

ABSTRACT

SANIA NUR FADZILLAH, 2023. *Analysis In Silico : Anti-Inflammatory Activities And Predictions Of Toxicity Of The Secondary Metabolite Compound Physalis peruviana L. As Biology Learning Resource.* Biologi of Education, Faculty of Teacher Training and Education, Siliwangi University, Tasikmalaya

The way of life back to nature, including in the field of health, forms the habit of using plants as traditional medicine. Traditional medicine is indicated to be able to cure a variety of diseases. As with the leaves of Ciplukan (Physalis peruviana L.) by the people of Desa Wanasuka Kecamatan Pangalengan Kabupaten Bandung is considered to be used as a traditional medicine for inflammatory diseases such as rheumatism, asthma, and gastritis (maag) due to side effects and toxicity produced relatively small when compared with modern medicine. The aim of this study is to identify the potential of the secondary metabolite compound found in the leaves of the Ciplukan (Physalis peruviana L.) as a candidate for anti-inflammatory drugs. These research methods are molecular methods of docking through physical chemical properties testing, pharmacokinetic profiles of test compounds through site Pre-ADMET (Absorption, distribution, metabolism, excretion, and toxicity) and Lipinski Rule of Five. The results of this study showed that the binding affinity of caffeic acid compounds with PTGS2 receptors (PDB ID: 5F19) showed a more negative result compared to the comparative drugs Aspirin and Ibuprofen -7.4. There was a molecular interaction similar to Aspirin, in which the addition of amino acid residues from ASN 382 and TYR 385 produces a strong irreversible inhibition of PTGS2 (PDB ID: 5F19) and is predicted to inhibit prostaglandin H synthase and indicate that caffeic acid is capable of producing irreversible inactivation of PTG2 (PDB ID:5F19). So potentially a candidate for a safer anti-inflammatory drug for the body. Because it has almost the same or close potential as Aspirin against inflammatory diseases.

Keywords: *Anti-inflammatory, In Silico, Physalis peruviana L., Predictions of drug candidates*