

INTISARI

Proses penuaan adalah proses alami yang terjadi pada seluruh manusia. Seluruh bagian tubuh manusia akan mengalami proses penuaan, termasuk organ kulit. Proses penuaan terjadi ketika degradasi protein kolagen dalam ECM meningkat dan produksinya menurun. Proses degradasi dilakukan oleh protein MMP. Pada penelitian ini, dilakukan penapisan virtual terhadap *database* ligan yang berisi senyawa aktif pada tanaman yang banyak tumbuh di Provinsi DIY dan Jawa Tengah. Penelitian ini bertujuan untuk melakukan penapisan virtual terhadap senyawa-senyawa tanaman lokal di DIY dan Jawa Tengah terhadap MMP-8, salah satu jenis enzim kolagenase, menggunakan perangkat lunak PyRx 0.8 dan menguji validitas hasilnya dengan uji penghambatan kolagenase secara enzimatik *in vitro* dan penetapan kadar golongan senyawa.

Penapisan virtual dilakukan dengan validasi MMP-8, penentuan *grid box*, penapisan terhadap ligan, analisis afinitas ikatan, dan penentuan tanaman sampel yang mengandung ligan dengan afinitas tinggi saat berikatan dengan protein MMP-8. Tanaman tersebut diekstraksi dengan etanol 70% dan dikeringkan dengan *freeze drying* untuk mendapatkan ekstrak serbuk. Uji penghambatan kolagenase dilakukan secara *non-cell based*, dilanjutkan dengan penetapan kadar flavonoid total. Hasil penelitian dianalisis menggunakan SPSS dengan taraf kepercayaan 95%.

Berdasarkan hasil penapisan virtual, senyawa liquiritigenin pada tumbuhan melati memiliki afinitas tinggi terhadap MMP-8 dengan nilai -9.4 kcal/mol. Hasil uji penghambatan kolagenase menunjukkan bahwa sampel ekstrak bunga melati mampu menghambat kolagenase. Persentase penghambatan tertinggi ditunjukkan pada konsentrasi 50 µg/mL dengan nilai ~97%. Ekstrak bunga melati memiliki nilai kadar flavonoid total sebesar 20.841 ± 0.588 mgQE/g.

Kata kunci: bunga melati, penapisan virtual, penghambatan kolagenase

ABSTRACT

The aging process is a natural process that occurs in all humans. All parts of the human body will experience the aging process, including the skin organs. The aging process occurs when the degradation of collagen protein in the ECM increases and its production decreases. The degradation process is carried out by the MMP protein. In this study, a virtual screening was carried out on a ligand database containing active compounds in plants that grow a lot in DIY and Central Java Provinces. This study aims to carry out a virtual screening of local plant compounds in DIY and Central Java for MMP-8, a type of collagenase enzyme, using PyRx 0.8 software and test the validity of the results by in vitro enzymatic collagenase inhibition test and assay of groups compound.

Virtual screening was carried out by MMP-8 validation, grid box determination, ligand screening, binding affinity analysis, and determination of sample plants containing high affinity ligands when binding to MMP-8 protein. The plant was extracted with 70% ethanol and freeze dried to obtain powder extract. The collagenase inhibition test was carried out on a non-cell based basis, followed by the determination of total flavonoid levels. The research results were analyzed using SPSS with a confidence level of 95%.

Based on the virtual screening results, the liquiritigenin compound in jasmine plants has a high affinity for MMP-8 with a value of -9.4 kcal/mol. The results of the collagenase inhibition test showed that the jasmine flower extract sample was able to inhibit collagenase. The highest inhibition percentage was shown at a concentration of 50 µg/mL with a value of ~97%. Jasmine flower extract has a total flavonoid content value of 20.841 ± 0.588 mgQE/g.

Keywords: anti collagenase, jasmine flower, virtual screening