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Molecular Docking Study of Quinazoline and Quinoline Derivatives against EGFR

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Abstract : With the development of computer tools over the past 20 years. Molecular modeling and, more precisely, molecular docking has very quickly entered field of pharmaceutical research. EGFR enzyme involved in cancer disease.Our work consists of studying the inhibition of EGFR (1M17) with deferent inhibitors derived from quinazoline and quinoline by molecular docking. The values of ligands L148 and L177 are the best ligands for inhibit the activity of 1M17 since it forms a stable complex with this enzyme by better binding to the active site. The results obtained show that the ligands L148 and L177 give weak interactions with the active site residues EGFR (1M17), which stabilize the complexes formed of this ligands, which gives a better binding at the level of the active site, and an RMSD of L148 [1,9563 Å] and of L177 [1,2483 Å]. [1, 9563, 1.2483] Å

Keywords : docking, EGFR, quinazoline, quinoliène, MOE
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