PEPTIDES OF NATURAL OCCURRENCE IN JATROPHA CURCAS SEEDS: INSIGHTS ON THE IN SILICO PROPERTIES

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INTRODUCTION: The field of finding polypeptides from plant biomass, even in rich sources such as species from the genus *Jatropha* is full of drawbacks to be explored, mainly due to sample preparation, appropriate fractionation and identification methods. Based on this, the discovery of polypeptides sequences with unknown properties represents a challenge even as valuable tool to design scaffolds that can be used to explore its biotechnological uses. **OBJECTIVES:** The aim of this study was to investigate and explore the properties *in silico* of twenty two polypeptide sequences deduced from de novo sequencing and genome search from *Jatropha curcas* seeds for further chemical synthesis uses. **MATERIALS AND METHODS:** SPE and RP-multi-steps chromatography with LC-MS procedures were performed to obtain polypeptide sequences. Kazuza and GenBank database were used for searching and identification. Two public bioinformatics tools (Peptide Property Calculator and ProtParam) were employed for explore *in silico* properties of peptide sequences. **RESULTS AND DISCUSSION:** All the sequences were confirmed in Jatropha genome and just one (CMGGV) not found significant similarity in GenBank database. The m/z ratio ranged from +1 (466.2) to +4 (480.74) yielding peptides with molecular weight of 465.2 to 1918.9 Da. Based on the *in silico* prediction properties was estimated: good solubility in water (sixteen sequences) while six were supposed have poor solubility; the net charge in pH 7 (ten negatively sequences, five positively sequences and six sequences with absence of charge); the isoelectric point (ranged from 4 to 11.7); stability (fifteen) and instability (seven); and absorbance at 280 nm (six sequences). The theoretical cyclization of sequences (head to tail) has changed dramatically its predicted properties. **CONCLUSIONS:** The approach utilized in this work is especially relevant because it opens perspectives for engineered analogues peptides with outstanding biotechnological uses to be explored.

Key-words: peptides, *Jatropha curcas*, peptides, mass spectrometry.
Acknowledgments: CNPq