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Molecular Docking Analysis of Novel Angiotensin-I Converting Enzyme (ACE) Inhibitory Peptides Isolated from Cultured Marine Microalga, *Nannochloropsis oculata*

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The high protein content in the cultured marine microalgae has been demanded to explore bioactive peptides in the functional food industry. Angiotensin-I converting enzyme (ACE) inhibitory active peptides isolated from the cultured marine microalga, *Nannochloropsis oculata* was subjected for molecular docking studies. The molecular docking system of the ACE-ligand complexes was used to assess the isolated peptides which are posed in the best orientation in the pocket of the ACE active site. Chemically synthesized (purity >98%) two novel peptides known as tri-peptide (LEQ) and hepta-peptide (GMNNLTP) were evaluated for ACE inhibitory activity using a commercial ACE assay kit. The relative IC_{50} values reported on LEQ and GMNNLTP were 70.53±0.17 µg/mL (191 µM) and 76.34±0.45µg/mL (105 µM), respectively. However, both peptides showed the lower ACE inhibitory activity compared to the positive control, captopril with an IC_{50} value of 4.2±0.02 µg/mL (19.5 µM). The docking studies using CDOCKER in Accelrys Discovery Studio 3.1, the calculated binding energy among the identified peptides, LEQ-I, indicated a lower binding energy (-216 kcal/mol) and CDOCK interaction energy (56.83 kcal/mol) compared to the LEQ-II and positive control, captopril. Binding energy and CDOCK interaction energy of the captopril were -53.21 and 30.90 kcal/mol, respectively. However, the association of amino acid residual interaction with a metal ion (Zn^{701}) and H-bond interactions, including Arg^{522}, Ala^{356}, Tyr^{523}, and Glu^{143} of the peptide, GMNNLTP-I showed comparatively lower (-461.55 kcal/mol) interactions and higher CDOCK interaction energy (128.24 kcal/mol) than GMNNLTP-II in the *in-silico* assay. Therefore, GMNNLTP isomer-1 showed the best-fit orientation with the direct coordination of the catalytic Zn (II) as observed in the lowest binding energy and the highest CDOCK interaction energy compared to the captopril. Consequently, these two novel peptides have the potential to use in therapeutic applications after further studies.

Keywords: *Nannochloropsis oculata, microalgae, ACE-I, molecular docking*