PENAMBATAN MOLEKULER DERIVAT KUERSETIN SEBAGAI SENYAWA ANTIKANKER PAYUDARA SECARA *IN SILICO*

SKRIPSI

FAUZIA NURUL IZZAH
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SEKOLAH TINGGI FARMASI INDONESIA
YAYASAN HAZANAH
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Sebagai salah satu syarat untuk memperoleh gelar Sarjana Farmasi

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ABSTRAK

Kuersetin adalah flavonoid alami yang telah terbukti memiliki aktivitas biologis, salah satunya adalah sebagai agen antikanker. Derivat yang digunakan pada penelitian ini diantaranya pentametil kuersetin, pentaasetat kuersetin, dan pentabenzil kuersetin. Penelitian ini bertujuan untuk mengevaluasi aktivitas antikanker payudara dari derivat kuersetin melalui metode penambatan molekuler terhadap tujuh reseptor kanker payudara, yaitu ERα, PR, HER2, HAC, PD-L1, FGFR, dan IGFR. Proses penambatan molekuler dilakukan menggunakan *AutodockTools* dan dianalisis lebih lanjut dengan *BIOVIA Discovery Studio Visualizer*. Validasi penambatan molekuler menunjukkan RMSD < 2 Å, menandakan bahwa metode yang digunakan valid. Hasil penambatan molekuler menunjukkan bahwa derivat pentabenzil kuersetin memiliki afinitas tertinggi, terutama terhadap reseptor ERα (-13,23 kcal/mol; 200,89 pM), HAC (-13,78 kcal/mol; 78,76 pM), dan PD-L1 (-12,55 kcal/mol; 633,59 pM); derivat pentaasetat kuersetin menunjukkan hasil penambatan yang baik terhadap reseptor HER2 (-10,16 kcal/mol; 35,68 nM); derivat pentametil kuersetin tidak memiliki hasil penambatan yang paling baik terhadap semua reseptor.

Kata kunci: kuersetin, derivat, kanker payudara, penambatan molekuler

ABSTRACT

Quercetin is a natural flavonoid that has been proven to possess biological activities, one of which is its anticancer potential. The derivatives used in this study include pentamethyl quercetin, pentaacetate quercetin, and pentabenzyl quercetin. This research aims to evaluate the breast cancer inhibitory activity of quercetin derivatives through molecular docking against seven breast cancer receptors, namely ERα, PR, HER2, HAC, PD-L1, FGFR, and IGFR. The molecular docking process was performed using AutoDockTools and further analyzed with BIOVIA Discovery Studio Visualizer. The docking validation showed an RMSD < 2 Å, indicating that the method used is valid. The molecular docking results revealed that the pentabenzyl quercetin derivative had the highest affinity, particularly towards receptors ERα (-13,23 kcal/mol; 200,89 pM), HAC (-13,78 kcal/mol; 78,76 pM), and PD-L1 (-12,55 kcal/mol; 633,59 pM); the pentaacetate quercetin derivative showed strong binding to the HER2 receptor (-10,16 kcal/mol; 35,68 nM); the pentamethyl quercetin derivative did not show the best binding results for any of the receptors.

***Keywords**: quercetin, derivative, breast cancer, molecular docking.*

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