ORIGINAL RESEARCH ARTICLES

TARGETED SEARCH FOR INHIBITORS OF THE EPIDERMAL GROWTH FACTOR RECEPTOR BY MOLECULAR DOCKING AND MOLECULAR DYNAMICS METHODS IN A SERIES OF HYDROXYPHENYL DERIVATIVES OF 4-OXOPYRIMIDINEBENZSULFONAMIDE

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ABSTRACT

Based on the results of molecular docking, it can be concluded that it is possible to study the binding of inhibitors to the active site of EGFR by this method, but docking does not accurately reproduce the binding of ligands to the active site, which is presumably due to limitations in the conformational mobility of molecules in this method. The molecular dynamics method can be used to search for chemical structures of epidermal growth factor receptor inhibitors. The reliability of predicting the biological activity of EGFR inhibitors is higher when using molecular dynamics in comparison with molecular docking. Cytostatic activity was investigated and a lead compound was found for new sodium salts of pyrimidinones.