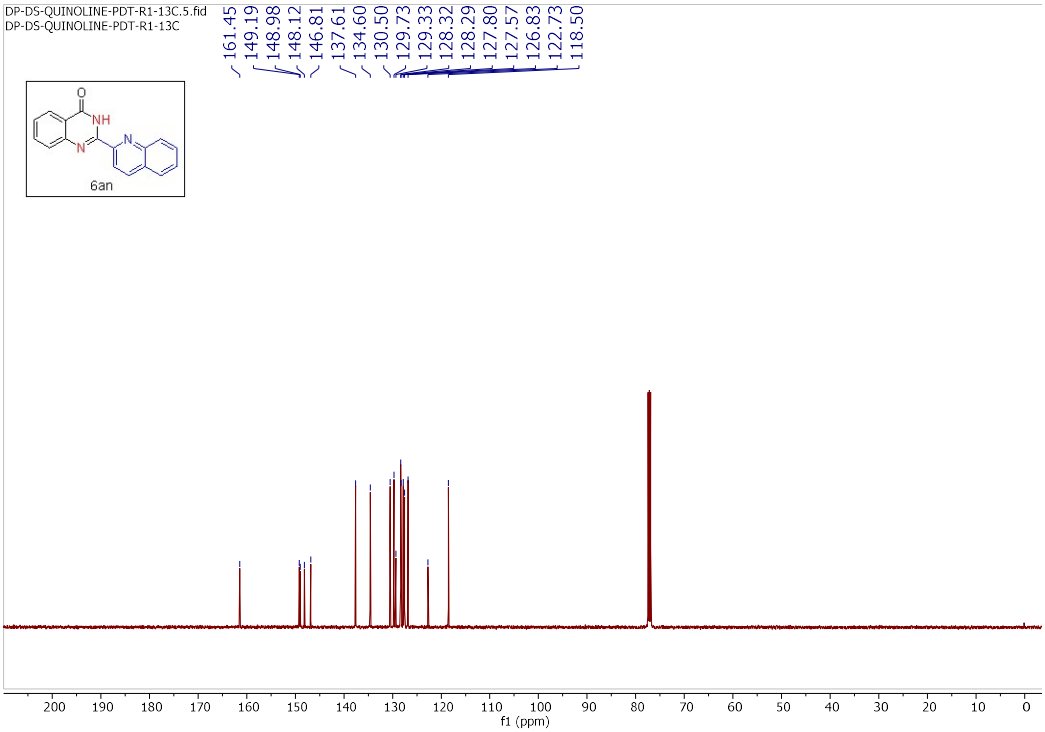


Figure S83. ^{13}C NMR Spectrum of 2-(quinolin-2-yl)quinazolin-4(3H)-one **(6an)** in $CDCl_3$.

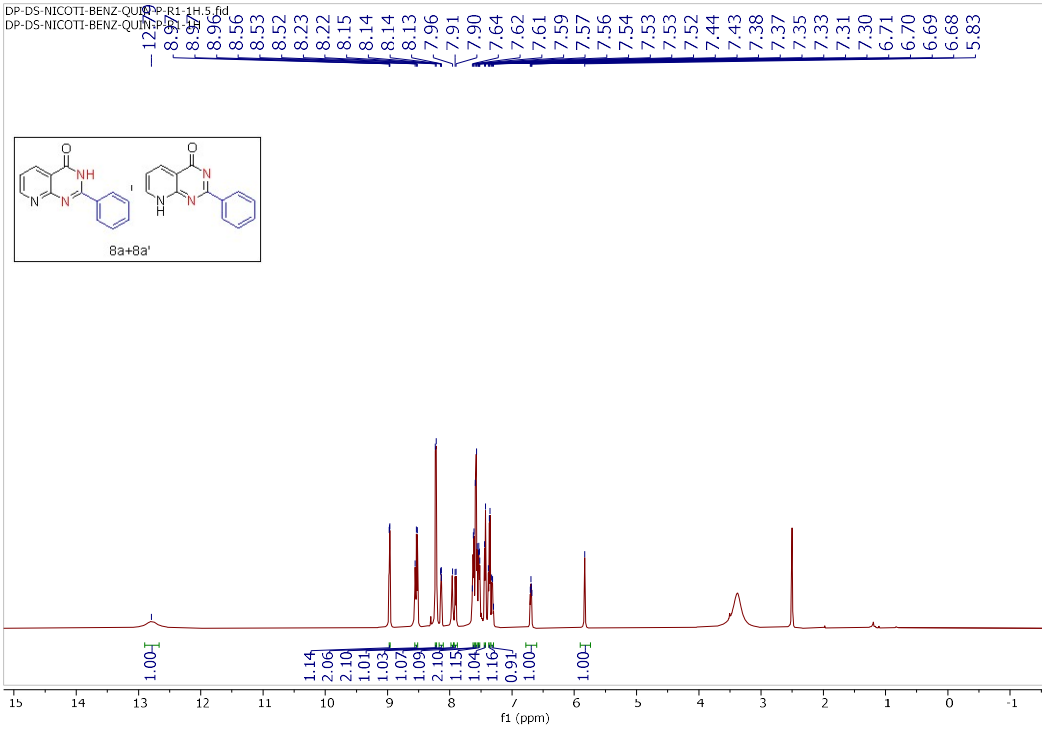


Figure S84. ^{1}H NMR Spectrum of 2-phenylpyrido[2,3-d]pyrimidin-4(3H)-one and 2-phenylpyrido[2,3-d]pyrimidin-4(8H)-one **(8a+8a')** in DMSO-d_6.

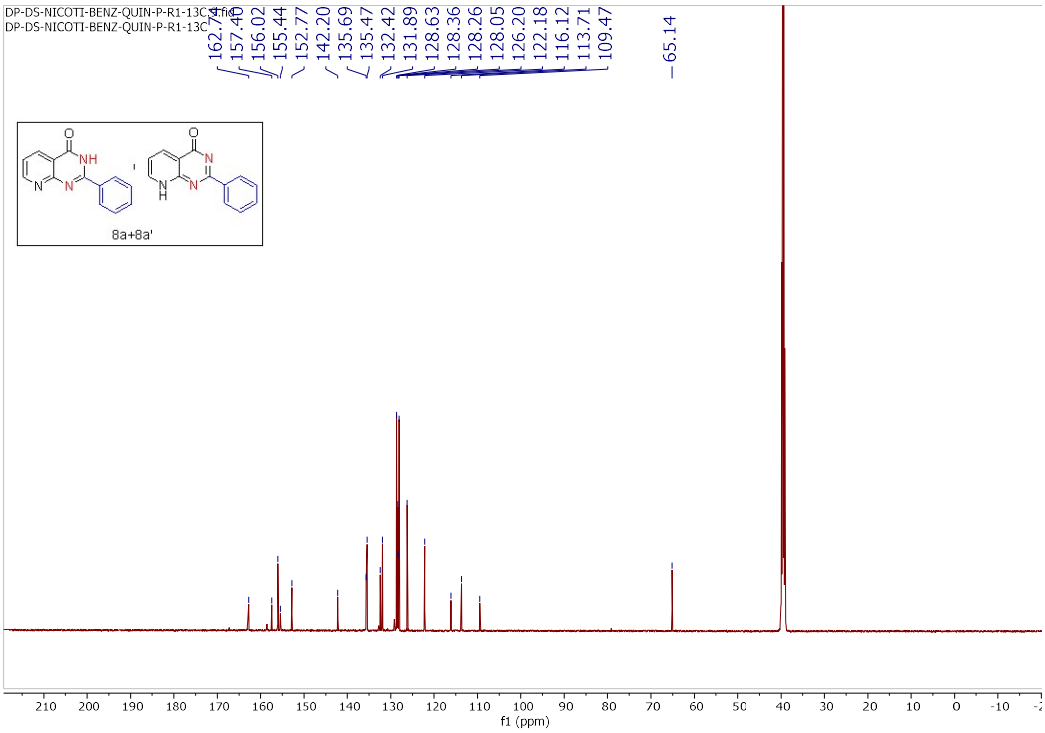


Figure S85. ^{13}C NMR Spectrum of 2-phenylpyrido[2,3-d]pyrimidin-4(3H)-one and 2-phenylpyrido[2,3-d]pyrimidin-4(8H)-one **(8a+8a')** in DMSO-d_6.

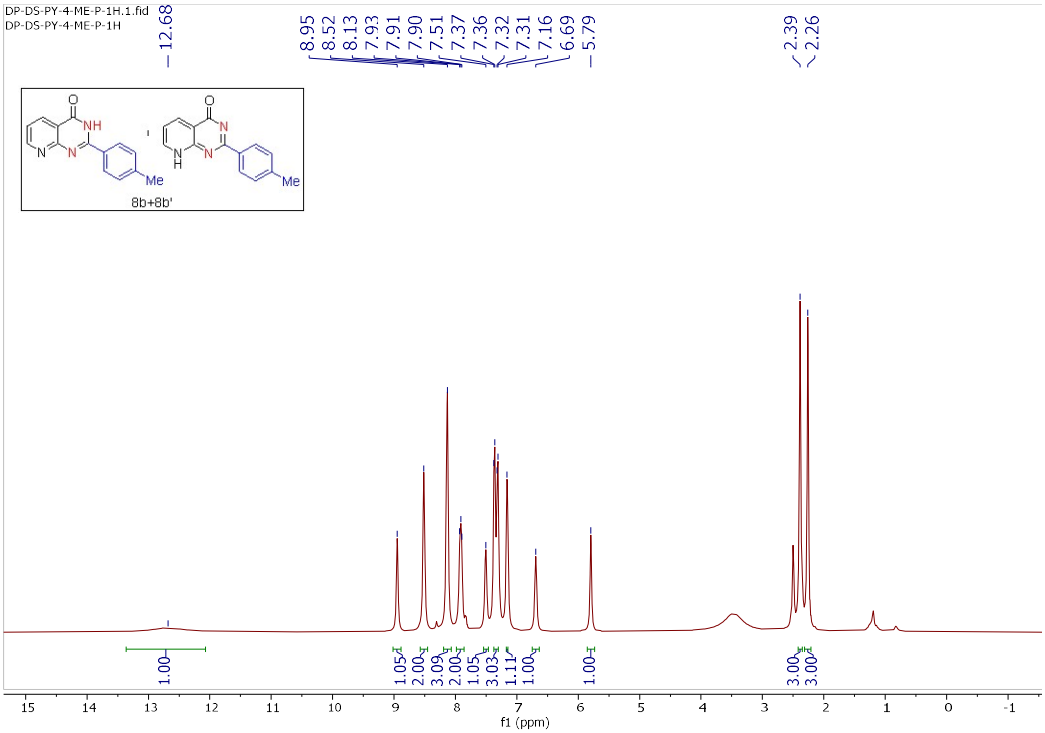


Figure S86. ^{1}H NMR Spectrum of 2-(p-tolyl)pyrido[2,3-d]pyrimidin-4(3H)-one and 2-(p-tolyl)pyrido[2,3-d]pyrimidin-4(8H)-one **(8b+8b')** in DMSO-d_6.

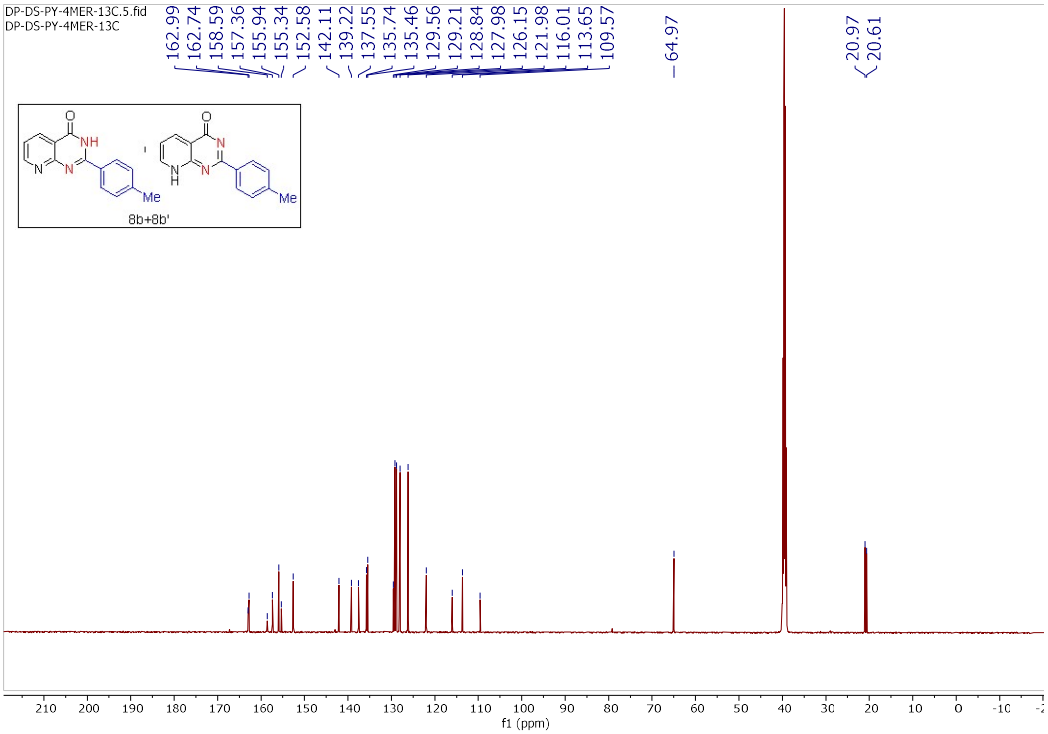


Figure S87. ^{13}C NMR Spectrum of 2-(p-tolyl)pyrido[2,3-d]pyrimidin-4(3H)-one and 2-(p-tolyl)pyrido[2,3-d]pyrimidin-4(8H)-one **(8b+8b')** in DMSO-d_6.

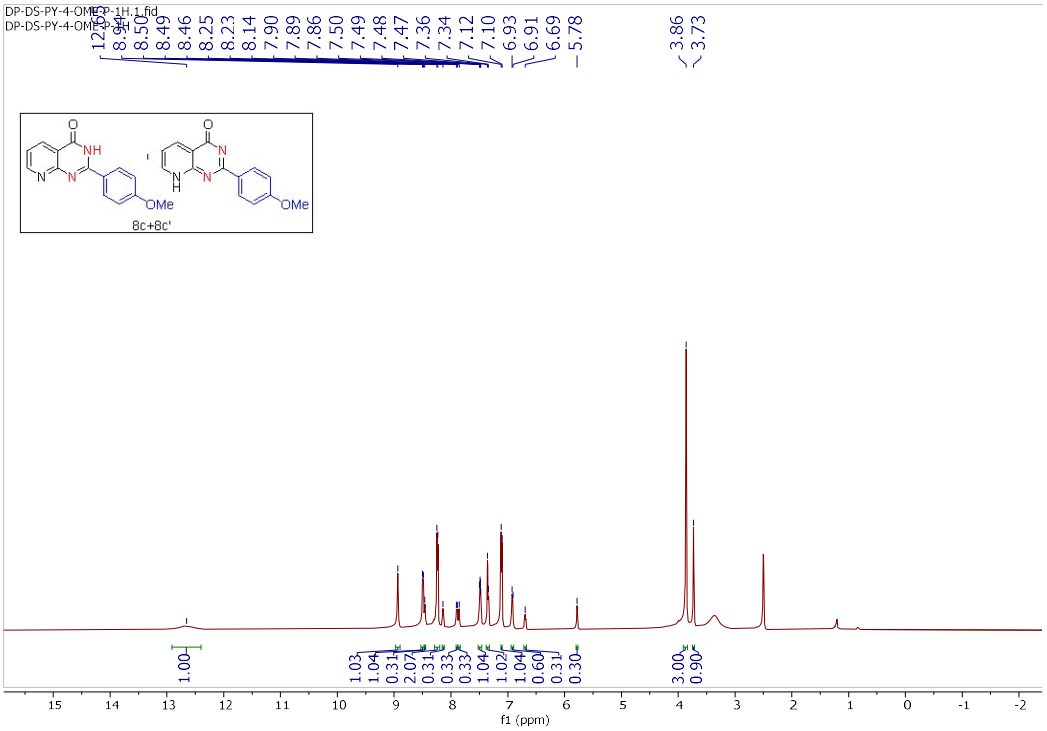


Figure S88. ^{1}H NMR Spectrum of 2-(4-methoxyphenyl)pyrido[2,3-d]pyrimidin-4(3H)-one and 2-(4-methoxyphenyl)pyrido[2,3-d]pyrimidin-4(8H)-one **(8c+8c')** in DMSO-d_6.

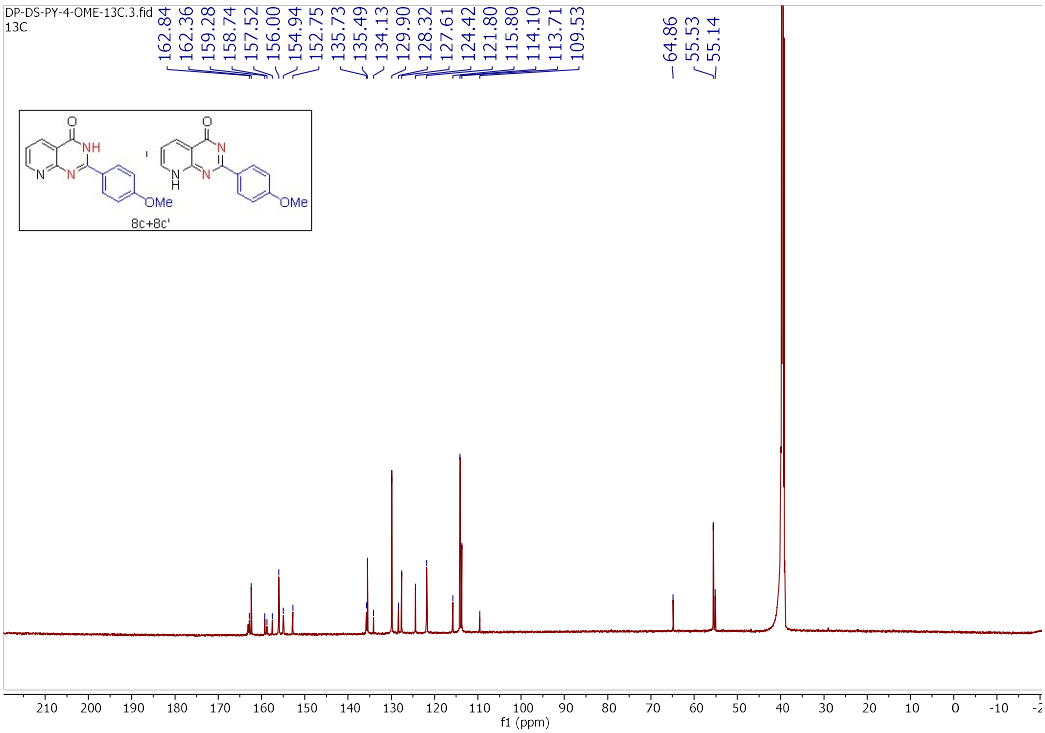


Figure S89. ^{13}C NMR Spectrum of 2-(4-methoxyphenyl)pyrido[2,3-d]pyrimidin-4(3H)-one and 2-(4-methoxyphenyl)pyrido[2,3-d]pyrimidin-4(8H)-one **(8c+8c')** in DMSO-*d*$_6$.

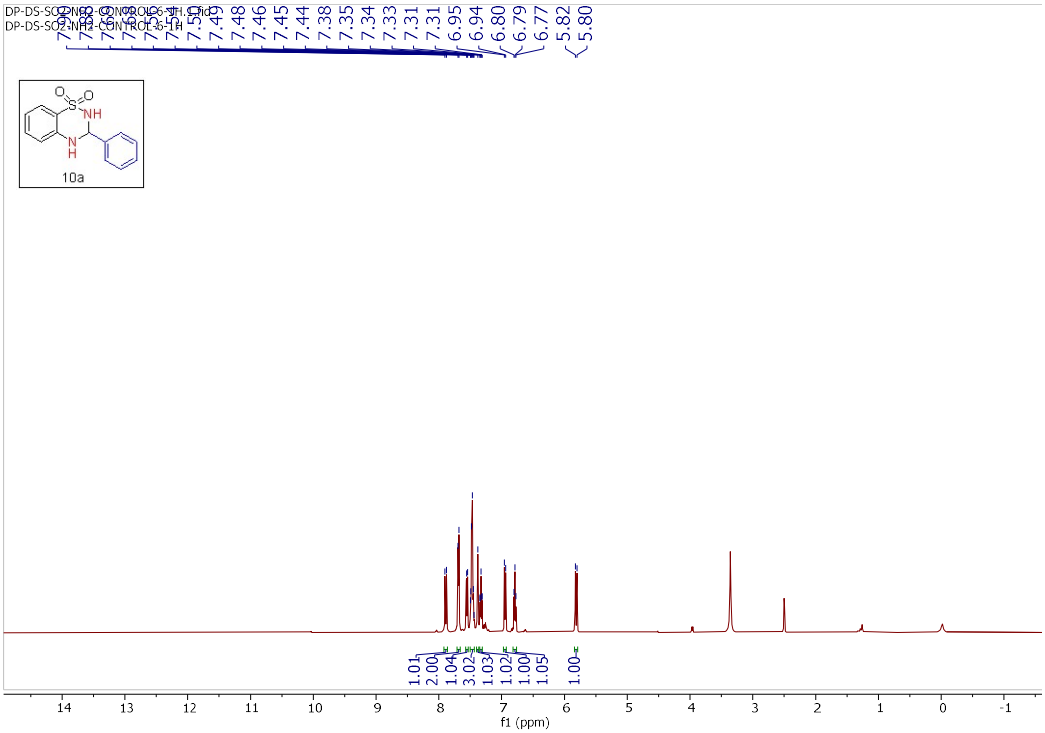


Figure S90. ^{1}H NMR Spectrum of 3-phenyl-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide **(10a)** in DMSO-*d*$_6$.

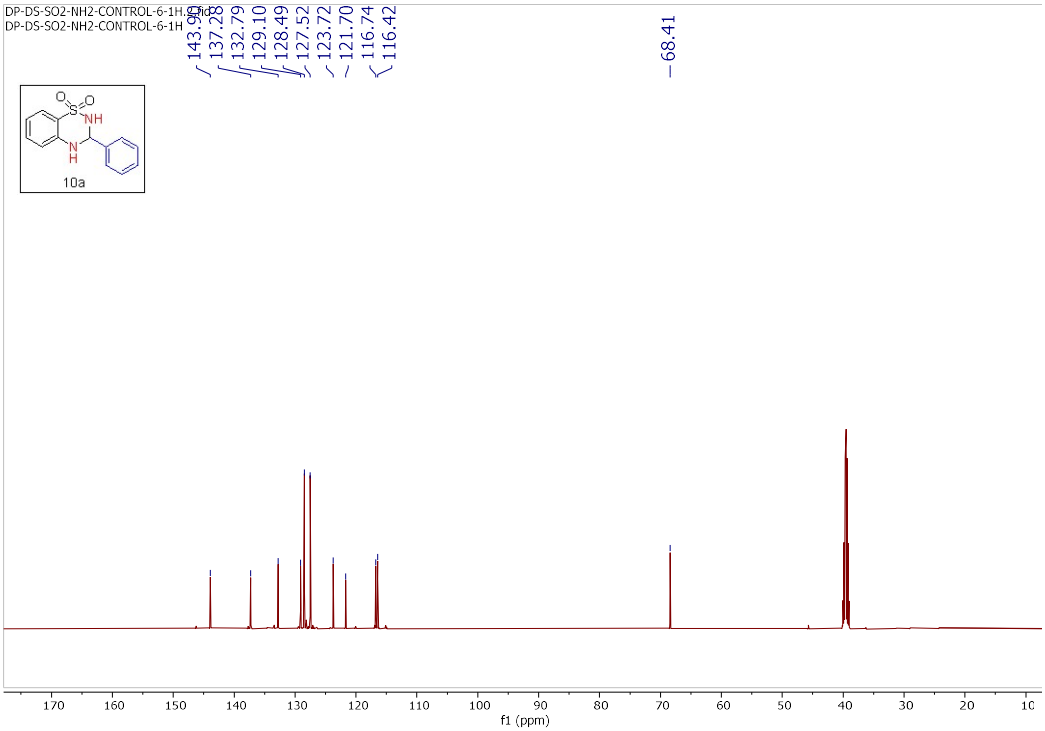


Figure S91. ^{13}C NMR Spectrum of 3-phenyl-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide **(10a)** in DMSO-d_6.

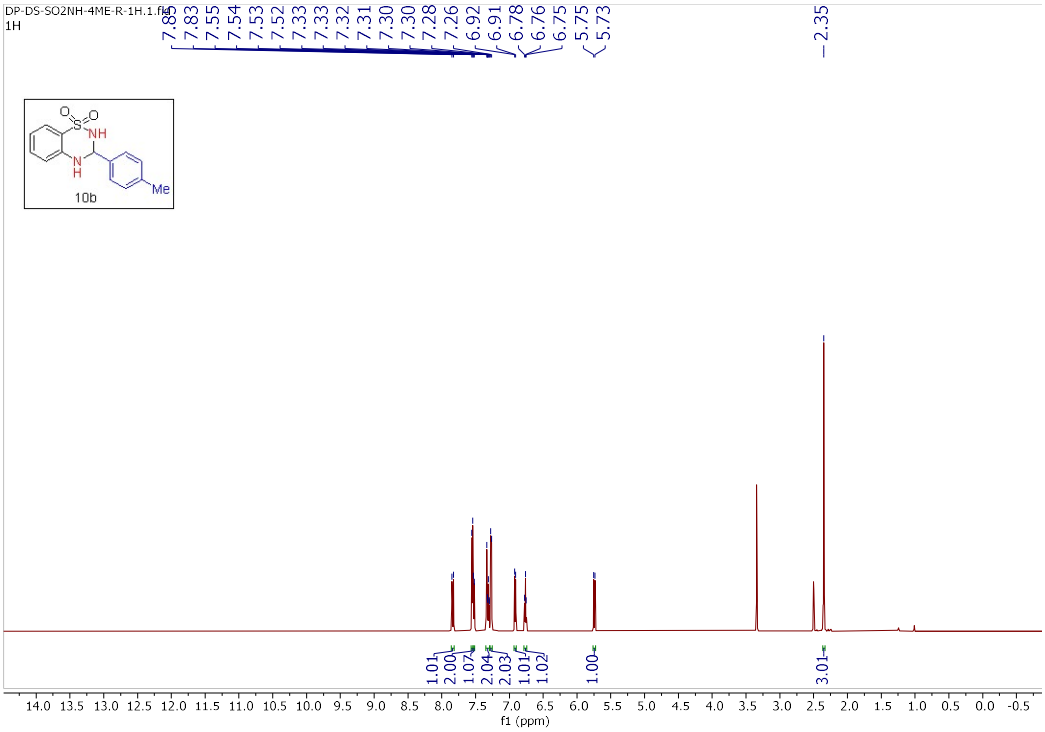


Figure S92. ^{1}H NMR Spectrum of 3-(p-tolyl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide **(10b)** in DMSO-d_6.

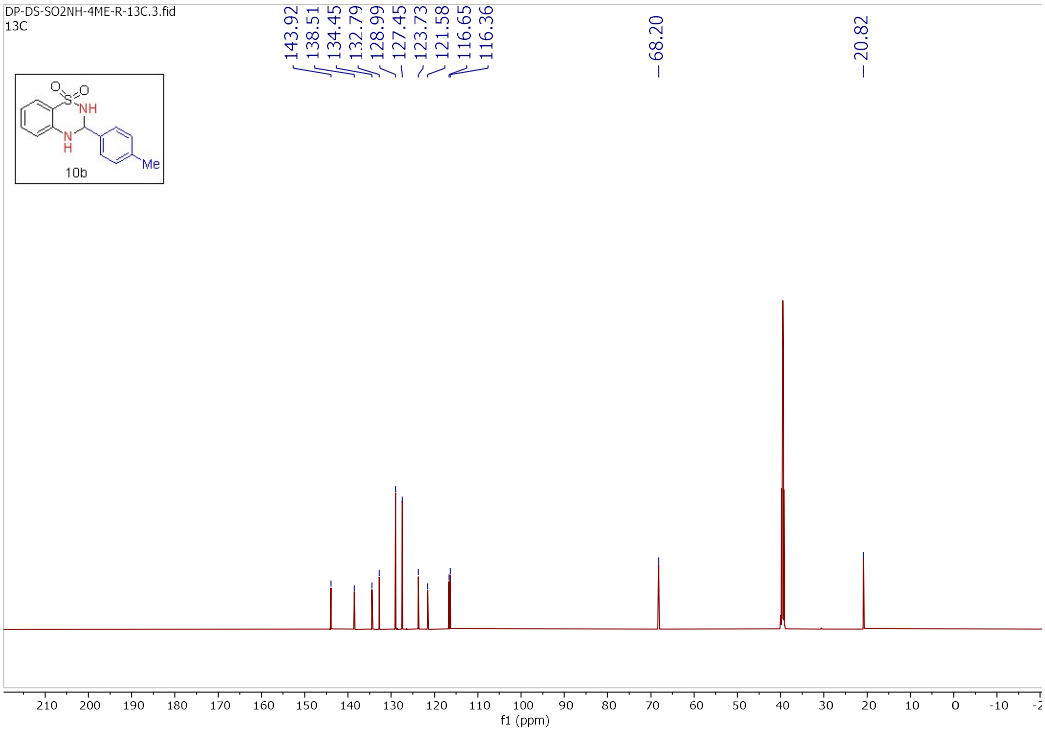


Figure S93. ^{13}C NMR Spectrum of 3-(p-tolyl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide **(10b)** in DMSO-d_6.

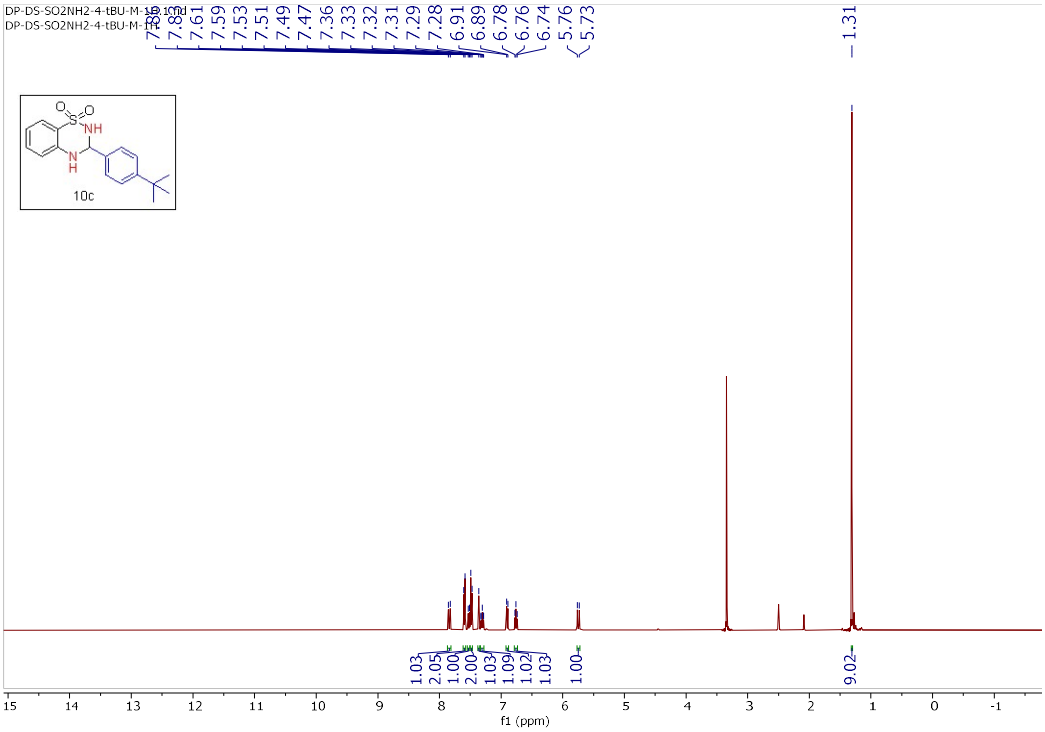


Figure S94. ^{1}H NMR Spectrum of 3-(4-(tert-butyl)phenyl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide **(10c)** in DMSO-d_6.

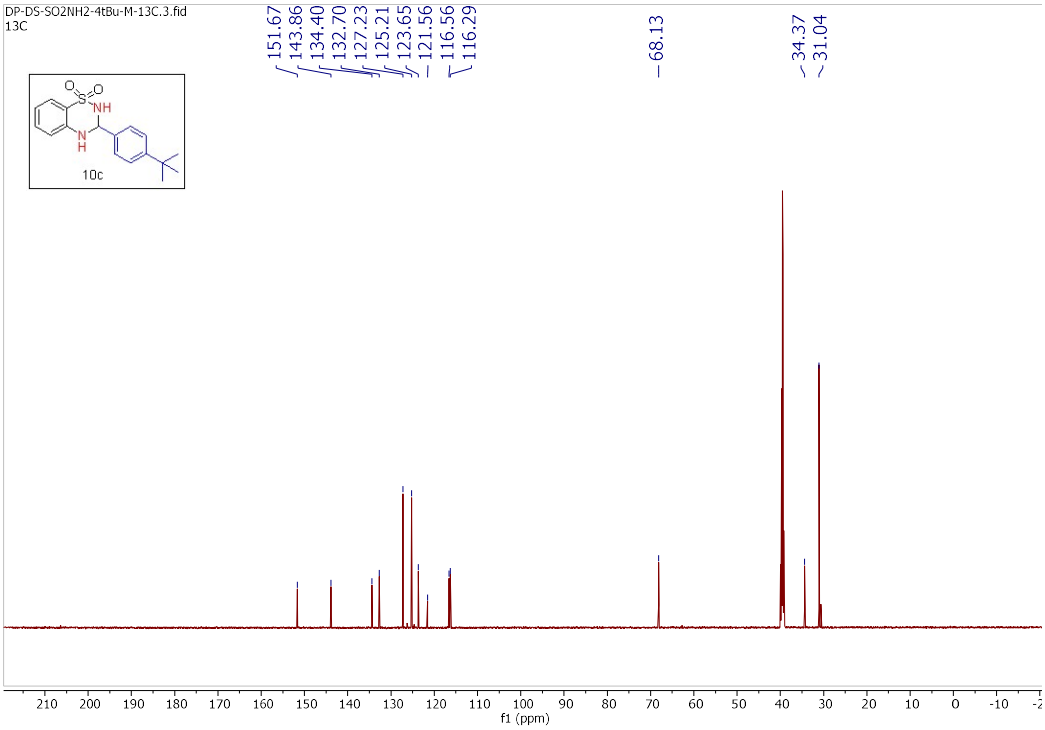


Figure S95. ^{13}C NMR Spectrum of 3-(4-(tert-butyl)phenyl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide **(10c)** in DMSO-d_6.

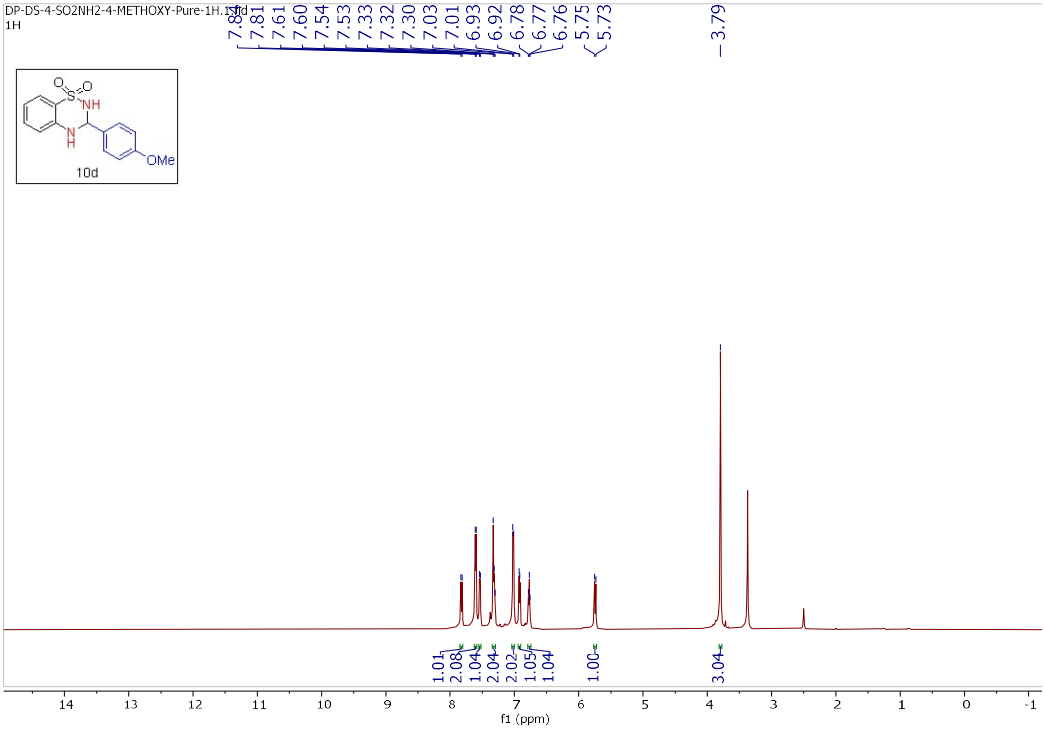


Figure S96. ^{1}H NMR Spectrum of 3-(4-methoxyphenyl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide **(10d)** in DMSO-d_6.

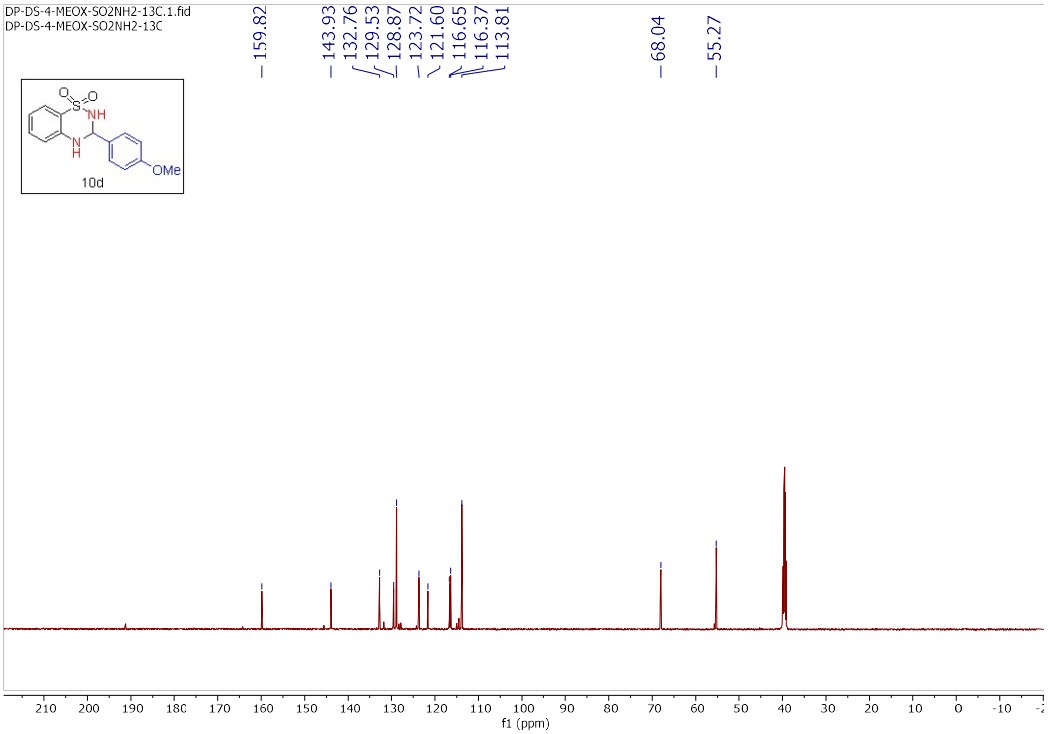


Figure S97. ^{13}C NMR Spectrum of 3-(4-methoxyphenyl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide **(10d)** in DMSO-d_6.

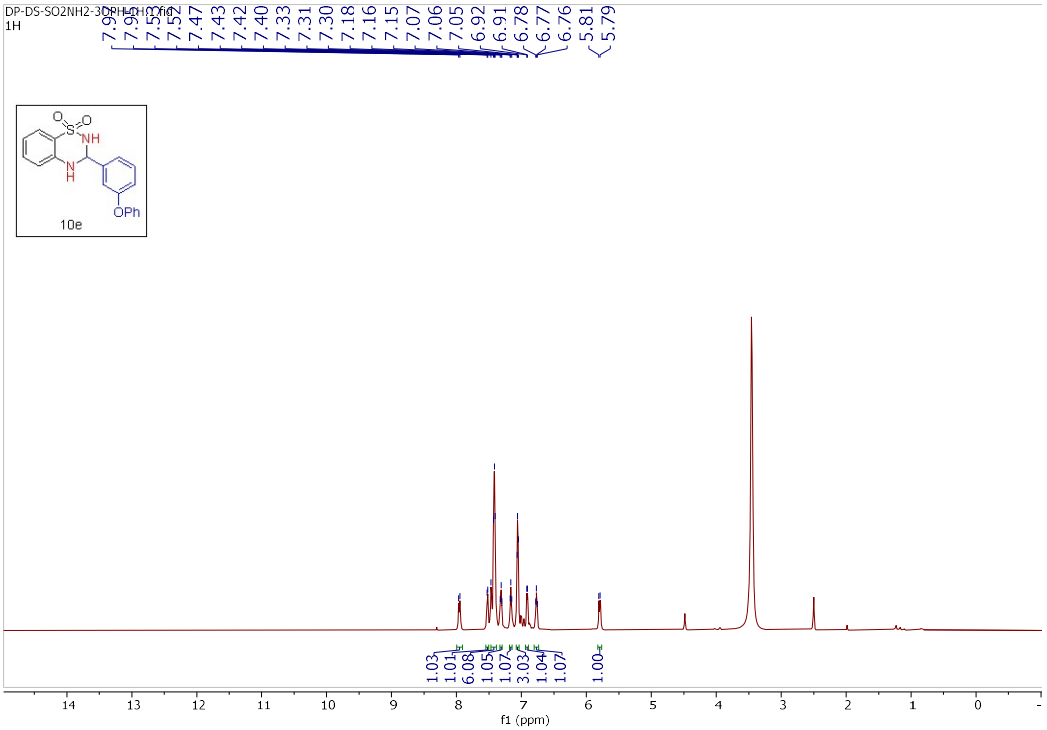


Figure S98. ^{1}H NMR Spectrum of 3-(3-phenoxyphenyl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide **(10e)** in DMSO-d_6.

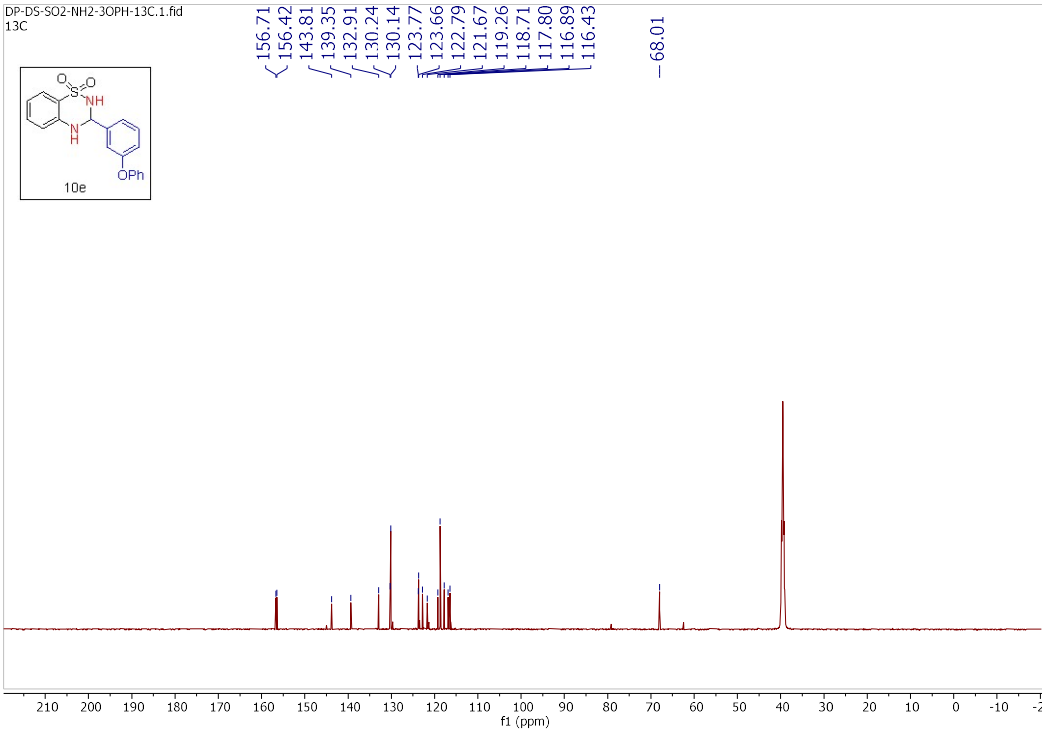


Figure S99. ^{13}C NMR Spectrum of 3-(3-phenoxyphenyl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide **(10e)** in DMSO-d_6.

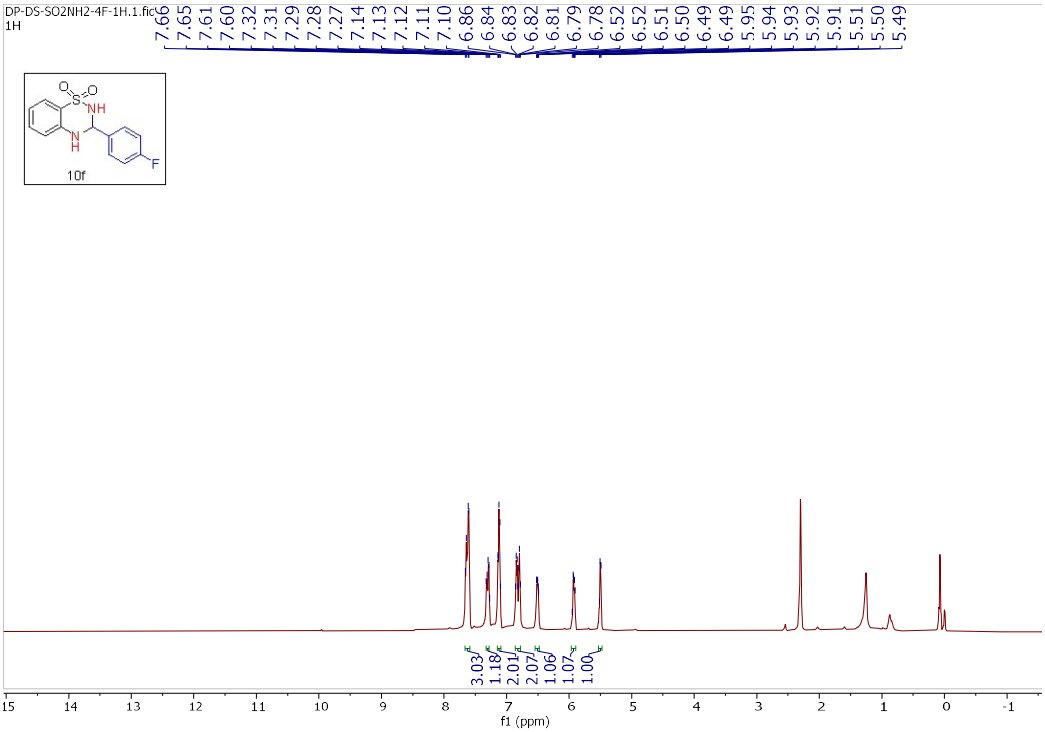


Figure S100. ^{1}H NMR Spectrum of 3-(4-fluorophenyl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide **(10f)** in $CDCl_3$ + DMSO-d_6.

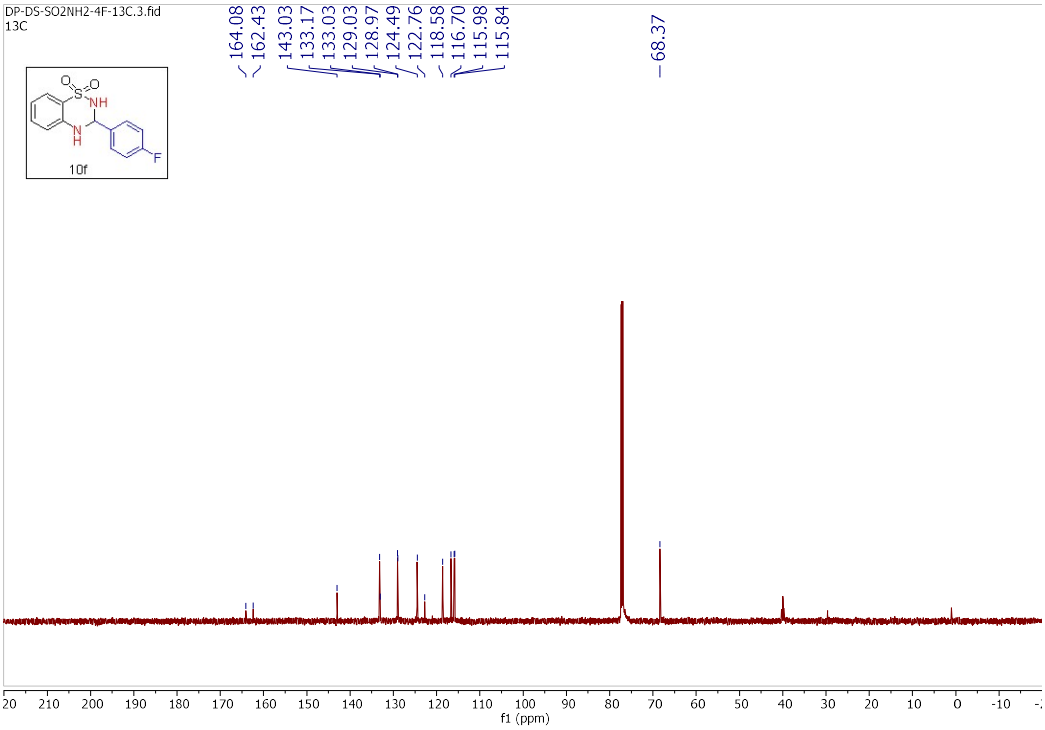


Figure S101. ^{13}C NMR Spectrum of 3-(4-fluorophenyl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide **(10f)** in $CDCl_3$ + DMSO-d_6.

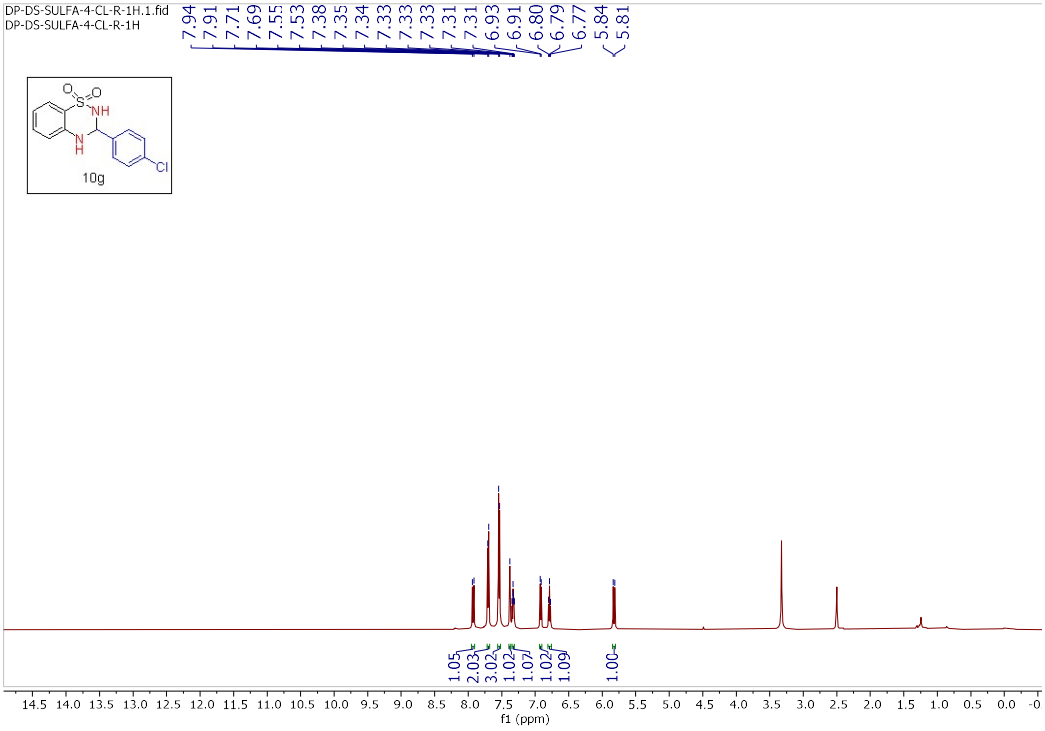


Figure S102. ^{1}H NMR Spectrum of 3-(4-chlorophenyl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide **(10g)** in DMSO-d_6.

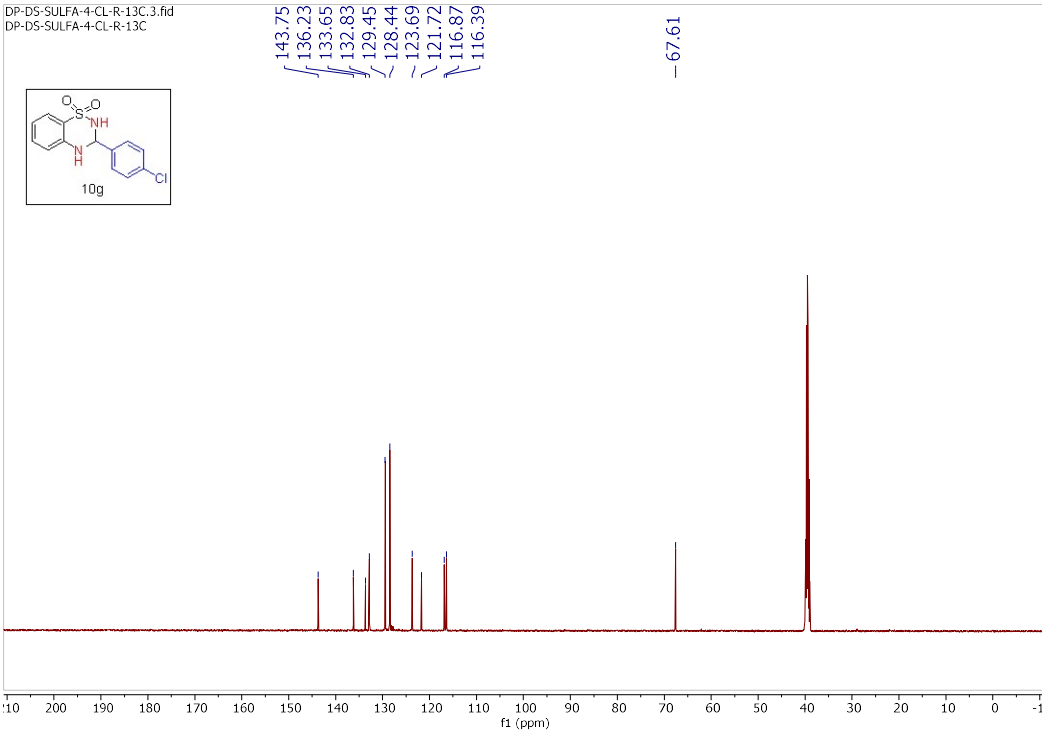


Figure S103. ^{13}C NMR Spectrum of 3-(4-chlorophenyl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide **(10g)** in DMSO-d_6.

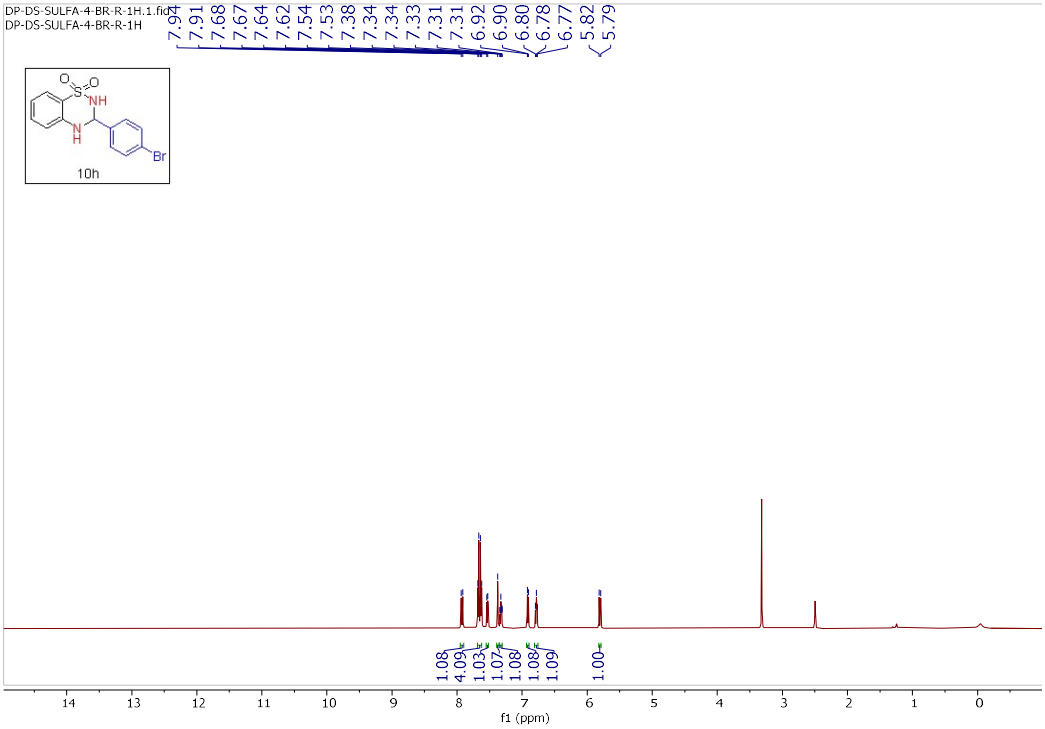


Figure S104. ^{1}H NMR Spectrum of 3-(4-bromophenyl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide **(10h)** in DMSO-d_6.

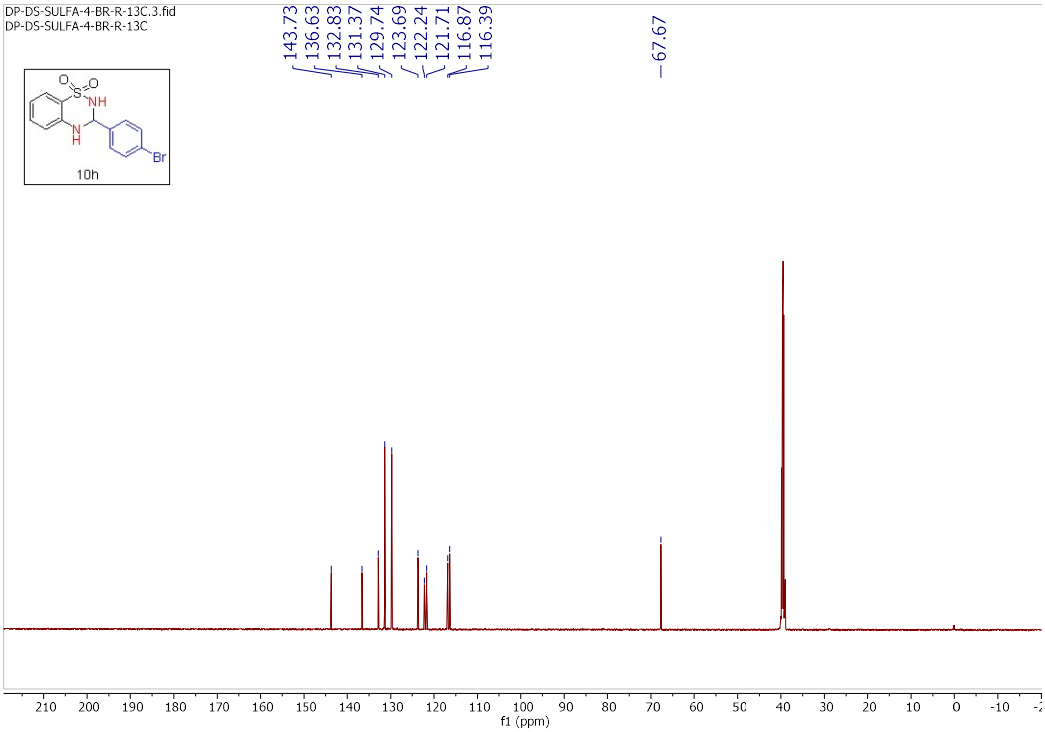


Figure S105. ^{13}C NMR Spectrum of 3-(4-bromophenyl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide **(10h)** in DMSO-d_6.

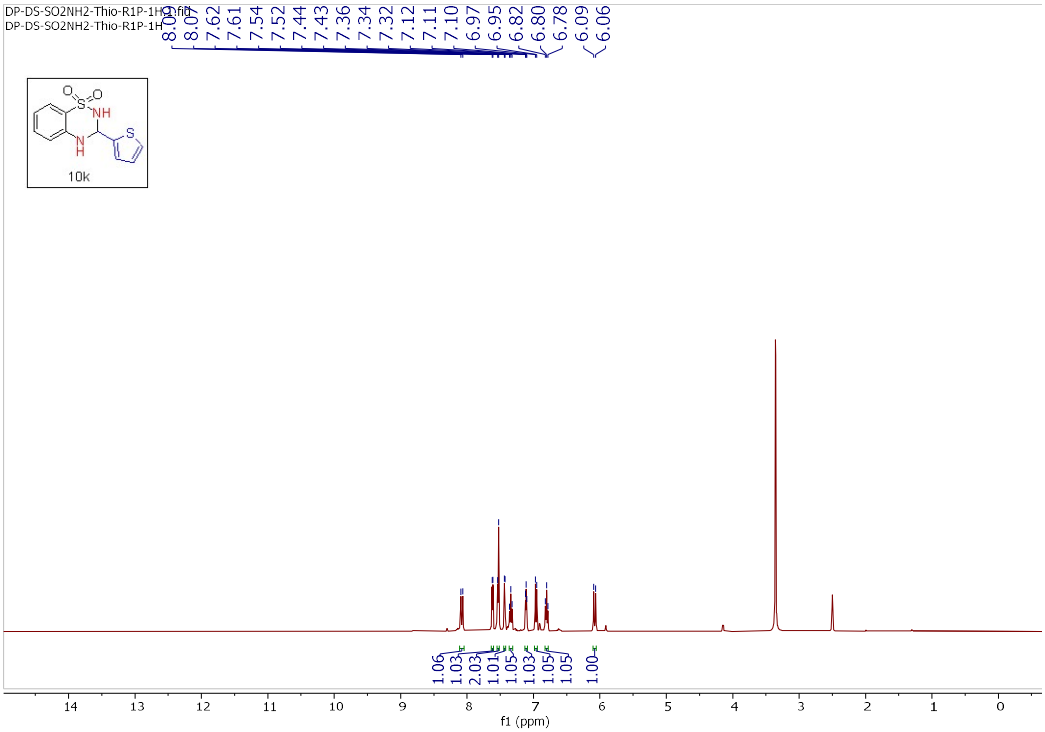


Figure S106. ^{1}H NMR Spectrum of 3-(thiophen-2-yl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide **(10k)** in DMSO-d_6.

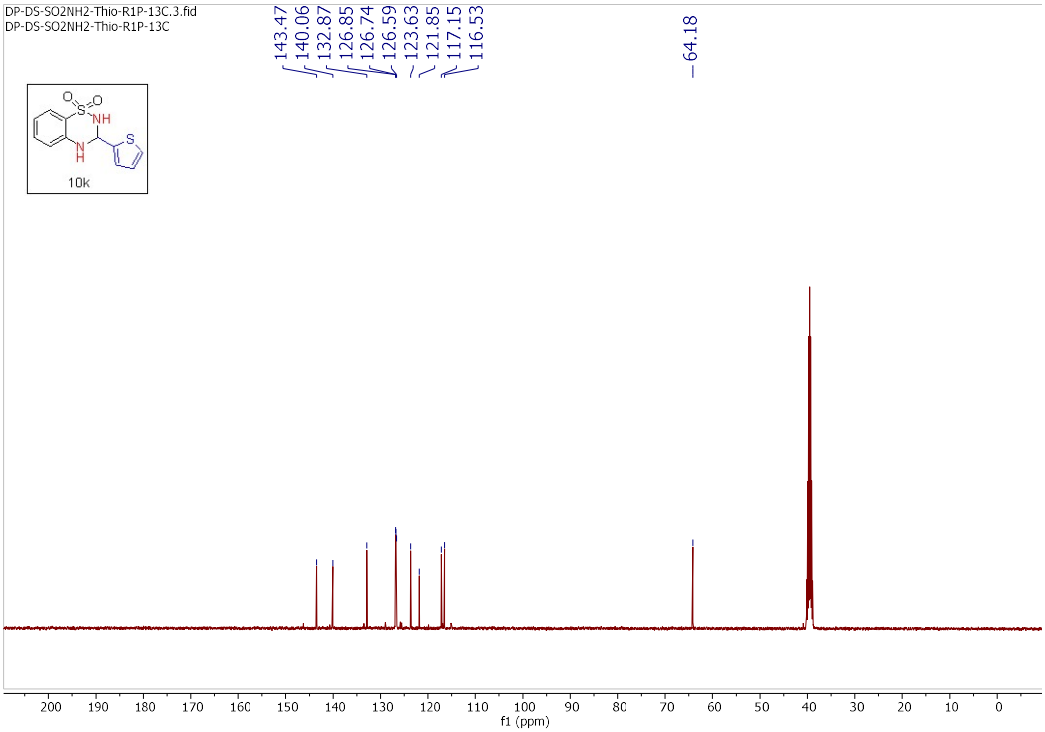


Figure S107. ^{13}C NMR Spectrum of 3-(thiophen-2-yl)-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide **(10k)** in DMSO-d_6.

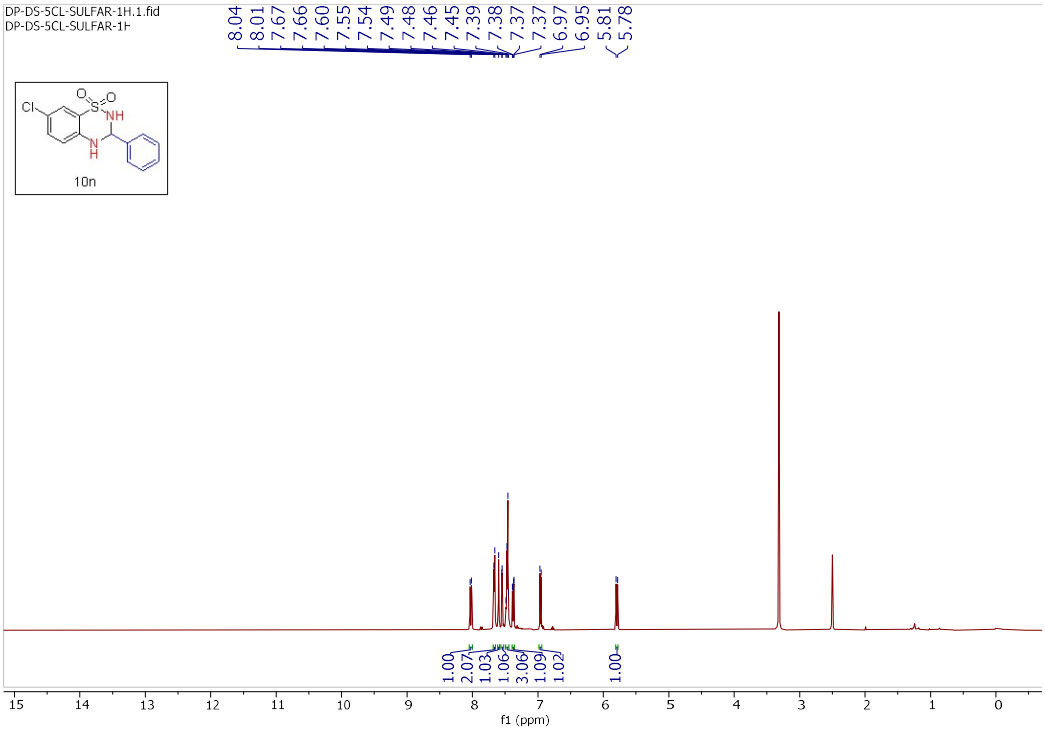


Figure S108. ^{1}H NMR Spectrum of 7-chloro-3-phenyl-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide **(10n)** in DMSO-d_6.

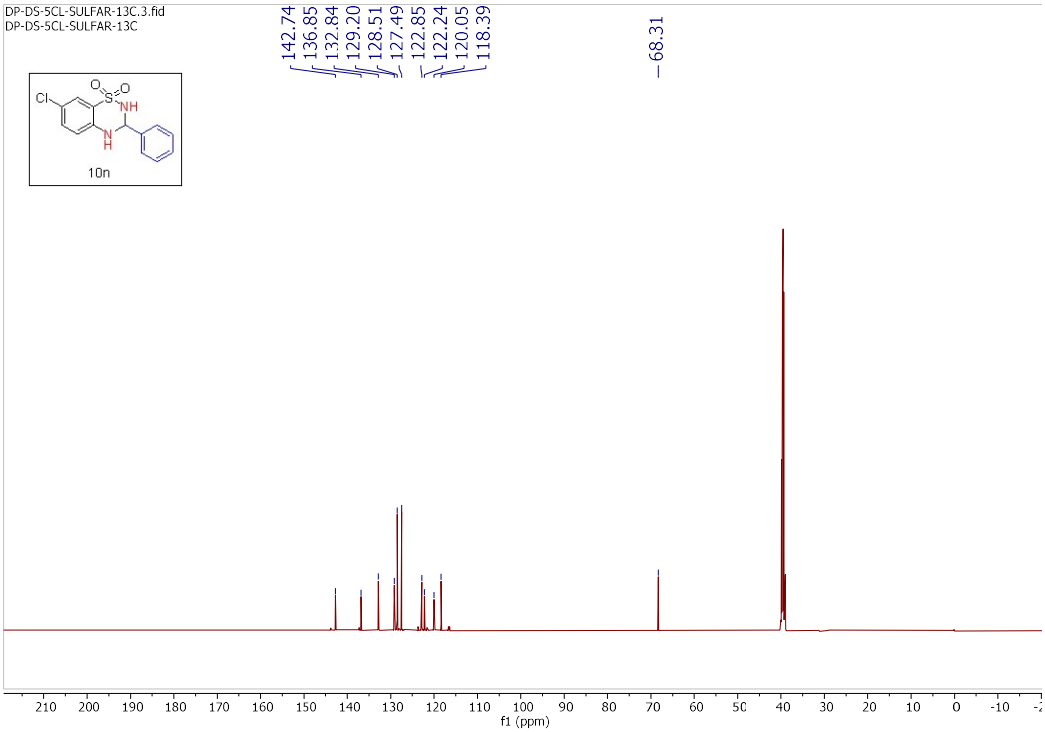


Figure S109. ^{13}C NMR Spectrum of 7-chloro-3-phenyl-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide **(10n)** in DMSO-d_6.

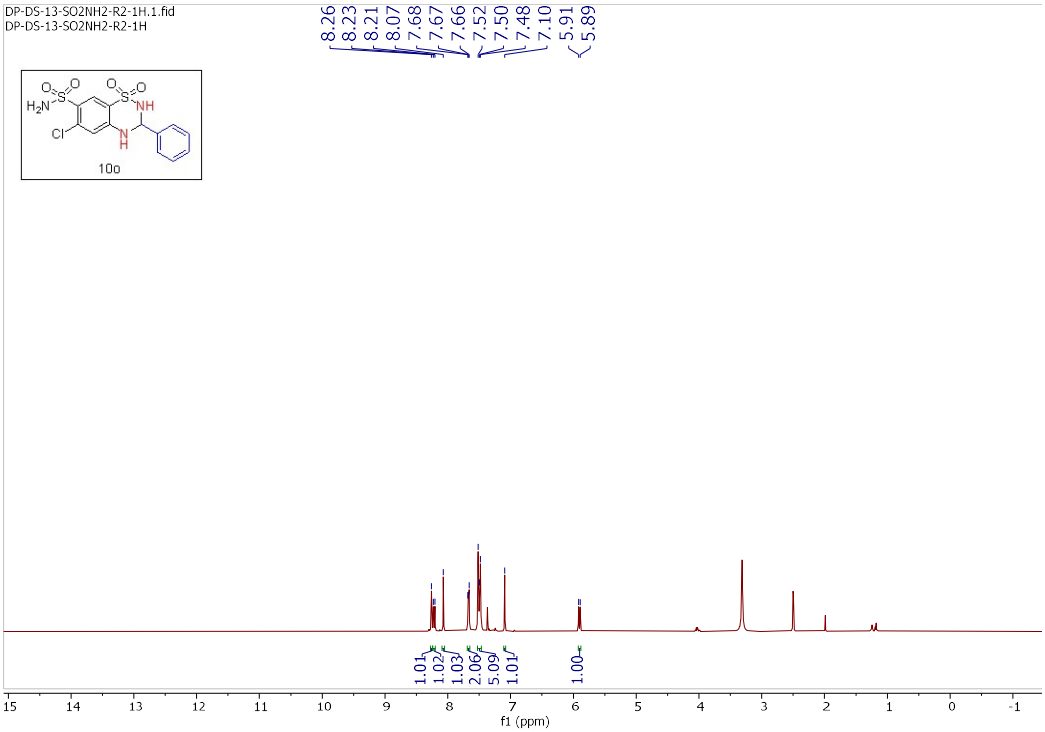


Figure S110. ^{1}H NMR Spectrum of 6-chloro-3-phenyl-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine-7-sulfonamide 1,1-dioxide **(10o)** in DMSO-d_6.

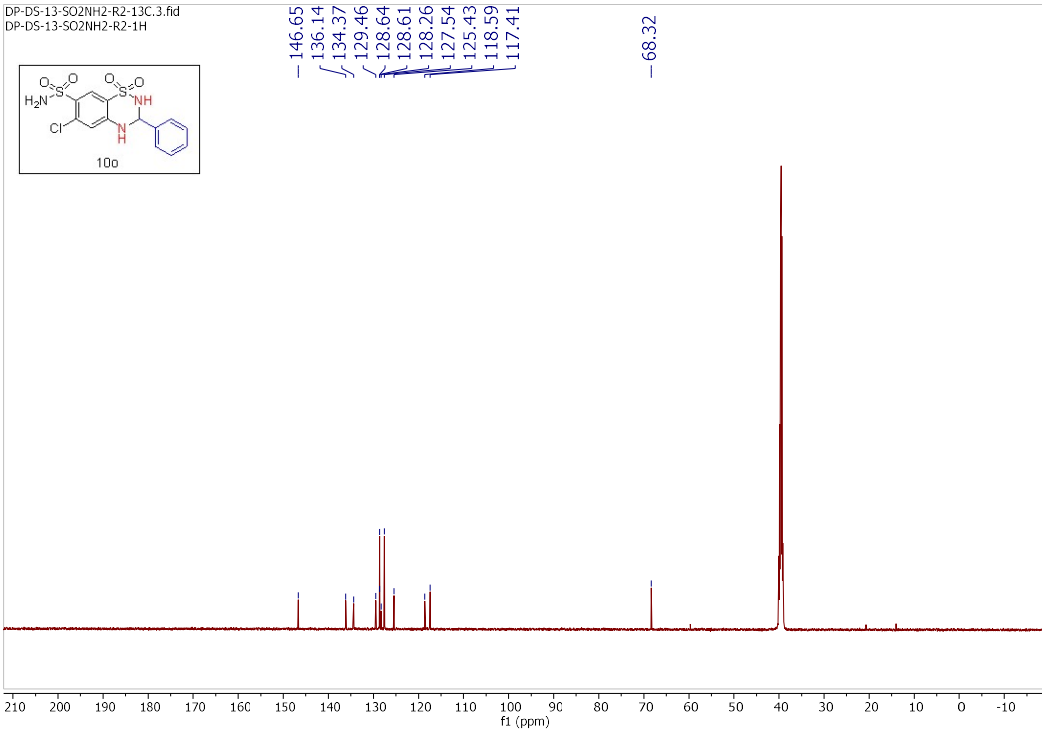


Figure S111. ^{13}C NMR Spectrum of 6-chloro-3-phenyl-3,4-dihydro-2*H*-benzo[e][1,2,4]thiadiazine-7-sulfonamide 1,1-dioxide **(10o)** in DMSO-d_6.

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