INTISARI

FADILLA, R., 2016, ANALISIS *DOCKING* MOLEKULER SENYAWA QUERSETIN, GUAIJAVARIN DAN MORIN-3-*O*-α-L-ARABOPIRANOSIDA SEBAGAI ANTIBAKTERI, TESIS, FAKULTAS FARMASI, UNIVERSITAS SETIA BUDI, SURAKARTA.

Daun jambu biji telah terbukti memiliki aktivitas antibakteri dan telah banyak digunakan untuk pencegahan dan terapi penanganan diare. Daun jambu biji banyak mengandung senyawa yang memiliki aktivitas antibakteri. Beberapa senyawa tersebut antara lain quersetin, guaijavarin dan morin-3-*O*-α-L-lyxopyranoside. Penelitian ini bertujuan untuk mengetahui interaksi dan pola interaksi senyawa quersetin, guaijavarin dan morin-3-O-α-L-arabopiranosida dari daun jambu biji (*P. guajava* L.) terhadap 9 molekul biologi target kerja antibakteri melalui *docking* molekuler. Molekul biologi target kerja antibakteri yang digunakan, antara lain protein SleB, protein SleL, maltoporin, AggA (*Aggregative Adherence Fimbriae*/1), Bc1960 peptidoglycan N-acetylglucosamine deacetylase, phosphatidylcholine-phospholipase C Bc, phospholipase C regulator + PapR, *penicillin binding protein 3 E.coli* (transferase) dan (gyrase + 4,5-dibromopyrolamide-based inhibitor (isomerase).

Pada penelitian ini, *docking* molekuler dilakukan pada senyawa quersetin, guaijavarin dan morin-3-*O*-α-L-lyxopyranoside dari daun jambu biji (*P. guajava* L.) sebagai ligan terhadap protein SleB (4F55), protein SleL (4S3J), maltoporin (1MPR), AggA (*Aggregative Adherence Fimbriae*/1) (4PH8), Bc1960 peptidoglycan N-acetylglucosamine deacetylase (4L1G), phosphatidylcholine-phospholipase C Bc (2HUC), phospholipase C regulator + PapR (2QFC), *penicillin binding protein 3 E.coli* (transferase) (4BJP) dan gyrase + 4,5-dibromopyrolamide-based inhibitor (isomerase) (4ZVI) sebagai target menggunakan perangkat lunak Autodock Vina serta PyMOL sebagai perangkat visualisasi.

Senyawa guaijavarin, morin-3-O-α-L-arabopiranosida dan quersetin dari daun jambu biji (*P. guajava* L.) memiliki interaksi yang baik terhadap 7 molekul biologi target kerja antibakteri karena mampu berikatan dengan sisi aktif dan residu protein dari makromolekul protein 4F55, 1MPR, 4L1G, 2HUC, 2QFC, 4ZVI dan 4BJP dengan rentang ΔG_{bind} -6,5-9,6 kkal/mol dan menunjukkan pola interaksi yang menyerupai ligan asli terhadap makromolekul protein 2QFC dan 4ZVI dilihat dari pengamatan visual.

Kata kunci: Diare, *docking* molekuler, AutoDock Vina, PyMOL, quersetin, guaijavarin, morin-3-*O*-α-L-lyxopyranoside

ABSTRACT

FADILLA, R., 2016, ANALYSIS OF MOLECULAR DOCKING QUERSETIN, GUAIJAVARIN AND MORIN-3-O-α-L-ARABOPYRANOSIDE AS ANTIBACTERIAL, THESIS, FACULTY OF PHARMACY, SETIA BUDI UNIVERSITY, SURAKARTA.

Guava leaves have been shown to have antibacterial activity and have been widely used for the prevention and therapeutic treatment of diarrhea. Guava leaves contain many compounds which possess antibacterial activity. Some of these compounds include quersetin, guaijavarin and morin-3-O-α-L-lyxopyranoside. This study aims to understand the interaction and interaction patterns quersetin, guaijavarin and morin-3-O-α-L-arabopiranosida of guava leaves (*P. guajava* L.) on 9 molecule biology antibacterial targets through molecular docking. Molecule biology antibacterial targets used, among other proteins SleB, protein SleL, maltoporin, Agga (aggregative adherence fimbriae/1), Bc1960 peptidoglycan N-acetylglucosamine deacetylase, phosphatidylcholine-phospholipase C Bc, phospholipase C regulator + PapR, penicillin binding protein 3 *E.coli* (transferase) and (gyrase + 4.5-dibromopyrolamide-based inhibitor (isomerase).

In this study, molecular docking performed on quersetin, guaijavarin and morin-3-O-α-L-lyxopyranoside of guava leaves (*P. guajava* L.) as ligands to the proteins SleB (4F55), protein SleL (4S3J), maltoporin (1MPR), Agga (aggregative adherence fimbriae/1) (4PH8), Bc1960 peptidoglycan N-acetylglucosamine deacetylase (4L1G), phosphatidylcholine-phospholipase C Bc (2HUC), phospholipase C regulator + PapR (2QFC), penicillin binding protein 3 *E. coli* (transferase) (4BJP) and gyrase + 4.5-dibromopyrolamide-based inhibitor (isomerase) (4ZVI) as a target using the software Autodock Vina and PyMOL as visualization tools.

Compounds guaijavarin, morin-3-O-α-L-arabopiranosida and quersetin of guava leaves (*P. guajava* L.) have a good interaction of 7 molecule biology antibacterial targets because it can bind to the active site and protein residues of protein macromolecules 4F55, 1MPR, 4L1G, 2HUC, 2QFC, 4ZVI and 4BJP with ΔG_{bind} range -6,5-9,6 kcal/mol and shows the interaction patterns that resemble the native ligand to the protein macromolecules 2QFC and 4ZVI seen from visual observation.

Keywords: Diarrhea, molecular docking, Autodock Vina, PyMOL, quersetin, guaijavarin, morin-3-O-α-L-lyxopyranoside