

Structural Characterization of TistH, a Multifunctional Peptide from the Scorpion *Tityus stigmurus*

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INTRODUCTION: Tityus stigmurus, also known as yellow scorpion, is a species of scorpion widely distributed in the Northeast region of Brazil, belonging to Buthidae family. Recently a new hypotensin identified in T. stigmurus scorpion venom, called TistH (T. stigmurus Hypotensin), had its three-dimensional structure resolved in silico by our group. OBJECTIVES: The present study aims to determine TistH structure by circular dichroism, as well as its stability to pH and temperature variation. MATERIAL AND METHODS: The synthetic peptide was custom ordered from Invitrogen Life Technologies, USA. Circular dichroism analyses were conducted at a temperature of 25 °C in water, TFE 20%, 50% or 70% (v/v), or sodium phosphate buffer (200 mM, pH 7.4) in a Jasco J-810 spectropolarimeter. Secondary structure of TistH was determined by deconvoluting CD data using SELCON3, CONTIN and CDSSTR at Dichroweb platform. The structural stability of the peptide was evaluated at pH ranging from 3 to 9 and temperature from 2°C to 98°C. RESULTS AND DISCUSSION: In water and phosphate buffer, the peptide presented a typical spectrum of disordered structure. However, in the presence of TFE (20 to 70%), it showed a general predominance of α -helical conformation. One can observe TistH stability to pH variations, since the percentage changes in peptide structure were minimal. When evaluating peptide structural profile at a fixed wavelength of 222 nm, the molar ellipticity increased proportionally to temperature, suggesting a partial loss of α -helix structure and increase of beta-sheet and random coil regions. CONCLUSIONS: This study contributes to a better understanding of the structure of TistH aiming to develop new classes of antihypertensive drugs, expanding the range of therapeutic agents on the market.

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