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MOLECULAR DOCKING ELLAGIC ACID AND CALCIUM PHOSPHATE AGAINST INFLAMMATORY PROTEIN TLR2 AND TLR4 *IN SILICO*

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ABSTRACT : Inflammation is an innate immune system response to various injury stimuli, such as pathogens, injury, or metabolic stress. Inflammatory proteins that play a role in inflammatory sterile conditions (trauma) or bacterial-induced circumstances, played by TLR2 and TLR4. Ellagic acid (EA) is one of the biological molecules found in pomegranate and it has the potential anti-inflammatory. Calcium phosphate is included as the main ingredient in osteogenesis bone graft. The activity test is done to determine the potential of ellagic acid and calcium phosphate as an anti-inflammatory agent. To test the potential of ellagic acid and calcium phosphate as an anti-inflammatory agent, the biological activity was tested using the PASS Server. To understand the interaction between ellagic acid and calcium phosphate with TLR2 and TLR4, molecular docking analysis specifically used PyRx software v.0.9.5. The results of the exploration of the PubChem database of 3D structures and data SMILE shows that ellagic acid has a Pa (probability of activity) as an anti-inflammatory by 0.749. Ellagic acid and calcium phosphate tend to bind strongly to TLR2 compared to TLR4, as indicated by the results of a stronger binding affinity. Ellagic acid and calcium phosphate will remain attached to TLR but do not have a strong potential for induction of inflammation.

Key words : Calcium phosphates, ellagic acid, medicine, socket preservation, *in silico*.

INTRODUCTION

Prevention of bone resorption after tooth extraction becomes very necessary to be discussed and strongly related to the dimensions of the alveolar bone (Assistant, 2012). Residual Ridge resorption is started immediately after extraction and can result in resorption of up to 50% even in 3 months resorption will continue. After tooth extraction, alveolar ridge resorption impact on the installation of dental implants for vertical and horizontal alveolar volume should be ideally suited to the site of insertion (Horváth *et al*, 2013). Alveolar Ridge Preservation indicated to minimize the loss of ridge volume that occurs after the tooth extraction (Avila-Ortiz *et al*, 2014; Prahasanti *et al*, 2020).

The ideal bone graft materials must be biocompatible, allowing the formation of new bone or bone replacement through the osteoconductive process (Nugraha *et al*, 2019; Sari *et al*, 2020). Bovine bone xenograft (BBX) has a chemical composition and geometry of the architecture is similar to human bone and can support new bone formation, regarded as material and as a bone graft biocompatible formation (Uzbek *et al*, 2014). Bovine bone xenograft basic materials are calcium phosphate, calcium phosphate general nature directed to the field of application Bioceramics (Canillas *et al*, 2017).

Use of BBX widely applied in alveolar bone destruction, but of several studies showed the use of alveolar bone xenograft on the vertical has very brittle nature and are not strong enough (Sheikh *et al*, 2015). Therefore, we need an innovation that is a stimulant osteoblastogenesis substance that stimulates the activity of bone graft to accelerate growth and as an anti-inflammatory that can inhibit bone resorption (Torre, 2017). Ellagic acid (EA) is one of the biological molecules found in pomegranate and have anti-inflammatory potential. Ellagic Acid detected not only in pomegranates but also in a wide variety of fruits and nuts (Usta *et al*, 2013). Ellagic acid is considered to have osteoblastogenesis stimulant is osteoinduction and has anti-inflammatory (Usta *et al*, 2013).