Review of: "Synthesis of 1, 2-Disubstituted Benzimidazoles at Ambient Temperature Catalyzed by 1-Methylimidazolium Tetraflouroborate ([Hmim] BF_4) and Investigating Their Anti-ovarian Cancer Properties Through Molecular Docking Studies and Calculations"

Angelika Długosz-Pokorska[1]

1 Medical University of Lodz

Potential competing interests: No potential competing interests to declare.

The research presented provides a comprehensive investigation into the catalytic performance of 1-methylimidazolium tetrafluoroborate ([Hmim] BF4) in the synthesis of 1,2-disubstituted benzimidazoles through a condensation reaction. The study meticulously explores various reaction conditions and catalyst parameters to optimize the yield and efficiency of the reaction. Furthermore, it integrates computational chemistry and drug design methods to evaluate the potential anti-ovarian cancer properties of the synthesized compounds. Here's an analysis of the key findings and implications:

Catalytic Performance: The experimental results elucidate the influence of different reaction parameters such as solvent, temperature, and catalyst quantity on the yield and reaction time. Through systematic evaluation, it is demonstrated that the best conditions for the synthesis involve using 10 mol % of the catalyst in a 1:1 mixture of EtOH:H2O solvent at room temperature. This optimization is crucial for maximizing the reaction yield and minimizing reaction time, contributing to the efficiency and practicality of the process.

Drug Design and Computational Chemistry: The study extends beyond conventional catalytic research by incorporating computational chemistry techniques to assess the potential pharmacological properties of the synthesized compounds. By adhering to Lee Pinsky's rules, the molecular properties of the compounds are evaluated, ensuring compatibility with drug design principles. Additionally, molecular docking studies reveal the interaction of synthesized compounds with the CD-125 protein associated with ovarian cancer, suggesting their potential as anti-cancer agents. The identification of hydrogen bonding interactions between ligands and specific residues further underscores the molecular mechanisms underlying their therapeutic potential.

Comparative Analysis: The research includes a comparative analysis of the catalytic efficiency of [Hmim] BF4 with other reported catalysts, demonstrating superior performance in terms of reaction time and yield. This comparison highlights the competitive advantage of [Hmim] BF4 as a highly efficient catalyst for the synthesis of benzimidazoles, underscoring its significance in green chemistry applications.

Implications and Future Directions: Overall, the study offers valuable insights into the synthesis of benzimidazoles

using [Hmim] BF4 as a catalyst, with implications for the development of efficient and sustainable chemical processes. Moreover, the investigation into the anti-ovarian cancer properties of synthesized compounds opens avenues for further research in medicinal chemistry and drug development. Future studies could focus on in vivo experiments to validate the efficacy and safety of these compounds as potential anti-cancer drugs.

Conclusion: In conclusion, the research represents a significant contribution to both catalytic chemistry and drug design, showcasing the versatility of [Hmim] BF4 as a catalyst and the potential therapeutic utility of synthesized benzimidazole compounds. The integration of experimental and computational approaches provides a comprehensive understanding of the reaction mechanism and pharmacological properties, laying the groundwork for future advancements in both fields.