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Molecular docking studies of 4-anilino quinazolines as inhibitors of epidermal growth factor receptor tyrosine kinase

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Original Article

Molecular Docking studies of 4-anilino quinazolines as inhibitors of Epidermal Growth Factor Receptor Tyrosine Kinase

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Abstract

A series of novel 4-anilino quinazoline derivatives were designed and optimized with AutoDock 4.2 to investigate the interaction between the target compounds and the amino acid residues of target protein Epidermal Growth Factor Receptor-Tyrosine Kinase. The free energies of binding and inhibition constants (Ki) of the docked ligands were calculated by the Lamarckian Genetic Algorithm (LGA). The docking results showed that the compounds SGQ4, DMUQ5, 6AUQ6 and PTQ8 produced significant docking affinity for the protein Tyrosine Kinase with the binding energy of -7.46, -7.31, -6.85 and -6.74 Kcal/mol, respectively compared to the standard Erlotinib (Binding energy: -3.84 Kcal/mol). The molecular descriptor properties and toxicity profile were predicted by the software. All the designed molecules passed the Lipinski rule of five successfully and they were found to be safe. The studied compounds are a promising class of compounds with potential anti-cancer activity against breast cancer cells and they can be recommended for further research to treat the disease. The prediction of acute toxicity in rats has been carried out in oral and intravenous routes of administration using the GUSAR program.

Key words: AnilinoQuinazoline, Erlotinib, GUSAR Molecular Docking, Tyrosine Kinase

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