



## AN EFFICIENT IONIC LIQUID, ONE-POT MULTICOMPONENT SYNTHESIS OF BIOLOGICALLY ACTIVE BENZO[4,5]THIAZOLO[3,2-A]PYRIMIDINES AND THEIR DERIVATIVES

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### ABSTRACT

The development of sustainable and efficient synthetic methodologies for heterocyclic scaffolds of biological significance remains a central focus in organic and medicinal chemistry. In this study, we report an efficient, green, and one-pot multicomponent protocol for the synthesis of benzo[4,5]thiazolo[3,2-a]pyrimidines and their derivatives employing anionic liquid as a recyclable catalyst and reaction medium. The reaction proceeds smoothly via the condensation of 2-aminobenzothiazole, substituted aromatic aldehydes, and  $\beta$ -dicarbonyl compounds under mild conditions, furnishing the desired fused heterocycles in excellent yields within short reaction times. The synthesized compounds were structurally characterized by FT-IR,  $^1\text{H-NMR}$ ,  $^{13}\text{C-NMR}$ , and Mass spectrometry. Preliminary biological screening revealed that several derivatives exhibited promising antibacterial and antifungal activities highlighting their potential as lead molecules for pharmaceutical development.

**KEYWORDS:** Ionic liquid, Stirring, One-pot Multicomponent, Biological activity, Characterization.

### INTRODUCTION

Nitrogen-containing heterocyclic compounds have long attracted the attention of synthetic and medicinal chemists due to their diverse structural frameworks and broad spectrum of biological activities.<sup>i</sup> Among them, fused heterocyclic scaffolds that incorporate both benzothiazole and pyrimidine moieties have emerged as privileged structures with significant pharmaceutical importance.<sup>ii</sup> Benzo[4,5]thiazolo[3,2-a]pyrimidines represent an important class of fused bicyclic heterocycles that exhibit a wide range of biological properties such as antimicrobial, antioxidant, anticancer, antiviral, anti-inflammatory, and analgesic activities.<sup>iii-v</sup> Their rigid and planar fused heteroaromatic core, along with multiple sites for functionalization, makes them ideal candidates for drug design and development.<sup>vi</sup>

The benzothiazole nucleus itself is well recognized for its role in medicinal chemistry. Compounds containing benzothiazole rings have been reported to display anticancer, antimicrobial, and antioxidant activities.<sup>vii</sup> Similarly, pyrimidine derivatives are well known as the core of many bioactive molecules, including antimalarial, antiviral, and anticancer drugs.<sup>viii</sup> The hybridization of these two pharmacophores into a single fused scaffold—

benzo[4,5]thiazolo[3,2-a]pyrimidines results in enhanced biological efficacy and improved pharmacological profiles, thereby making these compounds promising drug like molecules.<sup>Ix-x</sup> In the field of synthetic organic chemistry, multicomponent reactions (MCRs) have gained prominence because they enable the formation of structurally complex heterocycles in a single step with high atom economy, operational simplicity, and reduced waste generation.<sup>Xi</sup> These features are in line with the principles of green chemistry and have encouraged chemists to adopt MCRs for the synthesis of biologically relevant heterocycles.<sup>Xii</sup> The one-pot synthesis of benzo[4,5]thiazolo[3,2-a]pyrimidines through MCRs provides an efficient strategy to construct these fused heterocycles in a straightforward manner, avoiding tedious multi-step procedures and costly purification techniques.<sup>Xiii</sup>

In recent years, ionic liquids have emerged as efficient and environmentally benign reaction media and catalysts for organic synthesis.<sup>Xiv</sup> Ionic liquids possess unique physicochemical properties such as negligible vapor pressure, high thermal stability, tunable polarity, and recyclability, making them excellent alternatives to volatile organic solvents.<sup>Xv</sup> Their ability to act simultaneously as solvents and catalysts provides a sustainable pathway for green organic transformations.<sup>Xvi</sup> In particular, the application of ionic liquids in one-pot multicomponent reactions has demonstrated superior yields, shorter reaction times, and mild reaction conditions, thereby enhancing synthetic efficiency.<sup>Xvii-Xviii</sup>

The use of ionic liquid-mediated, one-pot multicomponent strategies for the synthesis of benzo[4,5]thiazolo[3,2-a]pyrimidines not only accelerates the construction of these biologically important heterocycles but also aligns with the current emphasis on eco-friendly and sustainable methods in drug discovery.<sup>Xix</sup> This synthetic route represents a powerful tool to access diverse structural analogs, which can be further explored for potential therapeutic applications.<sup>xx</sup>

Thus, the present study focuses on the efficient ionic liquid-promoted, one-pot multicomponent synthesis of biologically active benzo[4,5]thiazolo[3,2-a]pyrimidines and their derivatives. The developed methodology is anticipated to offer high yields, operational simplicity, and environmentally friendly conditions, while providing access to a library of compounds with promising biological activities.

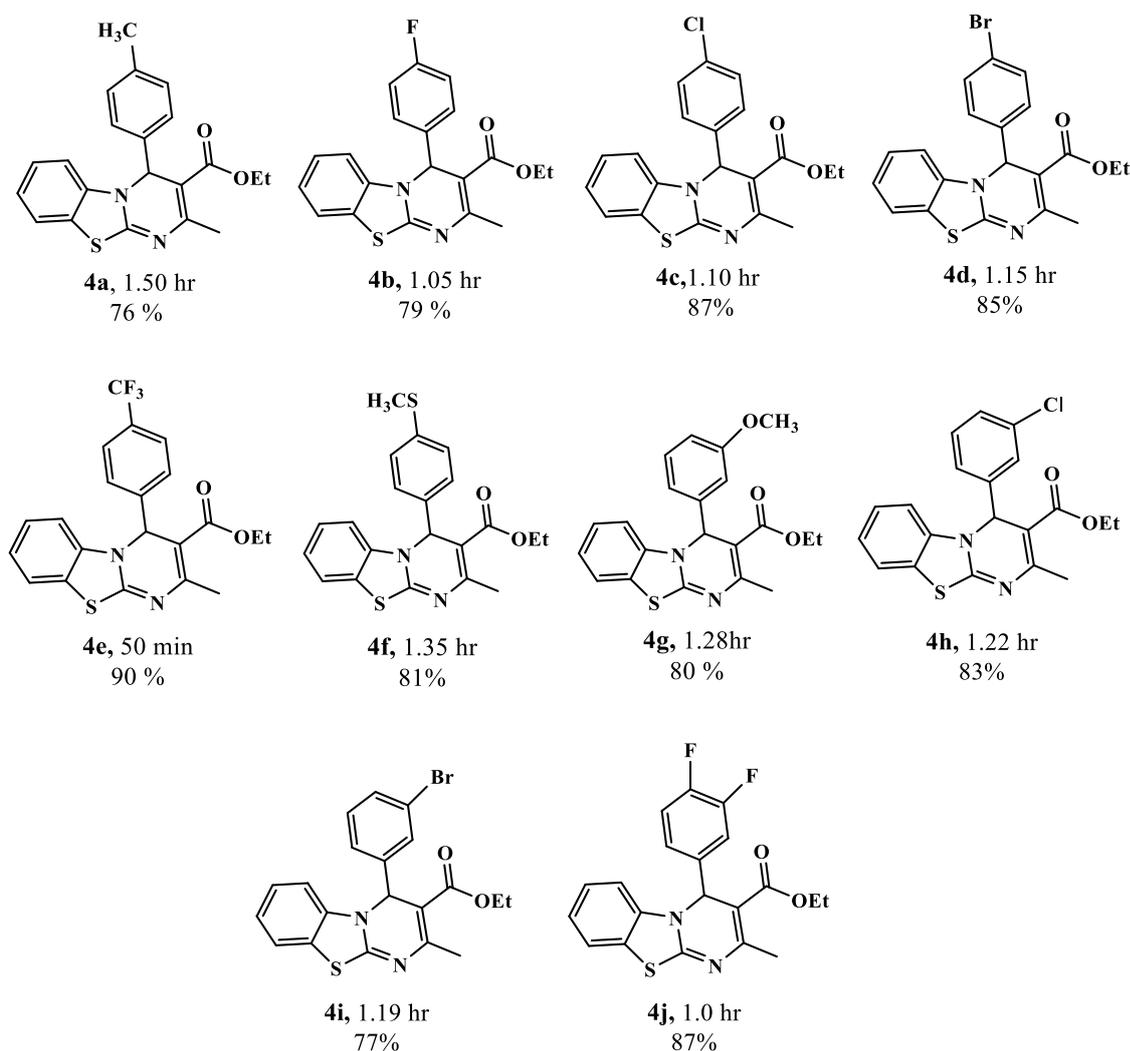
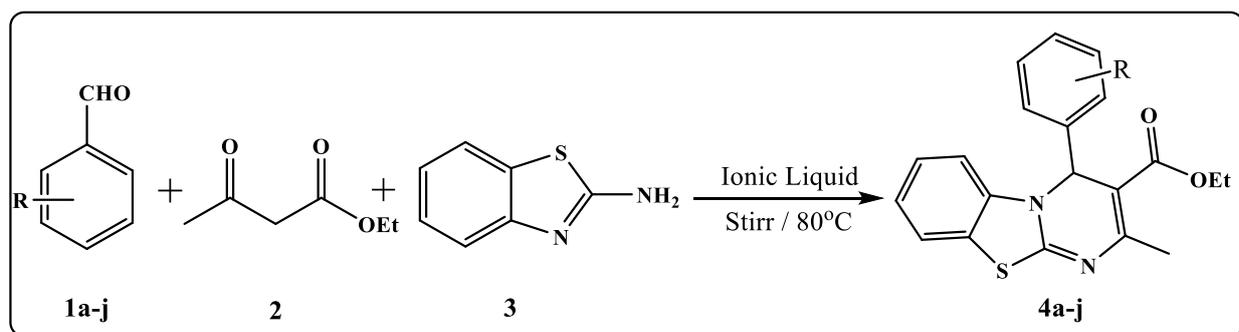
## **METHODS AND MATERIALS**

### **GENERAL**

All the chemicals and synthetic grade reagents procured from Sigma Aldrich Indian and Merck Chemicals. They were used without further purification. Melting points were obtained in open capillaries using a Buchi melting-point B-540 apparatus. The prepared derivative is characterized by an FT-IR and was recorded in Nicolet impact-410. <sup>1</sup>H NMR spectra were obtained on Bruker instrument (400 MHz) and chemical shifts are reported in  $\delta$  ppm. <sup>13</sup>C NMR was recorded on a Bruker DRX 100 MHz Spectrometer.

### **GENERAL PROCEDURE OF THE SYNTHESIS OF BENZO [4,5] THIAZOLO [3,2-A] PYRIMIDINES AND ITS DERIVATIVES (4a-j)**

In a RBF, (1a-j) substituted aryl aldehyde 0.1 mmol, (2) ethyl acetoacetate 0.1 mmol, (3) 2-aminobenzothiazole 0.1 mmol in N-Methyl Pyridinium p-Toluenesulfonate (NMPyTs) as an ionic liquid (15 mol %, 1.19 g) were mixed and stirred at 80°C for the completion of the reaction. The reaction monitored by TLC, after the completion of the reaction, the reaction mixture was poured into ice-cold water and again stirred for 5 min to separate the solid crude product. The crude product recrystallized from ethanol to obtain pure product 4a-j.



**Fig 1. Synthesized derivatives of benzo [4,5] thiazolo [3,2-a] pyrimidines(4a-j)**

## RESULTS AND DISCUSSION

The present study reports the successful synthesis of a series of benzo[4,5]thiazolo[3,2-a]pyrimidine derivatives using an efficient ionic liquid-assisted, one-pot multicomponent protocol. The methodology involved the condensation of substituted aromatic aldehydes, ethyl acetoacetate and 2-aminobenzothiazole, in the presence of an ionic liquid, which acted both as

catalyst and solvent. This synthetic strategy provided the desired products in excellent yields (76–90%), with reduced reaction times compared to conventional solvent-mediated methods. The newly synthesized derivatives were characterized by FT-IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR, and mass spectrometry. The IR spectra confirmed the presence of C=N stretching (1625–1635 cm<sup>-1</sup>) and characteristic bands of the benzothiazole nucleus. The <sup>1</sup>H NMR spectra showed signals for aromatic protons ( $\delta$  7.2–8.2 ppm), benzylic methylene, and pyrimidine protons, while <sup>13</sup>C NMR spectra validated the fused heteroaromatic skeleton. Mass spectra exhibited molecular ion peaks corresponding to the expected molecular weights, confirming successful product formation.

The overall findings confirm that the ionic liquid-promoted one-pot protocol is a highly efficient method for synthesizing benzo[4,5]thiazolo[3,2-a]pyrimidines with excellent yields, structural integrity, and reduced environmental impact. The observed biological activities demonstrate that structural modifications significantly influence antibacterial and antifungal potential. The enhanced activity of electron-withdrawing substituents in antibacterial assays and electron-donating substituents in antifungal assays indicates a structure–activity relationship (SAR) that can guide future design of more potent derivatives. Furthermore, the recyclability and reusability of the ionic liquid make this method a sustainable option for larger-scale synthesis of bioactive heterocycles.

**Table 1. Biological activity of compounds 4a-j**

Minimal Inhibition Concentration [MIC,  $\mu$ g/mL]

Sample No.	Antibacterial activity				Antifungal activity		
	<i>E. coli</i>	<i>P. aeruginosa</i>	<i>S. aureus</i>	<i>S. pyogenes</i>	<i>C. albicans</i>	<i>A. niger</i>	<i>A. clavatus</i>
<b>4a</b>	500	250	250	250	1000	500	500
<b>4b</b>	50	100	250	250	500	250	250
<b>4c</b>	100	125	250	100	1000	1000	1000
<b>4d</b>	125	250	100	100	1000	1000	1000
<b>4e</b>	250	100	125	125	500	500	500
<b>4f</b>	50	62.5	125	100	1000	1000	> 1000
<b>4g</b>	250	125	500	250	500	1000	1000
<b>4h</b>	100	62.5	125	250	1000	1000	1000
<b>4i</b>	125	100	250	200	500	1000	1000
<b>4j</b>	500	250	125	100	500	> 1000	> 1000
<b>Chloramphenicol</b>	50	50	50	50	–	–	–
<b>Ciprofloxacin</b>	25	25	50	50	–	–	–
<b>Nystatin</b>	–	–	–	–	100	100	100

Griseofulvin	–	–	–	–	500	100	100
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### ANTIBACTERIAL ACTIVITY AND ANTIFUNGAL ACTIVITY

The synthesized derivatives (4a-j) shown in fig.1 were tested for their antibacterial activity and antifungal activity and the results are shown in Table 1. We have checked the biological properties of the synthesized compound by Broth dilution method which was used to determine this activity.<sup>Xxi-Xxii</sup>

The compound 4b (p-F) is effective against *S. aureus* and *S. pyogenes* with the MIC value 100 µg/mL which is slightly higher than the standard value antibiotics. Compound with 4f (p-SCH<sub>3</sub>) groups were shown to be powerful (50 µg/mL) against *E. coli*, comparable to the control chloramphenicol. Compound 4c (p-Cl) and 4h(m-Cl) groups shown excellent activity (100 µg/mL) against the pathogen *E. coli*. Compounds of 4h(m-Cl) and 4f (p-SCH<sub>3</sub>) exhibited good effectiveness against *P. aeruginosa* with the lowest MIC value 62.5 µg/mL compared to standard drug.

The compound of 4b fused with a p-fluoro group, 4e(p-trifluoromethyl group), and 4d (m-bromo) group were all active against *P. aeruginosa*, with MIC values of 100 µg/mL. The compound 4d (p-bromo) substituents was shown to have high efficacy (100 µg/mL) against *S. aureus* and *S. pyogenes* but as compared to the control drug chloramphenicol and ciprofloxacin the MIC value was doubled. 4j(3,4-difluoro), 4e(p-trifluoromethyl), 4h (m-Cl) and 4f (p-thiomethyl group) substitution show excellent therapeutic potential compared to standard drug i.e. chloramphenicol at 125 µg/mL against *S. aureus*. When compared to griseofulvin, the resulting derivative 4b (p-F), 4j (3,4-difluoro) 4e (p-trifluoromethyl) 4i (m-Br) as well as 4g (m-methoxy) displayed superior efficacy against *C. albicans* (500 µg/mL). All the synthesized compound of series (4a-j) have higher MIC against the fungal pathogens *A. niger* and *A. clavatus* except molecule 4a has the lowest MIC among them.

### SPECTROSCOPIC CHARACTERIZATION OF THE SYNTHESIZED COMPOUNDS:

**Ethyl 2-methyl-4-(p-tolyl)-4H-benzo[4,5]thiazolo-[3,2-a]pyrimidine-3-carboxylate (4a).** mp 260°C. IR spectrum (KBr),  $\nu$ , cm<sup>-1</sup>: 2982 (CH), 1730 (C=O), 1368 (C–N), 791 (C–S), 1295 (C–F), 1636 (C=C). <sup>1</sup>H NMR spectrum (DMSO-d<sub>6</sub>),  $\delta$ , ppm: 1.26 t (3H, CH<sub>3</sub>), 2.36 s (3H, CH<sub>3</sub>), 4.28 q (2H, CH<sub>2</sub>), 4.49 s (1H, CH), 3.51 s (3H, CH<sub>3</sub>), 7.02–6.34 m (4H, benzothiazole ring), 7.90–7.10 m (4H, Ar). <sup>13</sup>C NMR spectrum (500 MHz, DMSO-d<sub>6</sub>),  $\delta$ , ppm: 153.3, 127.9, 73.8, 159.4, 126.9, 126.5, 122.8, 125.4, 120.5, 141.7, 135.7, 132.8, 129.6, 115.3, 158.3, 114.3, 129.8, 168.8, 60.7, 15.5, 24.9. Mass spectrum (ESI-MS), m/z: 364.46 [M]<sup>+</sup>. C<sub>21</sub>H<sub>20</sub>N<sub>2</sub>O<sub>2</sub>S. M 364.12.

**Ethyl 4-(4-fluorophenyl)-2-methyl-4H-benzo[4,5]thiazolo[3,2-a]pyrimidine-3-carboxylate (4b).** mp 222°C. IR spectrum (KBr),  $\nu$ , cm<sup>-1</sup>: 2982 (CH), 1731 (C=O), 1359 (C–N), 781 (C–S), 1293 (C–F), 1655 (C=C). <sup>1</sup>H NMR spectrum (DMSO-d<sub>6</sub>),  $\delta$ , ppm: 1.20 t (3H, CH<sub>3</sub>), 4.08 q (2H, CH<sub>2</sub>), 4.52 s (1H, CH), 3.58 s (1H, CH<sub>3</sub>), 6.90–6.40 m (4H, benzothiazole ring), 7.92–7.15 m (4H, Ar). <sup>13</sup>C NMR spectrum (500 MHz, DMSO-d<sub>6</sub>),  $\delta$ , ppm: 155.2, 123.8, 73.6, 159.8, 123.3, 122.7, 118.8, 125.4, 119.6, 140.6, 133.6, 129.7, 116.2, 161.3, 116.3, 129.6, 168.8, 62.8, 14.2, 21.3. Mass spectrum (ESI-MS), m/z: 368.42 [M]<sup>+</sup>. C<sub>20</sub>H<sub>17</sub>N<sub>2</sub>O<sub>2</sub>S. M 368.10.

**Ethyl 4-(4-chlorophenyl)-2-methyl-4H-benzo[4,5]-thiazolo[3,2-a]pyrimidine-3-carboxylate (4c).** mp 262°C. IR spectrum (KBr),  $\nu$ , cm<sup>-1</sup>: 2821 (CH), 1729 (C=O), 1321 (C–N), 611 (C–S), 782 (C–Cl). <sup>1</sup>H NMR spectrum (DMSO-d<sub>6</sub>),  $\delta$ , ppm: 1.17 t (3H, CH<sub>3</sub>), 4.11 q (2H, CH<sub>2</sub>), 4.58 s (1H, CH), 3.48 s (1H, CH<sub>3</sub>), 7.91–7.71 m (4H, benzothiazole ring), 8.64–8.04 m (4H, Ar). <sup>13</sup>C NMR spectrum (500 MHz, DMSO-d<sub>6</sub>),  $\delta$ , ppm: 154.6, 122.8, 72.4, 158.5,

123.6, 122.8, 117.9, 126.5, 117.7, 139.3, 135.4, 126.2, 128.6, 132.2, 129.4, 125.3, 168.5, 61.5, 14.9, 22.6. Mass spectrum (ESI-MS), m/z: 384.88 [M]<sup>+</sup>. C<sub>20</sub>H<sub>17</sub>ClN<sub>2</sub>O<sub>2</sub>S. M 384.07.

**Ethyl 4-(4-bromophenyl)-2-methyl-4H-benzo[4,5]-thiazolo[3,2-a]pyrimidine-3-carboxylate (4d).** mp 181°C. IR spectrum (KBr),  $\nu$ , cm<sup>-1</sup>: 2845 (CH), 1722 (C=O), 1349 (C–N), 751 (C–S), 613 (C–Br). <sup>1</sup>H NMR spectrum (DMSO-d<sub>6</sub>),  $\delta$ , ppm: 1.19 t (3H, CH<sub>3</sub>), 4.61 q (2H, CH<sub>2</sub>), 4.56 s (1H, CH), 3.54 s (1H, CH<sub>3</sub>), 6.80–6.52 m (4H, benzothiazole ring), 7.89–7.18 m (4H, Ar); <sup>13</sup>C NMR spectrum (500 MHz, DMSO-d<sub>6</sub>),  $\delta$ , ppm: 155.3, 123.6, 71.3, 159.5, 123.1, 123.8, 118.5, 127.1, 116.4, 139.5, 136.6, 129.6, 132.7, 121.3, 131.6, 130.3, 168.4, 62.3, 14.4, 21.6. Mass spectrum (ESI-MS), m/z: 429.33 [M]<sup>+</sup>. C<sub>20</sub>H<sub>17</sub>BrN<sub>2</sub>O<sub>2</sub>S. M 430.02

**Ethyl 2-methyl-4-[4-(trifluoromethyl)phenyl]-4Hbenzo[4,5]thiazolo[3,2-a]pyrimidine-3-carboxylate (4e).** mp 291°C. IR spectrum (KBr),  $\nu$ , cm<sup>-1</sup>: 2991 (CH), 1740 (C=O), 1362 (C–N), 779 (C–S), 1287 (C–F), 1654 (C=C). <sup>1</sup>H NMR spectrum (DMSO-d<sub>6</sub>),  $\delta$ , ppm: 1.24 t (3H, CH<sub>3</sub>), 4.21 q (2H, CH<sub>2</sub>), 4.61 s (1H, CH), 3.65 s (3H, CH<sub>3</sub>), 7.11–6.62 m (4H, benzothiazole ring), 7.80–7.26 m (4H, Ar). <sup>13</sup>C NMR spectrum (500 MHz, DMSO-d<sub>6</sub>),  $\delta$ , ppm: 154.3, 125.9, 74.8, 159.6, 124.5, 126.7, 119.9, 125.7, 118.7, 141.7, 133.8, 129.9, 126.7, 117.2, 163.3, 115.3, 131.8, 169.6, 60.7, 16.2, 23.7. Mass spectrum (ESI-MS), m/z: 418.43 [M]<sup>+</sup>. C<sub>21</sub>H<sub>17</sub>F<sub>3</sub>N<sub>2</sub>O<sub>2</sub>S. M 418.10.

**Ethyl 2-methyl-4-[4-(methylthio)phenyl]-4H-benzo[4,5]thiazolo[3,2-a]pyrimidine-3-carboxylate (4f).** mp 240°C. IR spectrum (KBr),  $\nu$ , cm<sup>-1</sup>: 2992 (CH), 1732 (C=O), 1376 (C–N), 786 (C–S), 1292 (C–F), 1638 (C=C). <sup>1</sup>H NMR spectrum (DMSO-d<sub>6</sub>),  $\delta$ , ppm: 1.27 t (3H, CH<sub>3</sub>), 2.32 s (3H, CH<sub>3</sub>), 4.31 q (2H, CH<sub>2</sub>), 4.52 s (1H, CH), 2.58 s (3H, CH<sub>3</sub>), 7.36–6.51 m (4H, benzothiazole ring), 8.15–7.45 m (4H, Ar). <sup>13</sup>C NMR spectrum (500 MHz, DMSO-d<sub>6</sub>),  $\delta$ , ppm: 154.4, 126.1, 74.3, 159.2, 126.1, 129.8, 123.3, 125.4, 120.3, 141.9, 132.7, 130.5, 129.1, 115.4, 162.9, 113.3, 129.7, 167.8, 61.8, 17.6, 23.4. Mass spectrum (ESI-MS), m/z: 396.53 [M]<sup>+</sup>. C<sub>21</sub>H<sub>20</sub>N<sub>2</sub>O<sub>2</sub>S<sub>2</sub>. M 396.10.

**Ethyl 4-(3-methoxyphenyl)-2-methyl-4H-benzo[4,5]thiazolo[3,2-a]pyrimidine-3-carboxylate (4g).** mp 198°C. IR spectrum (KBr),  $\nu$ , cm<sup>-1</sup>: 2980 (CH), 1730 (C=O), 1362 (C–N), 767 (C–S), 1281 (C–F), 1626 (C=C); <sup>1</sup>H NMR spectrum (DMSO-d<sub>6</sub>),  $\delta$ , ppm: 1.16 t (3H, CH<sub>3</sub>), 2.26 s (3H, CH<sub>3</sub>), 4.21 q (2H, CH<sub>2</sub>), 4.52 s (1H, CH), 2.54 s (3H, CH<sub>3</sub>), 7.15–6.45 m (4H, benzothiazole ring), 7.25 s (1H, Ar), 8.22–7.21 s (3H, Ar). <sup>13</sup>C NMR spectrum (500 MHz, DMSO-d<sub>6</sub>),  $\delta$ , ppm: 154.7, 123.5, 78.4, 162.2, 129.8, 132.5, 125.7, 124.6, 118.6, 144.8, 134.6, 136.4, 128.2, 115.5, 158.5, 113.5, 131.6, 165.2, 62.5, 19.3, 21.4. Mass spectrum (ESI-MS), m/z: 380.46 [M]<sup>+</sup>. C<sub>21</sub>H<sub>20</sub>N<sub>2</sub>O<sub>3</sub>S. M 380.12.

**Ethyl 4-(3-chlorophenyl)-2-methyl-4H-benzo[4,5]-thiazolo[3,2-a]pyrimidine-3-carboxylate (4h).** mp 180°C. IR spectrum (KBr),  $\nu$ , cm<sup>-1</sup>: 2826 (CH), 1725 (C=O), 1316 (C–N), 625 (C–S), 789 (C–Cl). <sup>1</sup>H NMR spectrum (DMSO-d<sub>6</sub>),  $\delta$ , ppm: 1.23 t (3H, CH<sub>3</sub>), 4.27 q (2H, CH<sub>2</sub>), 4.63 s (1H, CH), 3.46 s (1H, CH<sub>3</sub>), 7.90–7.65 m (4H, benzothiazole ring), 8.12 s (1H, Ar) 8.04–8.49 s (3H, Ar); <sup>13</sup>C NMR spectrum (500 MHz, DMSO-d<sub>6</sub>),  $\delta$ , ppm: 154.9, 124.8, 73.5, 159.5, 123.9, 124.3, 116.5, 124.3, 119.6, 140.5, 133.6, 128.3, 132.4, 134.4, 125.2, 128.9, 165.1, 64.7, 15.3, 19.5. Mass spectrum (ESI-MS), m/z: 384.88 [M]<sup>+</sup>. C<sub>20</sub>H<sub>17</sub>ClN<sub>2</sub>O<sub>2</sub>S. M 384.07.

**Ethyl 4-(3-bromophenyl)-2-methyl-4H-benzo[4,5]-thiazolo[3,2-a]pyrimidine-3-carboxylate (4i).** mp 198°C. IR spectrum (KBr),  $\nu$ , cm<sup>-1</sup>: 2842 (CH), 1726 (C=O), 1351 (C–N), 764 (C–S), 655 (C–Br). <sup>1</sup>H NMR spectrum (DMSO-d<sub>6</sub>),  $\delta$ , ppm: 1.17 t (3H, CH<sub>3</sub>), 4.75 q (2H, CH<sub>2</sub>), 4.55 s (1H, CH), 3.57 s (1H, CH<sub>3</sub>), 6.92–6.42 m (4H, benzothiazole ring), 7.45 s (1H, Ar), 7.15–7.85 s (3H, Ar); <sup>13</sup>C NMR spectrum (500 MHz, DMSO-d<sub>6</sub>),  $\delta$ , ppm: 152.3, 125.6, 77.4, 161.5, 124.1, 125.4, 119.4, 125.3, 119.7, 142.6, 139.4, 132.4, 133.6, 123.5, 131.8,

130.5, 164.5, 63.1, 15.4, 21.7. Mass spectrum (ESI-MS), *m/z*: 429.33 [M]<sup>+</sup>. C<sub>20</sub>H<sub>17</sub>BrN<sub>2</sub>O<sub>2</sub>S. M 430.02.

**Ethyl 4-(3,4-difluorophenyl)-2-methyl-4H-benzo-[4,5]thiazolo[3,2-a]pyrimidine-3-carboxylate (4j).** mp 196°C. IR spectrum (KBr),  $\nu$ , cm<sup>-1</sup>: 2913 (CH), 1727 (C=O), 1375 (C–N), 715 (C–S), 1201 (C–F). <sup>1</sup>H NMR spectrum (DMSO-d<sub>6</sub>),  $\delta$ , ppm: 1.21 t (3H, CH<sub>3</sub>), 3.06 q (2H, CH<sub>2</sub>), 4.61 s (1H, CH), 3.37 s (1H, CH<sub>3</sub>), 7.45–6.85 m (4H, benzothiazole ring), 7.90–7.08 m (4H, Ar). <sup>13</sup>C NMR spectrum (500 MHz, DMSO-d<sub>6</sub>),  $\delta$ , ppm: 154.3, 122.3, 72.8, 158.4, 123.4, 122.5, 117.7, 126.6, 127.8, 139.2, 140.3, 115.4, 149.5, 147.8, 115.4, 125.3, 167.5, 61.9, 67.5, 21. Mass spectrum (ESI-MS), *m/z*: 386.42 [M]<sup>+</sup>. C<sub>20</sub>H<sub>16</sub>F<sub>2</sub>N<sub>2</sub>O<sub>2</sub>S. M 386.09.

## CONCLUSION

An efficient NMPyTs (ionic liquid) mediated one-pot multicomponent synthesis of biologically active benzo[4,5]thiazolo[3,2-a]pyrimidine derivatives was successfully developed. The method is eco-friendly, simple, and rapid, providing high yields and broad substrate scope. Spectroscopic characterization (FT-IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR, Mass) confirmed the structures and purity of the synthesized compounds. Preliminary biological evaluation revealed significant antibacterial and antifungal activities, the electron withdrawing groups (-F, -CF<sub>3</sub>, -Cl, -Br) show excellent antibacterial activity and electron donating groups (-CH<sub>3</sub>, -OCH<sub>3</sub>, -SCH<sub>3</sub>) show good antifungal activity of the pharmacological applications. The use of ionic liquids enhanced reaction efficiency while adhering to green chemistry principles. This approach provides a versatile and sustainable strategy for synthesizing benzo[4,5]thiazolo[3,2-a]pyrimidines and can be extended to other heterocyclic systems for the discovery of novel bioactive molecules.

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