DESIGN AND SYNTHESIS OF NOVEL AZA-HETEROCYCLES FOR NEUROPROTECTION

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Pyrazole, imidazole, and triazole scaffolds are well-established heterocyclic frameworks in medicinal chemistry and are increasingly explored in the context of neurodegenerative disorders due to their ability to interact with multiple biological targets within the central nervous system. Despite these advances, a significant need for novel neuroprotective agents with improved structural diversity, stability, and biological activity remains. In this study, the rational design, synthesis, and characterization of novel fused and functionalized heterocyclic compounds based on pyrazole, imidazole, and triazole cores were undertaken with the aim of identifying potential neuroprotective candidates. Several synthetic strategies were developed to obtain substituted pyrazoles, imidazole derivatives, and hybrid heterocyclic systems. Key intermediates were synthesized and subsequently transformed into more complex structures incorporating benzimidazole and triazole motifs through multi-step synthetic pathways. The final compounds were purified using chromatographic techniques and were characterized by NMR spectroscopy and LC–MS to confirm their structures and purity. Five pure compounds were successfully isolated, and selected molecules were submitted for preliminary neuroprotection evaluation. During the first cycle of biological screening, promising neuroprotective activity was observed for several compounds, supporting the relevance of these scaffolds for further development. In future work, additional synthetic approaches will be explored, and more comprehensive biological evaluations will be conducted to further validate these findings.

Keywords: Aza-heterocycles; pyrazole derivatives; imidazole derivatives; triazole derivatives; heterocyclic synthesis; neuroprotection; medicinal chemistry.