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International Journal of Multidisciplinary Research in Science, Engineering and Technology (IJMRSET)

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Synthesis, Characterization and Biological Activity of Novel Benzothiazoles

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ABSTRACT: Benzothiazoles are a versatile and promising class of chemicals exhibiting a broad spectrum of pharmacological activities. Ongoing research and development may result in the identification of novel therapeutic compounds derived from benzothiazole, thereby making substantial contributions to medicinal chemistry. Notwithstanding the favorable pharmacological characteristics of benzothiazole derivatives, numerous obstacles and avenues for future investigation persist. Thorough investigations on the toxicity and safety profiles of benzothiazole derivatives are essential to ascertain their potential as medicinal agents. Additionally, further investigation is necessary to elucidate the structure-activity correlations of benzothiazole derivatives to enhance their pharmacological effects. Additional preclinical and clinical investigations are required to validate the efficacy and safety of benzothiazole-based pharmaceuticals in people. Examining the possibility of drug resistance and formulating measures to mitigate it is essential for the sustained efficacy of benzothiazole-based treatments. This study investigates the synthesis, characterization and biological activity of novel benzothiazole derivatives, with a particular focus on their potential applications as antifungal and analgesic.

KEYWORDS: Benzothiazole, synthesis, activity, compounds.

I. INTRODUCTION

Heterocyclic chemistry is fundamental to medical and organic chemistry, largely because of the prevalence of heterocyclic compounds in pharmaceuticals. These compounds frequently demonstrate therapeutic efficacy that can be optimized by altering the heterocyclic structure, resulting in substantial modifications to the drug's pharmacological characteristics. Benzothiazole is distinguished among heterocyclic compounds for its unique and adaptable features, rendering it a promising scaffold in experimental medication creation. Heterocyclic compounds, characterized by rings containing at least one non-carbon atom (such as nitrogen, oxygen, or sulfur), are essential in pharmaceutical development owing to their varied biological activity. Altering the heterocyclic ring can profoundly influence the compound's efficacy, selectivity, and pharmacokinetics. The distinctive amalgamation of sulfur and nitrogen atoms within the thiazole ring, united with a benzene ring, imparts benzothiazole its unique chemical characteristics and biological functions. This framework permits numerous replacements that can augment or alter its action, rendering it a flexible scaffold in pharmaceutical chemistry. It demonstrates aromaticity owing to the conjugation of π-electrons throughout the fused rings, enhancing its stability. Benzothiazole lacks applicability in domestic environments. Rather, it serves a vital function in industry and research, especially in the formulation of medicinal substances. Its distinctive chemical composition and biological properties render it an essential element in the formulation of pharmaceuticals with diverse therapeutic benefits. Benzothiazole is a compound of significant interest owing to its extensive applications and remarkable chemical characteristics. Benzothiazoles are utilized in industry as antioxidants and accelerators for vulcanization. Certain benzothiazoles, particularly 2-aryl benzothiazole, have garnered significant attention due to their unique structures and applications as anticancer and radioactive amyloid imaging agents. Creating benzothiazole compounds that offers novel alternatives for individuals who have acquired resistance to regular treatments. Benzothiazole derivatives not only possess direct anti-cancer properties but also augment the effectiveness of various therapeutic approaches.

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II. RESEARCH METHODOLOGY

Synthesis of Novel Derivatives: Stirring took place at room temperature for 12 hours using a solution of Reactant A (5 mmol), Reactant B (6 mmol), and sodium hydroxide (6 mmol) in N,N-dimethylformamide (10 mL). After evaporating 50% of the solvent, we added 50 mL of water to the solution before extracting it with 30% ethyl acetate. Over an anhydrous $MgSO_4$ bed, the ethyl acetate layer dried. After the solvent was evaporated, a crude product was obtained, which was then recrystallized from dichloromethane. A list of the synthesized compounds is given below in the table comprising Reactant A, Reactant B as well as the final product.

Characterization: Following techniques were used for characterization of novel synthesized benzothiazole derivatives.

Table 1: Techniques used for characterization

S. No.	Technique	Measurement
1	Elemental Analysis	Percentage of carbon, hydrogen, nitrogen and sulphur were analysed using CHN analyser EAGER 200 Thermoquest.
2	Mass Spectra	Mass spectra was analysed using GC MS.
3	M.P.	M.P. were determined in open capillaries with the help of VEGGO melting point apparatus.
4	IR	IR spectra was measured using Infra spectrophotometer Model RXIFTIR shimazdu.

Biological Activity: The antifungal activity of benzothiazole derivatives against *Candida albicans* (MTCC-183) and *C. glabrata* was assessed using the disc diffusion method. To identify the minimum concentration at which a compound is effective against a specific microbial strain, active compounds were further evaluated at progressively lower concentrations. The analgesic potential of novel benzothiazole compounds was evaluated in male albino Swiss mice by measuring the paw withdrawal latency on a hot plate set to 58°C.

Result and Discussion –

The current study focused on synthesizing novel derivatives of benzothiazoles. A total of 24 novel compounds were synthesized using the MAOS technique (Microwave assisted organic synthesis). The synthesized compounds were characterized using various techniques such as elemental analysis, M.P. determination, IR and mass spectrometry. Following novel compounds were synthesized.

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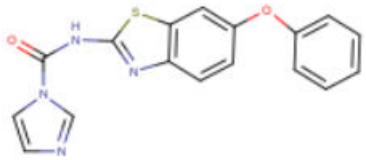
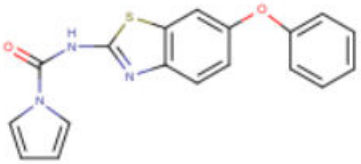
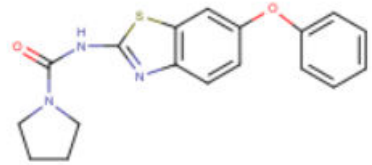
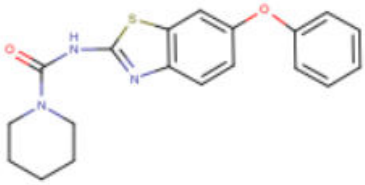
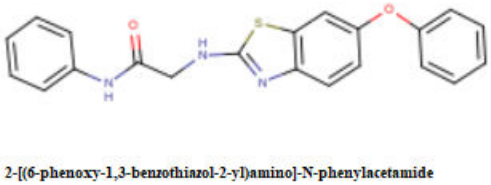
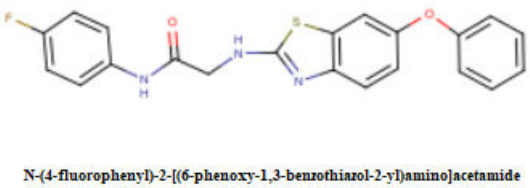
Table 2: Structure, elemental analysis and melting point of synthesized compounds

S. No.	IUPAC name of synthesized derivatives	Elemental analysis	Melting point
1	 N-(6-phenoxy-1,3-benzothiazol-2-yl)-1H-imidazole-1-carboxamide	C (60.70%), H (3.60%), N (16.66%), O (9.51%), S (9.53%)	177°C
2	 N-(6-phenoxy-1,3-benzothiazol-2-yl)-1H-pyrrole-1-carboxamide	C (65.57%), H (5.50%), N (13.49%), O (5.14%), S (10.30%)	175°C
3	 N-(6-phenoxy-1,3-benzothiazol-2-yl)pyrrolidine-1-carboxamide	C (63.70%), H (5.05%), N (12.38%), O (9.43%), S (9.45%)	179°C
4	 N-(6-phenoxy-1,3-benzothiazol-2-yl)piperidine-1-carboxamide	C (64.57%), H (5.42%), N (11.89%), O (9.05%), S (9.07%)	172°C
5	 2-[(6-phenoxy-1,3-benzothiazol-2-yl)amino]-N-phenylacetamide	C (67.18%), H (4.56%), N (11.19%), O (8.52%), S (8.54%)	173°C
6	 N-(4-fluorophenyl)-2-[(6-phenoxy-1,3-benzothiazol-2-yl)amino]acetamide	C (64.11%), H (4.10%), F (4.83%), N (10.68%), O (8.13%), S (8.15%)	176°C

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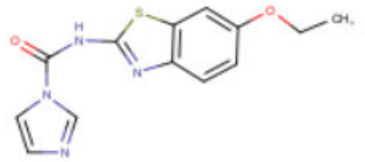
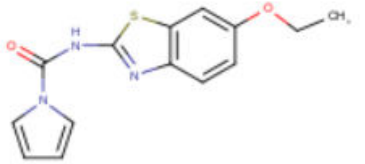
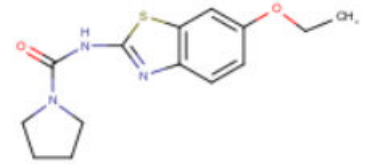
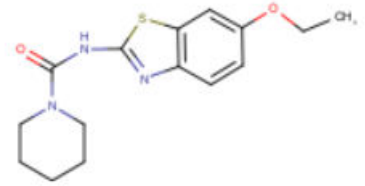
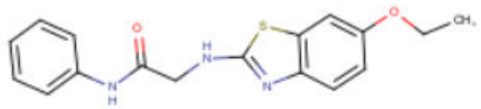
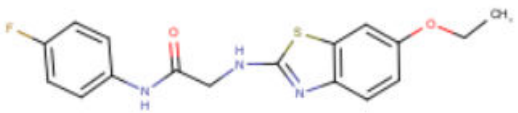
7	 N-(6-ethoxy-1,3-benzothiazol-2-yl)-1H-imidazole-1-carboxamide	C (54.16%), H (4.20%), N (19.43%), O (11.10%), S (11.12%)	184°C
8	 N-(6-ethoxy-1,3-benzothiazol-2-yl)-1H-pyrrole-1-carboxamide	C (58.52%), H (4.56%), N (14.62%), O (11.14%), S (11.16%)	183°C
9	 N-(6-ethoxy-1,3-benzothiazol-2-yl)pyrrolidine-1-carboxamide	C (57.71%), H (5.88%), N (14.42%), O (10.98%), S (11.00%)	181°C
10	 N-(6-ethoxy-1,3-benzothiazol-2-yl)piperidine-1-carboxamide	C (58.99%), H (6.27%), N (13.76%), O (10.48%), S (10.50%)	186°C
11	 2-[(6-ethoxy-1,3-benzothiazol-2-yl)amino]-N-phenylacetamide	C (62.37%), H (5.23%), N (12.83%), O (9.77%), S (9.79%)	184°C
12	 2-[(6-ethoxy-1,3-benzothiazol-2-yl)amino]-N-(4-fluorophenyl)acetamide	C (59.12%), H (4.67%), F (5.50%), N (12.17%), O (9.26%), S (9.28%)	188°C

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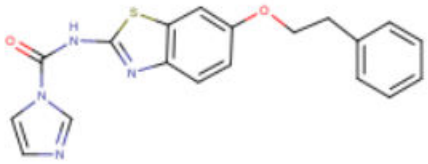
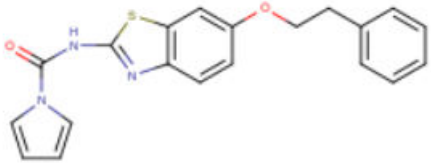
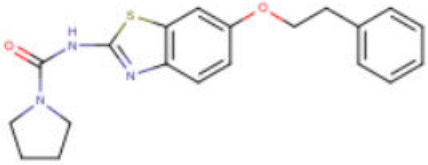
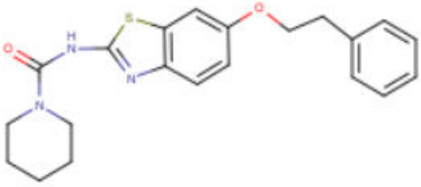
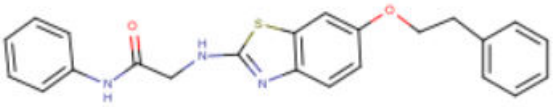
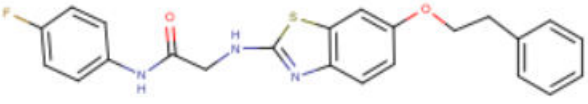
13	 N-[6-(2-phenylethoxy)-1,3-benzothiazol-2-yl]-1H-imidazole-1-carboxamide	C (62.62%), H (4.43%), N (15.37%), O (8.78%), S (8.80%)	175°C
14	 N-[6-(2-phenylethoxy)-1,3-benzothiazol-2-yl]-1H-pyrrole-1-carboxamide	C (66.10%), H (4.72%), N (11.56%), O (8.80%), S (8.82%)	176°C
15	 N-[6-(2-phenylethoxy)-1,3-benzothiazol-2-yl]pyrrolidine-1-carboxamide	C (65.37%), H (5.76%), N (11.44%), O (8.71%), S (8.72%)	179°C
16	 N-[6-(2-phenylethoxy)-1,3-benzothiazol-2-yl]piperidine-1-carboxamide	C (66.12%), H (6.08%), N (11.01%), O (8.39%), S (8.40%)	176°C
17	 N-phenyl-2-{[6-(2-phenylethoxy)-1,3-benzothiazol-2-yl]amino}acetamide	C (68.46%), H (5.25%), N (10.41%), O (7.93%), S (7.95%)	178°C
18	 N-(4-fluorophenyl)-2-{[6-(2-phenylethoxy)-1,3-benzothiazol-2-yl]amino}acetamide	C (65.54%), H (4.78%), F (4.51%), N (9.97%), O (7.59%), S (7.61%)	173°C

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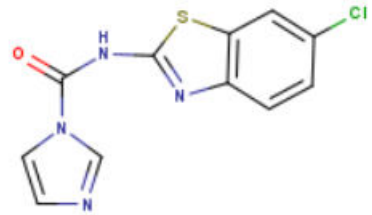
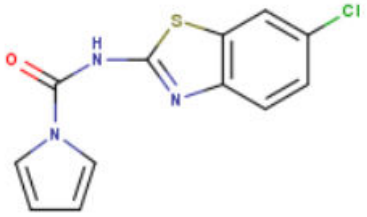
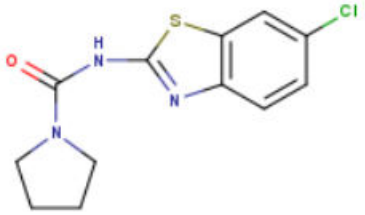
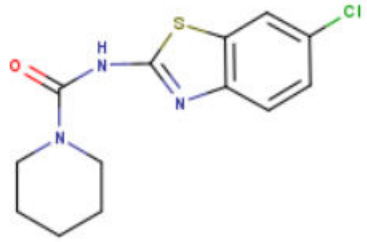
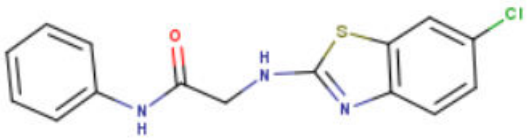
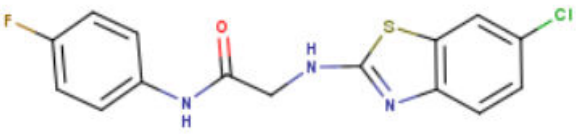
19	 N-(6-chloro-1,3-benzothiazol-2-yl)-1H-imidazole-1-carboxamide	C (47.40%), H (2.53%), Cl (12.72%), N (20.10%), O (5.74%), S (11.50%)	191°C
20	 N-(6-chloro-1,3-benzothiazol-2-yl)-1H-pyrrole-1-carboxamide	C (51.90%), H (2.90%), Cl (12.76%), N (15.13%), O (5.76%), S (11.54%)	189°C
21	 N-(6-chloro-1,3-benzothiazol-2-yl)pyrrolidine-1-carboxamide	C (51.15%), H (4.29%), Cl (12.58%), N (14.91%), O (5.68%), S (11.38%)	186°C
22	 N-(6-chloro-1,3-benzothiazol-2-yl)piperidine-1-carboxamide	C (52.79%), H (4.77%), Cl (11.99%), N (14.21%), O (5.41%), S (10.84%)	192°C
23	 2-[(6-chloro-1,3-benzothiazol-2-yl)amino]-N-phenylacetamide	C (56.69%), H (3.81%), Cl (11.16%), N (13.22%), O (5.03%), S (10.09%)	187°C
24	 2-[(6-chloro-1,3-benzothiazol-2-yl)amino]-N-(4-fluorophenyl)acetamide	C (53.66%), H (3.30%), Cl (10.56%), F (5.66%), N (12.51%), O (4.76%), S (9.55%)	193°C

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Table 3: Spectra data of synthesized compounds

Compounds	IR spectra (in cm^{-1})	Mass spectra
BZ-1	C-N: 1377.6 cm^{-1}, C-H: 1252.7 cm^{-1}	336: 1.00 337: 0.21 338: 0.07 339: 0.01
BZ-2	C=O: 1371.1 cm^{-1}, N-H: 1365.2 cm^{-1}	311: 1.00 312: 0.21 313: 0.07 314: 0.01
BZ-3	C-N: 1380.8 cm^{-1}, C=O: 1765.3 cm^{-1}	339: 1.00 340: 0.22 341: 0.07 342: 0.01
BZ-4	C-N: 1409.1 cm^{-1}	353: 1.00 354: 0.23 355: 0.07 356: 0.01
BZ-5	C=O: 1734.7 cm^{-1}	375: 1.00 376: 0.25 377: 0.08 378: 0.01
BZ-6	C-F: 772.7 cm^{-1}	393: 1.00 394: 0.25 395: 0.08 396: 0.01
BZ-7	C=O: 1780.2 cm^{-1}	288: 1.00 289: 0.17 290: 0.06 291: 0.01
BZ-8	C-N: 1283.3 cm^{-1}	287: 1.00 288: 0.17 289: 0.06 290: 0.01
BZ-9	C-O: 1129.8 cm^{-1}	291: 1.00 292: 0.17 293: 0.06 294: 0.01
BZ-10	C-N: 1404.4 cm^{-1}	305: 1.00 306: 0.18 307: 0.06 308: 0.01
BZ-11	C=O: 1747.2 cm^{-1}	327: 1.00 328: 0.21 329: 0.07 330: 0.01
BZ-12	C-F: 467.6 cm^{-1}	345: 1.00 346: 0.21 347: 0.07 348: 0.01
BZ-13	C=O: 1779.8 cm^{-1}	364: 1.00 365: 0.23 366: 0.07 367: 0.01
BZ-14	C=C: 1469.8 cm^{-1}	363: 1.00 364: 0.24 365: 0.08 366: 0.01
BZ-15	C-N: 1241.9 cm^{-1}	367: 1.00 368: 0.24 369: 0.08 370: 0.01
BZ-16	C-H: 601.3 cm^{-1}, C-C: 424.8 cm^{-1}	381: 1.00 382: 0.25 383: 0.08 384: 0.01
BZ-17	N-H: 1388.6 cm^{-1}, C=O: 1770.2 cm^{-1}	403: 1.00 404: 0.27 405: 0.08 406: 0.02
BZ-18	C-F: 776.5 cm^{-1}	421: 1.00 422: 0.27 423: 0.08 424: 0.02
BZ-19	C=O: 1783.7 cm^{-1}	278: 1.00 279: 0.14 280: 0.38 281: 0.05 282: 0.02
BZ-20	C=C: 1282.6 cm^{-1}	277: 1.00 278: 0.15 279: 0.38 280: 0.06 281: 0.02
BZ-21	C-H: 1240.9 cm^{-1}, N-H: 1378.7 cm^{-}	281: 1.00 282: 0.15 283: 0.38 284: 0.06 285: 0.02
BZ-22	C=O: 1764.2 cm^{-1}, C-C: 1108.0 cm^{-1}	295: 1.00 296: 0.16 297: 0.38 298: 0.06 299: 0.02
BZ-23	N-H: 1392.0 cm^{-1}, C=C: 1598.2 cm^{-1}	317: 1.00 318: 0.18 319: 0.38 320: 0.07 321: 0.02
BZ-24	C-F: 767.4 cm^{-1}	335: 1.00 336: 0.18 337: 0.38 338: 0.07 339: 0.02

Antifungal activity: In the biological evaluation of benzothiazole derivatives, their antifungal activity was assessed against *Candida albicans* (MTCC-183) and *C. glabrata* using the disc diffusion technique, followed by determination of minimal inhibitory concentration (MIC) values. The MIC results, which reflect the lowest concentration at which each compound inhibited fungal growth, were significantly high, indicating potent antifungal properties. Compounds BZ-1, BZ-7, BZ-14, BZ-18, and BZ-19 demonstrated particularly strong antifungal activity.

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Fig 1: Antifungal activity of compounds

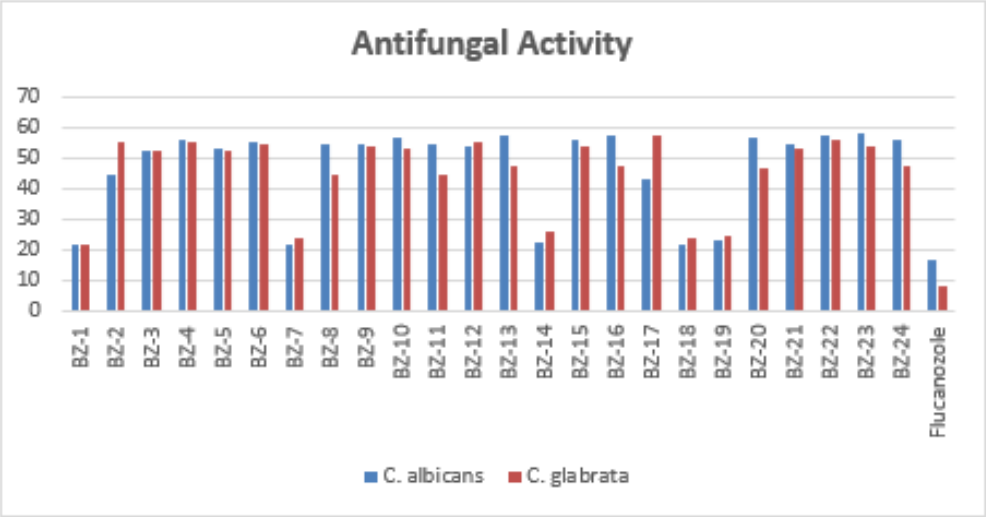
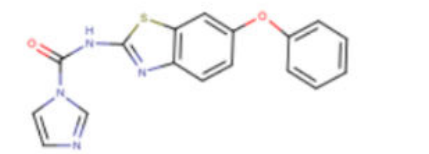
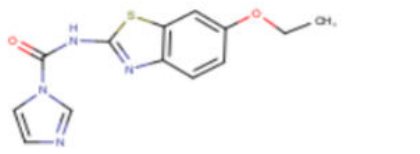


Fig 2: Compounds showing antifungal activity



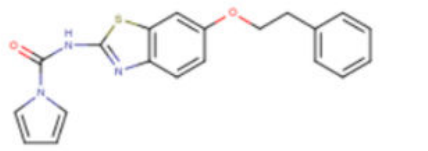
N-(6-phenoxy-1,3-benzothiazol-2-yl)-1H-imidazole-1-carboxamide

BZ-1



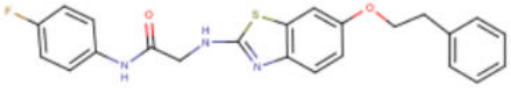
N-(6-ethoxy-1,3-benzothiazol-2-yl)-1H-imidazole-1-carboxamide

BZ-7



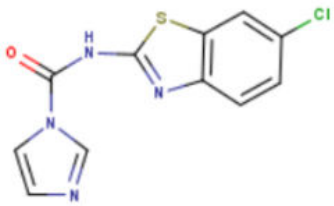
N-[6-(2-phenylethoxy)-1,3-benzothiazol-2-yl]-1H-pyrrole-1-carboxamide

BZ-14



N-(4-fluorophenyl)-2-[[6-(2-phenylethoxy)-1,3-benzothiazol-2-yl]amino]acetamide

BZ-18



N-(6-chloro-1,3-benzothiazol-2-yl)-1H-imidazole-1-carboxamide

BZ-19

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Analgesic activity: The study evaluated the analgesic activity of novel benzothiazole compounds in male albino Swiss mice by measuring their paw withdrawal latency on a hot plate at 58°C. Initial paw withdrawal times were recorded by testing at 0 and 30 minutes after intraperitoneal (i.p.) injection of each compound at doses ranging from 50 mg/kg. Pentazocine, a known analgesic, was used as a standard and showed a notable increase in latency time from 5.65 seconds to 8.5 seconds, demonstrating effective analgesic activity. Among the benzothiazole derivatives, several compounds displayed increased paw withdrawal latency after 30 minutes, indicating potential analgesic effects. Compounds BZ-1, BZ-8, BZ-14, BZ-18, and BZ-19 showed notable increases in latency times, with BZ-14 achieving the highest latency time of 7.9 seconds after 30 minutes. Although this value was slightly lower than that of pentazocine, it suggests that BZ-14 has a significant analgesic potential.

Fig 3: Analgesic activity of compounds

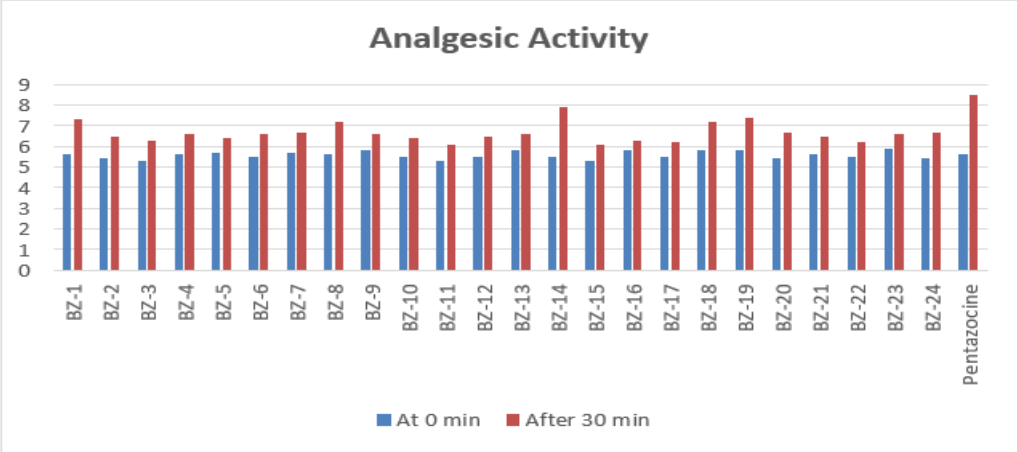
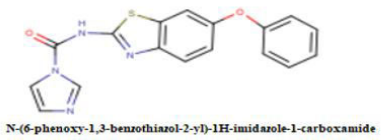
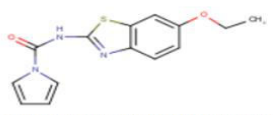


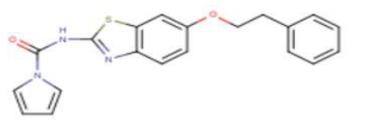
Fig 4: Compounds showing Analgesic activity



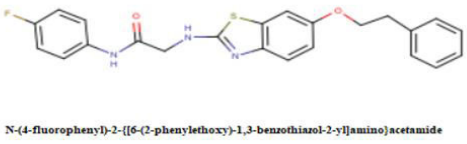
BZ-1



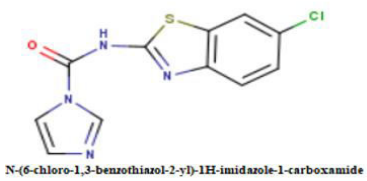
BZ-8



BZ-14



BZ-18



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III. CONCLUSION

The synthesis and characterization of novel benzothiazole derivatives revealed promising structural and functional properties that make these compounds valuable candidates for pharmacological applications. The biological assays conducted confirmed the efficacy of these benzothiazoles, particularly in their antifungal and analgesic activities, underscoring their potential as therapeutic agents. The results highlight the significance of benzothiazoles as versatile scaffolds, with the potential to be further modified for enhanced bioactivity and specificity.

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