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### **In silico design of analogue peptides derived of *bombina* species with improved antimycobacterial activity *in vitro***

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**T**uberculosis has become a major public health problem due to the emergence of multidrug resistant *Mycobacterium tuberculosis* strains; therefore, the development of new anti-TB compounds is necessary. The secretions from the skin of the *Bombina* species have antimicrobial peptides with broad-spectrum activity. In this work, using the server (<http://www.imtech.res.in/raghava/antibp/index.html>) and database (APD,<http://aps.unmc.edu/AP/main.php>), derived amino acid sequences of Bombinin and Maximin 1 that displayed the best antibacterial score, cationic and helical structure that improve their interaction with the mycobacterial membrane were obtained. The same analysis was used to modify the primary structure of the selected amino acid sequences in order to increase their antimycobacterial features. The designed peptides were synthesized by the Fmoc technique, characterized by MALDI-TOF and their activity was determined on *M. smegmatis* mc<sup>2</sup>155 cells using resazurin. In addition, were assessed the hemolytic activity, their ability to interfere the basal ATPase activity of *M. smegmatis* mc<sup>2</sup> 155 plasma membrane and cytotoxic activity on murine macrophages J774.

The experimental strategy allowed to find the 15 amino acid sequence derived of Bombinin and Maximin 1 with the best antibacterial characteristics and helical structure (peptide-A). The replacement of some amino acids of the peptide-A enabled to find a new sequence (peptide-B) with helical structure to be found, also improved positive charge and augmented antibacterial value. The peptide Maximin 1-B showed a lower MIC (2400µg/mL to 150µg/mL), and Maximin 1-A showed a higher inhibition of the basal ATPase activity of *M. smegmatis* mc<sup>2</sup>155 plasma membrane (24, 4%), and the peptides don't show toxicity over murine macrophages.

#### **Biography**

Sandra Milena Chingaté is Chemist, Magister in Biochemistry Science and doctoral student in Biochemistry Science at the Universidad Nacional De Colombia . Director of Career Technology in Industrial Chemistry at the Technological Corporation of Bogota. She has developed her research in the area of antimicrobial peptides as new anti-TB compounds in the research group Biochemistry and Molecular Biology of Mycobacterium at Universidad Nacional De Colombia.

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