Abstract

Precision Drug Discovery from Zingiber Officinalis: Unraveling Therapeutic Insights for Rheumatoid Arthritis through Innovative In Silico Approaches and Controlled Release Strategies †

Ujban Hussain 1,*, and Samiksha Sandeep Tammewar 2

1 Department of Pharmaceutical Sciences, The Rashtrasant Tukadoji Maharaj Nagpur University, Nagpur 440002, Maharashtra, India
2 Priyadarshini J. I College of Pharmacy, Nagpur 440002, Maharashtra, India; samutammewar@gmail.com
* Correspondence: ujbanhussain38441@gmail.com
† Presented at the 3rd International Electronic Conference on Biomolecules, 23–25 April 2024; Available online: https://sciforum.net/event/IECBM2024.

Keywords: controlled release strategies; precision drug delivery; in silico drug discovery; therapeutic insights; computational chemistry; novel drug development

1. Aim

• To pioneer an innovative in silico exploration of Zingiber officinalis for Rheumatoid Arthritis, employing virtual screening to discern the impact of its chemical constituents on the cyclo-oxygenase receptor.

2. Objectives

• To identify ligands from Zingiber officinalis that exhibit high binding affinity towards the Cyclooxygenase receptor, aiming to contribute valuable insights into potential therapeutic agents for Rheumatoid Arthritis.
• To investigate the structural and dynamic aspects of the ligand-receptor interactions, providing a comprehensive understanding of the molecular mechanisms underlying the potential therapeutic effects against Rheumatoid Arthritis.
• To explore and characterize novel chemical entities within Zingiber officinalis, uncovering previously unrecognized candidates with promising binding affinity and therapeutic potential for Rheumatoid Arthritis.

3. Material and Methodology

Ginger-derived ligands were prepared by retrieving smiles from Pubchem, sketching 2D structures on Chemsketch, and optimizing results with Avogadro.

COX1 and COX2 receptors, obtained from a protein data bank, were visualized in PyMol and prepared using Autodock Vina. Virtual screening in PyRx involved ligand and macromolecule conversion, grid selection, and Molinspiration for property calculation, including acute oral toxicity prediction with Protox II.

4. Result and Discussion

In silico studies revealed that all the synthesized molecules show good binding affinity toward the target protein ranging from −9.3 to −5.5.

5. Conclusions

The studies revealed that quercetin has higher binding as compared to the standard drug of rheumatoid arthritis i.e., ibuprofen. The ADME and toxicity studies also show...
positive results. Hence, this study has widened the scope of developing quercetin as a promising drug for rheumatoid arthritis.

Author Contributions: All the authors contributed equally. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Data available on request.

Conflicts of Interest: The authors declare no conflicts of interest.

Disclaimer/Publisher's Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.