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Synthesis And Molecular Docking Of Some Amic Acid Targeting Breast Cancer

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Abstract:

In this study, we synthesized and investigated interactions between three amic acid analogs and HER2(3PP0) by using virtual screening based on molecular docking to find potential compounds against HER2. The structures of the synthesized compounds were characterized based on a ^{1}HNMR, ^{13}CNMR, FT-IR and mass spectroscopy. The density function theory (DFT) calculation at the B3LYP method with 6-311++G(d,p) basis set are used to investigate the electronic structure and optimized geometrical structure of the mentioned compounds. Molecular docking against human epidermal growth factor receptor 2 (HER2) (PDB:3PP0) showed that compounds bind to the HER2. Binding involves hydrogen bonding for each compounds. The results revealed that the newly designed amic acid derivatives exhibited significant inhibition with HER2 exhibit anti breast cancer activity.

Keywords: Molecular docking; human epidermal growth factor receptor 2 (HER2); amic acid; Breast cancer

1- Introduction

Cancer is one of the serious threats to humans, causing deaths worldwide despite substantial advances in research for its diagnosis and treatment. Almost 20 million new cases are predicted by the year 2020 [1]. Breast cancer ranks as the second most common cancer for women and the most common cause of cancer deaths for women between ages 45–55 years old [2].