

***IN SILICO* PROTEOLYSIS AND MOLECULAR DOCKING FOR THE
EVALUATION OF JACK BEAN (*Canavalia ensiformis*) PROTEIN AS
PRECURSORS OF BIOACTIVE PEPTIDES WITH DUAL DIPEPTIDYL
PEPTIDASE-4 AND ANGIOTENSIN-I CONVERTING ENZYME
INHIBITORS**

Zulvana Anggraeni Harvian

17/419897/PTP/01562

ABSTRACT

Nowadays, there are many lifestyle disease which cause public health problems worldwide includes hypertension and diabetes type 2. Jack bean is one of underutilized legume in Indonesia, although it contains high protein. Amino acid profile analysis were conducted by using LC-MS/MS. Globular protein from jack bean analysed were derived from the BIOPEP for ACE and DPP-4 inhibitory activity during in silico proteolysis. A molecular docking study was occurred to confirm the inhibition activity between peptide as ligand and ACE and DPP-4 as receptor protein.

The results showed that Jack bean was contained 22.86% of protein. Furthermore, the analysis of amino acid residue was resulted that Histidine was the highest percent of abundance with 6.25% while the lowest value of 0.14% was obtained in Methionine. Based on BIOPEP-database screening Canavalin was obtained as the highest scores of ACEi overall (0.436 A). While the highest frequency value of DPP-4i was obtained in Concanvalin B with 0.641 A. The molecular docking study revealed that the ACE and DPP-4 inhibition of several peptides were mainly attributed to forming hydrogen bonds with the active pockets of ACE and DPP-4. These results indicate that Jack Bean is a potential source of bioactive peptides possessing ACE and DPP-4 inhibitors.

Keywords: Jack Bean in silico approach, DPP-4, ACE.

**PROTEOLISIS *IN SILICO* DAN MOLEKULAR DOCKING UNTUK
EVALUASI PROTEIN KACANG KORO PEDANG PUTIH (*Canavalia
ensiformis*) SEBAGAI PREKURSOR PEPTIDA BIOAKTIF DENGAN
DUAL INHIBITOR *DIPEPTIDYL PEPTIDASE-4* DAN *ANGIOTENSIN-I
CONVERTING ENZYME***

**Zulvana Anggraeni Harvian
17/419897/PTP/01562
INTISARI**

Saat ini, ada banyak penyakit akibat gaya hidup yang menyebabkan masalah kesehatan masyarakat di seluruh dunia termasuk hipertensi dan diabetes mellitus tipe 2. Kacang Koro Pedang Putih (KPP) adalah salah satu legum yang kurang dimanfaatkan di Indonesia, meskipun mengandung protein tinggi. Analisis profil asam amino dilakukan dengan menggunakan LC-MS / MS. Protein globular dari KPP yang dianalisis berasal dari BIOPEP terhadap aktivitas penghambatan ACE dan DPP-4 selama proteolysis *in silico*. *Molecular Docking* dilakukan untuk mengkonfirmasi aktivitas penghambatan antara peptida sebagai ligan dengan ACE dan DPP-4 sebagai protein reseptor.

Hasil penelitian berdasarkan LC-MS/MS menunjukkan bahwa KPP mengandung 22,86% protein. Selanjutnya, analisis residu asam amino menghasilkan bahwa Histidin memiliki persentase kelimpahan tertinggi dengan 6,25% sedangkan nilai terendah 0,14% diperoleh pada Metionin. Berdasarkan database BIOPEP, Canavalin diperoleh sebagai skor tertinggi ACEi keseluruhan (0,436 A). Sementara nilai frekuensi tertinggi DPP-4i diperoleh pada Concanvalin B dengan 0,641 A. Molekular docking mengungkapkan bahwa penghambatan ACE dan DPP-4 dari beberapa peptida ditunjukkan pada pembentukan ikatan hidrogen dengan sisi aktif ACE dan DPP-4. Hasil ini menunjukkan bahwa KPP adalah sumber potensial peptida bioaktif yang memiliki ACE dan DPP-4 inhibitor.

Kata Kunci: Kacang Koro Pedang Putih (KPP), pendekatan *in silico*, DPP-4, ACE