Purification, synthesis and conformational studies of "Jatrophidin I", a new cyclic peptide from the latex of *Jatropha curcas* L.

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Previously we have isolated cyclic peptides from the latex of *Jatropha* genus species (Euphorbiaceae). Continuing the quest to find new peptides, we studied the latex of *Jatropha curcas* L. through extraction with ethyl acetate, and posterior fractionation in Sephadex G-15 column. After this protocol, peptidic fractions, detected by Cl_2/*o*-tolidine reagent, were purified by RP- HPLC resulting in two different peptides. The structural elucidation by mass spectroscopy and 1D/2D NMR showed the known cyclic peptide Pohlianin A, and one new cyclic peptide, that has been named "Jatrophidin I" (GWLNLLGP). This octapeptide was synthethized using Fmoc strategy. NMR studies in $DMSO_{d6}$ revealed "*cis*/*trans*" conformations of Proline amide bond, and, to provide additional information to this equilibrium, studies of Molecular Dynamics/Simulated Annealing (MD/SA) simulations were realized considering the peptide with Proline in *cis* and *trans* orientations, resulting in two representations for the cyclic chain. Additionally, 2D NMR experiments of "Jatrophidin I" using different solvents and temperatures were obtained in order to visualize conformational changes in variable conditions. These data showed that the mainly conformation to this new peptide was found with Pro in cis configuration. Biological studies showed that the new peptide has week antifungal effect against *Candida albicans, C. krusei, C. parapsilosis and Cryptococcus neoformans*. New studies about antioxidant and antimalarial activities have been evaluated.

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