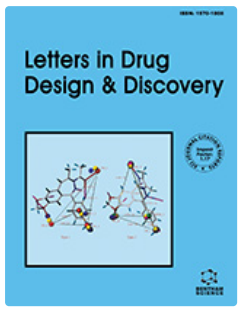

Letters in Drug Design & Discovery

Editor-in-Chief

ISSN (Print): 1570-1808
ISSN (Online): 1875-628X

Research Article

Discovery, Design, and Development of Effective and Stable Binding Compounds for Mutant EGFR Inhibition

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Volume 20, Issue 12, 2023

Published on: 03 September, 2022

Page: [1970 - 1981]

Pages: 12

DOI: 10.2174/1570180819666220613094708

Price: $65

Abstract

Background: The epidermal growth factor receptor of the tyrosine kinase family has been largely targeted in mutations associated with non-small cell lung cancer. EGFR inhibitors have been produced that bind allosterically to the C797S mutant EGFR enzyme.

Objective: Here, the Waterswap tool has been used for the interpretation and visualization of trajectories of mutant EGFR-ligand complexes. Virtual screening of the generated compounds has been carried out along with its molecular docking and ADMET analysis.

Methods: Out of the generated library of compounds, the top 15 have been selected. Waterswap calculated the binding free energies of the compounds and thermodynamic properties of the enumerated compounds were compared with that of standard EAI045.

Results: It was observed that compound KSK-1 stabilized better than EAI045.

Conclusion: Waterswap analysis offers a promising new path in the hunt for improved tools for analyzing and visualizing molecular driving forces in protein-ligand complex simulations.

Keywords: EGFR, Waterswap, virtual screening, molecular docking, ADMET, styrylquinoline.

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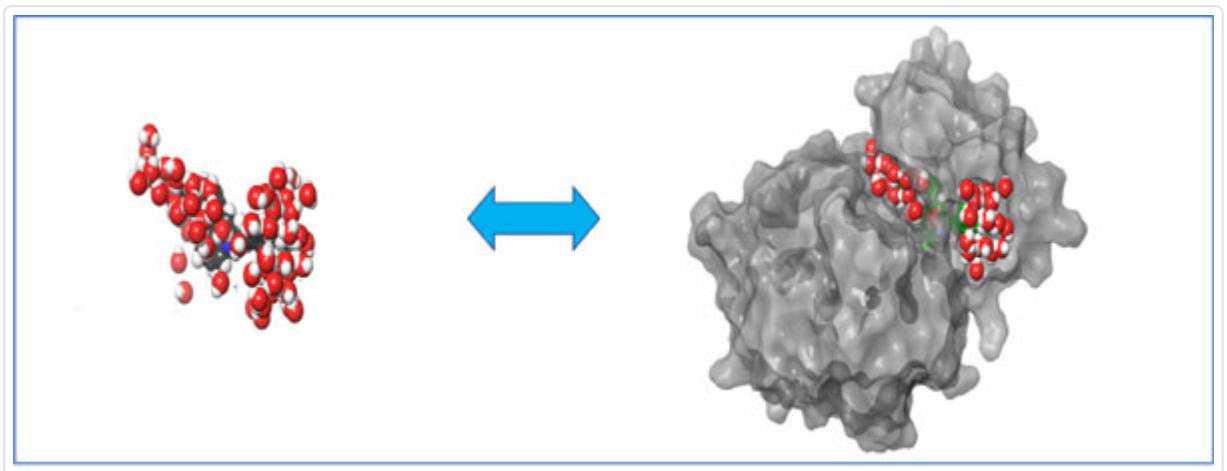
Graphical Abstract



Stable binding compounds for mutant EGFR inhibition.

References