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4th Annual Congress on

Drug Discovery & Designing

July 03-04, 2017   Bangkok, Thailand

An *in-silico* approach to study the binding interaction of coumarin derivatives to aromatase

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Human cytochrome P450 aromatase, which is an enzyme located in the endoplasmic reticulum of estrogen producing cells, plays a significant role of development of estrogen receptor positive breast cancer. The aromatase catalyzes the conversion of androgens (Androstenedione and Testosterone) to estrogens (Estrone and Estradiol). The third generation of aromatase inhibitors is found to be the most potent drugs for the leading breast cancer treatments and are in clinical use. Exemestane (EXM), Letrozole (LTZ), and Anastrozole (ANZ) have higher selectivity, less toxicity and improving potency over other drugs. The coumarins present in natural products shows high pharmacological activities for cancers such as anti-inflammatory, anti-tumor, anti- cancer, anti- viral, anti- depressant etc. Aromatase with PDB id: 3S79 was selected from the protein structure database for this study and visualized with Chimera 1.9 and VMD. Active site residues were identified as Arg 115, Ile 133, Phe 134, Phe 221, Trp 224, Ile 305, Ala 306, Asp 309, Thr 310, Val 313, Val 370, Leu 372, Val 373, Met 374, Ser 478, His 480, Glu 483 and Hem 600. Therefore, thirty different coumarin derivatives together with two different drug derivatives were designed and studied using Molecular Docking Simulations where as Exemestane and Androstenedione were used as References to observe the capability of the binding of coumarins to the aromatases. AutoDock Vina and AutoDock 4 were used to narrow down the ligands furthermore GEMEDOCK and DOCK6.7 were used to validate the results. The insight gained from the study herein have a compatible potential for the design of novel derivatives of coumarins for inhibition of aromatase.

Biography

Fourth year Undergraduate at the College of Chemical Sciences, Institute of Chemistry Ceylon. Involve with the computational aided research work and has an interest in the molecular biology, biochemistry, organic synthesis and nanotechnology. Tharushi has already presented in two occasions titled " International Conference on Computational Modeling and Simulation 2017" held in Colombo University and at 46th Annual Session of Institute of Chemistry Ceylon.

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Drug Des
ISSN: 2169-0138 DDO, an open access journal

Drug Discovery Congress
July 03-04, 2017

Volume 6, Issue 3 (Suppl)

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