

Summary of Peer Review for "Aliphatic Nucleophilic Substitution and Elimination Reactions: A Mechanistic and Computational Perspective"

14 December 2025

The manuscript under review provides a comprehensive and well-structured exploration of the fundamental principles governing aliphatic nucleophilic substitution and elimination reactions. The author skilfully navigates the complexities of the subject matter, elucidating the intricate details of reaction mechanisms, kinetics, and stereochemistry with exceptional clarity and depth.

The progressive structure of the article, commencing with the historical context and culminating in the cutting-edge computational approaches, is particularly effective in guiding the reader through the intricacies of the topic. The visual representations, including reaction schemes, energy profiles, and graphical analyses, are invaluable in illuminating key concepts, while the inclusion of Python code demonstrates a laudable commitment to reproducibility and transparency.

The nuanced discussion of the competition between reaction pathways highlights the delicate interplay of factors influencing reaction outcomes, providing a solid foundation for rational reaction design. The integration of modern computational methods and artificial intelligence, particularly the FlowER AI system, is a major strength of the work, offering a balanced perspective on the transformative potential and limitations of these approaches.

Minor refinements are suggested, including the addition of subheadings for enhanced readability, a more gradual introduction of the FlowER AI system, expansion of the conclusion to include broader applications, and rectification of minor typographical and formatting inconsistencies.

In summary, this exceptionally well-crafted manuscript makes a significant contribution to the field of organic chemistry, serving as an exemplar of interdisciplinary synthesis. Subject to the suggested minor revisions, this work is strongly recommended for publication and is expected to be of great interest to a wide readership, from students to seasoned researchers at the forefront of computational chemistry and artificial intelligence.

