World Academy of Science, Engineering and Technology
International Journal of Chemical and Materials Engineering
Vol:11, No:03, 2017

Microbiological Activity and Molecular Docking Study of Selected Steroid Derivatives of Biomedical Importance

Authors : Milica Karadzic, Lidija Jevric, Sanja Podunavac-Kuzmanovic, Strahinja Kovacevic, Sinisa Markov, Aleksandar Okljesa, Andrea Nikolic, Marija Sakac, Katarina Penov Gasi

Abstract : This study considered the microbiological activity determination and molecular docking study for selected steroid derivatives of biomedical importance. Minimal inhibitory concentration (MIC) was determined for steroid derivatives against Staphylococcus aureus using macrodilution method. Some of the investigated steroid derivatives express bacteriostatic effect against Staphylococcus aureus. Molecular docking approaches are the most widely used techniques for predicting the binding mode of a ligand. Molecular docking study was done for steroid derivatives for androgen receptor negative prostate cancer cell line (PC-3) toward Human Cytochrome P450 CYP17A1. The molecules that had the smallest experimental IC50 values confirmed their ability to dock into active place using suitable molecular docking procedure. The binding disposition of those molecules was thoroughly investigated. Microbiological analysis and molecular docking study were conducted with aim to additionally characterize selected steroid derivatives for future investigation regarding their biological activity and to estimate the binding-affinities of investigated derivatives. This article is based upon work from COST Action (TD1305), supported by COST (European Cooperation and Science and Technology).

Keywords : binding affinity, minimal inhibitory concentration, molecular docking, pc-3 cell line, staphylococcus aureus, steroids
Conference Title : ICCEA 2017 : International Conference on Chemical Engineering and Applications
Conference Location : Miami, United States
Conference Dates : March 09-10, 2017