

## A new clasification system of antibacterial peptides using Support Vector Machines (SVM)

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In recent years, pattern recognition has been applied to solve multiplicity of problems in several fields on computer science and technology. One example it is the design of pharmaceuticals *in silico*, or sequence analysis of proteins for identification or discovering of new biological targets. For example, this approach has been used in the prediction and design of new antimicrobial peptides, because these compounds could be used as an alternative to conventional antibiotics. For this reason, in this work is proposed to use machine learning tools such as support vector machines (SVM) linked to models of Quantitative Structure-Activity Relationships (QSAR), in order to carry out pattern recognition and create algorithm allowing identification of antibacterial activity of synthetic peptides.

In this study, we worked with a set of 2288 peptide sequences with and without antimicrobial activity (1144 by group), codifying the structural information of every sequence (charge, molecular weight, isoelectric point, hydrophobicity, size, secondary structure, twist tendency, and *in vitro* and *in vivo* aggregation). We developed a classifier in cascade, conformed by two SVMs. In the first one, peptides with and without antimicrobial activity are classified, filtering peptides with antimicrobial activity. In the second one, it is determined if these selected antimicrobial peptides are or not antibacterial ones. Our classification model showed an estimated precision of 80%, which allowed, based on structural descriptors and codification of sequences, to correlate peptide sequences with antibacterial activity by means of learning machines.

### Biography

Rodrigo Torres Sáez is a Biochemist with Ph.D. in Biochemistry and Molecular Biology. He obtained his Ph.D. in 2005 working on enzyme biotechnology at Universidad Autonoma de Madrid (Spain). In 2010 he moved to Cornell University (USA) working at the Nanobiotechnology Center (NBTC) in protein nanofiber synthesis. In 2011 he moved back to the School of Chemistry of the Universidad Industrial de Santander, Colombia, where he is currently an Associate Professor. His research interests include bioinformatics, proteomics, and nanobiotechnology. Currently he is working with both *in silico* design and synthesis of antimicrobial peptides as alternative antibiotics.

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