



Article

Ib-M6 Antimicrobial Peptide: Antibacterial Activity against Clinical Isolates of *Escherichia coli* and Molecular Docking

J. M. Flórez-Castillo ^{1,*} , P. Rondón-Villanar ^{2,*}, J. L. Ropero-Vega ¹ , S. Y. Mendoza-Espinel ³, J. A. Moreno-Amézquita ³, K. D. Méndez-Jalme ³, A. E. Farfán-García ³, S. Y. Gómez-Rangel ³ and Oscar Gilberto Gómez-Duarte ⁴

¹ Facultad de Ciencias Exactas, Naturales y Agropecuarias, Ciencias Básicas Aplicadas para la Sostenibilidad—CIBAS, Universidad de Santander, Calle 70 No. 55-210, C.P. Bucaramanga (Santander) 680003, Colombia; jose.ropero@udes.edu.co

² Facultad de Ciencias de la Salud, Grupo de Investigación en Biología Molecular y Biotecnología, Universidad de Santander, Calle 70 No. 55-210, C.P. 680003 Bucaramanga (Santander), Colombia

³ Facultad de Ciencias de la Salud, Grupo de Investigación en Manejo Clínico—CliniUdes, Universidad de Santander, Calle 70 No. 55-210, C.P. 680003 Bucaramanga (Santander), Colombia; buc14172051@mail.udes.edu.co (S.Y.M.-E.); july.moreno103@gmail.com (J.A.M.-A.); jlasendayana1402@gmail.com (K.D.M.-J.); afarfan@udes.edu.co (A.E.F.-G.); sergio.gomez@udes.edu.co (S.Y.G.-R.)

⁴ Division of Pediatric Infectious Diseases, Department of Pediatrics, Jacobs School of Medicine and Biomedical Sciences, University at Buffalo, Buffalo, NY 14203, USA; oscar.gom@buffalo.edu

* Correspondence: johanna.florez@udes.edu.co (J.M.F.-C.); diseno.molecular@udes.edu.co (P.R.-V.); Tel: +57-037-651-6500 (ext. 1665) (J.M.F.-C.)

Received: 28 November 2019; Accepted: 8 January 2020; Published: 12 February 2020



Abstract: The Ib-M6 peptide has antibacterial activity against non-pathogenic *Escherichia coli* K-12 strain. The first part of this study determines the antibacterial activity of Ib-M6 against fourteen pathogenic strains of *E. coli* O157:H7. Susceptibility assay showed that Ib-M6 had values of Minimum Inhibitory Concentration (MIC) lower than streptomycin, used as a reference antibiotic. Moreover, to predict the possible interaction between Ib-M6 and outer membrane components of *E. coli*, we used molecular docking simulations where PhuA protein and its complex with Lipopolysaccharide (LPS-PhuA) were used as targets of the peptide. PhuA/Ib-M6 complexes had energy values between −39.5 and −40.5 Rosetta Energy Units (REU) and only one hydrogen bond. In contrast, complexes between LPS-PhuA and Ib-M6 displayed energy values between −25.6 and −40.6 REU, and the presence of five possible hydrogen bonds. Hence, the antimicrobial activity of Ib-M6 peptide shown in the experimental assays could be caused by its interaction with the outer membrane of *E. coli*.

Keywords: antimicrobial peptides; *Escherichia coli*; molecular docking

1. Introduction

The discovery of antibiotics in the 1940s is considered the most significant advance of medicine in the 20th century since it allowed the treatment of common but deadly diseases such as tuberculosis and pneumonia [1,2]. Simultaneously and inevitably, a natural phenomenon produced by the defense mechanisms of microorganisms known as antimicrobial resistance (AMR) arose. Moreover, it has presented a disturbing increase, mainly caused by the indiscriminate use of antibiotics. For this reason, the difficulty in the treatment of infections has increased. Similarly, the cost and risk of medical and surgical procedures has increased [3]. According to the Department of Health of the United Kingdom,