New Anti-Inflammatory Agent from Genus artocarpus: A Prediction by Molecular Docking

Marvel Reuben Suwitono
Universitas Advent Indonesia

Abstract

Inflammation is a normal homeostatic mechanism of body for self-repair from cell damage. However, inflammation effect would give uncomfortable condition, thus drugs such as nonsteroidal anti-inflammatory drugs (NSAIDs), is needed to relieve it. Traditionally, Artocarpus spp., in which number of active compounds has been isolated, is believed to have anti-inflammatory activity. This study aims to identify the anti-inflammatory property of Artocarpus spp. Utilizing the computational method such as PyRx and AutoDock Vina. A total of 53 active structures (isolates) of genus Artocarpus were obtained from literature (as ligand). They were then studied by molecular docking with three enzymes, which is believed to be responsible for inflammation, such as cyclooxygenase-1 (COX-11), cyclooxygenase-2 (COX-12), and nuclear factor kappa beta (NF-κB) (as receptor). It was then compared to a common drug structures such as the nine NSAIDs classification and one public-pulled due to its increasing side effect. Data analysis utilizing the Analysis of Variance (ANOVA) revealed that each 63 ligand (53 Artocarpus isolates structure and 10 drugs) significantly differed each other according to its binding affinity (p = 0.000). A significant difference for macromolecules (receptor) (p=0.000) were also found out in this study. Duncan's multiple range test also showed that the highest rank were engelitin (a) (= -9.137 kcal/mol) and artonolD (b) (= -8.692 kcal/mol). Other isolates including common commercial drug were ranked lower. The findings of this study suggest studying these two substances further for their anti-inflammatory property.

Keywords: *Artocarpus, COX-1, COX-2, NF-kβ, PyRx, AutoDock Vina*