Title (32)	:	Potential angiotensin I-converting enzyme (ACE) peptides derived from Chlorella vulgaris applying bioinformatic approaches
Journal	:	AIP Conference Proceedings
Document Type	:	Conference Paper
Publisher	:	AIP Publishing
UniKL Author	:	Mohammad Zulkeflee Sabri; Kelly Yong Tau Len; Khairul Faizal Pa'ee
Link to Full Text	:	https://pubs.aip.org/aip/acp/article- abstract/2923/1/030004/3279782/Potential-angiotensin-I-converting- enzyme-ACE?redirectedFrom=fulltext
Link to Scopus Preview	:	https://www.scopus.com/inward/record.uri?eid=2-s2.0- 85190690551&doi=10.1063%2f5.0195655&partnerID=40&md5=671a8ed d027cff5512f670d690690454
Abstract	:	Microalgae has sparked interest in its potential application in various industries, including food, chemical, and pharmaceutical products. It consists of natural green biomass for biofuels and bioproducts. Chlorella vulgaris (C. vulgaris) is a natural algae found in freshwater, the sea, and land. It contains a high photosynthetic ability, allowing it to grow quickly in autotrophic, mixotrophic, and heterotrophic environments. Angiotensin I-converting enzyme (ACE; peptidyldipeptide hydrolase, EC 3.4.25.1) is a regulatory factor in the renin-angiotensin system (RAS), which regulates blood pressure and other aspects of cardiovascular homeostasis. ACE catalyse angiotensin I into angiotensin II, a potent vasoconstrictor, which mediates the effects of RAS. This study aimed to apply an in silico method to evaluate the ACE-inhibitory peptides derived from C. vulgaris. The main protein in C. sorokiniana was used to create an analogue protein precursor for C. vulgaris. AutoDock Vina was used to model the molecular interaction of ACE-inhibitory peptides and ACE to discern its inhibition pattern. The result shows that at least three main dipeptides, namely VE, AH and PP, were shown to exhibit the inhibitory properties of the ACE. The affinity of these dipeptides was compared with Lisinopril, a well-known medication of ACE inhibitor. The polarity of amino acids in each dipeptide was shown to be responsible for high binding affinity in the complex, in addition to the localisation of the peptide binding site in the complex.