Jurnal Farmasi Galenika (*Galenika Journal of Pharmacy*) (e-Journal) 2020; 6 (2): 347 – 355
ISSN: 2442-8744 (electronic); 2442-7284 (printed)
Journal Homepage: https://bestjournal.untad.ac.id/index.php/Galenika
DOI: 10.22487/j24428744.2020.v6.i2.15041

Pemodelan Molekuler Peptida Bioaktif Laut sebagai Antikoagulan Alami terhadap Enzim Sitokrom P450 (CYP) 2C9

(*Molecular Modelling of Marine Bioactive Peptides as Natural Anticoagulants against Cytochrome P450 (CYP) 2C9 Enzymes*)

Taufik Muhammad Fakih*, Mentari Luthfika Dewi

Program Studi Farmasi, Fakultas Matematika dan Ilmu Pengetahuan Alam, Universitas Islam Bandung, Bandung, Indonesia.
**E-mail: taufikmuhammadf@gmail.com*

Article Info:
Received: 18 Maret 2020
in revised form: 10 Mei 2020
Accepted: 04 Oktober 2020
Available Online: 04 Oktober 2020

Keywords:
Anticoagulant
Cytochrome P450 (CYP) 2C9
Marine Bioactive Peptides
Protein-Peptide Docking
In silico Study

Corresponding Author:
Taufik Muhammad Fakih
Program Studi Farmasi
Fakultas MIPA
Universitas Islam Bandung
Bandung
40116
Indonesia
email:
taufikmuhammadf@gmail.com

ABSTRACT

Anticoagulants are very important for the treatment and prevention of thrombotic disorders. The use of conventional anticoagulants like heparin and warfarin can cause bleeding complications. To find safer anticoagulant therapy agents, the development of isolation of new anticoagulant compounds has shifted towards natural sources. Bioactive peptides can be considered a better alternative because of their therapeutic potential in the treatment of various diseases. Several peptide molecules have been shown to inhibit the cytochrome P450 (CYP) 2C9 enzyme as a natural anticoagulant, such as bioactive peptides produced by yellowfin sole (*Limanda aspera*) and bioactive peptides in blue mussel (*Mytilus edulis*). This study aims to identify and evaluate the interactions that occur between peptide molecules with the cytochrome P450 (CYP) 2C9 enzyme using protein-peptide docking methods. Bioactive peptide sequencing was modeled using the PEP-FOLD software. The best conformation was chosen for an interaction study against the macromolecule of cytochrome P450 (CYP) 2C9 enzyme using PatchDock software. Further observations were made for the interactions by using BIOVIA Discovery Studio 2020 software. Based on the results of protein-peptide docking, the yellowfin sole peptide molecule has a good affinity against the macromolecule of cytochrome P450 (CYP) 2C9 enzyme, with an ACE score of −2527.01 kJ / mol. Therefore, the bioactive peptide is predicted to be used as a candidate for the cytochrome P450 (CYP) 2C9 enzyme inhibitor.

How to cite:
Fakih, T. M., & Dewi, M. L. (2020). Pemodelan Molekuler Peptida Bioaktif Laut sebagai Antikoagulan Alami terhadap Enzim Sitokrom P450 (CYP) 2C9. *Jurnal Farmasi Galenika :Galenika Journal of Pharmacy (e-Journal)*, *6*(2), 347-355. doi:10.22487/j24428744.2020.v6.i2.15041