

Structural bioinformatics of calcium-binding proteins associated with allergic diseases

Peter Lackner

Department of Molecular Biology, University of Salzburg, Hellbrunnerstr. 34, 5020 Salzburg, Austria. E-mail: Peter.Lackner@sbg.ac.at

Calcium binding proteins are involved in allergic diseases as allergens or in regulatory pathways. The increasing number of structurally resolved proteins facilitates the application of structure based bioinformatics (BI) approaches to study antigen recognition and processing or to support the development of therapeutic allergen derivatives.

The most relevant BI methods are structure comparison, structure modelling and prediction and In-Silico mutagenesis. For structure alignment we developed a new method which can deal with structural variability and permutation in sequence order. For structure modelling we apply standard methods such as MODELLER or SwissModel. In-Silico mutagenesis is based on a statistical potential approach.

Here we concentrate on allergens. We give a short introduction to the BI methods and present several examples how they have been used to investigate relations between allergens and for the development of hypoallergenic proteins potentially applicable for desensitization.