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Molecular Modeling Study of ErbBs (Epidermal Growth Factor Family of Receptor Tyrosine Kinases) with Derivatives of Erlotinib

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Abstract—*ErbBs (epidermal growth factor family of receptor tyrosine kinases) is critical in regulating cell proliferation, survival, differentiation and migration. The ErbB receptors are responsible for both restricted and redundant functions in the maintenance of tissues in adult mammals. ErbB or HER receptors out of all receptor tyrosine kinases is most comprehensively studied because of its role in development, physiology, and human cancer. Erlotinibis a quinazoline derivative and antineoplastic agent that functions as a Protein Kinase Inhibitor for EGFR associated tyrosine kinase. It is used in the treatment of non-small cell lung cancer.*

Hence, we have attempted with the help of virtual screening and molecular docking approach using Lamarckian Genetic Algorithm to see the binding mode of different classes of Erlotinib, selected on the basis of structural similarity. The study involved virtual screening of nearly 3200 molecules. Molecular docking using Lamarckian Genetic Algorithm was carried out for these ligands and the result gave binding energies which were in the range of -12.15 kcal/motto -1.17 kcal/mol. The top 10 best docked protein were visualized using UCSF chimera which resulted in finding intricate atomic scale properties between ligand and active site of target protein. The top molecules then were run for in-silico ADMET and drug likeness properties and 4 molecules showed promising results for Bioavailabity and Toxicity.

Further in-vitro and in-vivo study is required on these molecules as the binding mode provided hints for the future design of new inhibitors for EGFR tyrosine kinase with higher potency and specificity.