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# Synthesis, cytotoxic and antibacterial activities of 6bromobenzo[d]thiazol-2(3H)-one-[1,2,3] triazole hybrids

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**Abstract:** A series of new 6-bromobenzo[d]thiazol-2(3H)-one derived 1,2,3-triazole derivatives (**3a-j**) have been synthesized by 1,3-dipolar cycloaddition of 6-bromobenzo[d]thiazol-2(3H)-one (**2**) with propargyl bromide and different aryl azides in a copper catalyzed one-pot reaction. All the synthesized compounds (**3a-j**) were evaluated for their *in vitro* cytotoxic activity against two human cancer cell lines MCF-7 and HeLa. The results showed that these compounds showed good cytotoxicity against the tested cell lines as compared with that of standard drug Cisplatin. The antibacterial activity of the newly synthesized triazole derivatives (**3a-j**) were also studied against different bacteria. The activity results showed that majority of compounds showed good to moderate antibacterial activity compared with positive control drug Streptomycin.

**Keywords:** 6-bromobenzo[*d*]thiazol-2(3*H*)-one; 1, 2, 3-Triazole; Cytotoxicity; Antibacterial activity. © 2016 ACG Publications. All rights reserved.

# 1. Introduction

Cancer, the uninhibited growth of cells, and one of the main causes of fatality throughout the world, regardless of extensive development in the understanding of its biology and pharmacology. According to World Health Organization (WHO), it is expected that there will be 12 million deaths from cancer up to 2030. The conventional healing strategies for the treatment of cancer are radiotherapy, immunotherapy, surgery, and chemotherapy. Of them, chemotherapy is efficient, because it distributes anticancer drugs through the circulatory system.<sup>1</sup> Breast cancer is the most universally diagnosed tumor in women and clerical for approximately 23% of all female cancers and the second most deadly cancer in women worldwide today.<sup>2-4</sup> The search for a new anticancer agents which can selectively target the tumor cells is today's target of cancer therapy and is a never ending process, till the goal is reached. On the other hand, new antibacterial agents a in the field of medicinal chemistry. The focal point of such antibiotics research has moved to the finding of innovative chemical classes of bacterial targets. So, the discovery of new and effective antibacterial agents is the top way to overcome bacterial resistance and develop effective therapies.<sup>5</sup> In view of this, the development of novel chemotherapeutics, which selectively acts on the target without the side effects, has become a primary objective of medicinal chemists.

We are presently affianced in a plan aimed at development of new heterocycles containing 1,2,3-triazole moieties that decrease the development of tumor cells. Our previous efforts towards the synthesis and biological activity of new heterocycles containing 1,2,3-triazole hybrids as promising antimicrobial agents.<sup>6</sup> The triazole derivatives have been a subject of a lot investigation, because they are a group of totally synthetic pharmacological agents with different action. 1,2,3-triazole containing

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drug molecules, including tazobactam,<sup>7</sup> cefatrizine<sup>8</sup> and carboxyamidotriazole<sup>9</sup> are now available in the market (**Figure 1**).

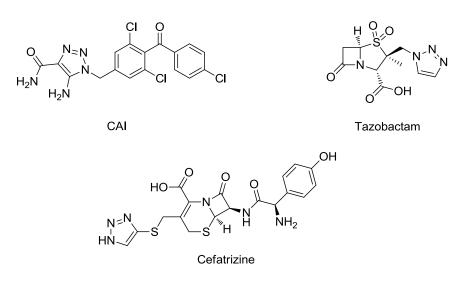
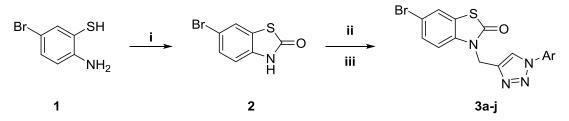


Figure 1. Some of 1,2,3-triazole containing drug molecules in the market

Recently, benzothiazoles and their derivatives have emerged as an important class of molecules due to their therapeutic and pharmacological properties such as anticancer,<sup>10</sup> antiinflammatory,<sup>13,14</sup> antimicrobial,<sup>15,16</sup> antitubercular<sup>17</sup> and antiviral activities.<sup>18</sup> Encouraged by the above facts herein, we report the synthesis of novel 6-bromobenzo[d]thiazol-2(3H)-one derived 1,2,3-triazole hybrids and evaluated for their *in vitro* anti cancer and antibacterial activities.

### 2. Results and discussion

The target 6-bromobenzo[d]thiazol-2(3H)-one derived 1,2,3-triazole derivatives (**a-j**) were synthesized using a reported synthetic route<sup>19</sup> as outlined in **Figure 2**. For this purpose first, the key compound **2** was prepared starting from the reaction of 2-amino-5-bromobenzenethiol (**1**) with COCl<sub>2</sub> in toluene at room temperature. Secondly, compound **2** and propargyl bromide with different aryl azides were refluxed in the presence of  $Cs_2CO_3$  in dry THF for 8-10 h. Thus, the 1,3-dipolar cycloaddition reaction between *in situ* generated alkyne and aryl azides in the presence of Cu(I) catalyst (Click reaction) produced novel 6-bromobenzo[d]thiazol-2(3H)-one derived 1,2,3-triazole derivatives (**3a-j**) in good to excellent yields. All these new synthesized compounds were fully characterized by <sup>1</sup>H NMR, <sup>13</sup>C NMR, IR, mass and elemental analysis (**Table 1**).



**Figure 2.** Reagents and reaction conditions: i) COCl<sub>2</sub> /Toluene/rt/4h; ii) Propargyl bromide/Cs<sub>2</sub>CO<sub>3</sub>;iii) ArN<sub>3</sub>/CuI/THF/rt/8-10h

Compound	ArN <sub>3</sub>	Time	Yield (%)
a	N <sub>3</sub>	8	84
b	Me Me Na	10	72
c	Me N <sub>3</sub>	8	70
d		8	69
e	CI N <sub>3</sub>	9	57
f	MeO N <sub>3</sub>	10	71
g	CF <sub>3</sub> N <sub>3</sub>	9	65
h	N <sub>3</sub>	10	65
i	NO <sub>2</sub> MeO CI	9	72
j	Br N <sub>3</sub>	9	68

 Table 1. 6-bromobenzo[d]thiazol-2(3H)-one based 1,2,3-triazoles.

### 2.1. Cytotoxic activity

In vitro cytotoxic activity of the synthesized triazole derivatives were carried out against two human cancer cell lines MCF-7(breast) and HeLa (cervical). Cisplatin was used as a reference drug. Cell viability in the presence of the test samples was measured by the MTT-micro cultured tetrazolium assay.<sup>20,21</sup> The response parameter calculated was the IC<sub>50</sub> value, which corresponds to the concentration required for 50% inhibition of cell viability.

The cytotoxic activity screening results (**Table 2**) revealed that, compound **3f** which contains 3-(trifluoromethyl)phenyl group on the triazole ring has exhibited very good activity against MCF-7 with IC<sub>50</sub> value 13.04  $\pm$  0.454  $\mu$ M, respectively. Similarly the compound derived from 4-methoxyphenyl group on the triazole ring has also exhibited good activity against both the cancer cell lines MCF-7 and HeLa with IC<sub>50</sub> values 17.54  $\pm$  1.189 & 12.15  $\pm$  0.563  $\mu$ M, respectively. Remaining triazole derivatives showed moderate activity against MCF-7 and HeLa with IC<sub>50</sub> values ranging from 23.56  $\pm$  0.677 to 78.43  $\pm$  2.888  $\mu$ M, respectively. Survival curves of **MCF-7** and **HeLa** are shown in **Figure 3** and **Figure 4**.

### 2.2. In vitro antibacterial activity

The newly synthesized 1,2,3-triazole derivatives (**3a-j**) were tested for their *in vitro* antibacterial activity against both gram-positive and gram-negative bacteria bacteria such as *Streptococcus pyogenes, Staphylococcus aureus, Pseudomonas aeruginosa* and *Klebsiella pneumonia* by using agar well diffusion method.<sup>22-24</sup> Streptomycin was used as positive control drug for comparison. The antibacterial results (**Table 3**) reveal that, compounds derived from 3-chlorophenyl

and 3,5-dichloro phenyl group on the triazole ring that is **3c** and **3d** showed excellent inhibition against *S. aureus* and *P. aeruginosa* on comparing with the standard drug streptomycin. Compound **3d** showed good activity against *S. pyogenes* and *K. pneumonia*. The rest of triazole derivatives showed moderate activity against all the tested bacteria.

Product	MCF-7	HeLa
<b>3</b> a	$69.09 \pm 2.540$	$42.64 \pm 2.139$
3b	$23.56 \pm 0.677$	$28.70 \pm 1.815$
3c	>200	>200
3d	$97.55 \pm 2.060$	>200
3e	$17.54 \pm 1.189$	$12.15 \pm 0.563$
3f	$13.04 \pm 0.454$	$44.30 \pm 1.910$
3g	$78.43 \pm 2.888$	>200
3h	>200	>200
<b>3i</b>	$43.73 \pm 2.157$	$35.61 \pm 2.600$
3j	$31.50 \pm 1.957$	$49.44 \pm 1.930$
Cisplatin	$11.44 \pm 0.5752$	$5.92 \pm 1.052$

Table 2. IC<sub>50</sub> values of 1,2,3-triazole derivatives (3a-j) on human tumor Cell lines MCF-7 and HeLa.

Anti cancer activity (MCF-7)

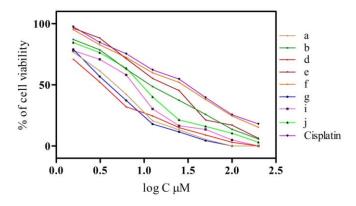


Figure 3.Survival curves of MCF-7 for active 1,2,3-triazole derivatives (3a-j)

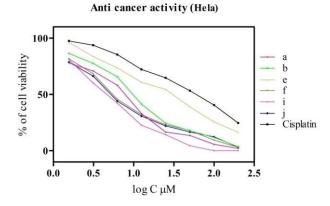


Figure 4. Survival curves of HeLa for active 1,2,3-triazole derivatives (3a-j)

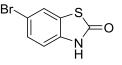
ZOI and MIC (µg/ml )						
Compound	S. aureus	S. pyogenes	P. aeruginosa	K. pneumoniae		
	ZOI MIC	ZOI MIC	ZOI MIC	ZOI MIC		
<b>3</b> a	08 200	08 200	08 200	08 200		
<b>3</b> b	14 100	15 100	08 200	08 200		
3c	19 25	17 50	20 25	18 50		
3d	20 25	19 25	18 25	20 50		
3e	10 200	10 200	14 100	10 200		
<b>3f</b>	13 100	13 100	12 100	16 50		
3g	13 100	10 200	16 50	11 200		
3h	15 100	15 100	11 200	15 100		
<b>3i</b>	08 200	10 200	10 200	08 200		
3ј	17 50	16 50	15 50	17 50		
Streptomycin	20 25	21 12.5	22 12.5	22 50		

 Table 3. Antibacterial activity of 1,2,3-triazole derivatives (3a-j).

#### 3. Experimental Section

All reactions were carried out in a round bottom flask under room temperature. All the reagents and solvents were purchased from S.D. Fine chemicals limited and used without further purification. Melting points were determined in open capillaries using Stuart SMP30 apparatus and are uncorrected. The progress of the reactions as well as the purity of the compounds was monitored by thin layer chromatography with F254 silica-gel precoated sheets using hexane /ethyl acetate (8:2) as eluent. NMR spectra were recorded on Bruker 400 MHz spectrometer using CDCl<sub>3</sub> (<sup>1</sup>HNMR), DMSO- $d_6$  (<sup>13</sup>C NMR) as solvent and TMS as internal standard. Elemental analyses were performed on a Perkin-Elmer 240CHN analyser. FTIR spectra were recorded on a Bruker spectrometer. Mass spectra were recorded using ESI-MS. Coupling constants (*J*) values are presented in Hertz and spin multiples are given as **s** (singlet), **d** (doublet), **t** (triplet), **dd** (doublet of doublets) and **m** (multiplet).

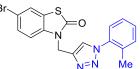
3.1. Synthesis of 6-bromobenzo[d]thiazol-2(3H)-one (2)



2-amino-5-bromobenzenethiol (1) (8.00 g, 0.039 mol) and oxalyl chloride (4.65g, 0.047mol) was dissolved in toluene and stirred at room temperature for 4h. The solvent was evaporated under vacuum and neutralized by Na<sub>2</sub>CO<sub>3</sub>. Crystallization by ethanol gave **2** as pale white crystals (7.4 g, 82 %): m.p. 122-124 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  11.45 (s, 1H, NH), 7.92 (s, 1H), 7.69 (d, *J* =8.2 Hz, 1H), 7.48 (d, *J* =8.2 Hz, 1H); MS: m/z 231 [M<sup>+</sup>].

# 3.2. General procedure for the synthesis of 6-bromo-3-((1-aryl-1H-1,2,3-triazol-4-yl)methyl) benzo[d]thiazol-2(3H)-ones (3a-j)

6-bromobenzo[d]thiazol-2(3H)-one (2) (2 mmol) along with cesium carbonate (5 mmol) was dissolved in 20 mL of dry THF and later propargyl bromide (3 mmol) was added slowly while stirring. Then, 2.6 mmol of aryl azide and 15 mol% of CuI were added into the mixture until complete consumption of the starting materials monitored by TLC. The reaction mixture was diluted with 25 mL of water, and extracted with ethylacetate (3x20 mL). The combined organic extracts were washed with brine and dried (Na<sub>2</sub>SO4). After removal of the solvent under reduced pressure, the residue was purified on silica gel with hexane/ethyl acetate (8:2) as eluent. 3.2.1. 6-bromo-3-((1-(2-methylphenyl)-1H-1,2,3-triazol-4-yl)methyl)benzo[d]thiazol-2(3H)-one (**3a**):



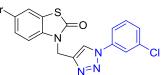
Pale yellow solid; mp 122-124 °C; IR (KBr): v 3131, 1767, 1594, 1495 cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>):  $\delta$  8.59 (s, 1H, triazole-H), 8.31 (d, *J* = 7.9 Hz, 1H), 8.16-8.05 (m, 2H), 7.74 (t, *J* = 8.1Hz, 1H), 7.47 (d, *J* = 8.4 Hz, 1H), 7.20-7.16 (m, 2H), 5.25 (s, 2H, N-CH<sub>2</sub>), 2.17 (s, 3H, Ar-CH<sub>3</sub>); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>):  $\delta$  163.9, 144.8, 143.0, 139.4, 136.5, 130.1, 129.9, 126.5, 125.6, 122.9, 122.5, 121.1, 119.7, 117.8, 111.3, 36.7, 28.7: MS: m/z: 402 [M<sup>+</sup>]. Anal. Calcd. for C<sub>17</sub>H<sub>13</sub>BrN<sub>4</sub>OS: C, 50.88; H, 3.27; N, 13.96; Found: C, 50.94; H, 3.23; N, 13.88.

*3.2.2.* 6-bromo-3-((1-(3,5-dimethylphenyl)-1H-1,2,3-triazol-4-yl)methyl)benzo[d]thiazol-2(3H)-one (**3b**):



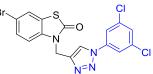
White solid; mp 135-137 °C; IR (KBr): v 3131, 1768, 1582, 1493 cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>):  $\delta$  8.21 (s, 1H, triazole-H), 8.09-8.00 (m, 2H), 7.95 (s, 1H), 7.86-7.79 (m, 2H), 7.75 (s, 1H), 5.34 (s, 2H, N-CH<sub>2</sub>), 3.07 (s, 6H, Ar-CH<sub>3</sub>); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>):  $\delta$  163.7, 145.7, 143.1, 139.3, 136.3, 129.9, 127.9, 125.2, 121.5, 119.2, 117.5, 117.3, 114.8, 36.3, 20.7; MS: m/z: 416 [M<sup>+</sup>]. Anal. Calcd. for C<sub>18</sub>H<sub>15</sub>BrN<sub>4</sub>OS; C, 52.06; H, 3.64; N, 13.49; Found C, 52.11; H, 3.66; N, 13.54.

3.2.3. 6-bromo-3-((1-(3-chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)benzo[d]thiazol-2(3H)-one (**3c**):



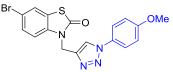
Pale yellow solid; mp 118-120 °C; IR (KBr): v 3140, 1753, 1584, 1494 cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>):  $\delta$  8.06 (s, 1H, triazole-H), 7.76 (s, 1H), 7.62 (d, *J* = 7.3 Hz, 1H), 7.51-7.40 (m, 3H), 7.20- 7.14 (m, 2H), 5.23 (s, 2H, N-CH<sub>2</sub>); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>):  $\delta$  163.6, 145.7, 143.5, 137.4, 134.1, 131.5, 128.4, 127.8, 125.2, 121.9, 119.6, 119.2, 118.5, 117.3, 114.8, 36.2; MS: m/z: 422 [M<sup>+</sup>]. Anal. Calcd. for C<sub>16</sub>H<sub>10</sub>BrClN<sub>4</sub>OS: C, 45.57; H, 2.39; N, 13.29; Found: C, 45.54; H, 2.42; N, 13.31.

*3.2.4.* 6-bromo-3-((1-(3,5-dichlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)benzo[d]thiazol-2(3H)-one (**3d**):



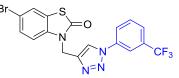
White solid; mp 129-131°C; IR (KBr): v 3130, 1742, 1580, 1495 cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>):  $\delta$  8.06 (s, 1H, triazole-H), 7.66 (s, 2H), 7.46-7.42 (m, 2H), 7.20-7.10 (m, 2H) 5.21 (s, 2H, N-CH<sub>2</sub>); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>):  $\delta$  163.6, 145.7, 143.7, 137.9, 135.1, 128.0, 127.8, 125.3, 122.0, 119.3, 118.5, 117.3, 114.8, 36.2; MS: m/z: 457 [M<sup>+</sup>]. Anal. Calcd. for C<sub>16</sub>H<sub>9</sub>BrCl<sub>2</sub>N<sub>4</sub>OS; C, 42.13; H, 1.99; N, 12.28; Found C, 42.17; H, 2.01; N, 12.31.

3.2.5.6-bromo-3-((1-(4-methoxyphenyl)-1H-1,2,3-triazol-4-yl)methyl)benzo[d]thiazol-2(3H)-one (**3e**):



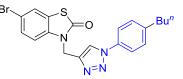
White solid; mp 104-106 °C; IR (KBr): v 3141,1742, 1589, 1496 cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>):  $\delta$  7.96 (s, 1H, triazole-H ), 7.60 (d, *J* =8.8 Hz, 2H), 7.52 (d, *J* =8.6 Hz, 1H),7.20-7.15 (m, 2H), 7.00 (d, *J* =8.8 Hz, 2H), 5.22 (s, 2H, N-CH<sub>2</sub>), 3.86 (s, 3H, OCH<sub>3</sub>); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>):  $\delta$  163.1, 159.2, 145.7, 143.0, 136.5, 129.8, 127.9, 125.2, 121.8, 121.6, 119.2, 117.4, 114.7, 55.5, 36.2; MS: m/z: 418 [M<sup>+</sup>]. Anal. Calcd. for C<sub>17</sub>H<sub>13</sub>BrN<sub>4</sub>O<sub>2</sub>S: C, 48.93; H, 3.14; N, 13.43; Found C, 48.98; H, 3.17; N, 13.48.

3.2.6.(6-bromo-3-((1-(3-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)methyl)benzo[d]thiazol-2(3H)-one (**3f**):



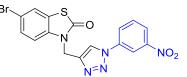
Pale yellow solid; mp 113-115 °C; IR (KBr): v 3144, 1745, 1598, 1492 cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>):  $\delta$  8.13 (s, 1H), 8.00(s, 1H, triazole-H), 7.94 (d, *J* =7.9 Hz, 1H), 7.73-7.62 (m, 2H), 7.48(d, *J* = 8.6 Hz, 1H), 7.20-7.15 (m, 1H), 7.14 (d, *J* = 2.1Hz,1H), 5.24 (s, 2H, N-CH<sub>2</sub>); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>):  $\delta$  163.6, 145.7, 143.6, 136.8, 131.2, 130.6, 130.3,127.9, 125.2, 124.8, 123.9, 122.1, 119.3, 117.3, 116.6, 114.8, 36.2; MS: m/z: 456 [M<sup>+</sup>]. Anal. Calcd. for C<sub>17</sub>H<sub>10</sub>BrF<sub>3</sub>N<sub>4</sub>OS; C, 44.85; H, 2.21; N, 12.31; Found C, 44.81; H, 2.27; N, 12.35.

3.2.7. 6-bromo-3-((1-(4-butylphenyl)-1H-1,2,3-triazol-4-yl)methyl)benzo[d]thiazol-2(3H)-one (3g):



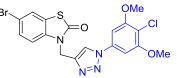
White solid; mp 145-147 °C IR (KBr): v 3140, 1747, 1585, 1496 cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>):  $\delta$  8.19 (s, 1H, triazole-H), 7.65-7.49 (m, 2H), 7.38-7.25(m, 3H), 7.20-7.10 (m, 2H), 5.23 (s, 2H, N-CH<sub>2</sub>), 2.66 (t, J = 7.7 Hz, 2H, Ar-CH<sub>2</sub>), 1.65-1.52 (m, 2H), 1.41-1.29 (m, 2H), 0.93 (t, J = 7.3 Hz,3H); <sup>13</sup>C NMR (DMSO- $d_6$ ):  $\delta$  163.7, 145.7, 143.2, 143.1, 134.6, 129.5, 127.9, 125.2, 121.6, 119.8, 119.2, 117.4, 114.8, 36.2, 34.1, 32.8, 21.6, 13.6; MS: m/z: 444 [M<sup>+</sup>]. Anal. Calcd. for C<sub>20</sub>H<sub>19</sub>BrN<sub>4</sub>OS; C, 54.18; H, 4.32; N, 12.64; Found C, 54.22; H, 4.37; N, 12.61.

*3.2.8.* 6-*bromo-3-((1-(3-nitrophenyl)-1H-1,2,3-triazol-4-yl)methyl)benzo[d]thiazol-2(3H)-one* (**3h**):



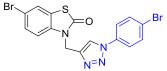
White solid; mp 140-142 °C; IR (KBr): v 31317, 1767, 1589, 1493 cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>):  $\delta$  8.05 (s, 1H, triazole-H), 8.02 (s, 1H), 7.72-7.61 (m, 2H), 7.58-7.43 (m, 2H), 7.19 (s, 1H), 7.08-7.01(m, 1H), 5.33 (s, 2H, N-CH<sub>2</sub>); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>):  $\delta$  163.6, 145.7, 143.5, 137.4, 134.1, 131.5, 128.4, 127.8, 125.2, 121.9, 119.6, 119.2, 118.5, 117.3, 114.8, 36.2; MS: m/z: 433 [M<sup>+</sup>]. Anal. Calcd. for C<sub>16</sub>H<sub>10</sub>BrN<sub>5</sub>O<sub>3</sub>S: C, 44.46; H, 2.33; N, 16.20; Found: C, 44.39; H, 2.37; N, 16.23.

3.2.9.6-bromo-3-((1-(4-chloro-3,5-dimethoxyphenyl)-1H-1,2,3-triazol-4-yl)methyl)benzo[d] thiazol-2(3H)-one (**3i**):



Yellow solid; mp 124-126 °C; IR (KBr): v 3141, 1751, 1573, 1494 cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>):  $\delta$  8.20 (s, 1H, triazole-H), 7.60-7.45 (m, 2H), 7.20-7.08 (m, 3H), 5.24 (s, 2H, N-CH<sub>2</sub>), 3.90 (s, 3H, O-CH<sub>3</sub>), 3.85 (s, 3H, O-CH<sub>3</sub>); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>):  $\delta$  163.7, 158.9, 158.8, 145.8, 141.9, 127.9, 125.7, 125.2, 124.4, 122.3, 119.3, 117.5, 115.1, 114.8, 110.1, 56.9, 56.7, 35.9; MS: m/z: 482[M<sup>+</sup>]. Anal. Calcd. for C<sub>18</sub>H<sub>14</sub>BrClN<sub>4</sub>O<sub>3</sub>S; C, 44.88; H, 2.93; N, 11.63; Found C, 44.94; H, 2.97; N, 11.65.

3.2.10. 6-bromo-3-((1-(4-bromophenyl)-1H-1,2,3-triazol-4-yl)methyl)benzo[d]thiazol-2(3H)-one (**3j**):



White solid; mp 149-151 °C; IR (KBr): v 3144, 1766, 1598, 1495 cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>):  $\delta$  8.04 (s, 1H, triazole-H), 7.73-7.58 (m, 4H), 7.48 (d, J = 8.6 Hz, 1H), 7.23-7.11(m, 2H), 5.22 (s, 2H, N-CH<sub>2</sub>); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>):  $\delta$  163.6, 144.3, 142.5, 138.5, 131.2, 129.5, 126.1, 125.2, 122.6, 121.4, 120.8, 114.5, 111.1, 36.2: MS: m/z: 467 [M<sup>+</sup>]. Anal. Calcd. for C<sub>16</sub>H<sub>10</sub>Br<sub>2</sub>N<sub>4</sub>OS: C, 41.23; H, 2.16; N, 12.02; Found : C, 41.19; H, 2.11; N, 12.05.

# 3.3. Cytotoxic activity

The newly synthesized 1,2,3-triazole derivatives (**3a-j**) were evaluated for their *in vitro* anti cancer activity against two human cancer cell lines that is MCF-7(breast) and HeLa (cervical) as described in our previous study.<sup>25</sup> The IC<sub>50</sub> values were calculated from the percentage of cell viability and compared with the reference drug Cisplatin (**Table 2**).

### 3.4. Antibacterial activity

All the synthesized compounds were screened for their *in vitro* antibacterial activity against against the two gram-positive and two gram-negative micro organisms by agar well diffusion method. Streptomycin was used as a standard drug. Serial dilutions of the test compounds as well as standards were performed at concentrations ranging from 150 to 0.97 mg mL<sup>-1</sup> in a 200 mL culture medium final volume. Afterwards each well was seeded with a 50  $\mu$ L microbial suspension of 0.5 MacFarland density. In each test a microbial culture control and a sterility control (negative) were performed. The plates were incubated for 24 h at 37 °C. The lowest concentration which inhibited the visible microbial growth was considered the MIC.

### 4. Conclusion

In conclusion, a series of novel 6-bromobenzo [d] thiazol-2(3H)-one derived 1,2,3-triazole hybrids (3a-j) were synthesized in one pot [3+2] cycloaddition reaction and screened for their in vitro anti cancer and antibacterial activities. The compounds **3e** and **3f** have shown better cytotoxic activity than the remaining compounds as compared with the standard drug cisplatin. Similarly, the compounds **3c** and **3d** have shown highest antibacterial activity against all tested micro organisms. This activity result advises that a simple modification in structure, a potent anti cancer and antibacterial agents can be generated with good efficacy.

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