

Review of: "A Novel One-Pot Three-Component Approach to Orthoaminocarbonitrile Tetrahydronaphthalenes Using Triethylamine (Et₃N) as a Highly Efficient and Homogeneous Catalyst Under Mild Conditions and Investigating Its Anti-cancer Properties Through Molecular Docking Studies and Calculations"

Sajjad H. Sumrra¹

¹ University of Gujrat

Potential competing interests: No potential competing interests to declare.

[Review Report for Qeios]

The manuscript entitled "Novel One-Pot Three-Component Approach to Orthoaminocarbonitrile Tetrahydronaphthalenes Using Triethylamine (Et₃N) as a Highly Efficient and Homogeneous Catalyst Under Mild Conditions and Investigating Its Anti-cancer Properties Through Molecular Docking Studies and Calculations" brings interesting information on the title compounds, but extended studies and significant improvements are required to be published in the journal Qeios. This manuscript continues to be rather poor in scientific and English writing. I would encourage the authors to carry out a series of additional experimental work and submit it at a later, more advanced state. Some of my serious concerns are given below:

1. The introduction part of the manuscript is not appealing and must be revised. Cite the following papers for molecular docking simulation studies:

<https://doi.org/10.1016/j.molstruc.2022.134780>

<https://doi.org/10.1080/07391102.2023.2293260>

<https://doi.org/10.1007/s10534-022-00385-6>

2. In the introduction section, emphasize the importance of the medicinal chemistry of heterocyclic compounds. Authors can refer to the following studies for more information:

<https://doi.org/10.1016/j.molstruc.2022.133044>

<https://doi.org/10.3109/14756366.2011.582686>

<https://doi.org/10.1007/s00044-012-0388-0>

<https://doi.org/10.1007/s11696-022-02123-1>

3. Cite the method adopted for the synthesis of orthoaminocarbonitrile tetrahydronaphthalenes. What about their recrystallization? Have the authors tried to obtain crystals? Discuss the steps and solvents used for their recrystallization.
4. Recheck this sentence; "The precipitate was separated from the filtrate and washed with ethanol. Afterwards, the mixture was concentrated under reduced pressure....". How was the mixture concentrated after the filtration of precipitates?
5. Add melting points and details of elemental analysis in the representative spectral data. Mention IUPAC names of compounds instead of "Compound 4a, 4b...".
6. Instead of repeating the same unit "at four temperatures 50°C, 60°C, 70°C, and 80°C", just mention at the end.
7. What is the methodology used for selecting the protein in molecular docking studies?
8. Improve the resolution of docking figures (1-3). It's better to use a white background.
9. The data is not represented in a well-structured and presentable manner. The text of the manuscript must be properly aligned and formatted.
10. Use an equal number of significant digits in tables.
11. The conclusion section needs improvement. Rewrite it and make it meaningful.