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Study of the antihypertensive peptides derived from alpha-lactalbumin hydrolysate after simulation of digestion

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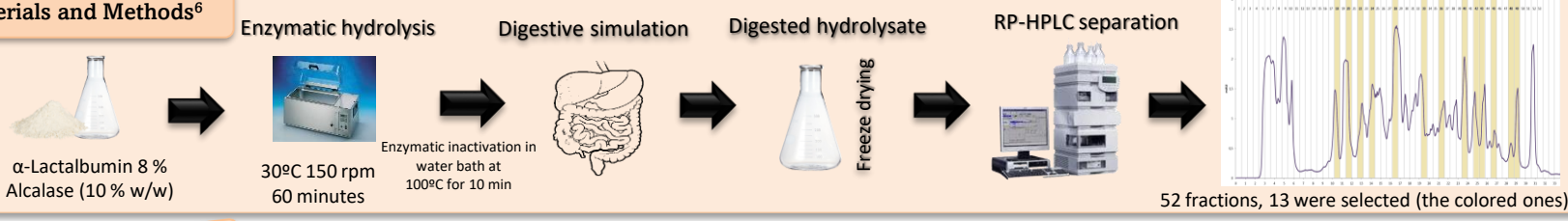
Introduction and Objective

Oxidative stress and free radical generation have been linked to a multitude of Noncommunicable Chronic Diseases (NCDs)[1]. Dietary antioxidants can help the body reduce oxidative stress[2]. Protein hydrolysates, sources of bioactive peptides, are widely used in food technology for their nutritional and functional properties (antioxidant, antihypertensive, etc) that depend on their physicochemical and structural characteristics[4,5]. The aim of this work was to correlate the antihypertensive activity found *in vitro* with *in silico* studies and to evaluate possible structure-activity relationships and possible mechanisms of antihypertensive capacity of the obtained peptides.

Materials and Methods[6]



-Fractions identification by nano-HPLC associated with a quadruple-orbitrap hybrid mass spectrometer
-Synthesis of peptides
-*In vitro* antihypertensive studie
-*In silico* studies
-Results analysis

Results and Discussion

Peptide	Sequence	Nº of amino acids	Isoelectric point	Charge at pH=7.4	Weight (Da)	GRAVY
1	IWCKDDQNPH	10	4.94	-1.4	1254.370	-1.66
2	KFLDDDLTDDIM	12	3.39	-4	1436.558	-0.44
3	DKFLDDDLTDDIM	13	3.3	-5	1550.638	-0.67

Table 1. General characteristics and physicochemical properties of peptides. Weight, isoelectric point, and charge at physiological pH were assessed with MOE's QSAR package. GRAVY index was calculated through GRAVY calculator (http://www.gravy-calculator.de/).

ACE inhibitory activity of **P1**
IC_{50} (mg/mL) : 3,9
(the only one that show activity)

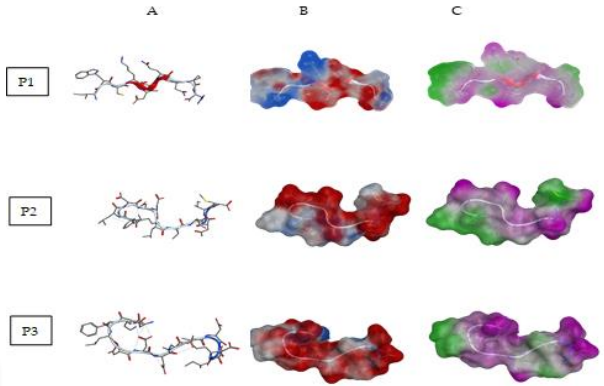


Figure 1. 3D representation of P1 (IWCKDDQNPH), P2 (DKFLDDDLTDDIM) and P3 (DKFLDDDLTDDIM) rendered by MOE showing conformations at 50ns of the simulation. P1 region that adopts alpha helix structure contains KDDQ residues (A) and two molecular surfaces showing electrostatics (B) lipophilicity (C).

Conclusions

Three peptides were obtained from the hydrolysis of alpha-lactalbumin with Alcalase enzyme, and their antihypertensive potential was studied using in vitro and in silico methods. The peptide IWCKDDQNPH (P1) was the only one that presented antihypertensive activity in vitro. The evaluation of P1 structure and amino acid composition through in silico studies showed accordance with what was obtained experimentally in the laboratory

Acknowledgements

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POS_NAC_M_2020_1_164417

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