

Synthesis and Molecular Docking Studies of Hydrazone Derivatives Potent Inhibitors as a Human Carbonic Anhydrase IX

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Abstract : Hydrazone scaffold is important to design new drug groups and is found to possess numerous uses in pharmaceutical chemistry. Besides, hydrazone derivatives are also known for biological activities such as anticancer, antimicrobial, antiviral, and antifungal. Hydrazone derivatives are promising anticancer agents because they inhibit cancer proliferation and induce apoptosis. Human carbonic anhydrase IX has a high potential to be an antiproliferative drug target, and targeting this protein is also important for obtaining potential anticancer inhibitors. The protein construct was retrieved as a PDB file from the RCSB protein database. This binding interaction of proteins and ligands was performed using Discovery Studio Visualizer. In vitro inhibitory activity of hydrazone derivatives was tested against enzyme carbonic anhydrase IX on the PyRx programme. Most of these molecules showed remarkable human carbonic anhydrase IX inhibitory activity compared to the acetazolamide. As a result, these compounds appear to be a potential target in drug design against human carbonic anhydrase IX.

Keywords : cancer, carbonic anhydrase IX enzyme, docking, hydrazone

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