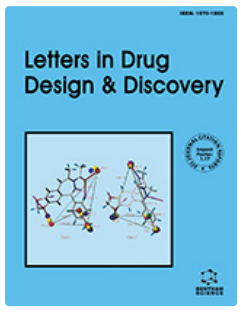

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Research Article

Assessment of Binding Site and Development of Small Molecule Inhibitors Targeting Epidermal Growth Factor Receptor Mutations in Non-Small Cell Lung Cancer (NSCLC)

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Abstract

Background: Mutations occurring in the epidermal growth factor receptor of the tyrosine kinase family concerned with non-small cell lung cancer have been specifically targeted.

Objectives: The library design and R-group enhancement technique have been carried out on the preexisting marketed drugs to increase the binding affinity of the designed novel compounds. The screening of compounds was done using a flexible docking protocol.

Methods: Molecular docking studies provided information about binding pockets and interactions of molecules with the mutant (PDB: 4I1Z) as well as wild-type (PDB: 4I23) EGFR enzymes. The flexible docking was well supported by ADMET and molecular dynamic simulation studies.

Results: On the basis of docking score and protein-ligand interactions, the highest-scoring molecule was selected for molecular dynamics simulation, providing a complete insight into the ligand interaction and saturation.

Conclusion: The screened molecules can act as potential EGFR inhibitors in the management of drug resistance.

Keywords: Non-small cell lung cancer, EGFR, library design, virtual screening, molecular docking, molecular dynamics simulations.

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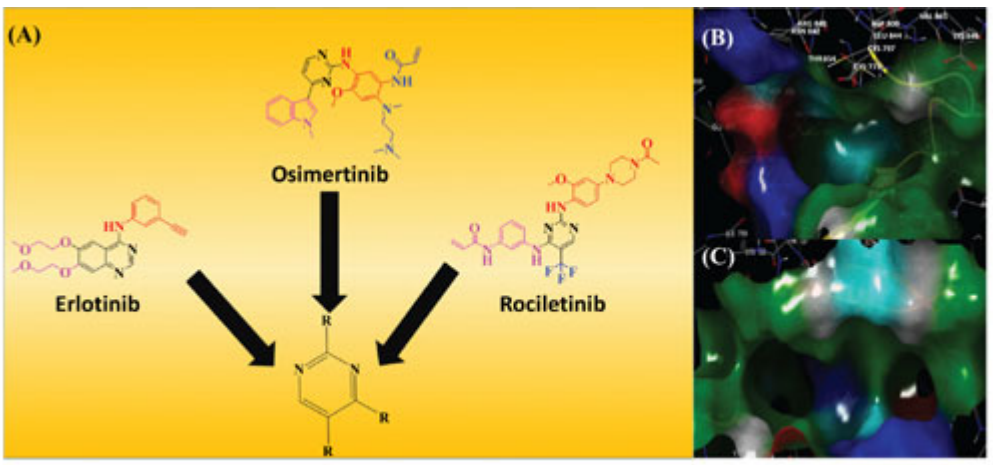
Graphical Abstract



Evaluation of the binding location and creation of small molecule inhibitors aimed at non-small lung cancer epidermal growth factor receptor mutations (NSCLC).

References

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