

# Supporting Information

## Rhodium (II) catalyzed synthesis of 2-aminoquinoline derivatives from 2-quinolone and *N*-sulfonyl-1, 2, 3-triazoles

Nilesh M. Kahar<sup>a</sup>, Pankaj P. Jadhav<sup>a</sup>, Sudam G. Dawande<sup>b\*</sup>

<sup>a</sup>*Department of Chemistry, Institute of Chemical Technology, Mumbai, Maharashtra, India-400019*

<sup>b</sup>*Department of Chemistry, Indian Institute of Technology, Madras, Tamilnadu, India-600036*

Email: [sg.dawande@iitm.ac.in](mailto:sg.dawande@iitm.ac.in)

### Contents:

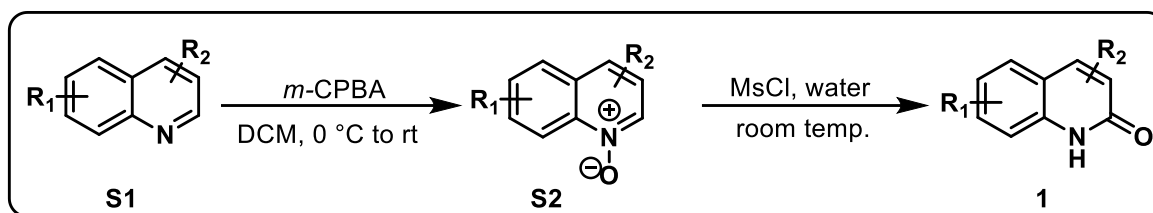
1.	General Methods	02
2.	Preparation of Starting Materials	03
3.	Optimization table	06
4.	General procedure for synthesis of 2-aminoquinoline derivatives	07
5.	Characterization data	08
6.	Preparation of 4-methyl- <i>N</i> -(quinolin-2-yl)benzenesulfonamide ( <b>4</b> )	20
7.	Reaction of deuterated <i>N</i> -sulfonyl-1,2,3-triazole with 2-quinolone	21
8.	Crystal data of <b>3g</b>	22
9.	References	23
10.	NMR Spectra	23

## 1. General methods

All the reactions were performed in oven-dried glassware under a nitrogen atmosphere. Solvents were dried using standard methods. Tetrahydrofuran was dried over sodium metal. Acetonitrile, dichloromethane, and toluene were distilled over calcium hydride. Unless otherwise stated, all the commercial reagents were used as received. Progress of the reaction was monitored by thin-layer chromatography (Merck Silica gel 60 F-254, pre-coated plates on alumina). Column chromatographic purifications were performed using Merck silica gel (100-200 mesh). Melting points were recorded on a digital melting point apparatus and are uncorrected. Spectroscopic characterizations were carried at the Central Instrumentation Facility (CIF), Indian Institute of Science Education and Research (IISER) Bhopal, and Institute of Chemical Technology Matunga Mumbai Maharashtra. <sup>1</sup>H-NMR spectra were recorded on Bruker Avance III FT-NMR and Agilent spectrometers at 400MHz and 500 MHz. <sup>13</sup>C-NMR spectra were recorded at 101 MHz, 126 MHz. <sup>1</sup>H-NMR chemical shifts are reported in ppm relative to the TMS (=0) and are abbreviated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), br (broad). <sup>13</sup>C-NMR chemical shifts are reported in ppm relative to the residual CDCl<sub>3</sub> signal (= 77.16). IR spectra were recorded on a Perkin Elmer FT-IR spectrometer. HRMS data were obtained on Bruker microTOF-QII or Agilent 5975C high-resolution mass spectrometers.

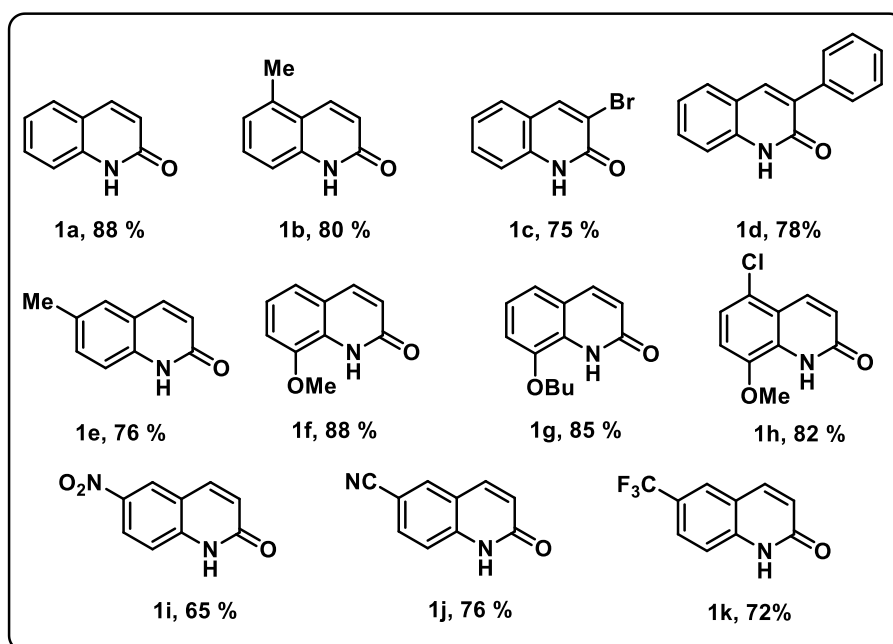
## 2. Preparation of starting materials:

### 2.1a Preparation of 2-quinolone (**1a-1k**): Prepared according to the literature procedure.<sup>1</sup>

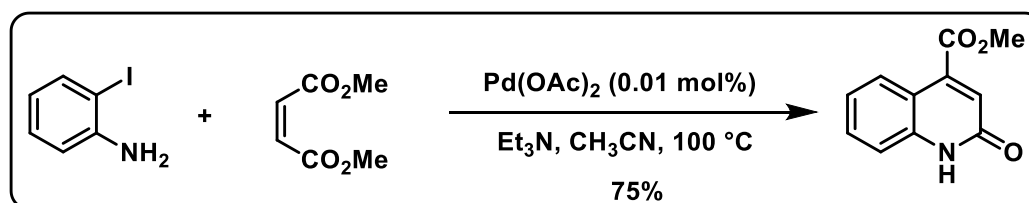


To a solution of corresponding quinoline **S1** (0.65 g, 5 mmol) in DCM (30 ml) *m*-chloroperbenzoic acid (2.35 g, 7.5 mmol, 1.5 equiv.) was added at 0 °C. The reaction mixture is allowed to stir at room temperature for 24 h. Next saturated aqueous NaHCO<sub>3</sub> solution (100 ml) was added to the reaction mixture. Then it was extracted with DCM (50 ml × 3) and the organic layers were washed with water, brine and was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel to obtain the pure quinoline-*N*-oxide **S2**.

In a vial placed quinoline *N*-oxide **S2** (435 mg, 3 mmol, 1 equiv.) and then added H<sub>2</sub>O (35 ml) followed by MsCl (0.47 mL, 6 mmol, 2 equiv.). The reaction mixture was stirred vigorously at room temperature. The progress of the reaction was monitored by TLC. After completion of the reaction, the mixture was filtered and vacuum dried to obtain 2-quinolone **1a** as white solid. The 2-quinolone **1b-1k** were also obtained with 65-88% yield by following similar reaction conditions.

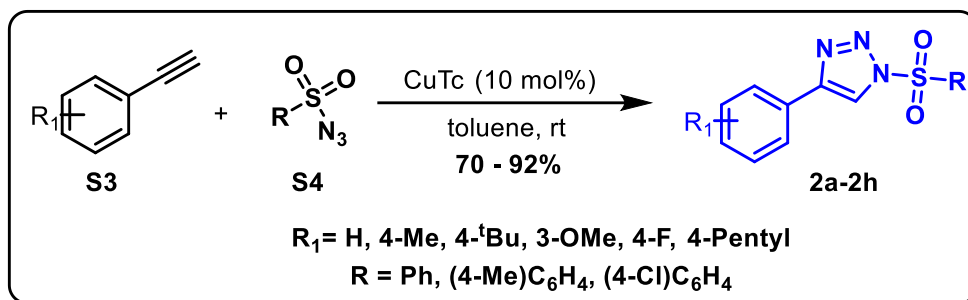


**2.1b Preparation of methyl 2-oxo-1,2-dihydroquinoline-4-carboxylate (II):** Prepared by following literature procedure.<sup>2</sup>



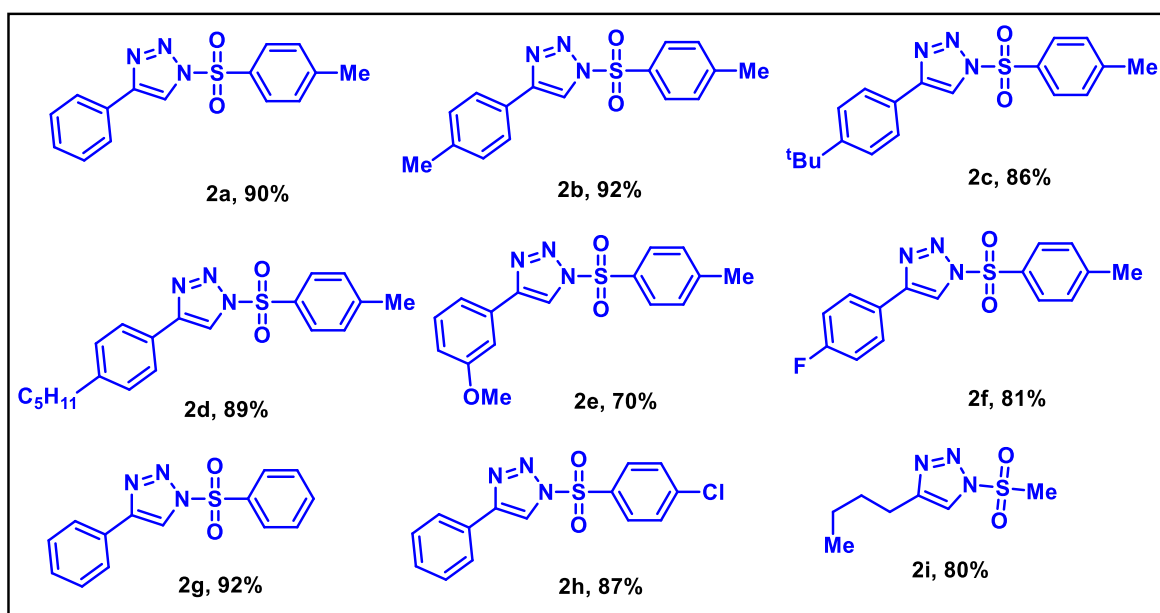
In a 10 ml Schlenk tube placed 2-iodoaniline (1.095 g, 5 mmol), dimethyl maleate (0.937 g, 6.5 mmol), triethylamine (0.55 mL, 4 mmol), palladium diacetate (11 mg, 0.05 mmol) and 3 mL acetonitrile. The tube was flushed with nitrogen. The Schlenk tube was heated at 100° for 3.5 h then cooled to room temperature. The tube was opened and the resulting solids filtered and washed with acetonitrile. The solids were dissolved in chloroform and the solvent removed under vacuum. The crude product was purified by column chromatography to obtain a white solid with 75% yield.

**2.2 Preparation of *N*-sulfonyl-1,2,3-triazoles:** The *N*-sulfonyl-1,2,3-triazoles were prepared according to the literature procedure.<sup>3</sup>

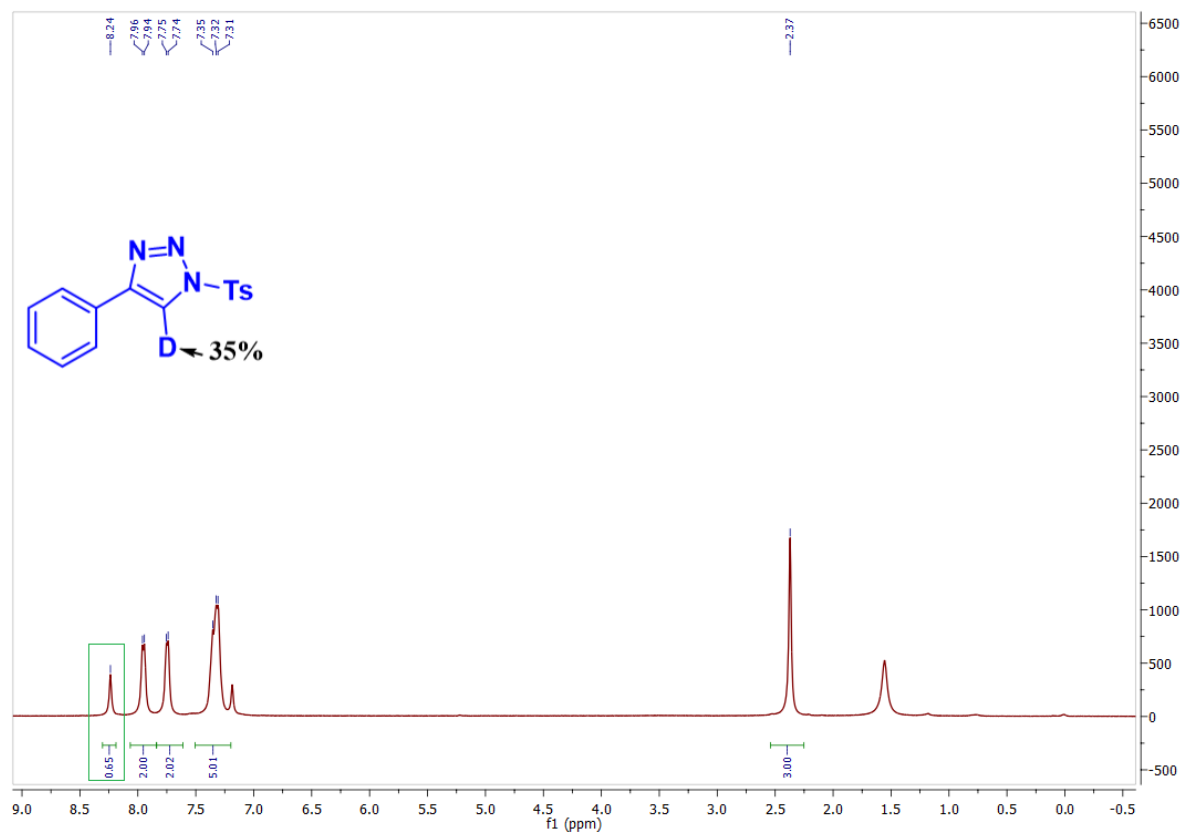
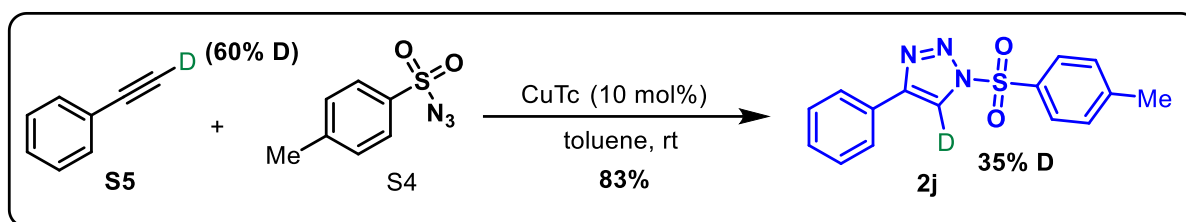


To an oven dried 50 ml round bottom flask containing solution of alkyne **S3** (510 mg, 5.0 mmol, 1 equiv.) and aryl sulfonyl azide **S4** (985 mg, 5.0 mmol, 1 equiv) in toluene (15 mL) added CuTC (81 mg, 0.5 mmol, 10 mol%). The resulting reaction mixture allowed to stir for 2 h at room temperature and then diluted with saturated aqueous  $\text{NH}_4\text{Cl}$  (25 mL). Then extracted with ethyl acetate and the combined organic layers were washed with brine and dried over anhydrous  $\text{Na}_2\text{SO}_4$ . The solvents were removed under reduced pressure. The concentrates were washed with a mixture of DCM and hexane to afford *N*-sulfonyl-1,2,3-triazoles **2a** in 90% yield.

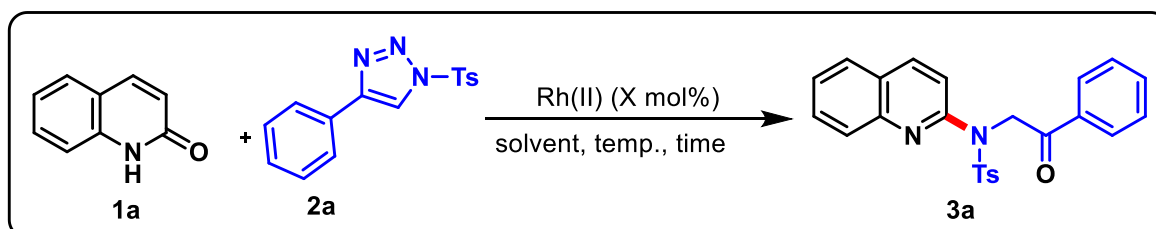
The *N*-sulfonyl-1,2,3-triazoles **2b-2i** were also obtained with 70-92% yield by following similar reaction conditions.



**Preparation of *N*-sulfonyl-1,2,3-triazoles (2j):** The *N*-sulfonyl-1,2,3-triazole (2j) is prepared from deuterated phenyl acetylene according to the literature procedure.<sup>3</sup>



### 3. Optimization for Rh(II) catalyzed synthesis of 2-aminoquinoline derivatives:

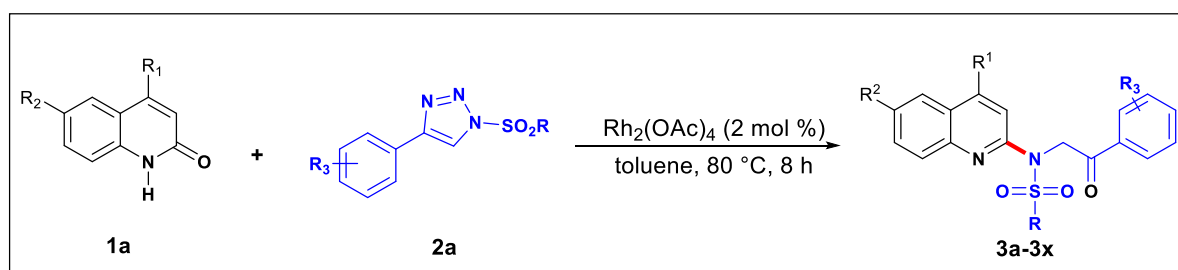


Entry	Rh <sub>2</sub> L <sub>4</sub> (2%)	Solvent	Temp. °C	Time (h)	yield (%) <sup>b</sup>
1	Rh <sub>2</sub> (OAc) <sub>4</sub>	CHCl <sub>3</sub>	r.t.	24	-
2	Rh <sub>2</sub> (OAc) <sub>4</sub>	CHCl <sub>3</sub>	80	8	65

<b>3</b>	Rh <sub>2</sub> (OAc) <sub>4</sub>	DCM	80	8	58
<b>4</b>	Rh <sub>2</sub> (OAc) <sub>4</sub>	DCE	80	8	74
<b>5</b>	<b>Rh<sub>2</sub>(OAc)<sub>4</sub></b>	<b>toluene</b>	<b>80</b>	<b>8</b>	<b>88</b>
<b>6</b>	Rh <sub>2</sub> (OAc) <sub>4</sub>	Cl-benzene	80	8	64
<b>7</b>	Rh <sub>2</sub> (Oct) <sub>4</sub>	toluene	80	8	86
<b>8</b>	Rh <sub>2</sub> (esp) <sub>2</sub>	toluene	80	8	82
<b>9</b>	Rh <sub>2</sub> (TFA) <sub>4</sub>	toluene	80	8	-
<b>10</b>	Rh <sub>2</sub> (OAc) <sub>4</sub>	toluene	110	8	72
<b>11</b>	Rh <sub>2</sub> (OAc) <sub>4</sub>	toluene	80	8	90
<b>12</b>	-	toluene	80	24	-
<b>13</b>	CuOTf	toluene	80	24	-
<b>14</b>	Cu(MeCN) <sub>4</sub> BF <sub>4</sub>	toluene	80	24	-
<b>15</b>	FeCl <sub>3</sub>	toluene	80	24	-

<sup>a</sup>Reaction conditions: **1a** (0.2 mmol), **2a** (0.24 mmol), Rh(II) catalysts (X mmol), solvent (2 mL). <sup>b</sup>Isolated yield, <sup>c</sup>5 mol% Rh<sub>2</sub>(OAc)<sub>4</sub>.

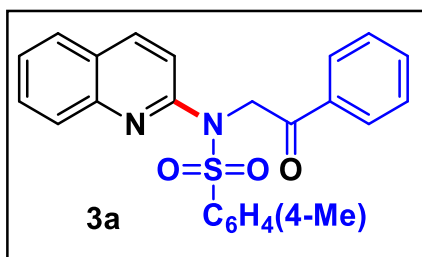
#### 4. General procedure for synthesis of 2-aminoquinoline derivatives:



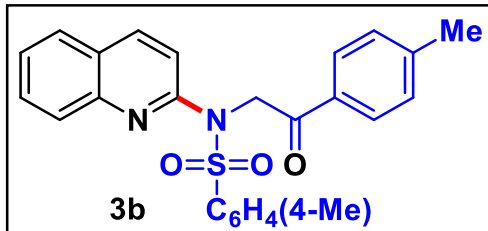
To a sealed tube charged with a stirring bar, was added 2-quinolone **1** (29 mg, 0.2 mmol), triazole (72 mg, 0.24 mmol) **2**, Rh<sub>2</sub>(OAc)<sub>4</sub> (2 mol %), and toluene (2 mL). The reaction mixture was stirred under inert atmosphere at 80 °C until the complete consumption of starting material (monitored by TLC). The organic solvents were removed under reduced pressure and the crude product was purified by column chromatography using petroleum ether / ethyl acetate as an eluent to give **3a** with 88% yield.

By following above general method compound **3b-3x** are prepared.

## 5. Characterization data

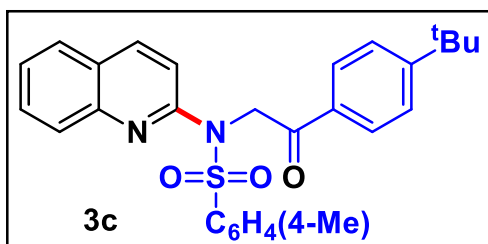


**4-methyl-*N*-(2-oxo-2-phenylethyl)-*N*-(quinolin-2-yl)benzenesulfonamide (3a):** Obtained as a white solid; Yield = 73 mg (88%); m. p. = 154-156 °C;  $R_f$  = 0.5 (Ethyl Acetate/Hexane : 30/70);  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.01-7.92 (m, 3H), 7.85-7.74 (m, 3H), 7.60 (d,  $J$  = 8.0 Hz, 1H), 7.52 (t,  $J$  = 7.4 Hz, 1H), 7.43-7.36 (m, 4H), 7.30-7.26 (m, 1H), 7.19 (d,  $J$  = 8.1 Hz, 2H), 5.54 (s, 2H), 2.29 (s, 3H);  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  193.8, 150.9, 146.3, 144.4, 137.9, 136.6, 135.8, 133.5, 129.9, 129.8, 128.8, 128.2, 128.1, 127.9, 127.4, 125.8, 125.6, 115.9, 53.4, 21.7; **IR (neat):** 2930, 1692, 1604, 1359, 1205, 775  $\text{cm}^{-1}$ ; **HRMS-ESI ( $m/z$ ):** Calculated for:  $\text{C}_{24}\text{H}_{20}\text{N}_2\text{O}_3\text{SNa}$  [ $\text{M}+\text{Na}$ ] $^+$ : 439.1089; found: 439.1088.



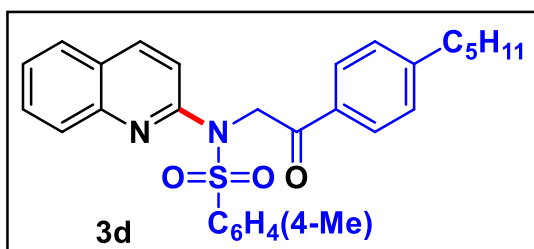
**4-methyl-*N*-(2-oxo-2-(*p*-tolyl)ethyl)-*N*-(quinolin-2-yl)benzenesulfonamide (3b):** Obtained as a white solid; Yield = 73 mg (85%); m. p. = 152-154 °C;  $R_f$  = 0.5 (Ethyl Acetate/Hexane : 30/70);  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.03 (d,  $J$  = 9.0 Hz, 1H), 7.92 (d,  $J$  = 8.2 Hz, 2H), 7.88 (d,  $J$  = 8.3 Hz, 2H), 7.84 (d,  $J$  = 9.0 Hz, 1H), 7.68 (d,  $J$  = 8.0 Hz, 1H), 7.60-7.45 (m, 2H), 7.39-7.34 (m, 1H), 7.32 – 7.24 (m, 4H), 5.60 (s, 2H), 2.44 (s, 3H), 2.38 (s, 3H);  $^{13}\text{C NMR}$  (126 MHz,  $\text{CDCl}_3$ )  $\delta$  193.3, 151.0, 146.4, 144.3, 137.9, 136.7, 133.2, 129.9, 129.7, 129.5, 128.4, 128.3, 128.2, 127.9, 127.3, 125.8, 125.6, 116.0, 53.3, 21.9, 21.7; **IR (neat):** 2927, 1691, 1600, 1355, 1200, 753  $\text{cm}^{-1}$ ; **HRMS-ESI ( $m/z$ ):** Calculated for:  $\text{C}_{25}\text{H}_{22}\text{N}_2\text{O}_3\text{SNa}$  [ $\text{M}+\text{Na}$ ] $^+$ : 453.1243; found: 453.1243.





***N*-(2-(4-(tert-butyl)phenyl)-2-oxoethyl)-4-methyl-*N*-(quinolin-2-yl)benzenesulfonamide**

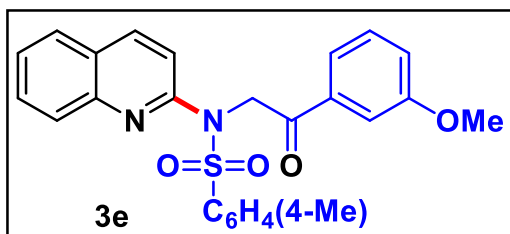
**(3c):** Obtained as a white solid; Yield = 81 mg (86%); m. p. = 122-124 °C;  $R_f$  = 0.5 (Ethyl Acetate/Hexane : 30/70);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.03 (d,  $J$  = 8.4 Hz, 1H), 7.96 (d,  $J$  = 8.0 Hz, 2H), 7.86 (dd,  $J$  = 8.4, 8.8 Hz, 3H), 7.69 (d,  $J$  = 8.0 Hz, 1H), 7.56-7.45 (m, 4H), 7.38 (t,  $J$  = 7.6 Hz, 1H), 7.27 (d,  $J$  = 8.4 Hz, 2H), 5.63 (s, 2H), 2.39 (s, 3H), 1.36 (s, 9H);  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  193.2, 157.3, 151.1, 146.4, 144.3, 137.8, 136.7, 133.1, 129.9, 129.7, 128.2, 128.15, 127.9, 127.3, 125.9, 125.8, 125.6, 116.1, 53.4, 35.4, 31.3, 21.7; **IR (neat):** 2932, 1688, 1609, 1360, 1190, 767  $\text{cm}^{-1}$ ; **HRMS-ESI ( $m/z$ ):** Calculated for:  $\text{C}_{28}\text{H}_{28}\text{N}_2\text{O}_3\text{SNa}$   $[\text{M}+\text{Na}]^+$ : 495.1713; found: 495.1714.



**4-methyl-*N*-(2-oxo-2-(4-pentylphenyl)ethyl)-*N*-(quinolin-2-yl)benzenesulfonamide (3d):**

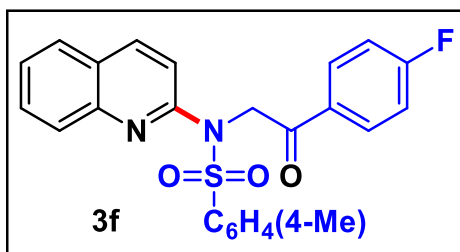
Obtained as a white solid; Yield = 81 mg (83%); m. p. = 165-167 °C;  $R_f$  = 0.5 (Ethyl Acetate/Hexane : 30/70);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.03 (d,  $J$  = 9.2 Hz, 1H), 7.94 (d,  $J$  = 8 Hz, 2H), 7.86 (dd,  $J$  = 8, 9.2 Hz, 3H), 7.69 (d,  $J$  = 8 Hz, 1H), 7.56 – 7.46 (m, 2H), 7.37 (t,  $J$  = 8 Hz, 1H), 7.33 – 7.26 (m, 3H), 7.18 (s, 1H), 5.62 (s, 2H), 2.68 (t,  $J$  = 7.2 Hz, 2H), 2.39 (s, 3H), 1.70 – 1.60 (m, 3H), 1.37 – 1.31 (m, 3H), 0.91 (t,  $J$  = 6.0 Hz, 3H);  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  193.3, 151.0, 149.3, 146.4, 144.3, 137.9, 136.6, 133.4, 129.9, 129.7, 128.9, 128.3, 128.2, 127.9, 127.3, 125.8, 125.6, 116.1, 53.3, 36.2, 31.6, 30.9, 22.6, 21.7, 14.2; **IR (neat):**

2921, 1697, 1600, 1355, 1210, 781  $\text{cm}^{-1}$ ; **HRMS-ESI** ( $m/z$ ): Calculated for:  $\text{C}_{29}\text{H}_{30}\text{N}_2\text{O}_3\text{SNa}$   $[\text{M}+\text{Na}]^+$ : 509.1871; found: 509.1870.



***N*-(2-(3-methoxyphenyl)-2-oxoethyl)-4-methyl-*N*-(quinolin-2-yl)benzenesulfonamide**

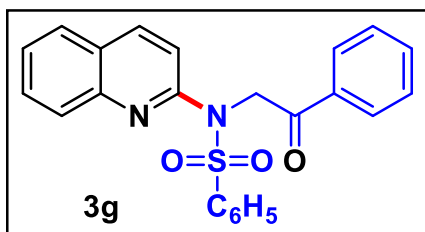
**(3e)**: Obtained as a white solid; Yield = 71 mg (80%); m. p. = 136-138  $^{\circ}\text{C}$ ;  $R_f$  = 0.4 (Ethyl Acetate/Hexane : 30/70);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.03 (d,  $J$  = 8.8 Hz, 1H), 7.86 (t,  $J$  = 8.4 Hz, 3H), 7.66 (dd,  $J$  = 8, 7.2 Hz, 2H), 7.58 – 7.32 (m, 5H), 7.27 (d,  $J$  = 8 Hz, 2H), 7.15 (d,  $J$  = 7.6 Hz, 1H), 5.61 (s, 2H), 3.83 (s, 3H), 2.37 (s, 3H);  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  193.6, 159.9, 150.8, 146.3, 144.4, 137.9, 137.0, 136.5, 129.9, 129.8, 129.7, 128.1, 127.8, 127.3, 125.7, 125.6, 120.6, 120.1, 115.8, 112.4, 55.6, 53.5, 21.7; **IR** (neat): 2934, 1682, 1621, 1353, 1189, 770  $\text{cm}^{-1}$ ; **HRMS-ESI** ( $m/z$ ): Calculated for:  $\text{C}_{25}\text{H}_{22}\text{N}_2\text{O}_4\text{SNa}$   $[\text{M}+\text{Na}]^+$ : 469.1194; found: 469.1193.



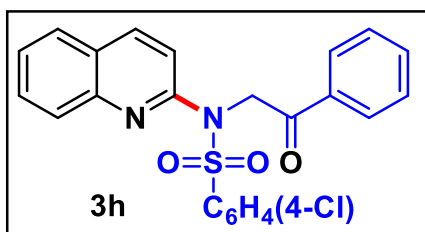
***N*-(2-(4-fluorophenyl)-2-oxoethyl)-4-methyl-*N*-(quinolin-2-yl)benzenesulfonamide** **(3f)**:

Obtained as a white solid; Yield = 71 mg (82%); m. p. = 135-137  $^{\circ}\text{C}$ ;  $R_f$  = 0.6 (Ethyl Acetate/Hexane : 30/70);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.10-8.0 (m, 3H), 7.86 (t,  $J$  = 8.0 Hz, 3H), 7.69 (d,  $J$  = 8.0 Hz, 1H), 7.54-7.45 (m, 2 H), 7.38 (t,  $J$  = 6.8 Hz, 1H), 7.28 (d,  $J$  = 8.0 Hz, 2H), 7.18 (t,  $J$  = 8.4 Hz, 2H), 5.58 (s, 2H), 2.39 (s, 3H);  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.4, 167.3, 164.7, 150.8, 146.3, 144.5, 138.0, 136.4, 132.1, 130.9 (d,  $J$  = 36.8 Hz), 129.9 (d,  $J$  = 31.6 Hz), 128.0, 127.9, 127.4, 125.8 (d,  $J$  = 35.2 Hz), 116.1, 115.9, 115.8, 53.2, 21.7; **IR** (neat):

2930, 1675, 1600, 1361, 1203, 771  $\text{cm}^{-1}$ ; **HRMS-ESI** ( $m/z$ ): Calculated for:  $\text{C}_{24}\text{H}_{20}\text{FN}_2\text{O}_3\text{S}$   
[ $\text{M}+\text{H}$ ] $^+$ : 435.1175; found: 435.1173.

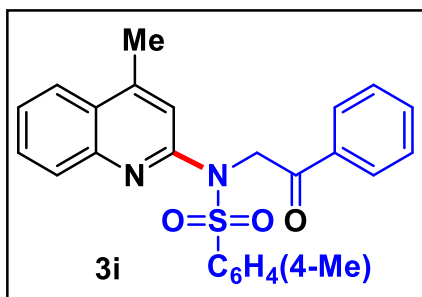


***N*-(2-oxo-2-phenylethyl)-*N*-(quinolin-2-yl)benzenesulfonamide (3g)**: Obtained as a white solid; Yield = 89 mg (86%); m. p. = 140-142  $^{\circ}\text{C}$ ;  $R_f$  = 0.5 (Ethyl Acetate/Hexane : 30/70);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.12-7.91 (m, 5H), 7.84 (d,  $J$  = 8.8 Hz, 1H), 7.70 (d,  $J$  = 8.0 Hz, 1H), 7.66 – 7.44 (m, 8H), 7.41 – 7.36 (m, 1H), 5.64 (s, 2H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  193.7, 150.8, 146.3, 139.5, 138.0, 135.7, 133.6, 133.5, 129.8, 129.3, 128.9, 128.2, 128.1, 127.8, 127.4, 125.8, 125.7, 115.9, 53.4; **IR** (neat): 2931, 1682, 1609, 1350, 1210, 765  $\text{cm}^{-1}$ ; **HRMS-ESI** ( $m/z$ ): Calculated for:  $\text{C}_{23}\text{H}_{19}\text{N}_2\text{O}_3\text{S}$  [ $\text{M}+\text{H}$ ] $^+$ : 403.1112; found: 403.1112; (CCDC 2254798).



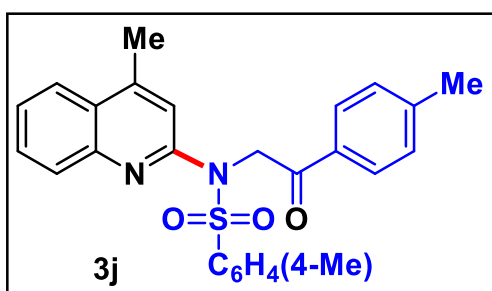
**4-chloro-*N*-(2-oxo-2-phenylethyl)-*N*-(quinolin-2-yl)benzenesulfonamide (3h)**: Obtained as a white solid; Yield = 73 mg (84%); m. p. = 149-151  $^{\circ}\text{C}$ ;  $R_f$  = 0.55 (Ethyl Acetate/Hexane : 30/70);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.07 (d,  $J$  = 9.0 Hz, 1H), 8.03 (d,  $J$  = 7.8 Hz, 2H), 7.97 (d,  $J$  = 8.0 Hz, 2H), 7.80 (d,  $J$  = 8.4 Hz, 1H), 7.71 (d,  $J$  = 8.1 Hz, 1H), 7.64 (t,  $J$  = 7.3 Hz, 1H), 7.58-7.45 (m, 5H), 7.46 (d,  $J$  = 8.6 Hz, 1H), 7.40 (m, 1H), 5.63 (s, 2H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  193.6, 150.6, 146.4, 140.1, 138.2, 138.0, 135.6, 133.7, 131.5, 130.0, 129.5, 129.48, 128.9, 128.2, 128.15, 127.4, 125.9, 115.8, 53.5; **IR** (neat): 2929, 1670, 1611, 1359, 1211, 767

cm<sup>-1</sup>; **HRMS-ESI** (*m/z*): Calculated for: C<sub>23</sub>H<sub>17</sub>ClN<sub>2</sub>O<sub>3</sub>SNa [M+Na]<sup>+</sup>: 459.0542; found: 459.0542.



**4-methyl-*N*-(4-methylquinolin-2-yl)-*N*-(2-oxo-2-phenylethyl)benzenesulfonamide (3i):**

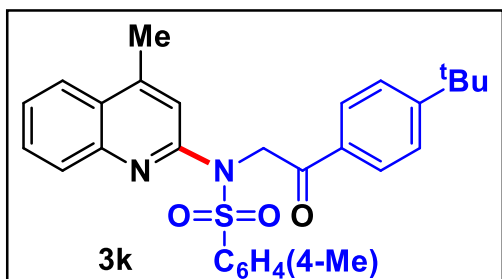
Obtained as a white solid; Yield = 73 mg (84%); m. p. = 144-146 °C; R<sub>f</sub> = 0.5 (Ethyl Acetate/Hexane : 30/70); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.00 (d, *J* = 7.4 Hz, 2H), 7.92-7.82 (m, 3H), 7.73 (s, 1H), 7.66-7.56 (m, 1H), 7.55-7.45 (m, 4H), 7.45-7.35 (m, 1H), 7.28 (d, *J* = 7.4 Hz, 2H), 5.59 (s, 2H), 2.64 (s, 3H), 2.38 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 193.8, 150.8, 146.3, 146.2, 144.3, 136.6, 135.8, 133.4, 129.8, 129.4, 128.8, 128.7, 128.2, 127.9, 126.1, 125.5, 123.7, 116.7, 53.4, 21.7, 19.3; **IR (neat):** 2927, 1682, 1604, 1355, 1221, 774 cm<sup>-1</sup>; **HRMS-ESI** (*m/z*): Calculated for: C<sub>25</sub>H<sub>23</sub>N<sub>2</sub>O<sub>3</sub>S [M+H]<sup>+</sup>: 431.1425; found: 431.1424.



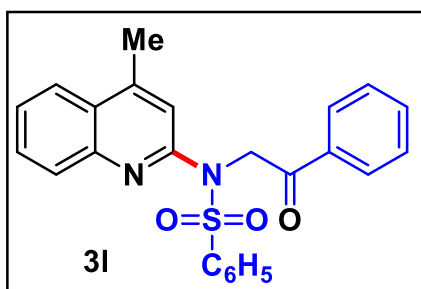
**4-methyl-*N*-(4-methylquinolin-2-yl)-*N*-(2-oxo-2-(*p*-tolyl)ethyl)benzenesulfonamide (3j):**

Obtained as a white solid; Yield = 71 mg (80%); m. p. = 138-140 °C; R<sub>f</sub> = 0.5 (Ethyl Acetate/Hexane : 30/70); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.90 (d, *J* = 8 Hz, 2H), 7.87- 7.80 (m, 3H), 7.72 (s, 1H), 7.56-7.44 (m, 2H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.37-7.20 (m, 4H), 5.57 (s, 2H), 2.64 (s, 3H), 2.43 (s, 3H), 2.38 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 193.3, 150.9, 146.3, 146.2, 144.3, 144.2, 136.7, 133.3, 129.8, 129.5, 129.4, 128.8, 128.3, 127.9, 126.2, 125.4, 123.7,

116.8, 53.3, 21.9, 21.7, 19.3; **IR (neat):** 2920, 1670, 1600, 1354, 1210, 771  $\text{cm}^{-1}$ ; **HRMS-ESI** ( $m/z$ ): Calculated for:  $\text{C}_{26}\text{H}_{25}\text{N}_2\text{O}_3\text{S}$   $[\text{M}+\text{H}]^+$ : 445.1593; found: 445.1593.

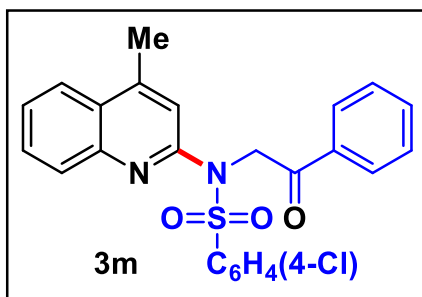


***N*-(2-(4-(tert-butyl)phenyl)-2-oxoethyl)-4-methyl-*N*-(4-methylquinolin-2-yl) benzenesulfonamide (3k):** Obtained as a white solid; Yield = 76 mg (78%); m. p. = 132-134  $^{\circ}\text{C}$ ;  $R_f$  = 0.6 (Ethyl Acetate/Hexane : 30/70);  **$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )**  $\delta$  7.94 (d,  $J$  = 8.1 Hz, 2H), 7.90-7.80 (m, 3H), 7.72 (s, 1H), 7.59 – 7.45 (m, 4H), 7.39 (t,  $J$  = 6.1 Hz, 1H), 7.26 (d,  $J$  = 8.2 Hz, 2H), 5.59 (s, 2H), 2.65 (s, 3H), 2.38 (s, 3H), 1.36 (s, 9H);  **$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )**  $\delta$  193.2, 157.2, 151.0, 146.3, 146.2, 144.2, 136.6, 133.1, 129.8, 129.4, 128.8, 128.1, 127.9, 126.2, 125.8, 125.4, 123.7, 116.9, 53.3, 35.3, 31.2, 21.7, 19.30; **IR (neat):** 2934, 1670, 1601, 1349, 1210, 779  $\text{cm}^{-1}$ ; **HRMS-ESI** ( $m/z$ ): Calculated for:  $\text{C}_{29}\text{H}_{31}\text{N}_2\text{O}_3\text{S}$   $[\text{M}+\text{H}]^+$ : 487.2051; found: 487.2051.



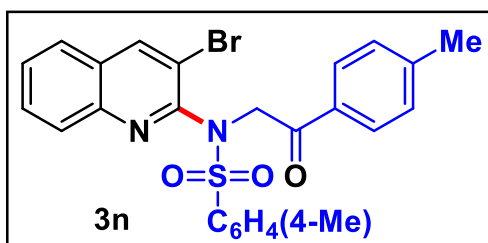
***N*-(4-methylquinolin-2-yl)-*N*-(2-oxo-2-phenylethyl)benzenesulfonamide (3l):** Obtained as a white solid; Yield = 68 mg (81%); m. p. = 136-138  $^{\circ}\text{C}$ ;  $R_f$  = 0.45 (Ethyl Acetate/Hexane : 30/70);  **$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )**  $\delta$  8.05-7.95 (m, 4H), 7.84 (d,  $J$  = 8.0 Hz, 1H), 7.72 (s, 1H), 7.62 – 7.45 (m, 7H), 7.44-7.29 (m, 2H), 5.60 (s, 2H), 2.64 (s, 3H);  **$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )**  $\delta$  193.7, 150.8, 146.4, 146.2, 139.5, 135.7, 133.5, 133.4, 129.5, 129.2, 128.8, 128.7, 128.2, 127.8, 126.2, 125.5, 123.7, 116.7, 53.4, 19.3; **IR (neat):** 2925, 1677, 1609, 1348, 1211,

767  $\text{cm}^{-1}$ ; **HRMS-ESI** ( $m/z$ ): Calculated for:  $\text{C}_{24}\text{H}_{21}\text{N}_2\text{O}_3\text{S}$   $[\text{M}+\text{H}]^+$ : 417.1277; found: 417.1275.



**4-chloro-N-(4-methylquinolin-2-yl)-N-(2-oxo-2-phenylethyl)benzenesulfonamide (3m):**

Obtained as a white solid; Yield = 74 mg (82%); 168-170  $^{\circ}\text{C}$ ;  $R_f = 0.6$  (Ethyl Acetate/Hexane : 30/70);  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.00 (d,  $J = 6.9$  Hz, 2H), 7.93 (d,  $J = 7.9$  Hz, 2H), 7.86 (d,  $J = 7.7$  Hz, 1H), 7.67 (s, 1H), 7.61 (t,  $J = 6.2$  Hz, 1H), 7.56 – 7.35 (m, 7H), 5.58 (s, 2H), 2.66 (s, 3H);  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  193.7, 150.5, 146.7, 146.2, 140.0, 138.0, 135.6, 133.6, 129.7, 129.5, 129.4, 128.9, 128.7, 128.2, 126.2, 125.7, 123.7, 116.6, 53.5, 19.3; **IR** (neat): 2981, 1662, 1607, 1359, 1195, 765  $\text{cm}^{-1}$ ; **HRMS-ESI** ( $m/z$ ): Calculated for:  $\text{C}_{24}\text{H}_{20}\text{ClN}_2\text{O}_3\text{S}$   $[\text{M}+\text{H}]^+$ : 451.0885; found: 451.0889.

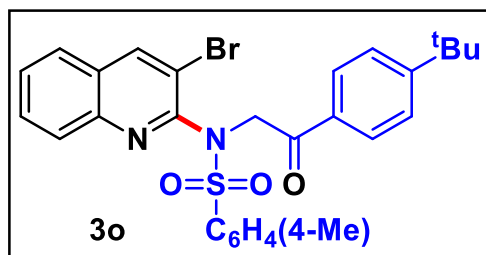


**N-(3-bromoquinolin-2-yl)-4-methyl-N-(2-oxo-2-(p-tolyl)ethyl)benzenesulfonamide (3n):**

Obtained as a white solid; Yield = 82 mg (80%); m. p. = 126-128  $^{\circ}\text{C}$ ;  $R_f = 0.6$  (Ethyl Acetate/Hexane : 30/70);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.50 (s, 1H), 7.69 (m, 5H), 7.61 (t,  $J = 6.2$  Hz, 1H), 7.52 (t,  $J = 6.4$  Hz, 1H), 7.36-7.23 (m, 3H), 7.17 (d,  $J = 6.8$  Hz, 2H), 5.14 (s, 2H), 2.45 (s, 3H), 2.35 (s, 3H);  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  191.6, 150.8, 145.3, 144.8, 144.4, 141.4, 134.5, 132.4, 130.0, 129.6, 129.5, 129.0, 128.7, 128.6, 128.3, 128.0, 126.7, 120.1,

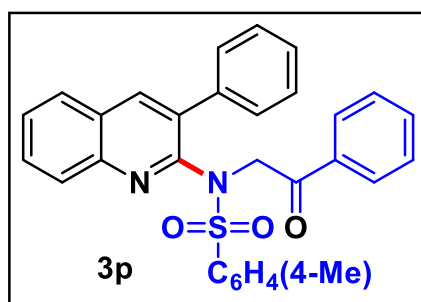
56.3, 21.8, 21.77; **IR (neat):** 2932, 1689, 1591, 1357, 1210, 768  $\text{cm}^{-1}$ ; **HRMS-ESI ( $m/z$ ):**

Calculated for:  $\text{C}_{25}\text{H}_{21}\text{BrN}_2\text{O}_3\text{SNa}$   $[\text{M}+\text{Na}]^+$ : 533.0335; found: 533.0334.



***N*-(3-bromoquinolin-2-yl)-*N*-(2-(4-(tert-butyl)phenyl)-2-oxoethyl)-4-methylbenzenesulfonamide (3o):** Obtained as a white solid; Yield = 84 mg (76%); m. p. = 124-126  $^{\circ}\text{C}$ ;  $R_f$  = 0.5

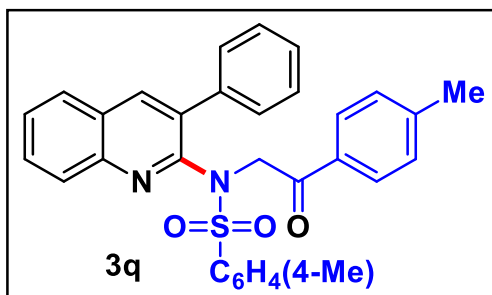
(Ethyl Acetate/Hexane : 30/70);  **$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )**  $\delta$  8.53 (s, 1H), 7.85-7.74 (m, 3H), 7.74-7.66 (m, 3H), 7.63 (t,  $J$  = 6.0 Hz, 1H), 7.55 (t,  $J$  = 6.2 Hz, 1H), 7.42 (d,  $J$  = 8.4 Hz, 2H), 7.32 (d,  $J$  = 8.0 Hz, 2H), 5.18 (s, 2H), 2.47 (s, 3H), 1.29 (s, 9H);  **$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )**  $\delta$  191.6, 157.7, 150.8, 145.3, 144.4, 141.5, 134.6, 132.3, 129.9, 129.6, 129.0, 128.71, 128.7, 128.1, 128.0, 126.7, 125.8, 120.2, 56.4, 35.3, 31.1, 21.8; **IR (neat):** 2927, 1672, 1601, 1356, 1205, 772  $\text{cm}^{-1}$ ; **HRMS-ESI ( $m/z$ ):** Calculated for:  $\text{C}_{28}\text{H}_{27}\text{BrN}_2\text{O}_3\text{SNa}$   $[\text{M}+\text{Na}]^+$ : 573.0818; found: 573.0818.



**4-methyl-*N*-(2-oxo-2-phenylethyl)-*N*-(3-phenylquinolin-2-yl)benzenesulfonamide (3p):**

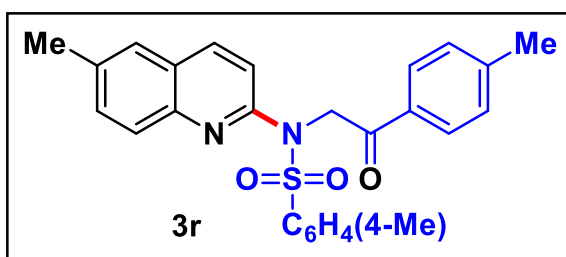
Obtained as a white solid; Yield = 73 mg (74%); m. p. = 150-152  $^{\circ}\text{C}$ ;  $R_f$  = 0.6 (Ethyl Acetate/Hexane : 30/70);  **$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**  $\delta$  8.20 (s, 1H), 7.98 (d,  $J$  = 5.6 Hz, 2H), 7.86 – 7.81 (m, 3H), 7.77 (d,  $J$  = 8.4 Hz, 1H), 7.64 – 7.58 (m, 1H), 7.57 – 7.51 (m, 2H), 7.50 – 7.45 (m, 2H), 7.44 – 7.38 (m, 5H), 7.21 (d,  $J$  = 8.0 Hz, 2H), 5.21 (s, 2H), 2.41 (s, 3H);  **$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )**  $\delta$  192.7, 150.8, 145.8, 144.1, 139.4, 139.1, 135.3, 135.1, 135.0,

133.7, 130.1, 129.5, 129.4, 128.82, 128.8, 128.6, 128.4, 128.1, 127.9, 127.6, 127.55, 127.1, 55.2, 21.7; **IR (neat)**: 2930, 1667, 1612, 1349, 1200, 768  $\text{cm}^{-1}$ ; **HRMS-ESI ( $m/z$ )**: Calculated for:  $\text{C}_{30}\text{H}_{24}\text{N}_2\text{O}_3\text{SNa}$  [ $\text{M}+\text{Na}$ ] $^+$ : 515.1403; found: 515.1403.



**4-methyl-N-(2-oxo-2-(p-tolyl)ethyl)-N-(3-phenylquinolin-2-yl)benzenesulfonamide (3q):**

Obtained as a white solid; Yield = 79 mg (78%); m. p. = 156-158  $^{\circ}\text{C}$ ;  $R_f$  = 0.6 (Ethyl Acetate/Hexane : 30/70);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.17 (s, 1H), 7.98 (d,  $J$  = 7.2 Hz, 2H), 7.80 (d,  $J$  = 7.8 Hz, 1H), 7.77-7.64 (m, 3H), 7.57 (t,  $J$  = 6.8 Hz, 1H), 7.52-7.42 (m, 3H), 7.42-7.32 (m, 3H), 7.18-7.08 (m, 4H), 5.20 (s, 2H), 2.39 (s, 3H), 2.36 (s, 3H);  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.3, 150.8, 145.7, 144.6, 144.0, 139.3, 139.2, 135.3, 135.1, 132.8, 130.1, 129.5, 129.4, 129.3, 128.7, 128.5, 128.4, 128.2, 127.8, 127.5, 127.48, 127.0, 55.1, 21.8, 21.7; **IR (neat)**: 2940, 1662, 1610, 1356, 1195, 765  $\text{cm}^{-1}$ ; **HRMS-ESI ( $m/z$ )**: Calculated for:  $\text{C}_{31}\text{H}_{26}\text{N}_2\text{O}_3\text{SNa}$  [ $\text{M}+\text{Na}$ ] $^+$ : 529.1560; found: 529.1561.

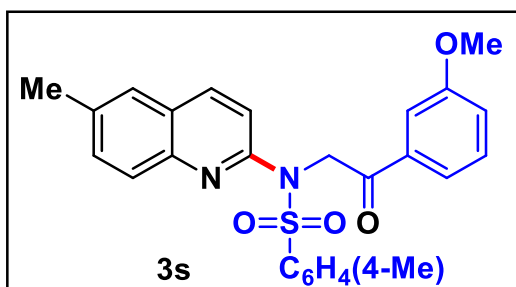


**4-methyl-N-(6-methylquinolin-2-yl)-N-(2-oxo-2-(p-tolyl)ethyl)benzenesulfonamide (3r):**

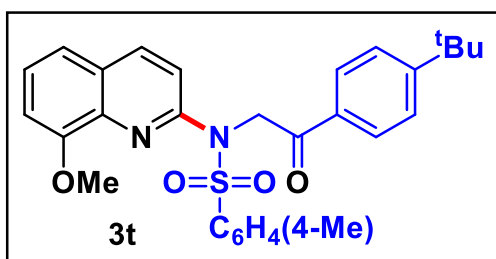
Obtained as a white solid; Yield = 69 mg (77%); m. p. = 143-145  $^{\circ}\text{C}$ ;  $R_f$  = 0.45 (Ethyl Acetate/Hexane : 30/70);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  = 8.07 (s, 1H), 8.03 – 7.93 (m, 1H), 7.93 – 7.89 (m, 1H), 7.85 – 7.78 (m, 2H), 7.64-7.54 (m, 1H), 7.43 (t,  $J$  = 6.6, 2H), 7.37-7.22 (m, 4H), 7.18 (d,  $J$  = 7.8, 1H), 5.57 (s, 2H), 2.43 (s, 6H), 2.37 (s, 3H);  $^{13}\text{C NMR}$  (101 MHz,



$\text{CDCl}_3$ )  $\delta$  = 193.4, 150.4, 144.3, 144.2, 137.2, 135.5, 133.8, 131.9, 130.32, 130.3, 129.9, 129.82, 129.8, 129.5, 128.3, 127.9, 126.3, 116.5, 53.4, 21.8, 21.7, 21.5; **IR (neat)**: 2925, 1669, 1600, 1349, 1201, 755  $\text{cm}^{-1}$ ; **HRMS-ESI** ( $m/z$ ): Calculated for:  $\text{C}_{26}\text{H}_{25}\text{N}_2\text{O}_3\text{S}$   $[\text{M}+\text{H}]^+$ : 445.1584; found: 445.1583.

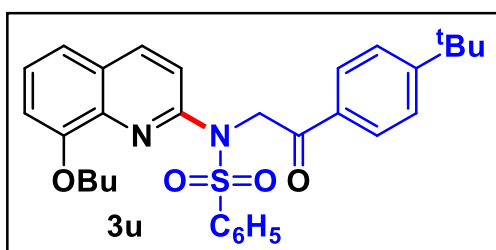


***N*-(2-(3-methoxyphenyl)-2-oxoethyl)-4-methyl-*N*-(6-methylquinolin-2-yl)benzenesulfonamide (3s)**: Obtained as a white solid; Yield = 72 mg (78%); m. p. = 147-149 °C;  $R_f$  = 0.4 (Ethyl Acetate/Hexane : 30/70);  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  = 8.09 (s, 1H), 7.99 (d,  $J=7.7$ , 1H), 7.96 (d,  $J=9.0$ , 1H), 7.83 (t,  $J=8.5$ , 2H), 7.62 (d,  $J=7.2$ , 1H), 7.58 (d,  $J=7.5$ , 1H), 7.50 (s, 1H), 7.46 (s, 1H), 7.46-7.35 (m, 1H), 7.34 (d,  $J=9.2$ , 1H), 7.28 – 7.23 (m, 1H), 7.15 (d,  $J=8.0$ , 1H), 5.57 (s, 2H), 3.83 (s, 3H), 2.44 (s, 3H), 2.37 (s, 3H);  $^{13}\text{C NMR}$  (126 MHz,  $\text{CDCl}_3$ )  $\delta$  = 193.7, 160.0, 150.4, 144.8, 144.3, 137.3, 135.6, 133.9, 132.0, 130.4, 130.0, 129.9, 129.8, 128.4, 127.9, 126.3, 120.7, 120.1, 116.4, 112.5, 55.6, 53.6, 21.7, 21.5; **IR (neat)**: 2929, 1672, 1596, 1349, 1203, 771  $\text{cm}^{-1}$ ; **HRMS-ESI** ( $m/z$ ): Calculated for:  $\text{C}_{26}\text{H}_{24}\text{N}_2\text{O}_4\text{SNa}$   $[\text{M}+\text{Na}]^+$ : 483.1352; found: 483.1352.



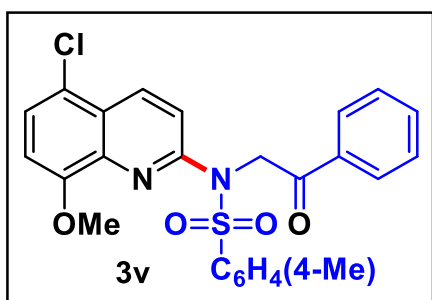
***N*-(2-(4-(tert-butyl)phenyl)-2-oxoethyl)-*N*-(8-methoxyquinolin-2-yl)-4-methylbenzenesulfonamide (3t)**: Obtained as a white solid; Yield = 70 mg (70%); m. p. = 166-168 °C;  $R_f$  = 0.4 (Ethyl Acetate/Hexane : 30/70);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.00 (d,  $J$  = 8.1 Hz, 2H), 7.96

(d,  $J = 8.9$  Hz, 2H), 7.84 (d,  $J = 9.0$  Hz, 1H), 7.52 (d,  $J = 8.3$  Hz, 2H), 7.32-7.18 (m, 5H), 6.86 (d,  $J = 6.2$  Hz, 1H), 5.67 (s, 2H), 3.60 (s, 3H), 2.38 (s, 3H), 1.37 (s, 9H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  193.7, 157.0, 154.8, 149.9, 144.3, 138.1, 137.9, 137.0, 133.6, 129.8, 128.4, 128.1, 126.8, 125.6, 125.55, 119.2, 115.5, 109.1, 55.8, 53.3, 35.3, 31.3, 21.7; IR (neat): 2920, 1652, 1587, 1350, 1215, 776  $\text{cm}^{-1}$ ; HRMS-ESI ( $m/z$ ): Calculated for:  $\text{C}_{29}\text{H}_{30}\text{N}_2\text{O}_4\text{SNa}$   $[\text{M}+\text{Na}]^+$ : 525.1821; found: 525.1821.

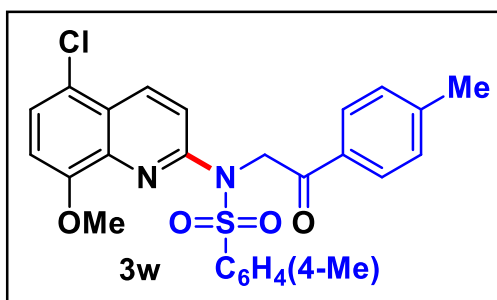


***N*-(8-butoxyquinolin-2-yl)-*N*-(2-(4-(tert-butyl)phenyl)-2-oxoethyl)benzenesulfonamide**

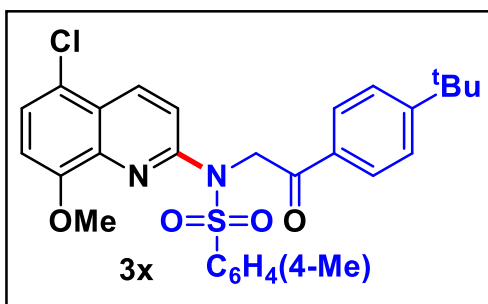
**(3u)**: Obtained as a white solid; Yield = 69 mg (66%); m. p. = 170-172  $^{\circ}\text{C}$ ;  $R_f = 0.4$  (Ethyl Acetate/ Hexane: 30/70);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.04 (d,  $J = 8.0$  Hz, 2H), 8.00 – 7.93 (m, 3H), 7.81 (d,  $J = 8.0$  Hz, 1H), 7.58 – 7.43 (m, 5H), 7.26 – 7.22 (m, 2H), 7.00 – 6.78 (m, 1H), 5.79 (s, 2H), 3.86 (t,  $J = 6.5$  Hz, 2H), 1.47 – 1.38 (m, 2H), 1.36 (s, 9H), 1.18 (dt,  $J = 14.5$ , 7.4 Hz, 2H), 0.74 (t,  $J = 7.4$  Hz, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta = 192.8$ , 157.2, 154.3, 149.8, 140.0, 137.9, 133.3, 133.0, 129.2, 128.2, 127.9, 127.0, 125.7, 125.69, 119.2, 115.6, 110.7, 68.8, 53.5, 35.3, 31.2, 31.0, 29.8, 19.2, 13.9; IR (neat): 2930, 1682, 1611, 1352, 1195, 770  $\text{cm}^{-1}$ ; HRMS-ESI ( $m/z$ ): Calculated for:  $\text{C}_{31}\text{H}_{34}\text{N}_2\text{O}_4\text{SNa}$   $[\text{M}+\text{Na}]^+$ : 553.2138; found: 553.2137.



***N*-(5-chloro-8-methoxyquinolin-2-yl)-4-methyl-*N*-(2-oxo-2-phenylethyl)benzenesulfonamide (3v):** Obtained as a white solid; Yield = 67 mg (69%); m. p. = 152-154 °C;  $R_f$  = 0.5 (Ethyl Acetate/Hexane : 30/70);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.35 (d,  $J$  = 8.2 Hz, 1H), 8.06 (d,  $J$  = 8.4 Hz, 2H), 8.00-7.90 (m, 3H), 7.64 – 7.56 (m, 1H), 7.51 (t,  $J$  = 7.2 Hz, 2H), 7.32-7.22 (m, 3H), 6.73 (d,  $J$  = 8.2 Hz, 1H), 5.68 (s, 2H), 3.52 (s, 3H), 2.38 (s, 3H);  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  194.0, 153.8, 150.0, 144.6, 138.6, 136.6, 136.1, 135.1, 133.3, 129.9, 128.6, 128.4, 128.1, 125.1, 124.1, 122.0, 115.4, 108.8, 55.8, 53.3, 21.7. **IR (neat):** 2931, 1651, 1614, 1352, 1205, 765  $\text{cm}^{-1}$ ; **HRMS-ESI ( $m/z$ ):** Calculated for:  $\text{C}_{25}\text{H}_{22}\text{ClN}_2\text{O}_4\text{S}$   $[\text{M}+\text{H}]^+$ : 481.0990; found: 481.0988.

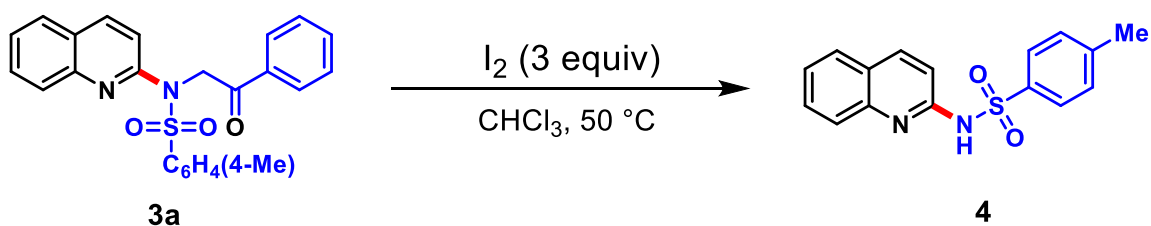


***N*-(5-chloro-8-methoxyquinolin-2-yl)-4-methyl-*N*-(2-oxo-2-(*p*-tolyl)ethyl)benzenesulfonamide (3w):** Obtained as a white solid; Yield = 72 mg (73%); m. p. = 146-148 °C;  $R_f$  = 0.35 (Ethyl Acetate/Hexane : 30/70);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.35 (d,  $J$  = 9.2 Hz, 1H), 8.01 – 7.87 (m, 5H), 7.35-7.19 (m, 5H), 6.74 (d,  $J$  = 8.4 Hz, 1H), 5.68 (s, 2H), 3.56 (s, 3H), 2.44 (s, 3H), 2.38 (s, 3H);  $^{13}\text{C NMR}$  (126 MHz,  $\text{CDCl}_3$ )  $\delta$  193.5, 153.9, 150.2, 144.5, 144.1, 138.7, 136.8, 135.1, 133.5, 129.9, 129.3, 128.5, 128.1, 125.1, 124.2, 122.1, 115.6, 109.0, 55.9, 53.2, 21.9, 21.7; **IR (neat):** 2927, 1691, 1614, 1353, 1203, 771  $\text{cm}^{-1}$ ; **HRMS-ESI ( $m/z$ ):** Calculated for:  $\text{C}_{26}\text{H}_{24}\text{ClN}_2\text{O}_4\text{S}$   $[\text{M}+\text{H}]^+$ : 495.1147; found: 495.1146.



***N*-(2-(4-(tert-butyl)phenyl)-2-oxoethyl)-*N*-(5-chloro-8-methoxyquinolin-2-yl)-4-methylbenzenesulfonamide (3x):** Obtained as a white solid; Yield = 77 mg (71%); m. p. = 157-159 °C;  $R_f$  = 0.45 (Ethyl Acetate/Hexane : 30/70);  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.35 (d,  $J$  = 7.6 Hz, 1H), 8.05-7.95 (m, 4H), 7.92 (d,  $J$  = 7.6 Hz, 1H), 7.53 (d,  $J$  = 6.8 Hz, 2H), 7.32-7.24 (m, 3H), 6.73 (d,  $J$  = 6.4 Hz, 1H), 5.68 (s, 2H), 3.53 (s, 3H), 2.38 (s, 3H), 1.37 (s, 9H);  $^{13}\text{C NMR}$  (126 MHz,  $\text{CDCl}_3$ )  $\delta$  193.5, 157.1, 153.9, 150.2, 144.5, 138.7, 136.8, 135.1, 133.5, 129.9, 128.3, 128.1, 125.6, 125.1, 124.2, 122.0, 115.6, 108.8, 55.8, 53.2, 35.3, 31.3, 21.7; **IR (neat):** 2932, 1681, 1611, 1358, 1202, 770  $\text{cm}^{-1}$ ; **HRMS-ESI ( $m/z$ ):** Calculated for:  $\text{C}_{29}\text{H}_{29}\text{ClN}_2\text{O}_4\text{SNa}$   $[\text{M}+\text{Na}]^+$ : 559.1433; found: 559.1433.

**6. Preparation of 4-methyl-*N*-(quinolin-2-yl)benzenesulfonamide (4) from 4-methyl-*N*-(2-oxo-2-phenylethyl)-*N*-(quinolin-2-yl)benzenesulfonamide (3a) with molecular iodine:**

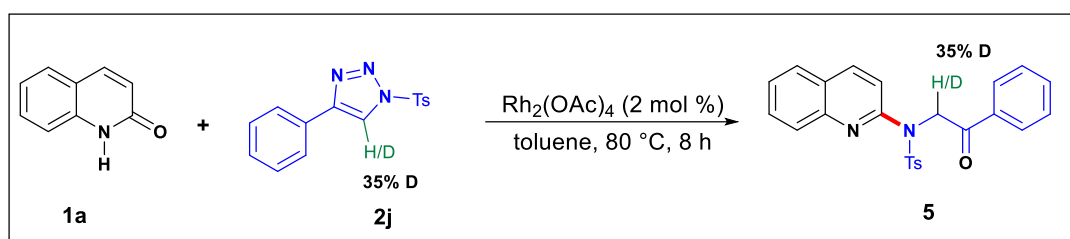


To a 10 mL round bottom flask containing solution of 2-aminoquinoline derivative **3a** (83 mg, 0.2 mmol) in 1,2-dichloroethane (2 mL) was added molecular iodine (153 mg, 3 equiv.) and the reaction mixture was stirred at 50 °C for 5 hours. Then the reaction mixture diluted with chloroform, washed with aqueous solution of sodium bisulfite and sat. aqueous solution

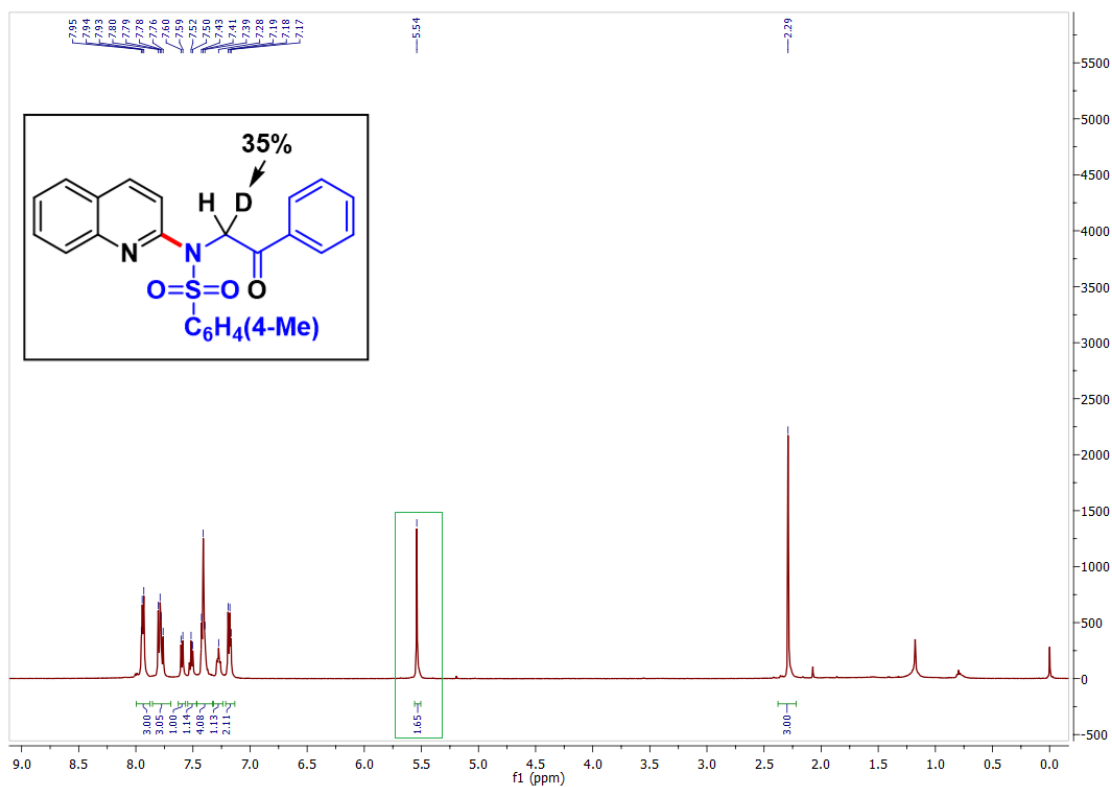
of sodium chloride. Then organic layers were concentrated under reduced pressure. The crude product was purified by using silica gel column chromatography to obtain product **4** as white solid with 55 mg (92%) yield. The product **4** was further characterized as follows;

**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)** δ 11.98 (bs, 1H), 7.89 (d, *J* = 8.2, 2H), 7.87 (d, *J* = 8.2, 1H), 7.60 (t, *J* = 8.0 Hz, 2H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.05 (d, *J* = 9.5 Hz, 1H), 2.37 (s, 3H); **<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>)** δ 154.6, 142.8, 140.9, 140.1, 136.8, 131.8, 129.5, 128.2, 126.4, 124.8, 121.5, 120.4, 117.7, 21.6; **IR (neat):** 2991, 1650, 1529, 1239, 765 cm<sup>-1</sup>; **HRMS-ESI (*m/z*):** Calculated for: C<sub>16</sub>H<sub>15</sub>N<sub>2</sub>O<sub>2</sub>S [M+H]<sup>+</sup>: 299.0842; found: 299.0842.

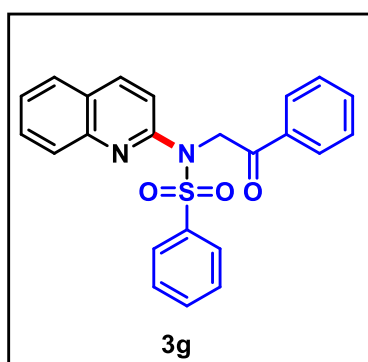
### 7. Reaction of deuterated *N*-sulfonyl-1,2,3-triazole with 2-quinolone:



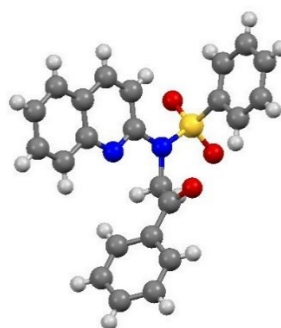
To a sealed tube charged with a stirring bar, was added 2-quinolone **1a** (29 mg, 0.2 mmol), triazole (72 mg, 0.24 mmol) **2j**, Rh<sub>2</sub>(OAc)<sub>4</sub> (2 mol %), and toluene (2 mL). The reaction mixture was stirred under inert atmosphere at 80 °C until the complete consumption of starting material (monitored by TLC). The organic solvents were removed under reduced pressure and the crude product was purified by column chromatography using petroleum ether / ethyl acetate as an eluent to give **5**.



## 8. Crystallographic data of compound 3g



(CCDC: 2254798)



ORTEP DIAGRAM

Data	Compound (3g) (CCDC: 2254798)
Solvent system for crystal growth	Ethyl acetate-Pet. Ether
Crystal growth method	Solvent evaporation
Formula	C <sub>23</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub> S
Formula Weight	402.1038
Wavelength	0.71073
Temperature(K)	296 K
Ellipsoid counter probability	50%

Space Group	P 21/c
Hall Group	-2 ybc
a (Å)	8.0778(5)
b(Å)	20.7672(14)
c(Å)	11.4161(8)
$\alpha(^{\circ})$	90
$\beta(^{\circ})$	98.705(5)
$\gamma(^{\circ})$	90
V(cm <sup>3</sup> )	1893.0(2)
Z	4
Density(g cm <sup>-3</sup> )	1.412
$\mu(\text{mm}^{-1})$	0.200
F (000)	840
$\theta$ (max)	28.794
$h_{\text{min,max}}/ k_{\text{min,max}}/ l_{\text{min,max}}$	10,28,15
No. unique ref./ obs. ref.	4927/4892
No. of parameters	262
R(reflections)	0.0523 (3397)
wR <sub>2</sub> (reflections)	0.1216 (4892)
Data completeness	0.993
S	1.050

### 9. References:

- 1) L.-Y. Xie, Y. Duan, L.-H. Lu, Y.-J. Li, S. Peng, C. Wu, K.-J. Liu, Z. Wang, W.-M. He, *ACS Sustainable Chem. Eng.* 2017, **5**, 10407.
- 2) R. F. Heck, *Org. React.* 1982, **27**, 345.
- 3) J. Raushel, V. V. Fokin, *Org. Lett.* 2010, **12**, 4952.

### 10. NMR Spectra:

