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MOLECULAR DOCKING STUDY AND ADME/T PREDICTIONS OF 2 PHENYLAMINOIMIDAZO[4,5-H]ISOQUINOLIN-9-ONES WITH POTENT ANTI-AROMATASE CYTOCHROME P450 ACTIVITY IN BREAST CANCER THERAPY

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Post-menopausal women with hormone dependent breast cancer in the past were treated with tamoxifen, which mediates its action by blocking estrogen binding to the estrogen receptor thereby preventing estrogen induced proliferation. Unfortunately, tamoxifen is a partial agonist in many tissue types. Alternatively, aromatase inhibitors represent the first successful class of cancer therapeutics by inhibiting estrogen synthesis. However, recent studies have shown that the first, second and third generation of aromatse inhibitors although potent yet present with adverse reactions such as nausea, abdominal pain, baldness, joint pain, diarrhea, vaginal dryness etc. This study explored 2 phenylaminoimidazo[4,5-h]isoquinolin-9-ones for their inhibitory activities against aromatase cytochrome p450 in breast cancer therapy via molecular docking approach and evaluated their drug-likeness properties and ADME/T predictions. Docking study by PyRx tools reveals that 17 out of 30 of the 2 phenylaminoimidazo[4,5-h] isoquinolin-9-ones compounds showed stable binding complex with higher binding affinity values when compared with the co-crystallized ligand (reference compound). However, only 5 of these compounds (CHEMBL26409, CHEMBL26864, CHEMBL2799, CHEMBL27302 and CHEMBL27485) satisfy the ADME/T predictions and the drug-likeness according to the lipinsky rule.

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