UNIVERSITI TEKNOLOGI MARA

MOLECULAR DOCKING OF BETA-SITOSTEROL WITH COX-1 AND COX-2

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ABSTRACT

Cyclooxygenase (COX) is known as prostaglandin endoperoxide synthase, which responsible in converting arachidonic acid to prostaglandins. COX-1 protects stomach from acid and digestive chemicals while COX-2 plays major role in inflammation via binding to arachidonic acid. Inhibition of COX-1 reduces the inflammation, but causes the loss of protection in stomach lining. Whereas there is much less gastric irritation associated with COX-2 inhibition. Inhibition of COX-1 causes undesirable side effects rather than COX-2. This experiment is conducted to identify the potential of beta-sitosterol in reducing inflammation by inhibiting cyclooxygenase enzymes via molecular docking using Autodock Vina. The purpose of this study to identify the potential of beta-sitosterol to bind to COX-2 more than COX-1. Molecular docking studies revealed that beta-sitosterol has lower binding affinity with COX-2 compared with COX-1 which are -10.1 and -9.1 respectively. The best dock score refers to lowest binding affinity obtained. Molecular docking studies reported that beta-sitosterol was found to treat the inflammation that caused by COX-2 without any undesirable effects within the body.

CHAPTER ONE:

INTRODUCTION

1.1 BACKGROUND

Beta-sitosterol is very useful in medicine production as its uses can be explored and gives many benefits. Beta-sitosterol basically is a compound that contained in plants. It is also known as "plant sterol ester" by chemists. It is highly rich in vegetables, fruits, nuts and seeds. It is very useful in medicine production. Beta-sitosterol can be used to treat heart disease and overcome the high cholesterol-related disease. Beta-sitosterol also known as good chemopreventive in treating carcinogenesis of colon as it can be used as anti-oxidant in biological activity carcinogenesis. Beta-sitosterol gives important effect in neurodegenerative disorder, especially Alzheimer disease. Other than that, beta-sitosterol is found to be used in treating the diabetic disease.

Stigmasterol has its role on the production of hormone such as androgens, estrogens, progesterone and corticoids. With its function, stigmasterol is being used to become part of medication purpose. Stigmasterol is found to be important compound in treating the cancer. Besides, the combination of stigmasterol and beta-sitosterol itself exhibit synergistic effect in hypoglycaemic activity. Similar to beta-sitosterol, stigmasterol are used as antioxidant. One of stigmasterol's activities is inhibit the inflammatory action thus made it as anti-inflammatory agent.