

## Electronic Supplementary Information (ESI)

### Visible light triggered, catalyst free approach for the synthesis of thiazoles and imidazo[2,1-b]thiazoles in EtOH : H<sub>2</sub>O green medium

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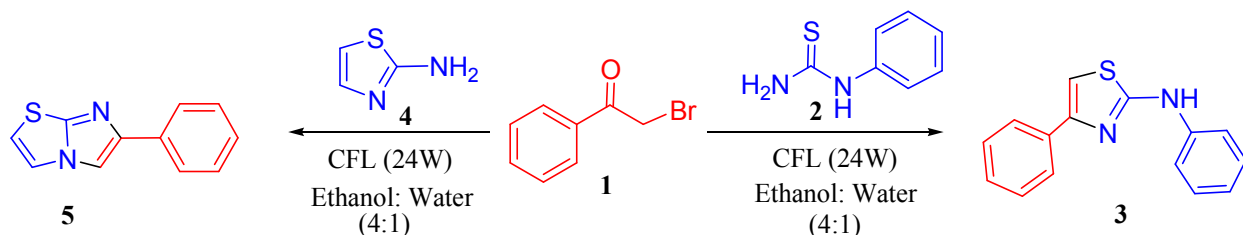
### Experimental

**General Information:** Reagents were obtained from commercial suppliers, and used without further purification unless otherwise specified by a reference. All reactions were performed using oven-dried glass wares. Organic solutions were concentrated using a Buchi rotary evaporator. TLC was performed using silica gel GF254 (Merck) plates. Melting points were determined by open glass capillary method and are uncorrected. IR spectra in KBr were recorded on a Perkin-Elmer 993 IR spectrophotometer, <sup>1</sup>H NMR spectra were recorded on a Bruker AVII 400 spectrometer in DMSO-d<sub>6</sub> and CDCl<sub>3</sub> using TMS as internal reference with chemical shift value being reported in ppm. All coupling constants (*J*) are reported in Hertz (Hz). Elemental analysis were carried out in a Coleman automatic carbon, hydrogen and nitrogen analyzer.

**General method:** A mixture of 1 mmol of phenacyl bromide (**1**) and N-phenylthiourea (**2**) was added in ethanol and water (**4: 1**, 10ml). The mixture was irradiated with 24 W CFL stirring at rt. for 5–10min. After the completion of the reaction (monitored by TLC), water (10 ml) was added and the mixture was filtered. Solid was washed with water and a yield of 81–96% was obtained. Same procedure was applied for the formation of **5a-5g**. The aqueous layer was extracted with ethyl acetate (3 ×10 ml). The combined organic layers were extracted with water, dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The combined organic layers were evaporated under reduced pressure and the resulting crude product was purified by column chromatography by using ethyl acetate and hexane as eluent. The product was confirmed by IR, <sup>1</sup>H and mass spectra. All the compounds

that were obtained are known and were characterized by comparison of their spectral data with those reported in literature.

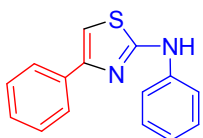
**Table 2 optimization table of reaction conditions<sup>a</sup>**



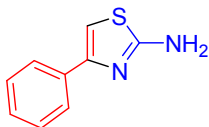
Entry	Reaction Condition	Time(min)	Yield <sup>b</sup> (3a)	Time(h)	Yield <sup>b</sup> (5a)
1	24W, CFL, air, no catalyst	10	95	5	60
2	Daylight, air, no catalyst	10	43	5	18
3	No light, air, no catalyst	10	34	5	10
4	CFL, degassed	10	54	5	- <sup>c</sup>
5	CFL, N <sub>2</sub>	10	36	5	- <sup>c</sup>
6	20W, CFL, air, no catalyst	10	87	5	52
7	18 W, CFL, air, no catalyst	10	80	5	40
8	White LED (7W), no catalyst	10	76	5	23
9	CFL, air, eosinY (0.5 mol %)	10	96	5	60
10	CFL, air, eosin Y (1mol %)	10	96	5	60
11	CFL, Air, Benzoquinone <sup>d</sup>	10	52	5	16

<sup>a</sup>Reaction condition: **1a** (1.0 mmol), **2a** (1.0 mmol) in ethanol: water irradiated using CFL under open air at room temperature. <sup>b</sup>Yield of the product (%). <sup>c</sup>not detected. <sup>d</sup>2 mmol.

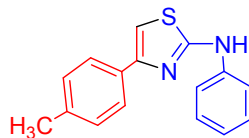
### Structure of the Products (3)



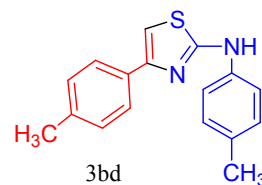
3aa  
Yield=95%  
Time=8min



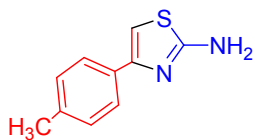
3ab  
Yield=88%  
Time=10min



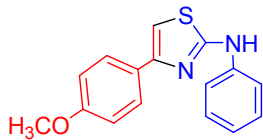
3ba  
Yield=85%  
Time=10min



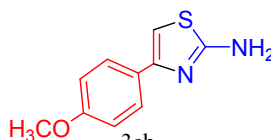
3bd  
Yield=82%  
Time=10min



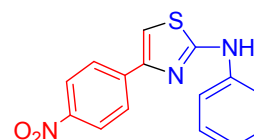
3bb  
Yield=82%  
Time=10min



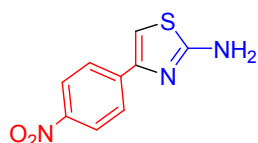
3ca  
Yield=87%  
Time=9min



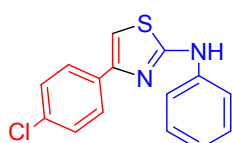
3cb  
Yield=85%  
Time=9min



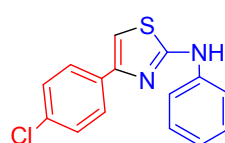
3da  
Yield=96%  
Time=5min



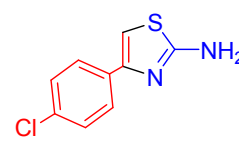
3db  
Yield=94%  
Time=5min



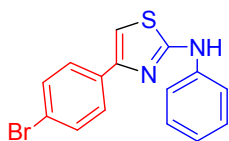
3ea  
Yield=94%  
Time=7min



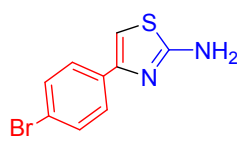
3ec  
Yield=94%  
Time=7min



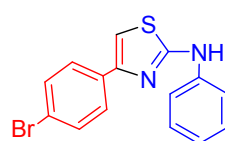
3eb  
Yield=90%  
Time=9min



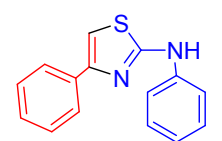
3fa  
Yield=89%  
Time=9min



3fb  
Yield=87%  
Time=10min

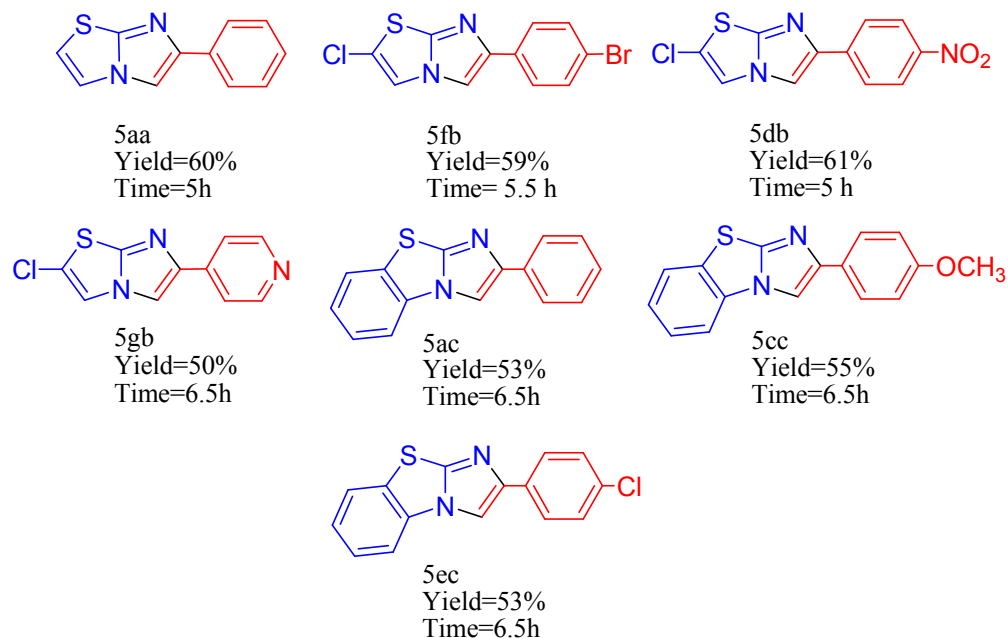


3fc  
Yield=89%  
Time=8min



3ae  
Yield=81%  
Time=10min

### Structure of the Products (5)



Spectral data and Melting Point of isolated and purified compounds are summarized below:

#### (3aa) *N*-4-Diphenylthiazol-2-amine: (m.p. 133-135 °C; lit. m.p. 134-136 °C)

White solid; IR (KBr)  $\nu_{\max}$  (cm<sup>-1</sup>): 3387, 3102, 3058, 2935, 1601, 1584, 1520, 1480, 1458; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>):  $\delta$  7.13 (s, 1H), 6.97-7.02 (m, 1H), 7.26-7.30 (m, 5H), 7.31-7.40 (m, 2H), 7.86 (d, *J* = 7.6 Hz, 2H), 10.13 (s, 1H); MS (ESI) *m/z*: 253 [M+H]; Anal. Calcd. for C<sub>15</sub>H<sub>12</sub>N<sub>2</sub>S: C, 71.40; H, 4.79; N, 11.10; Found: C, 71.20; H, 4.82; N, 11.26.

#### (3ab) 4-Phenylthiazol-2-amine: (m.p. 149-151 °C; lit. m.p. 150-152 °C)

White solid; IR (KBr)  $\nu_{\max}$  (cm<sup>-1</sup>): 3441, 3256, 3145, 3120, 1588, 1536, 1516, 1485, 1444; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>):  $\delta$  7.00 (s, 1H), 7.06 (s, 2H), 7.24 (t, *J* = 7.6 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 2H), 7.80 (d, *J* = 7.6 Hz, 2H); MS (ESI) *m/z*: 177 [M+H]; Anal. Calcd. for C<sub>9</sub>H<sub>8</sub>N<sub>2</sub>S: C, 61.34; H, 4.58; N, 15.90; Found: C, 61.24; H, 4.63; N, 15.61.

#### (3ba) *N*-Phenyl-4-*p*-tolylthiazol-2-amine: (m.p. 103-105 °C; lit. m.p. 102-103 °C)

White solid; IR (KBr)  $\nu_{\max}$  (cm<sup>-1</sup>): 3376, 3116, 3048, 2915, 2850, 1612, 1585, 1555, 1488, 1452, 1403; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>):  $\delta$  2.34 (s, 3H), 6.95 (t, *J* = 7.6 Hz, 1H), 7.25 (d, *J* = 7.6

Hz, 2H), 7.24 (s, 1H), 7.36 (t,  $J = 7.6$  Hz, 2H), 7.73 (d,  $J = 8.0$  Hz, 2H), 7.83 (d,  $J = 8.0$  Hz, 2H), 10.22 (s, 1H); MS (ESI)  $m/z$ : 267 [M+H]; Anal. Calcd. for  $C_{16}H_{14}N_2S$ : C, 72.15; H, 5.30; N, 10.52; Found: C, 72.22; H, 5.14; N, 10.38.

**(3bb) 4-*p*-Tolylthiazol-2-amine: (m.p. 133-135 °C; lit. m.p. 135-136 °C)**

Pale yellow solid; IR (KBr)  $\nu_{\max}$  ( $cm^{-1}$ ): 3451, 3293, 3122, 2753, 1630, 1532, 1524, 1488;  $^1H$  NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  2.30 (s, 3H), 6.92 (s, 1H), 7.02 (s, 2H), 7.17 (d,  $J = 8.0$  Hz, 2H), 7.66 (d,  $J = 8.0$  Hz, 2H); MS (ESI)  $m/z$ : 191 [M+H]; Anal. Calcd. for  $C_{10}H_{10}N_2S$ : C, 63.13; H, 5.30; N, 14.72; Found: C, 63.04; H, 5.38; N, 14.78.

**(3ca) 4-(4-Methoxyphenyl)-*N*-phenylthiazol-2-amine: (m.p. 136-137 °C; lit. m.p. 138-139 °C)**

White solid; IR (KBr)  $\nu_{\max}$  ( $cm^{-1}$ ): 3355, 3102, 2955, 2940, 2838, 1591, 1553, 1510, 1480, 1465, 1422, 1245;  $^1H$  NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  3.80 (s, 3H), 6.95-7.01 (m, 3H), 7.15 (s, 1H), 7.33 (t,  $J = 7.6$  Hz, 2H), 7.71 (d,  $J = 8.0$  Hz, 2H), 7.84 (d,  $J = 8.0$  Hz, 2H), 10.24 (s, 1H); MS (ESI)  $m/z$ : 283 [M+H]; Anal. Calcd. for  $C_{16}H_{14}N_2OS$ : C, 68.06; H, 5.00; N, 9.92; Found: C, 67.70; H, 5.11; N, 10.01.

**(3cb) 4-(4-Methoxyphenyl) thiazol-2-amine: (m.p. 202-205 °C; lit. m.p. 204-206 °C)**

White solid; IR (KBr)  $\nu_{\max}$  ( $cm^{-1}$ ): 3442, 3261, 3122, 2955, 2830, 1628, 1613, 1532, 1529, 1488, 1242;  $^1H$  NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  3.79 (s, 3H), 6.83 (s, 1H), 6.91 (d,  $J = 8.8$  Hz, 2H), 7.00 (s, 2H), 7.72 (d,  $J = 8.8$  Hz, 2H); MS (ESI)  $m/z$ : 207 [M+H]; Anal. Calcd. for  $C_{10}H_{10}N_2OS$ : C, 58.23; H, 4.89; N, 13.58; Found: C, 58.10; H, 4.70; N, 13.65.

**(3da) 4-(4-Nitrophenyl)-*N*-phenylthiazol-2-amine: (m.p. 204-206 °C; lit. m.p. 206-207 °C)**

Orange solid; IR (KBr)  $\nu_{\max}$  ( $cm^{-1}$ ): 3336, 3113, 3076, 2921, 1611, 1596, 1546, 1529, 1488, 1441, 1412, 1315;  $^1H$  NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  7.01 (t,  $J = 7.2$  Hz, 1H), 7.38 (t,  $J = 7.2$  Hz, 2H), 7.74 (d,  $J = 7.2$  Hz, 2H), 7.76 (s, 1H), 8.17 (d,  $J = 8.8$  Hz, 2H), 8.31 (d,  $J = 8.8$  Hz, 2H), 10.42 (s, 1H); MS (ESI)  $m/z$ : 298 [M+H]; Anal. Calcd. for  $C_{15}H_{11}N_3O_2S$ : C, 60.59; H, 3.73; N, 14.13; Found: C, 60.40; H, 3.60; N, 14.02.

**(3db) 4-(4-Nitrophenyl)thiazol-2-amine: (m.p. 284-285 °C; lit. m.p. 284-286 °C)**

Orange solid; IR (KBr)  $\nu_{\max}$  (cm<sup>-1</sup>): 3392, 3310, 3146, 3122, 2928, 1646, 1596, 1532, 1512, 1508, 1415, 1326; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>):  $\delta$  7.25 (s, 2H), 7.41 (s, 1H), 8.06 (d, *J* = 8.8 Hz, 2H), 8.23 (d, *J* = 8.8 Hz, 2H); MS (ESI) *m/z*: 222 [M+H]; Anal. Calcd. for C<sub>9</sub>H<sub>7</sub>N<sub>3</sub>O<sub>2</sub>S: C, 48.86; H, 3.19; N, 18.99; Found: C, 48.59; H, 3.26; N, 18.62.

**(3ea) 4-(4-Chlorophenyl)-*N*-phenylthiazol-2-amine: (m.p. 143-145 °C; lit. m.p. 144-146 °C)**

White solid; IR (KBr)  $\nu_{\max}$  (cm<sup>-1</sup>): 3386, 3108, 3062, 2931, 1587, 1568, 1488, 1475, 1449, 1408, 689; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>):  $\delta$  7.01 (t, *J* = 7.6 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.42 (s, 1H), 7.50 (d, *J* = 7.6 Hz, 2H), 7.72 (d, *J* = 8.0 Hz, 2H), 7.95 (d, *J* = 8.0 Hz, 2H), 10.22 (s, 1H); MS (ESI) *m/z*: 287 [M+H]; Anal. Calcd. for C<sub>15</sub>H<sub>11</sub>ClN<sub>2</sub>S: C, 62.82; H, 3.87; N, 9.77; Found: C, 62.73; H, 3.71; N, 9.62.

**(3eb) 4-(4-Chlorophenyl) thiazol-2-amine: (m.p. 165-167 °C; lit. m.p. 167–168 °C)**

White solid; IR (KBr)  $\nu_{\max}$  (cm<sup>-1</sup>): 3443, 3276, 3118, 3025, 2752, 1629, 1578, 1538, 1473, 1409, 726; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>):  $\delta$  7.14 (s 2H), 7.44 (d, *J* = 8.4 Hz, 2H), 7.56 (s, 1H), 7.80 (d, *J* = 8.4 Hz, 2H); MS (ESI) *m/z*: 211 [M+H]; Anal. Calcd. for C<sub>9</sub>H<sub>7</sub>ClN<sub>2</sub>S: C, 51.31; H, 3.35; N, 13.30; Found: C, 51.10; H, 3.42; N, 13.43.

**(3fa) 4-(4-Bromophenyl)-*N*-phenylthiazol-2-amine: (m.p. 231-233 °C; lit. m.p. 230-232 °C)**

White solid; IR (KBr)  $\nu_{\max}$  (cm<sup>-1</sup>): 3450, 2965, 1626, 1603, 1575, 1561, 1535, 1505, 590; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>):  $\delta$  6.99 (t, *J* = 7.2 Hz, 1H), 7.36 (t, *J* = 7.2 Hz, 2H), 7.44 (s, 1H), 7.62 (d, *J* = 8.4 Hz, 2H), 7.73 (d, *J* = 7.2 Hz, 2H), 7.89 (d, *J* = 8.4 Hz, 2H), 10.24 (s, 1H); MS (ESI) *m/z*: 332 [M+H]; Anal. Calcd. for C<sub>15</sub>H<sub>11</sub>BrN<sub>2</sub>S: C, 54.39; H, 3.35; N, 8.46; Found: C, 54.17; H, 3.25; N, 8.30.

**(3fb) 4-(4-Bromophenyl)thiazol-2-amine: (m.p. 181-183 °C; lit. m.p. 182-184 °C)**

White solid; IR (KBr)  $\nu_{\max}$  (cm<sup>-1</sup>): 3436, 3277, 3118, 3048, 2752, 1629, 1575, 1538, 1465, 1401, 572; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>):  $\delta$  7.06 (s, 2H), 7.14 (s, 1H), 7.56 (d, *J* = 8.4 Hz, 2H), 7.75

(d,  $J = 8.4$  Hz, 2H); MS (ESI)  $m/z$ : 256 [M+H]; Anal. Calcd. for  $C_9H_7BrN_2S$ : C, 42.37; H, 2.77; N, 10.98; Found: C, 42.15; H, 2.65; N, 10.76.

**(5aa) 6-phenylimidazo [2, 1-b]thiazole: (m.p. 134-137 °C)**

IR (KBr)  $\nu_{\max}$  ( $cm^{-1}$ ): 3031, 2810, 1615, 1560, 1526, 1459, 1408;  $^1H$  NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  7.18-7.20 (1H, d,  $J=4.44$ ), 7.23 (1H, t); 7.35-7.39 (2H, t), 7.80-7.83 (2H, d), 7.87-7.88 (1H, d,  $J=4.48$ ), 8.15 (1H, s); MS (ESI)  $m/z$ : 201[M+H]; Anal. Calcd. for  $C_{11}H_8N_2S$ : C, 65.97; H, 4.03; N, 13.99; Found: C, 65.39; H, 3.82; N, 13.26.

**(5fb) 6-(4-bromophenyl)-2-chloroimidazo[2, 1-b]thiazole: (m.p. 231-233 °C; lit. m.p. 233-235 °C)**

IR (KBr)  $\nu_{\max}$  ( $cm^{-1}$ ): 1542, 1193, 979, 738;  $^1H$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  7.60 (2H, d,  $J=8.4$ ), 7.80 (2H, d,  $J=8.4$ ), 8.28 (1H, s), 8.31 (1H, s); MS (ESI)  $m/z$ : 312 [M+H]; Anal. Calcd. for  $C_{11}H_6BrClN_2S$ : C, 42.13; H, 1.93; N, 8.93; Found: C, 39.58; H, 1.72; N, 8.01.

**(5ac) 2-Phenyl-benzo[d]imidazo[2,1-b]thiazole: (m.p. 101-103 °C; lit. m.p. 102-104 °C)**

IR (KBr)  $\nu_{\max}$  ( $cm^{-1}$ ): 3420, 2342, 1574;  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  6.47-7.00 (m, 6H), 7.59-7.60 (m, 1H), 7.66-7.69 (m, 1H), 7.89-7.90 (m, 1H), 7.96 (s, 1H); MS (ESI)  $m/z$ : 251 [M+H]; Anal. Calcd. for  $C_{15}H_{10}N_2S$ : C, 71.97; H, 4.03; N, 11.19; Found: C, 71.65; H, 3.91; N, 10.59.

**(5cc) 2-(4-Methoxyphenyl)-benzo[d]imidazo[2,1-b]thiazole: (m.p. 174-176 °C; lit. m.p. 175-177 °C)**

IR (KBr)  $\nu_{\max}$  ( $cm^{-1}$ ): 3424, 2938, 1602, 1495;  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  3.84 (s, 3H), 6.95-6.99 (m, 2H), 7.27-7.35 (m, 2H), 7.45-7.48 (m, 1H), 7.52-7.53 (m, 1H), 7.68-7.75 (m, 2H), 7.86 (s, 1H); MS (ESI)  $m/z$ : 281 [M+H]; Anal. Calcd. for  $C_{16}H_{12}N_2OS$ : C, 68.55; H, 4.31; N, 9.99; Found: C, 68.34; H, 4.16; N, 9.72.