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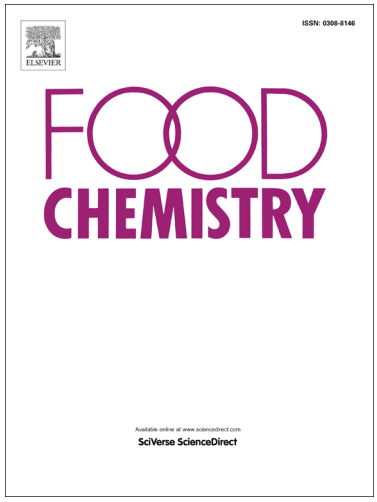

Identification of Pinto bean peptides with inhibitory effects on α-amylase and angiotensin converting enzyme (ACE) activities using an integrated bioinformatics-assisted approach

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PII: S0308-8146(17)30746-X
DOI: http://dx.doi.org/10.1016/j.foodchem.2017.04.166
Reference: FOCH 21039

To appear in: *Food Chemistry*

Received Date: 15 December 2016
Revised Date: 17 March 2017
Accepted Date: 26 April 2017

Please cite this article as: Ngoh, Y-Y., Gan, C-Y., Identification of Pinto bean peptides with inhibitory effects on α-amylase and angiotensin converting enzyme (ACE) activities using an integrated bioinformatics-assisted approach, *Food Chemistry* (2017), doi: http://dx.doi.org/10.1016/j.foodchem.2017.04.166

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Identification of Pinto bean peptides with inhibitory effects on α-amylase and angiotensin converting enzyme (ACE) activities using an integrated bioinformatics-assisted approach

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ABSTRACT

Five Pinto bean peptides with α-amylase and angiotensin converting enzyme (ACE) inhibitory activities were successfully identified using the integrated bioinformatics approach. By using PEAKS studio, 511 peptide sequences were first shortlisted based on their *de novo* sequence property and average local confidence (ALC) yield of ≥ 60%. Subsequently, only five peptides were found to have high potential (score≥0.80) for contributing bioactivy. The important sites which were potentially bound by the peptides: (a) Trp58, Trp59, Tyr 62, Asp96, Arg195, Asp197, Glu233, His299, Asp300 and His305 for α-amylase; (b) His353, Ala354, His383, Glu384, His387, Glu411, Lys511, His513, Tyr520 and Tyr523 for ACE had corresponded to the catalytic and substrate binding sites of the two enzymes.A validation assay was then conducted and IC_{50} values were determined. The range of the values for α-amylase inhibitory activity was 10.03–23.33 mM, whereas the values for ACE inhibitory activity were of 1.52–31.88 μM.

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