

Author's Accepted Manuscript

Antimicrobial Potency of Cationic Antimicrobial Peptides can be Predicted from their Amino Acid Composition: Application to the Detection of “Cryptic” Antimicrobial Peptides

Katia Pane, Lorenzo Durante, Orlando Crescenzi, Valeria Cafaro, Elio Pizzo, Mario Varcamonti, Anna Zanfardino, Viviana Izzo, Alberto Di Donato, Eugenio Notomista



www.elsevier.com/locate/jtbi

PII: S0022-5193(17)30068-1
DOI: <http://dx.doi.org/10.1016/j.jtbi.2017.02.012>
Reference: YJTBI8968

To appear in: *Journal of Theoretical Biology*

Received date: 23 June 2016
Revised date: 23 January 2017
Accepted date: 11 February 2017

Cite this article as: Katia Pane, Lorenzo Durante, Orlando Crescenzi, Valeria Cafaro, Elio Pizzo, Mario Varcamonti, Anna Zanfardino, Viviana Izzo, Alberto Di Donato and Eugenio Notomista, Antimicrobial Potency of Cationic Antimicrobial Peptides can be Predicted from their Amino Acid Composition Application to the Detection of “Cryptic” Antimicrobial Peptides, *Journal of Theoretical Biology*, <http://dx.doi.org/10.1016/j.jtbi.2017.02.012>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting galley proof before it is published in its final citable form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Antimicrobial Potency of Cationic Antimicrobial Peptides can be Predicted from their Amino Acid Composition: Application to the Detection of “Cryptic” Antimicrobial Peptides.

Katia Pane^{a 1}, Lorenzo Durante^{a1}, Orlando Crescenzi^b, Valeria Cafaro^a, Elio Pizzo^a, Mario Varcamonti^a, Anna Zanfardino^a, Viviana Izzo^c, Alberto Di Donato^a, Eugenio Notomista^{a*}

^aDepartment of Biology, Università degli Studi di Napoli Federico II, Napoli, Italy

^bDepartment of Chemical Sciences, Università degli Studi di Napoli Federico II, Napoli, Italy

^cDepartment of Medicine, Surgery and Dentistry, Università degli Studi di Salerno, Baronissi, Italy

*Corresponding author: notomist@unina.it

Abstract

Cationic antimicrobial peptides (CAMPs) are essential components of innate immunity. Here we show that antimicrobial potency of CAMPs is linearly correlated to the product $C^m H^n L$ where C is the net charge of the peptide, H is a measure of its hydrophobicity and L its length. Exponents m and n define the relative contribution of charge and hydrophobicity to the antimicrobial potency. Very interestingly the values of m and n are strain specific. The ratio $n/(m+n)$ can vary between ca. 0.5 and 1, thus indicating that some strains are sensitive to highly charged peptides, whereas others are particularly susceptible to more hydrophobic peptides. The slope of the regression line for the describing the correlation “antimicrobial potency”/“ $C^m H^n L$ product” changes from strain to strain indicating that some strains acquired a higher resistance to CAMPs than others. Our analysis provides also an effective and computationally not demanding computational strategy to identify search for CAMPs contained included inside the structure of larger proteins or precursors, which can be defined as “cryptic” CAMPs. We demonstrate that it is not only possible to identify and locate localize with very good precision the position of cryptic peptides, but also to analyze the internal structure of long CAMPs, thus allowing to draw an accurate map of the molecular determinants of their antimicrobial activity. A spreadsheet, provided in the Supplementary Material,

¹ These authors contributed equally to this work

Download English Version:

<https://daneshyari.com/en/article/5760140>

Download Persian Version:

<https://daneshyari.com/article/5760140>

[Daneshyari.com](https://daneshyari.com)