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Understanding the binding affinites of the sulfonanilide derivaties on aromatase

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Breast cancer is one of the main causes of deaths in women and is the second largest cancer deaths in US. In the development of the breast cancer, the estrogen plays a key role. The enzyme Aromatase belongs to the Cytochrome P450 super family and is involved in the conversion of androgens to estrogens. The enzyme is however found to be in increasing levels in humans during the breast cancer conditions in contrast to the normal conditions. Aromatase Inhibitors are known to have a role in breast cancer and are hence considered as the drug molecules. They act by either inhibiting the production of estrogen or the action of estrogen on receptors. One such known inhibitor is the Sulfonanilide derivatives. The present paper deals with the assessment and understanding of the binding affinities of these derivatives on Aromatase. The investigation proceeds in silico. The target enzyme, Aromatase was selected from the Protein Data Bank (PDB) Id: 3EQM. The potential 81 Sulfonanilide derivatives were drawn in the Marvin Sketch tool. The molecular docking was performed with the Aromatase and the ligands in the Molegro Virtual Docker (MVD) and the binding affinities were analysed. It was observed that the highest binding affinity was shown by the 78th molecule with the Moldock score grid -181.665, and the lowest was reported by the 4th molecule, Moledock score grid, -112.211.

Biography

Shailima RD Vardhini is currently working as the Head, Department of Biochemistry, St. Mary's College, Yousufguda, Hyderabad, AP, India. She has published research articles in various reputed international journals and is also on the Reviewer and Editorial Board of reputed Journals. Her research interests include Cancer Biology, Nanotechnology and Bioinformatics.

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