COCOA AS A SOURCE OF BIOACTIVE PROTEINS AND PEPTIDES: AN *IN SILICO* APROACH

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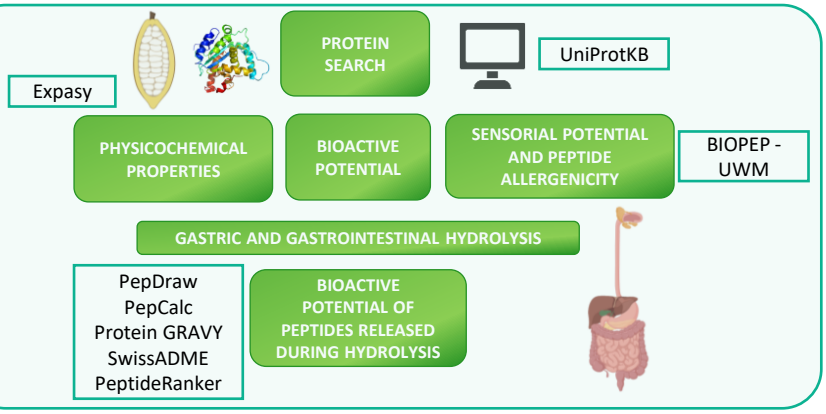
1. INTRODUCTION

Cocoa is known worldwide for its health-promoting properties, mainly attributed to compounds such as flavanols. However, cocoa may also be of interest due to its protein fraction, although there are currently few studies, as it represents 10 - 15% of the cocoa bean [1]. The search for new sources of bioactive peptides has gained interest in recent years. The prediction of the bioactive potential of proteins subjected to *in silico* digestion using bioinformatics tools allows the characterization of peptides without using *in vitro* or *in vivo* assays [2]. The **objective** of this work was to study cocoa proteins using bioinformatics tools as a source of bioactive peptides.

2. MATERIALS AND METHODS



3. RESULTS

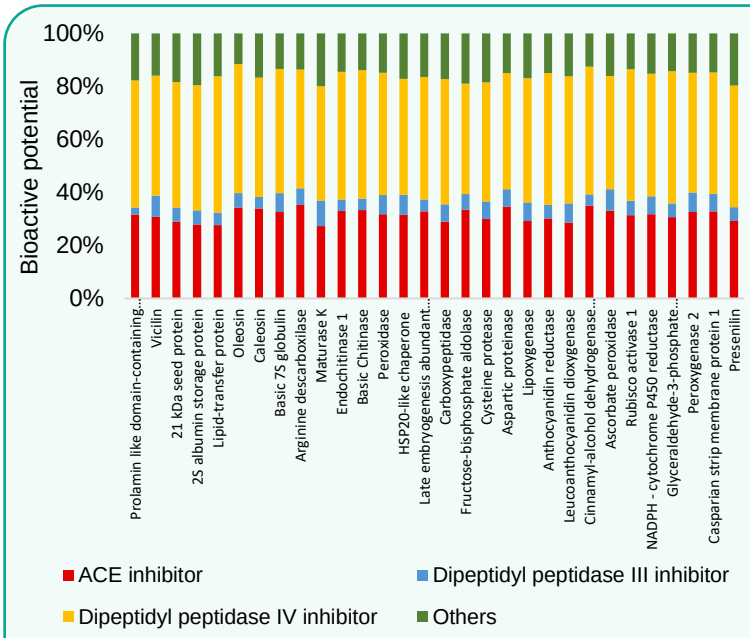


Figure 1. Bioactive potential of cocoa protein amino acid sequences (%)

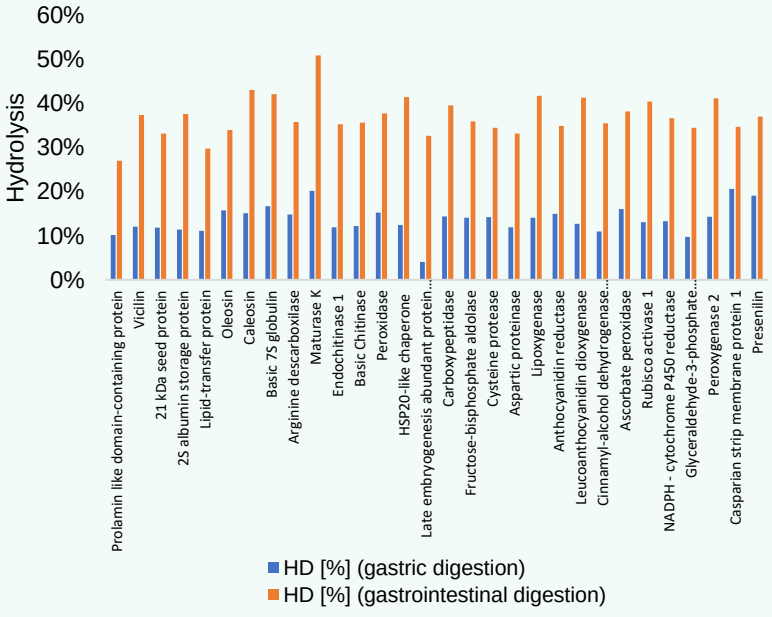


Figure 2. Hydrolysis degree (%) of cocoa proteins after *in silico* digestion

- Cocoa proteins presented different sizes (10-90 kDa) and pI values (5-7), highlighting the storage proteins of the seed as the major fraction. More than 60% of cocoa proteins, mainly defense and stress proteins and essential proteins, are stable, and most of them are thermostable. The amino acids with the highest frequency in all cocoa proteins are apolar aliphatic, and therefore hydrophobic.
- The potential active sequences in cocoa proteins (**Figure 1**) showed mainly DPP IV and ACE inhibitory activity, as well as DPP III inhibitory activity. None of the protein sequences exhibited allergenic epitopes. Bitter sequences were the most common, followed by sweet sequences.
- Cocoa protein hydrolysis by *in silico* digestion (**Figure 2**) displayed higher efficiency in the gastrointestinal phase than the gastric phase due to the utilization of several enzymes.
- The peptides released during *in silico* gastrointestinal digestion revealed mainly DPP IV inhibitory activity and ACE inhibitory activity, as well as antioxidant activity.

4. CONCLUSIONS

- Bioinformatic tools provide an advantage in the study of proteins and peptides released during gastrointestinal digestion.
- The use of cocoa proteins may be a promising strategy in preventing cardiometabolic diseases by utilizing the bioactive peptides released during gastrointestinal digestion according to *in silico* digestion.

REFERENCES

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