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"

Adel S. Girgis[1]

1 National Research Centre

Potential competing interests: No potential competing interests to declare.

The current study, titled “Synthesis of 1, 2-Disubstituted Benzimidazoles at Ambient Temperature Catalyzed by 1-Methylimidazolium Tetrafluoroborate ([Hmim] BF_4) and Investigating Their Anti-ovarian Cancer Properties Through Molecular Docking Studies and Calculations,” deals with the synthesis of the titled compounds. Most of the study is directed towards the synthesis of benzimidazolyl analogs (which were previously reported using other conventional techniques) utilizing a green technique. Little was mentioned about the experimentally supported bio-properties. Computational ADME was mentioned as the supporting profile of the targeted agents, with no experimentally evidenced results. Intensive/major revisions are needed considering the following items.

- The first paragraph of the introduction section should be intensively revised. It should emphasize the ration design of the adopted analogs with special interest in the expected bio-properties and mode of action relative to other analogs and compared to others previously reported in this subject. Enhancement of the bio-properties considered in the current study should be highlighted based on their expected biochemical behavior. Actually, no correlation was mentioned between the targeted agents and approved ovarian cancer therapeutics.

- Experimentally determined anti-proliferation properties against the targeted cancer cell line(s) are so needed for supporting the hypothesized phenomenon for this study.

- The mode of action of the promising agents mentioned should be experimentally evidenced.

- Docking observations should be compared to the co-crystallized ligand and/or drug.

- Better docking figures are needed. The interacted amino acid(s) should be identified with names/numbers. Maybe the black background should be altered to a white one that can enhance the appearance of these figures. A short table of docking results (including hydrogen bonding, pi-interaction, and docking scores) is highly needed.

The author can go to any of the following articles for conducting the antiproliferation properties and presenting the docking observations. https://doi.org/10.1016/j.ejmech.2023.115563

https://doi.org/10.1038/s41598-022-17883-9

https://doi.org/10.1016/j.bioorg.2021.105466