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Study of the physicochemical properties of potential and clinically approved popular selective estrogen receptor modulators with aromatase

Breast cancer is a disease caused by the disordered multiplication of breast cells, statistical data show that in 2018 about 2.1 million new cases were registered, which corresponds to 11.6% of all registered cancer cases worldwide, being more incident in women. Researches for the development of new drugs that prevent the aromataze protein responsible for hormonal imbalance, which consequently generates this uncontrolled multiplication, have been developed. Some drugs already on the market, classified as selective estrogen receptor modulators, are used to control the development of cancer or for prevention in menopausal women. In the present work we use the molecular docking tool, Auto Dock Vina. With this, the binding energies, expressed in kilo calories per mol, were compared to the original ligand present in the target protein, using it as a parameter to determine the potential of interaction between the drug and the protein. The energy present in the original ligand (4-hydroxytamoxiphene) was (-9.6), if compared to those of the ligands, Anastrozole (-7.1), Exemestane (-8.6), Lestrozole (-8.2) and Tamoxifen (-9.4). It is concluded that they have a weaker intermolecule interaction than the original ligand, making it necessary to study other similar compounds for the analysis of interactions with the target protein.

Keywords: SERMs; hormonal inbalançe; physicochemical properties; breats cancer.