

**Electronic Supplementary Information**

**A simple access to *N*-(un)substituted isoquinolin-1(2*H*)-ones: unusual formation of regioisomeric isoquinolin-1(4*H*)-ones**

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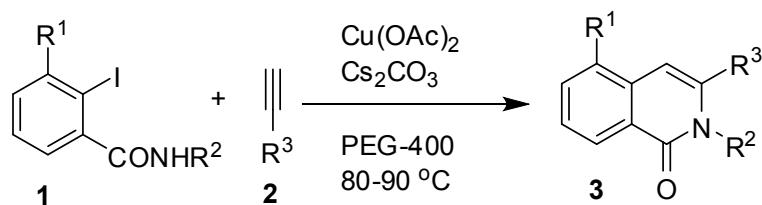
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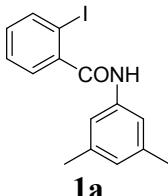
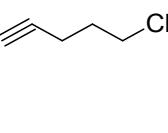
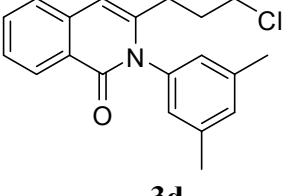
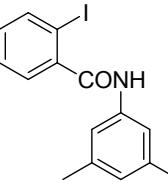
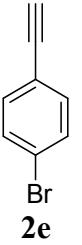
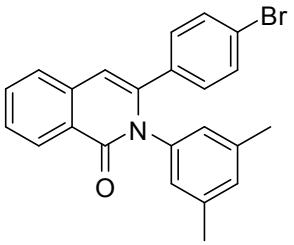
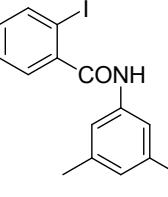
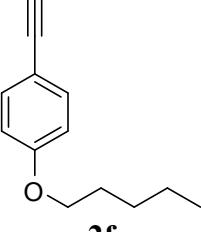
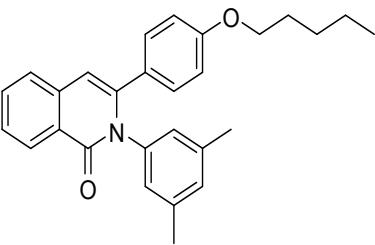
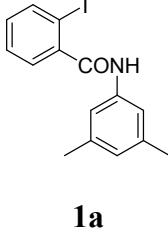
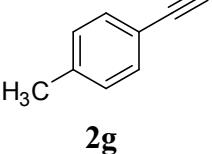
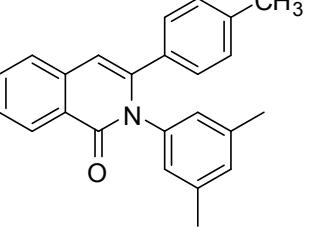
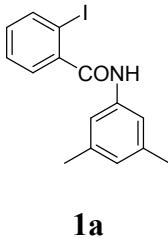
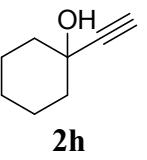
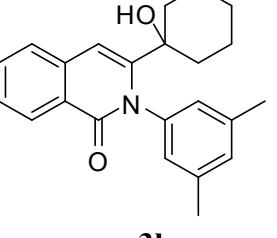
<sup>c</sup>*Dr Reddy's Institute of Life Sciences, University of Hyderabad Campus, Gachibowli, Hyderabad 500 046, India*

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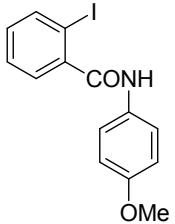
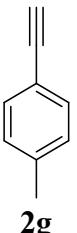
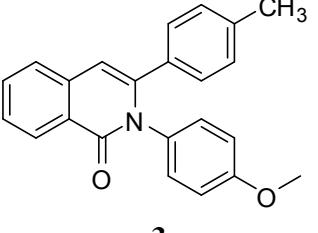
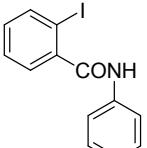
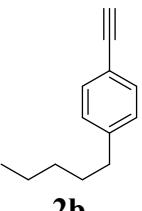
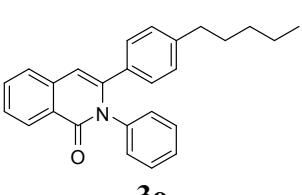
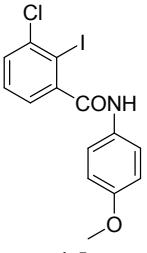
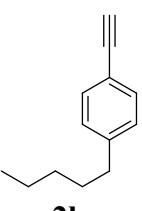
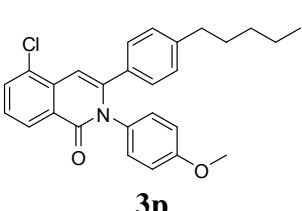
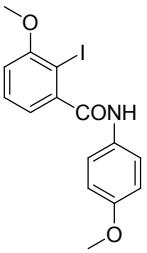
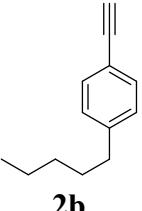
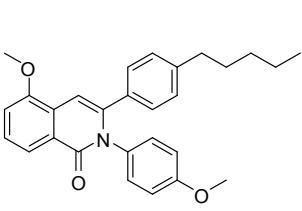
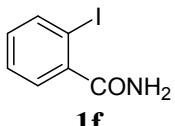
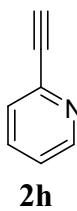
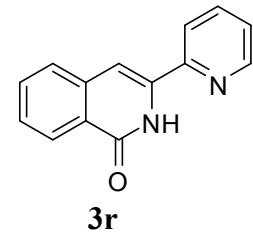
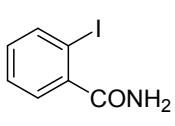
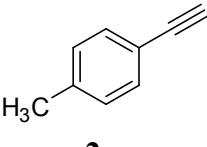
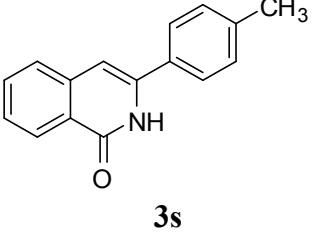
**Table S-1.** Cu-mediated synthesis of isoquinolin-1(2*H*)-ones (**3**)<sup>a</sup>.

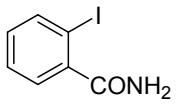
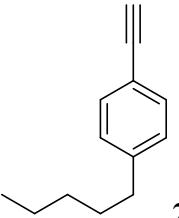
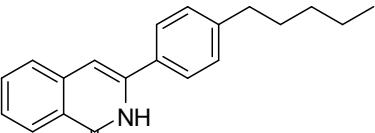
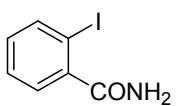
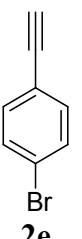
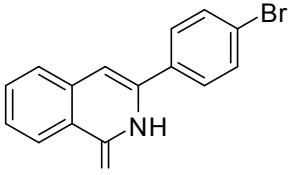


Entry	Iodoamide ( <b>1</b> )	Terminal alkyne ( <b>2</b> )	Product ( <b>3</b> )	Time (h)	Yield <sup>b</sup> (%)
1.				3.0	81.0
2.				3.0	76.0
3.				3.0	68

4.				4.0	71.0
5.				4.0	83
6.				4.0	79.0
7.				4.0	75.0
8.				4.0	68.0

9.				3.0	82.0
10.				3.0	77
11.				3.0	75
12.				3.0	82
13.				4.0	79.0

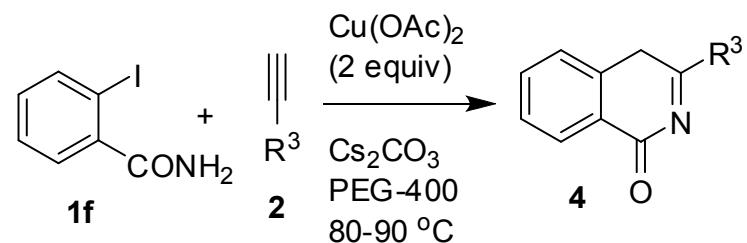
14.				4.0	73.0
15.				3.0	56.0
16.				3.0	63.0
17.				3	73
18.				3.0	93
19.				3.0	84.0

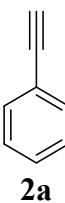
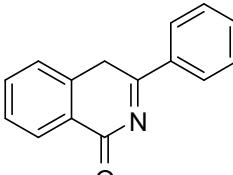
20.				3.0	87.0
21.				3.0	83

<sup>a</sup>All the reactions were carried out by using **1** (1.0 mmol), terminal **2** (1.0 mmol),  $\text{Cs}_2\text{CO}_3$  (2.0 mmol), and anhyd  $\text{Cu}(\text{OAc})_2$  (0.2 mmol) in PEG-400 (5.0 mL) at 80-90 °C under nitrogen.

<sup>b</sup>Isolated yield.

**Table S-2.** Synthesis of isoquinolin-1(4*H*)-ones (**4**)<sup>a</sup>



Entry	Terminal alkyne ( <b>2</b> )	Product ( <b>4</b> )	Time (h)	Yield <sup>b</sup> (%)
1.			4.0	81

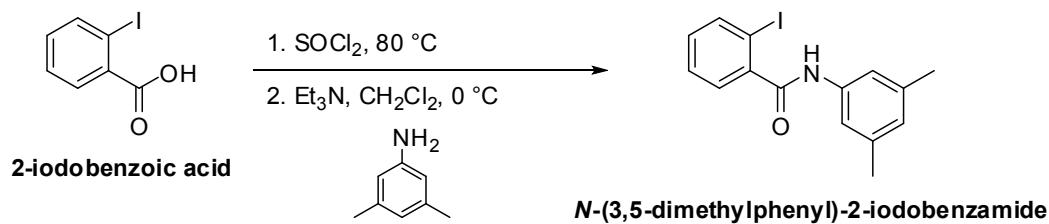
2.			3.5	78
2g				
3.			3.5	81.0
2b				
4.			4.0	76
2c				
5.			5.0	57
2h				
6.			4.5	62
2e				

<sup>a</sup>All the reactions were carried out by using **1** (1.0 mmol), terminal **2** (1.0 mmol), Cs<sub>2</sub>CO<sub>3</sub> (2.0 mmol), and anhyd Cu(OAc)<sub>2</sub> (2.0 mmol) in PEG-400 (5.0 mL) at 80-90 °C under nitrogen.

<sup>b</sup>Isolated yield.

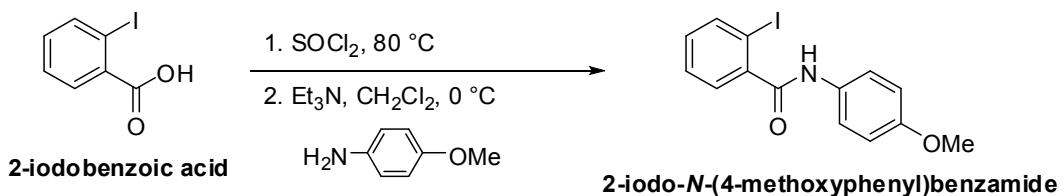
**General methods:** Unless stated otherwise, solvents and chemicals were obtained from commercial sources and were used without further purification. Reactions were monitored by thin layer chromatography (TLC) on silica gel plates (60 F254), visualizing with ultraviolet light or iodine spray. Flash chromatography was performed on silica gel (230-400 mesh) using hexane and ethyl acetate.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were determined in  $\text{DMSO}-d_6$  and  $\text{CDCl}_3$  solutions by using 400 or 100 MHz spectrometers, respectively. Proton chemical shifts ( $\delta$ ) are relative to tetramethylsilane (TMS,  $\delta = 0.00$ ) as internal standard and expressed in ppm. Spin multiplicities are given as s (singlet), d (doublet), t (triplet) and m (multiplet) as well as b (broad). Coupling constants ( $J$ ) are given in hertz. Infrared spectra were recorded on a FT-IR spectrometer. Melting points were determined using melting point B-540 apparatus and are uncorrected. HRMS was determined using waters LCT premier XEOTF ARE-047 apparatus.

#### Preparation of *N*-(3,5-dimethylphenyl)-2-iodobenzamide (1a):



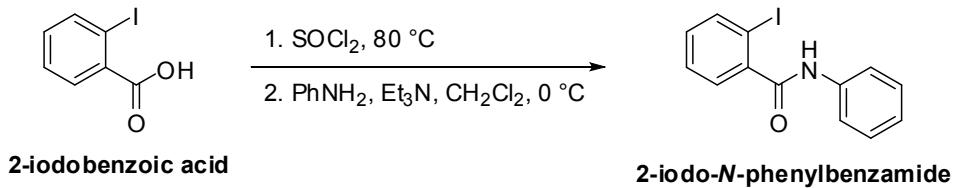
To a suspension of 2-iodobenzoic acid (20 mmol) in dry toluene was added  $\text{SOCl}_2$  (120 mmol) and the mixture was heated at  $80^\circ\text{C}$  for 3 h. After evaporation of the volatile materials,  $\text{CH}_2\text{Cl}_2$  (40 mL) and triethylamine (50 mmol) were added. The solution was cooled to  $0^\circ\text{C}$  and was added 3,5-dimethylaniline (20 mmol). After 1 h at room temperature, a saturated aqueous solution of  $\text{NaHCO}_3$  (50 mL) was added to this mixture. The white precipitate formed was filtered, washed with water and dried to give the title compound as a white powder (yield 88%);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.92 (d,  $J=7.8$  Hz, 1H), 7.52 (dd,  $J=7.4$  Hz, 1.5 Hz, 1H), 7.44 (t,  $J=7.3$  Hz, 1H), 7.33 (s, 1H), 7.27 (s, 2H), 7.15 (td,  $J=7.8, 1.5$  Hz, 1H), 6.82 (s, 1H), 2.34 (s, 6H).

#### Preparation of 2-ido-*N*-(4-methoxyphenyl)benzamide<sup>1</sup> (1b):



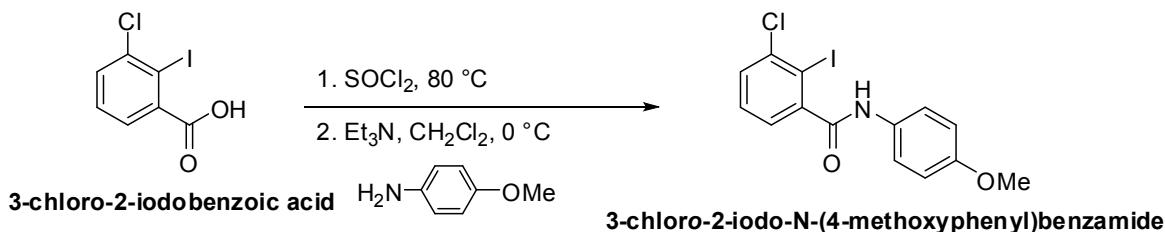
To a suspension of 2-iodobenzoic acid (20 mmol) in dry toluene was added  $\text{SOCl}_2$  (120 mmol) and the mixture was heated at 80 °C for 3 h. After evaporation of the volatile materials,  $\text{CH}_2\text{Cl}_2$  (40 mL) and triethylamine (50 mmol) were added. The solution was cooled to 0 °C and was added 4-methoxy aniline (20 mmol). After 1 h at room temperature, a saturated aqueous solution of  $\text{NaHCO}_3$  (50 mL) was added to this mixture. The white precipitate formed was filtered, washed with water and dried to give the title compound as a white powder (yield 86%);  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d^6$ )  $\delta$  10.24 (s, 1H), 7.92 (d,  $J=7.8$  Hz, 1H), 7.62 (d,  $J=8.8$  Hz, 2H), 7.44-7.51 (m, 2H), 7.22 (td,  $J=7.8, 0.2$  Hz, 1H), 6.92 (d,  $J=8.8$  Hz, 2H), 3.74 (s, 3H).

#### Preparation of 2-iodo-N-phenylbenzamide (1c)<sup>1</sup>:



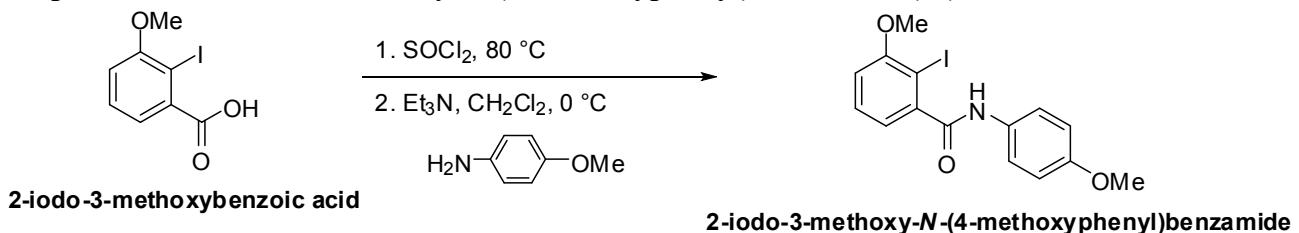
To a suspension of 2-iodobenzoic acid (20 mmol) in dry toluene was added  $\text{SOCl}_2$  (120 mmol) and the mixture was heated at 80 °C for 3 h. After evaporation of the volatile materials,  $\text{CH}_2\text{Cl}_2$  (40 mL) and triethylamine (50 mmol) were added. The solution was cooled to 0 °C and was added aniline (20 mmol). After 1 h at room temperature, a saturated aqueous solution of  $\text{NaHCO}_3$  (50 mL) was added to this mixture. The white precipitate formed was filtered, washed with water and dried to give the title compound as a white powder (yield 83%);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.51-7.54 (m, 4H), 7.32-7.38 (m, 6H).

#### Preparation of 3-chloro-2-ido-N-(4-methoxyphenyl)benzamide (1d):



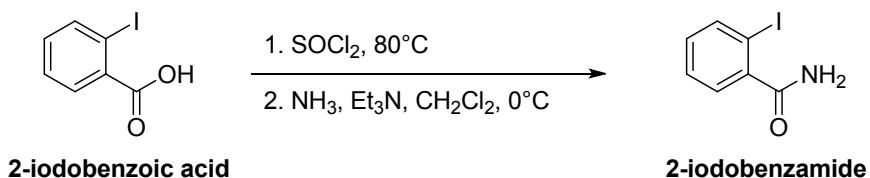
To a suspension of 3-chloro-2-iodo-benzoic acid (5 mmol) in dry toluene was added  $\text{SOCl}_2$  (30 mmol) and the mixture was heated at  $80^\circ\text{C}$  for 3 h. After evaporation of the volatile materials,  $\text{CH}_2\text{Cl}_2$  (20 mL) and triethylamine (12 mmol) were added. The solution was cooled to  $0^\circ\text{C}$  and was added 4-methoxy aniline (20 mmol). After 1 h at room temperature, a saturated aqueous solution of  $\text{NaHCO}_3$  (50 mL) was added to this mixture. The white precipitate formed was filtered, washed with water and dried to give the title compound as a white powder (yield 78%);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.91 (d,  $J=8.3$  Hz, 1H), 7.68 (t,  $J=8.3$  Hz, 1H), 7.55 (d,  $J=8.8$  Hz, 1H), 7.19 (d,  $J=7.3$  Hz, 2H), 6.98 (d,  $J=8.3$  Hz, 2H), 3.85 (s, 3H).

#### **Preparation of 2-iodo-3-methoxy-N-(4-methoxyphenyl)benzamide (1e):**



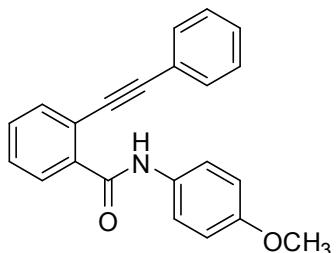
To a suspension of 2-Iodo-3-methoxybenzoic acid (5 mmol) in dry toluene was added  $\text{SOCl}_2$  (30 mmol) and the mixture was heated at  $80^\circ\text{C}$  for 3 h. After evaporation of the volatile materials,  $\text{CH}_2\text{Cl}_2$  (20 mL) and triethylamine (12 mmol) were added. The solution was cooled to  $0^\circ\text{C}$  to which was added 4-methoxy aniline (5 mmol). After 1 h at room temperature a saturated aqueous solution of  $\text{NaHCO}_3$  (25 mL) was added to this mixture. The brown precipitate formed was filtered, washed with water and dried to give the title compound as a brown powder (yield 65%);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.55 (dd,  $J=7.3$  Hz, 2Hz, 2H), 7.35-7.39 (m, 2H), 7.09 (dd,  $J=7.3$ , 1.5 Hz, 1H), 6.86-6.93 (m, 3H), 3.92 (s, 3H), 3.82 (s, 3H).

#### **Preparation of 2-iodobenzamide (1f):**



To a suspension of 2-iodobenzoic acid (20 mmol) in dry toluene was added  $\text{SOCl}_2$  (120 mmol) and the mixture was heated at 80°C for 3 h. After evaporation of the volatile materials,  $\text{CH}_2\text{Cl}_2$  (40 mL) and triethylamine (50 mmol) were added. The solution was cooled to 0 °C and bubbled with gaseous ammonia. After 1 h at room temperature, a saturated aqueous solution of  $\text{NaHCO}_3$  (50 mL) was added to this mixture. The white precipitate formed was filtered, washed with water and dried to give the title compound as a white powder (yield 85%);  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ )  $\delta$  7.86 (dd,  $J=7.8, 1$  Hz, 1H), 7.80 (s, 1H), 7.49 (s, 1H), 7.42 (td,  $J=7.3, 1.0$  Hz, 1H), 7.34 (dd,  $J=7.4, 1.5$  Hz, 1H), 7.14 (td,  $J=7.8, 1.9$  Hz, 1H).

***N*-(4-methoxyphenyl)-2-(phenylethyynyl)benzamide (5):**



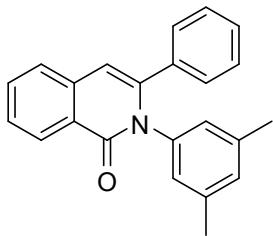
Yellow color solid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.18 (d,  $J=7.3$  Hz, 1H), 7.84 (d,  $J=7.4$  Hz, 1H), 7.78 (t,  $J=7.4$  Hz, 1H), 7.62 (t,  $J=7.4$  Hz, 1H), 7.11 (s, 1H), 6.89-6.99 (m, 7H), 6.67 (d,  $J=8.3$  Hz, 2H), 3.66 (s, 3H); ES-MS:  $m/z$ [M + 1]: 328.40.

**General procedure for the preparation of compound 3:**

To a mixture of 2-iodobenzamide **1** (1.0 mmol),  $\text{Cu}(\text{OAc})_2$  (0.2 mmol) and  $\text{Cs}_2\text{CO}_3$  (2.0 mmol) in polyethylene glycol (5.0 mL) was added terminal alkyne **2** (1.0 mmol) at room temperature and the mixture was stirred for 10-15 min under nitrogen at the same temperature. The mixture was then heated to 80-90 °C and stirred under nitrogen for the time mentioned in Table 2 (or Table S-

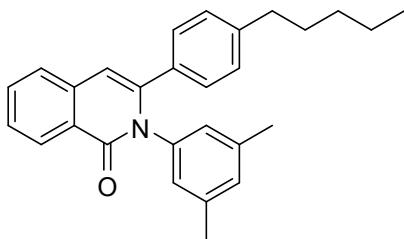
1). The reaction was monitored by TLC After completion of the reaction the mixture was diluted with EtOAc (10 mL) and filtered through celite. The filtrate was collected and washed with water (2 x 20 mL). The EtOAc layer was collected, and concentrated under low vacuum. The residue obtained was purified by column chromatography (petroleum ether-EtOAc) to give the desired product **3**.

**2-(3,5-Dimethylphenyl)-3-phenylisoquinolin-1(2H)-one (3a)**



White color solid; Yield: 81%; mp: 136-138 °C; IR (CHCl<sub>3</sub>): 3019, 1691, 1654, 1599 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.07 (d, *J*=7.3 Hz, 1H), 7.79 (d, *J*=7.4 Hz, 2H), 7.72 (d, *J*=7.8 Hz, 1H), 7.62 (t, *J*= 7.8 Hz, 1H), 7.54 (t, *J*=7.4 Hz, 1H), 7.35 (t, *J*=7.4 Hz, 3H), 7.54 (t, *J*=7.4 Hz, 2H), 6.88 (s, 1H), 6.29 (s, 1H), 2.40 (s, 6H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 153.7, 148.1, 145.2, 138.2 (2C), 137.4, 134.0, 132.0, 129.6, 129.5, 129.1 (2C), 128.5 (2C), 127.4, 126.7, 123.7, 121.9 (2C), 119.5, 103.1, 21.3 (2C); HRMS: *m/z*[M +1] calcd for C<sub>23</sub>H<sub>20</sub>NO: 326.1545; found: 326.1561

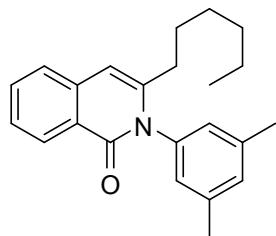
**2-(3,5-Dimethylphenyl)-3-(4-pentylphenyl)isoquinolin-1(2H)-one (3b)**



Pale yellow solid; Yield: 76%; mp: 85-90 °C; IR (CHCl<sub>3</sub>): 3018, 1687, 1656, 1602 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.02 (d, *J*=7.3 Hz, 1H), 7.70 (d, *J*= 8.3 Hz, 3H), 7.57-7.62 (m, 1H), 7.49-7.53 (m, 1H), 7.21 (s, 2H), 7.15 (d, *J*=7.8 Hz, 2H), 6.87 (s, 1H), 6.25 (s, 1H), 2.61 (t, *J*=7.3 Hz, 2H), 2.40 (s, 6H), 1.34-1.39 (m, 2H), 1.26-1.32 (m, 2H), 1.11-1.15 (m, 2H), 0.88 (t, *J*=7.3 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 154.0, 147.5, 145.2, 142.6, 138.2, 137.5, 132.0, 131.3,

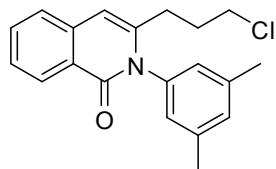
129.4, 129.3 (2C), 129.1 (3C), 128.7, 126.7, 123.7, 121.9 (2C), 119.4, 103.3, 35.7, 31.4, 31.0, 22.5, 21.3 (2C), 14.0; HRMS:  $m/z$ [M + 1] calcd for C<sub>28</sub>H<sub>30</sub>NO: 396.2327; found: 396.2345.

**2-(3,5-Dimethylphenyl)-3-hexylisoquinolin-1(2H)-one (3c)**



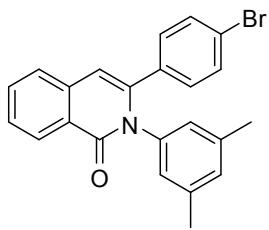
Colorless liquid; Yield: 68%; IR (CHCl<sub>3</sub>): 3017, 1697, 1666, 1593 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.37 (d,  $J$ =7.3 Hz, 1H), 7.49 (t,  $J$ =7.4 Hz, 1H), 7.36 (t,  $J$ =7.4 Hz, 1H), 7.18 (d,  $J$ =7.9 Hz, 1H), 6.85 (s, 2H), 6.75 (s, 1H), 5.99 (s, 1H), 2.31-2.36 (m, 8H), 1.53-1.61 (m, 2H), 1.26-1.37 (m, 6H), 0.88 (t,  $J$ =7.3 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  156.3, 150.2, 146.4, 137.9, 134.0, 132.1, 127.3 (2C), 125.1, 124.5, 123.4, 120.5 (3C), 101.7, 33.1, 31.6, 28.5, 26.8, 22.5, 21.3 (2C), 14.0; HRMS:  $m/z$ [M + 1] calcd for C<sub>23</sub>H<sub>28</sub>NO: 334.2171; found: 334.2189

**3-(3-Chloropropyl)-2-(3,5-dimethylphenyl)isoquinolin-1(2H)-one (3d)**



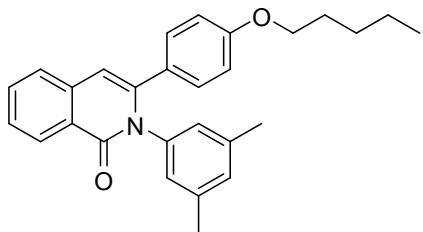
Gummy mass; Yield: 71.0%; IR (CHCl<sub>3</sub>): 3015, 1695, 1662, 1595 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.30 (d,  $J$ =7.8 Hz, 1H), 7.50 (t,  $J$ =7.8 Hz, 1H), 7.37 (t,  $J$ =7.8 Hz, 1H), 7.18 (d,  $J$ =7.8 Hz, 1H), 6.79 (s, 2H), 6.74 (s, 1H), 6.03 (s, 1H), 3.52 (t,  $J$ =6.3 Hz, 2H), 2.52 (t,  $J$ =7.4 Hz, 2H), 2.32 (s, 6H), 1.99-2.05 (m, 2H); <sup>13</sup>C NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  154.2, 149.8, 146.3, 138.1, 133.6, 132.2, 127.7, 127.3, 125.2, 124.7, 123.4, 120.2 (3C), 102.7, 43.7, 30.3, 29.7, 21.4 (2C); HRMS:  $m/z$ [M + 1] calcd for C<sub>20</sub>H<sub>21</sub>NOCl: 326.1312; found: 326.1329.

**5. 3-(4-Bromophenyl)-2-(3,5-dimethylphenyl)isoquinolin-1(2H)-one (3e)**



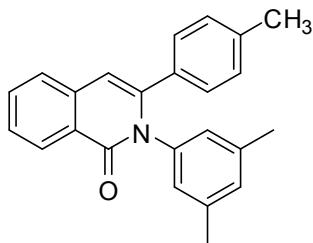
Off-white color solid; Yield: 83%; mp: 122-124; IR (CHCl<sub>3</sub>): 3014, 1692, 1655, 1590 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.02 (d, *J*=7.9 Hz, 1H) 7.70 (d, *J*=7.9 Hz, 1H), 7.59-7.65 (m, 3H), 7.48-7.56 (m, 2H), 7.43-7.46 (m, 1H), 7.15 (s, 2H), 6.88 (s, 1H), 6.19 (s, 1H), 2.39 (s, 6H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 148.6, 145.2, 138.3, 137.6, 137.2, 133.0, 132.1, 131.7 (2C), 130.7, 130.5, 129.8 (2C), 126.8, 123.7, 121.6 (3C), 121.2, 119.5, 101.8, 21.3 (2C); HRMS: *m/z*[M + 1]calcd for C<sub>23</sub>H<sub>19</sub>NOBr: 404.0650; found: 404.0633.

### **2-(3,5-Dimethylphenyl)-3-(pentyloxy)phenylisoquinolin-1(2H)-one (3f)**



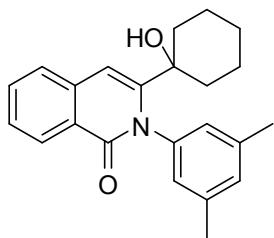
Yellow color solid; Yield: 79%; mp: 80-84 °C; IR (CHCl<sub>3</sub>): 3015, 1685, 1603, 1510 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.00 (d, *J*=7.3 Hz, 1H), 7.72 (d, *J*=8.3 Hz, 2H), 7.68 (d, *J*=7.3 Hz, 1H), 7.59 (t, *J*=7.3 Hz, 1H), 7.49 (t, *J*=7.4 Hz, 1H), 7.2 (s, 2H), 6.86 (d, *J*=8.3 Hz, 3H), 6.22 (s, 1H), 3.97 (t, *J*=6.9 Hz, 2H), 2.39 (s, 6H), 1.76-1.83 (m, 2H), 1.34-1.52 (m, 4H), 0.96 (t, *J*=7.4 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 158.6, 154.0, 146.5, 145.4, 138.1, 137.7, 131.9, 130.9, 130.5 (2C), 129.2, 129.1, 128.8, 126.5, 123.6, 121.8 (2C), 119.2, 114.6 (2C), 103.0, 67.9, 28.9, 28.1, 22.4, 21.3 (2C), 14.0; HRMS: *m/z*[M+1]calcd for C<sub>28</sub>H<sub>30</sub>NO<sub>2</sub>: 412.2277; found: 412.2291.

### **2-(3,5-Dimethylphenyl)-3-(p-tolyl)isoquinolin-1(2H)-one (3g)**



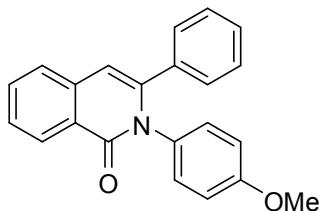
Yellow color solid; Yield: 75%; mp: 124-126 °C; IR (CHCl<sub>3</sub>): 3014, 1680, 1602, 1505 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.01 (d, *J*=7.8 Hz, 1H), 7.62-7.70 (m, 3H), 7.60 (t, *J*=7.8 Hz, 1H), 7.51 (t, *J*=6.5 Hz, 1H), 7.26 (s, 2H), 7.15 (d, *J*=7.8 Hz, 2H), 6.87 (s, 1H), 6.24 (s, 1H), 2.40 (s, 6H), 2.36 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 153.7, 147.4, 145.3, 138.1, 137.5, 137.4, 131.9, 131.1, 129.5, 129.4, 129.3 (2C), 129.2, 129.0 (2C), 126.6, 123.6, 121.9 (2C), 119.3, 103.1, 21.3 (3C); HRMS: *m/z*[M+1] calcd for C<sub>24</sub>H<sub>22</sub>NO : 340.1701; found: 340.1718.

### **2-(3,5-Dimethylphenyl)-3-(1-hydroxycyclohexyl)isoquinolin-1(2H)-one (3h)**



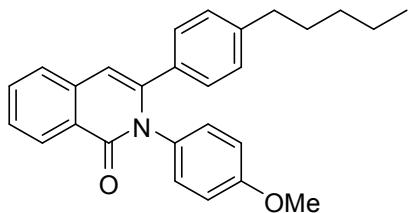
Light yellow solid; Yield: 68%; mp: 116-119 °C; IR (Neat): 3586, 3017, 1597, 1666, 1593 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.97 (d, *J*=7.3 Hz, 1H), 7.58 (d, *J*=3.2 Hz, 2H), 7.50-7.53 (m, 1H), 7.00 (s, 2H), 6.81 (s, 1H), 5.56 (s, 1H), 2.33 (s, 6H), 1.85-1.92 (m, 2H), 1.68-1.79 (m, 4H), 1.46-1.56 (m, 4H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 153.2, 147.5, 145.1, 138.1, 136.9, 132.1, 132.0, 129.6, 129.3, 126.5, 123.5, 121.5 (2C), 119.5, 110.5, 71.5, 38.3 (2C), 25.3, 22.3 (2C), 21.2 (2C); HRMS: *m/z*[M + 1]calcd for C<sub>23</sub>H<sub>26</sub>NO<sub>2</sub>: 348.1964; found: 348.1963.

### **2-(4-Methoxyphenyl)-3-phenylisoquinolin-1(2H)-one (3i)**



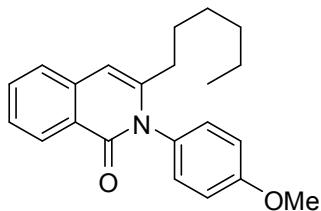
Yellow color solid; Yield: 82%; mp: 168-170 °C, IR (CHCl<sub>3</sub>): 3020, 1690, 1654, 1502 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.01 (d, *J*=7.8 Hz, 1H), 7.78 (d, *J*= 7.9 Hz, 2H), 7.72 (d, *J*=7.9 Hz, 1H), 7.50-7.62 (m, 4H), 7.37 (t, *J*=7.4 Hz, 2H), 7.26 (s, 1H), 6.98 (d, *J*=8.8 Hz, 2H), 6.27 (s, 1H), 3.88 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 157.1, 153.0, 148.2, 138.5, 137.3, 134.0, 131.9, 129.6, 129.0 (2C), 128.6 (3C), 127.4, 125.5 (2C), 123.5, 119.5, 113.9 (2C), 102.8, 55.4; HRMS: *m/z*(M + 1) calcd for C<sub>22</sub>H<sub>18</sub>NO<sub>2</sub>: 328.1338; found 328.1351.

### **2-(4-Methoxyphenyl)-3-(4-pentylphenyl)isoquinolin-1(2H)-one (3j)**



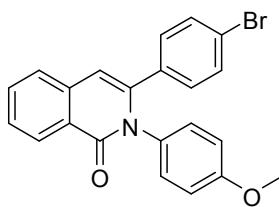
Yellow color solid; Yield: 77%; mp: 101-103 °C; IR (CHCl<sub>3</sub>): 3019, 1690, 1655, 1505 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.99 (d, *J*=7.8 Hz, 1H), 7.70 (d, *J*=7.8 Hz, 2H), 7.50-7.59 (m, 5H), 7.18 (d, *J*=8.4 Hz, 2H), 6.98 (dd, *J*= 6.8, 2 Hz, 2H), 6.25 (s, 1H), 3.88 (s, 3H), 2.61 (t, *J*=7.8 Hz, 2H), 1.54-1.63 (m, 2H), 1.24-1.38 (m, 4H), 0.90 (t, *J*=7.6 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 157.0, 153.0, 147.5, 142.5, 138.6, 137.4, 131.7, 131.3, 129.5, 129.3, 129.0 (2C), 128.6 (2C), 125.5 (2C), 123.4, 119.3, 113.9 (2C), 102.9, 55.4, 35.7, 31.3, 31.0, 22.5, 14.0; HRMS: *m/z*[M + 1] calcd for C<sub>27</sub>H<sub>28</sub>NO<sub>2</sub>: 398.2120; found: 398.2116.

### **3-Hexyl-2-(4-methoxyphenyl)isoquinolin-1(2H)-one (3k)**



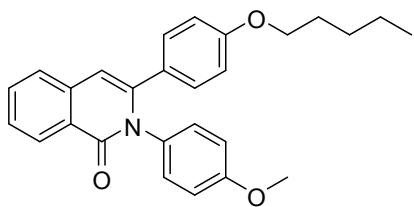
Pale yellow Colored liquid; Yield: 75%; IR (neat): 3019, 1692, 1652, 1505 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.31 (d, *J*=7.8 Hz, 1H), 7.42-7.49 (m, 1H), 7.32-7.36 (m, 1H), 7.22-7.25 (m, 2H), 7.24 (dd, *J*=6.8, 2 Hz, 1H), 6.89 (dd, *J*= 6.9, 2.0 Hz, 2H), 5.97 (s, 1H), 3.83 (s, 3H), 2.36 (t, *J*=7.8 Hz, 2H), 1.41-1.48 (m, 2H), 1.04-1.24 (m, 6H), 0.89 (t, *J*=7.6 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 156.2, 149.8, 139.4, 134.6, 133.9, 131.9, 129.4, 127.3, 127.1, 124.5, 124.4, 123.6, 113.7 (2C), 101.7, 55.3, 33.0, 31.4, 28.5, 26.6, 22.4, 14.0; HRMS: *m/z*[M + 1]calcd for C<sub>22</sub>H<sub>26</sub>NO<sub>2</sub>: 336.1964; found: 333.1967.

### **3-(4-Bromophenyl)-2-(4-methoxyphenyl)isoquinolin-1(2H)-one (3l)**



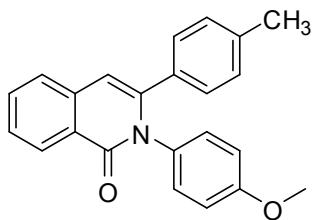
Yellow color solid; Yield: 82%; mp: 122-125 °C; IR (CHCl<sub>3</sub>): 3019, 1690, 1652, 1506 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.00 (d, *J*=7.8 Hz, 1H), 7.55-7.70 (m, 4H), 7.46-7.54 (m, 5H), 6.95-6.99 (m, 2H), 6.19 (s, 1H), 3.88 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 157.2, 148.6, 138.3, 137.7, 137.0, 134.2, 132.9, 132.0, 131.7 (2C), 130.4 (2C), 129.8, 125.3 (2C), 123.6, 121.2, 119.5, 114.0 (2C), 101.6, 55.4; HRMS: *m/z*(M+1) calcd for C<sub>22</sub>H<sub>17</sub>NO<sub>2</sub>Br : 406.0443; found: 406.0461.

### **2-(4-Methoxyphenyl)-3-(4-(pentyloxy)phenyl)isoquinolin-1(2H)-one (3m)**



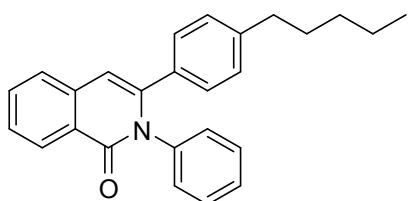
Pale yellow color solid; Yield: 79%; mp: 114-116°C; IR (CHCl<sub>3</sub>): 3018, 1688, 1656, 1604, 1510 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.99 (d, *J*=7.3 Hz, 1H), 7.71 (d, *J*=8.8 Hz, 3H), 7.49-7.58 (m, 4H), 6.97 (d, *J*=8.8 Hz, 2H), 6.89 (d, *J*=8.8 Hz, 2H), 6.22 (s, 1H), 3.99 (t, *J*=6.3 Hz, 2H), 3.88 (s, 3H), 1.78-1.83 (m, 2H), 1.41-1.46 (m, 4H), 0.95 (t, *J*=7.2 Hz, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 158.6, 156.9, 153.3, 146.5, 138.7, 137.5, 131.7, 130.4 (2C), 129.2, 129.0, 126.5, 125.4 (2C), 123.4, 119.1, 114.6 (2C), 113.9 (2C), 102.8, 67.9, 55.4, 28.9, 28.1, 22.4, 14.0; HRMS: *m/z*[M + 1]calcd for C<sub>27</sub>H<sub>28</sub>NO<sub>3</sub>: 414.2069; found: 414.2089.

### **2-(4-Methoxyphenyl)-3-(p-tolyl)isoquinolin-1(2H)-one (3n)**



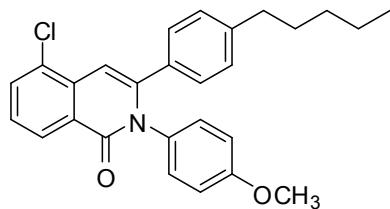
Yellow color solid; Yield: 73%; mp: 140-143 °C; IR (CHCl<sub>3</sub>): 3019, 1689, 1656, 1505 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.99 (d, *J*=7.8 Hz, 1H), 7.66-7.40 (m, 3H), 7.48-7.61 (m, 4H), 7.18 (d, *J*=7.8 Hz, 2H), 6.98 (d, *J*=8.8 Hz, 2H), 6.24 (s, 1H), 3.88 (s, 3H), 2.37 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 157.0, 147.5, 138.5, 137.5, 137.4, 131.8, 131.1, 129.4 (3C), 129.3 (2C), 129.0 (2C), 125.5 (2C), 123.5, 119.3, 113.9 (2C), 103.0, 55.4, 21.2; HRMS: *m/z*[M + 1]calcd for C<sub>23</sub>H<sub>20</sub>NO<sub>2</sub>: 342.1494; found: 342.1487.

### **3-(4-Pentylphenyl)-2-phenylisoquinolin-1(2H)-one (3o)**



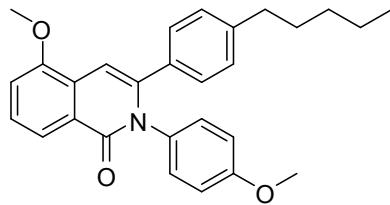
Off-white color solid; Yield: 56%; mp: 102-104 °C; IR (CHCl<sub>3</sub>): 3004, 1708, 1630, 1598, 1510 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.02 (d, *J*=7.3 Hz, 1H), 7.71 (d, *J*=7.8 Hz, 1H), 7.63 (t, *J*=8.4 Hz, 3H), 7.41-7.50 (m, 5H), 7.21-7.23 (m, 1H), 7.14 (d, *J*=8.3 Hz, 2H), 6.25 (s, 1H), 2.59 (t, *J*=8.3 Hz, 2H), 1.59-1.63 (m, 2H), 1.31-1.35 (m, 4H), 0.90 (t, *J*=7.6 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 154.2, 147.4, 145.9, 142.6, 137.7, 132.1, 131.2, 129.4, 129.1 (2C), 128.7 (5C), 124.7, 123.7, 123.6 (2C), 119.4, 103.4, 35.7, 31.5, 31.0, 22.5, 14.0; HRMS: *m/z*[M + 1] calcd for C<sub>26</sub>H<sub>25</sub>NO : 368.2014; found: 368.2003.

### **5-Chloro-2-(4-methoxyphenyl)-3-(4-pentylphenyl)isoquinolin-1(2*H*)-one (3p)**



Pale Yellow color solid; Yield: 63%; mp: 118-120 °C; IR (CHCl<sub>3</sub>): 2929, 1682, 1654, 1607 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.91 (d, *J*=8.3 Hz, 1H), 7.68 (d, *J*=8.3 Hz, 3H), 7.55 (d, *J*=8.8 Hz, 2H), 7.46 (d, *J*=8.3 Hz, 1H), 7.19 (d, *J*=7.3 Hz, 2H), 6.98 (d, *J*=8.3 Hz, 2H), 6.23 (s, 1H), 3.88 (s, 3H), 2.62 (t, *J*=7.8 Hz, 2H), 1.61-1.65 (m, 2H), 1.33-1.35 (m, 4H), 0.90 (t, *J*=6.8 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 177.1, 157.2, 146.3, 143.1, 138.9, 138.2, 137.0, 131.0, 129.8, 129.2 (2C), 128.8 (2C), 128.0, 125.6 (2C), 124.7, 119.4, 114.0 (2C), 104.1, 55.5, 35.7, 31.5, 31.0, 22.5, 14.0; HRMS: *m/z*[M + 1] calcd for C<sub>27</sub>H<sub>27</sub>NO<sub>2</sub>Cl : 432.1730; found: 432.1718.

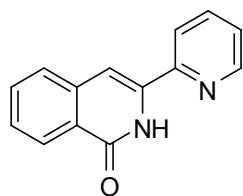
### **5-Methoxy-2-(4-methoxyphenyl)-3-(4-pentylphenyl)isoquinolin-1(2*H*)-one (3q)**



Pale Yellow color solid; Yield: 73%; mp: 129-130 °C; IR (CHCl<sub>3</sub>): 3016, 1686, 1650, 1594, 1506 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.70 (d, *J*=8.3 Hz, 2H), 7.59 (d, *J*=7.3 Hz, 1H), 7.53-7.56 (m, 2H), 7.43 (t, *J*=7.8 Hz, 1H), 7.16 (d, *J*=7.8 Hz, 2H), 7.05 (d, *J*=7.8 Hz, 1H), 6.95-6.98

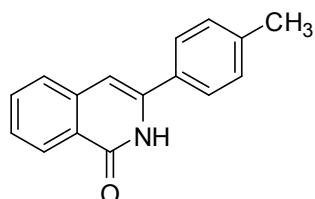
(m, 2H), 6.68 (s, 1H), 4.04 (s, 3H), 3.87 (s, 3H), 2.61 (t,  $J=7.3$  Hz, 2H), 1.56-1.63 (m, 2H), 1.32-1.35 (m, 4H), 0.90 (t,  $J=6.8$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.0, 155.2, 148.2, 141.1, 138.7, 137.1, 133.7, 131.8, 130.1, 129.7, 129.0 (2C), 128.3 (2C), 127.0 (2C), 123.3, 119.3, 113.3 (2C), 102.0, 55.6, 55.2, 35.5, 31.3, 31.2, 22.4, 13.9; HRMS:  $m/z$ [M + 1] calcd for  $\text{C}_{28}\text{H}_{30}\text{NO}_3$  : 428.2226; found: 428.2213.

### 3-(Pyridin-2-yl)isoquinolin-1(2*H*)-one (**3r**)



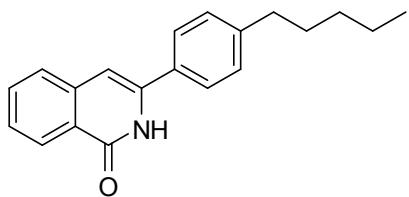
Red color solid; Yield: 93%; mp: 134-136 °C; IR ( $\text{CHCl}_3$ ): 1709, 1614, 1590  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  11.22 (s, 1H), 8.60 (d,  $J=4.4$  Hz, 1H), 7.89 (d,  $J=7.4$  Hz, 1H), 7.77 (d,  $J=7.3$  Hz, 1H), 7.68 (t,  $J=7.8$  Hz, 1H), 7.62 (t,  $J=7.8$  Hz, 1H), 7.54 (t,  $J=7.3$  Hz, 1H), 7.29 (d,  $J=7.9$  Hz, 1H), 7.11-7.14 (m, 1H), 6.35 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  168.6, 155.5, 148.9, 137.9, 137.7, 136.5, 131.0, 129.5, 129.3, 124.2, 123.4, 120.9, 119.9, 101.8; HRMS:  $m/z$ [M + 1] calcd for  $\text{C}_{14}\text{H}_{11}\text{N}_2\text{O}$  : 223.0871; found: 223.0873.

### 3-(*p*-Tolyl)isoquinolin-1(2*H*)-one (**3s**)



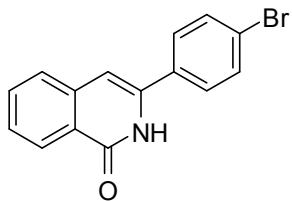
White color solid; Yield: 84%; mp: 220-222 °C; IR ( $\text{CHCl}_3$ ): 3036, 1689, 1556, 1611  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.00 (s, 1H), 7.88 (d,  $J=7.4$  Hz, 1H), 7.78 (d,  $J=7.8$  Hz, 1H), 7.64 (t,  $J=7.9$  Hz, 1H), 7.52 (t,  $J=6.9$  Hz, 1H), 7.34 (d,  $J=8.3$  Hz, 2H), 7.25 (d,  $J=8.3$  Hz, 2H), 6.54 (s, 1H), 2.39 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  169.0, 138.2, 137.7, 132.3, 132.1, 132.0, 129.9, 128.9 (2C), 128.5, 128.3 (2C), 123.5, 119.6, 106.1, 21.2; HRMS:  $m/z$ [M + 1] calcd for  $\text{C}_{16}\text{H}_{14}\text{NO}$  : 236.1075; found: 236.1083.

**3-(4-Pentylphenyl)isoquinolin-1(2*H*)-one (3t)**



White color solid; Yield: 87%; mp: 136-138°C; IR (CHCl<sub>3</sub>): 2925, 1713, 1649, 1612 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.10 (s, 1H), 7.88 (d, *J*=7.3 Hz, 1H), 7.79 (d, *J*=7.3 Hz, 1H), 7.63 (t, *J*=7.8 Hz, 1H), 7.51 (t, *J*=7.8 Hz, 1H), 7.36 (d, *J*=7.8 Hz, 2H), 7.25 (d, *J*=7.8 Hz, 2H), 6.54 (s, 1H), 2.64 (t, *J*=7.8 Hz, 2H), 1.60-1.68 (m, 2H), 1.33-1.39 (m, 4H), 0.91 (t, *J*=6.4 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 169.0, 142.7, 138.3, 132.3, 132.2, 132.1, 129.2 (2C), 128.9, 128.5, 128.4 (2C), 123.4, 119.6, 106.1, 35.6, 31.4, 30.9, 22.4, 14.0; HRMS: *m/z*[M + 1] calcd for C<sub>20</sub>H<sub>22</sub>NO: 292.1701; found: 292.1689.

**3-(4-Bromophenyl)isoquinolin-1(2*H*)-one (3u)**



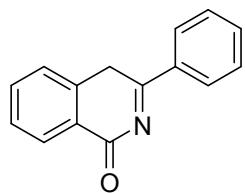
Pale yellow color solid; Yield: 83%; mp: 255-257 °C; IR (CHCl<sub>3</sub>): 3036, 1685, 1651, 1591 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.03 (s, 1H), 7.88 (d, *J*=7.3 Hz, 1H), 7.78 (d, *J*=7.8 Hz, 1H), 7.65 (t, *J*=7.3 Hz, 1H), 7.52-7.58 (m, 3H), 7.32 (d, *J*=8.3 Hz, 2H), 6.47 (s, 1H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) δ 169.1, 138.6, 133.9, 133.1, 132.3, 131.5 (2C), 131.0 (2C), 129.3, 128.2, 122.7, 120.4, 120.2, 104.5; HRMS: *m/z*[M + 1] calcd for C<sub>15</sub>H<sub>11</sub>BrNO: 300.0024; found: 300.0019.

**General procedure for the preparation of compound 4:**

To a mixture of 2-iodobenzamide **1f** (1.0 mmol), Cu(OAc)<sub>2</sub> (2.0 mmol) and Cs<sub>2</sub>CO<sub>3</sub> (2.0 mmol) in polyethylene glycol (5.0 mL) was added terminal alkyne **2** (1.0 mmol) at room temperature and the mixture was stirred for 10-15 min under nitrogen at the same temperature. The mixture

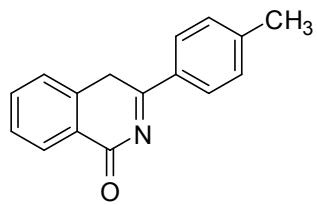
was then heated to 80-90 °C and stirred under nitrogen for 3.5-5 h. The reaction was monitored by TLC. After completion of the reaction, the mixture was diluted with EtOAc (10 mL) and filtered through celite. The filtrate was collected and washed with water (2 x 20 mL). The EtOAc layer was collected, and concentrated under low vacuum. The residue obtained was purified by column chromatography (petroleum ether-EtOAc) to give the desired product (**4**).

### **3-Phenylisoquinolin-1(4H)-one (**4a**)**



White color solid; Yield: 81%; mp: 110-113 °C; IR (CHCl<sub>3</sub>): 3019, 1691, 1599 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.06 (d, *J*=7.8 Hz, 2H), 7.70 (d, *J*=7.3 Hz, 1H), 7.56 - 7.64 (m, 2H), 7.51 (t, *J*= 7.8 Hz, 2H), 7.39 (t, *J*=7.8 Hz, 2H), 4.56 (s, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 195.3, 138.5, 136.2, 133.6, 132.7 (2C), 131.0, 128.8 (2C), 128.3 (2C), 127.5, 117.8, 113.6, 43.5; HRMS: *m/z*[M + 1] calcd for C<sub>15</sub>H<sub>12</sub>NO: 222.0919; found: 222.0925.

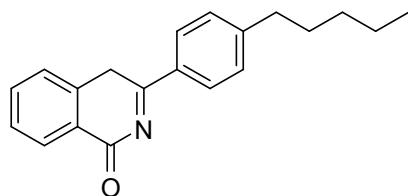
### **3-(*p*-Tolyl)isoquinolin-1(4H)-one (**4b**)**



White color solid; Yield: 78%; mp: 105-108 °C; IR (CHCl<sub>3</sub>): 3036, 1689, 1556 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.95 (d, *J*=8.3 Hz, 2H), 7.69 (dd, *J*= 8.4, 1.5 Hz, 1H), 7.56 (td, *J*=7.8,1.0 Hz, 1H), 7.37-7.41 (m, 2H), 7.30 (d, *J*=8.4 Hz, 2H), 4.53 (s, 2H), 2.43 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 195.0, 144.5, 138.7, 133.7, 132.7 (2C), 130.9, 129.4 (2C), 128.5

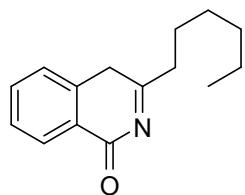
(2C), 127.5, 117.9, 113.5, 43.4, 21.6; HRMS:  $m/z$ [M + 1] calcd for C<sub>16</sub>H<sub>14</sub>NO : 236.1075; found: 236.1079.

### **3-(4-Pentylphenyl)isoquinolin-1(4H)-one (4c)**



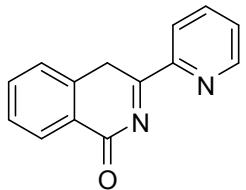
White color solid; Yield: 81%; mp: 99-101 °C; IR (CHCl<sub>3</sub>): 2925, 1713, 1612 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.97 (d,  $J$ =8.3 Hz, 2H), 7.69 (d,  $J$ =7.3 Hz, 1H), 7.57 (t,  $J$ =7.3 Hz, 1H), 7.37-7.41 (m, 2H), 7.30 (d,  $J$ =8.3 Hz, 2H), 4.53 (s, 2H), 2.67 (t,  $J$ =7.8 Hz, 2H), 1.60-1.68 (m, 2H), 1.30-1.37 (m, 4H), 0.89 (t,  $J$ =6.3 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  195.0, 149.5, 138.7, 133.9, 132.7 (2C), 131.0, 128.8 (2C), 128.5 (2C), 127.4, 117.9, 113.5, 43.4, 35.9, 31.3, 30.7, 22.4, 13.9; HRMS:  $m/z$ [M + 1] calcd for C<sub>20</sub>H<sub>22</sub>NO: 292.1701; found: 292.1703.

### **3-Hexylisoquinolin-1(4H)-one (4d)**



Pale yellow liquid; Yield: 76%; IR (CHCl<sub>3</sub>): 1684, 1593, 1579 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  7.80 (d,  $J$ =7.4 Hz, 1H), 7.65 (td,  $J$ = 7.7, 1.0 Hz, 1H), 7.40-7.47 (m, 2H), 4.05 (s, 2H), 2.57 (t,  $J$ = 7.4 Hz, 2H), 1.48-1.53 (m, 2H), 1.23-1.29 (m, 6H), 0.86 (t,  $J$ =6.4 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  206.0, 138.3, 132.8 (2C), 132.7, 130.9, 127.5, 113.3, 47.7, 43.0, 31.5, 28.7, 23.6, 22.4, 14.0; HRMS:  $m/z$ [M + NH<sub>4</sub>] calcd for C<sub>15</sub>H<sub>23</sub>N<sub>2</sub>O: 247.1810; found: 247.1822.

### **3-(Pyridin-2-yl)isoquinolin-1(4H)-one (4e)**



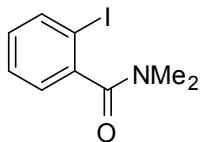
Gummy solid; Yield: 57% ; IR (CHCl<sub>3</sub>): 3021, 1690, 1598 cm<sup>-1</sup>; <sup>1</sup>HNMR (400 MHz, CDCl<sub>3</sub>): δ 8.62 (d, *J*=4.4 Hz, 1H), 7.98 (d, *J*=7.4 Hz, 1H), 7.77 (d, *J*=7.3 Hz, 1H), 7.66 (t, *J*=7.8 Hz, 1H), 7.65 (t, *J*=7.8 Hz, 1H), 7.56 (t, *J*=7.3 Hz, 1H), 7.31 (d, *J*=7.9 Hz, 1H), 7.10-7.13 (m, 1H), 4.57 (s, 2H) ppm; <sup>13</sup>CNMR (100 MHz, CDCl<sub>3</sub>): δ 195.3, 155.5, 148.9, 137.9, 137.7, 136.5, 131.0, 129.5, 129.3, 124.2, 123.4, 120.8, 119.9, 43.5 ppm; HRMS: *m/z*[M + 1] calcd for C<sub>14</sub>H<sub>11</sub>N<sub>2</sub>O: 223.0871; found: 223.0861

### **3-(4-Bromophenyl)isoquinolin-1(4H)-one (4f)**



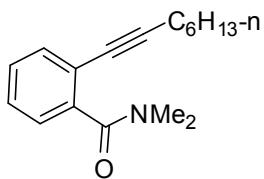
Gummy solid; Yield: 62%; IR (CHCl<sub>3</sub>): 1686, 1590, 1580cm<sup>-1</sup>; <sup>1</sup>HNMR (400 MHz, CDCl<sub>3</sub>): δ 7.89 (d, *J*=7.3 Hz, 1H), 7.79 (d, *J*=7.8 Hz, 1H), 7.66 (t, *J*=7.3 Hz, 1H), 7.51-7.59 (m, 3H), 7.31 (d, *J*=8.3 Hz, 2H), 4.6 (s, 2H) ppm; <sup>13</sup>CNMR (100 MHz, DMSO-d<sub>6</sub>): δ 196.0, 138.6, 133.9, 133.0, 132.3, 131.5 (2C), 131.0 (2C), 129.3, 128.2, 122.7, 120.4, 120.2, 44.2 ppm; HRMS: *m/z*[M + H] calcd for C<sub>15</sub>H<sub>11</sub>BrNO: 300.0024; found: 300.0011

### **2-Iodo-N,N-dimethylbenzamide (1g):**



<sup>1</sup>HNMR (400 MHz, CDCl<sub>3</sub>): δ 7.83 (d, *J* = 7.8 Hz, 1H), 7.39 (t, *J* = 7.8 Hz, 1H), 7.72 (t, *J* = 7.8 Hz, 1H), 7.05 (d, *J* = 7.8 Hz, 1H), 3.14 (s, 3H), 2.85 (s, 3H) ppm; ESMS- (M+H): 276.2

### ***N,N*-dimethyl-2-(oct-1-yn-1-yl)benzamide (6):**



<sup>1</sup>HNMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.37-7.41 (m, 1H), 7.24-7.32 (m, 3H), 3.12 (s, 3H), 2.87 (s, 3H), 2.38 (t, *J* = 7.4Hz, 2H), 1.57-1.60 (m, 2H), 1.38-1.46 (m, 2H), 1.27-1.36 (m, 4H), 0.90 (t, *J* = 6.9Hz, 3H) ppm;

## References

1. S. Goswami A. K. Adak, R. Mukherjee, S. Jana<sup>a</sup>, S. Dey, J. F. Gallagher *Tetrahedron* **2005**, 61 4289.