

Bioinformatics applied to allergy: Allergen databases, from collecting sequence information to data integration. The Allergome platform as a model

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Abstract

Allergens are proteins or glycoproteins that are recognized by IgE produced by the immune system of allergic individuals. Until now around 1,500 allergenic structures have been identified and this number seems not have reached a plateau after 3–4 decades of research and the advent of molecular biology. Several allergen databases are available on Internet. Different aims and philosophies lead to different products. Here we report about main feature of web sites dedicated to allergens and we describe in more details our current work on the Allergome platform.

The web server Allergome (www.allergome.org) represent a free independent open resource whose goal is to provide an exhaustive repository of data related to all the IgE-binding compounds. The main purpose of Allergome is to collect a list of allergenic sources and molecules by using the widest selection criteria and sources. A further development of the Allergome platform has been represented by the Real Time Monitoring of IgE sensitization module (ReTiME) that allows uploading of raw data from both *in vivo* and *in vitro* testing, thus representing the first attempt to have IT applied to allergy data mining. More recently, a new module (RefArray) representing a tool for literature mining has been released.

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1. Introduction

Diseases such as asthma, rhinitis, urticaria, eczema, anaphylaxis are among the most common health problems of people living in developed countries, affecting more than 30% of the population [1]. Allergic diseases are tightly related to the pathological production of specific IgE antibodies recognizing a number of sensitizing organisms and compounds in the environment, namely the allergens [2]. Allergens act as primary sensitizers of the immune system,

inducing, by still not completely known mechanisms, an IgE production towards structures otherwise safe for normal subjects. Secondly, tissue specific allergic reactions are triggered by the same allergenic compounds reaching the effector cells of the immune systems, the mast cells, within body tissues. Route of exposure may vary greatly from allergen to allergen, being the most common ones contact, inhalation, ingestion, injection. Allergens bind the IgE antibodies that specifically recognize part of the allergenic molecules, the epitope. In the last forty years, and mostly in the last fifteen, research on allergens lead to the identification of more than 1300 structures [2] and to a wealth of knowledge that nowadays is spread on more than 7000 papers [3]. This increasing knowledge on

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Table 1

1. IUIS Allergen Nomenclature (http://www.allergen.org)	Official web site for allergen nomenclature, recently updated and renewed, is devoted to assign the correct names to new allergens [16]
2. Allergen Database for Food Safety (http://allergen.nihs.go.jp/ADFS/)	A database with computational tools to be used to define allergenicity of new compounds. Includes an original database containing information on allergen structures and epitopes
3. AllAllergy (http://allallergy.net/database.htm)	A comprehensive database merging and displaying information on high and low molecular weight allergens, to be consulted by non specialists
4. ALLERDB (http://research.i2r.a-star.edu.sg/Templar/DB/Allergen/)	A computational resource
5. The Allergen Database (http://allergen.csl.gov.uk/index.htm)	A basic database for allergen structures
6. Allergome (http://www.allergome.org/)	An integrated platform collecting information and data for allergens
7. Allermatch (http://www.allermatch.org/)	A computational tool associated to a database
8. Biotechnology information for food safety database (http://www.iit.edu/~sgendel/fa.htm)	Among the very first allergen database to appear on the web. It maintains and implement the original list of allergens
9. FARRP Allergen Database (http://www.allergenonline.com/)	Both an independent dataset and a site for computational needs
10. IMGT Marie-Paule Allergen page (http://imgt.cines.fr/textes/IMGTeducation/IMGTlexique/A/AllergensBiochemicalData.html)	An allergen database integrated in a large data system
11. The Immune Epitope Database (http://www.immuneepitope.org/)	A recently released database dedicated to allergenic epitopes
12. InformAll (http://foodallergens.ifr.ac.uk/)	A European Union project for a database dedicated to food allergens
13. Structural Database of Allergenic Proteins (http://fermi.utmb.edu/SDAP/sdap_src.html)	One of the most comprehensive allergen database having several powerful computational tools for sequence comparison and allergenicity evaluation
14. WebAllergen (http://weballergen.bii.a-star.edu.sg/)	A web-based resource for computational needs

allergenic molecules has given further stimuli for a precise identification and a comprehensive classification of allergen sources. The spreading of this knowledge has been further improved by the widely adoption of Internet resources [3]. Biochemical, immunochemical techniques and molecular biology methods are allowing the identification of increasing number of allergenic structures and in a parallel way information technology is allowing us to create online databases that can be easily reached by worldwide users.

2. Allergen databases

Starting from the first release of the International Union of Immunological Societies Allergen Nomenclature subcommittee web site [4], several research groups and institutions have started to accumulate information and data from available sources in order to create databases of scientific knowledge on allergens. A number of allergen databases are now accessible. Table 1 reports the most updated list of allergen-dedicated web-based resources. There are several other databases available supporting computational tools [5,6], or from web sites of companies involved in the allergy field. The philosophy of each of the databases briefly described in Table 1 differs. Selection criteria for including a protein as allergen may range from

authors' active submission to literature screening, leading to a different number of structures available in each database.

Five main features may be present or not in allergen databases: (a) allergenic organisms, in the attempt to classify allergens on the basis of the source releasing them; (b) allergenic molecules and sub-molecular structures (epitopes), in the attempt to classify sensitizing and triggering allergenic structures at the molecular level; (c) literature on allergens (text mining), collecting all the periodical bibliographic sources and having simple and practical search tools for reference retrieval; (d) raw data on allergen reactivity (data mining), an increasing interesting use of information technology resources, enabling to collect raw clinical data on a condition. In the specific field of allergic diseases, it should support the data transfer from clinical and laboratory settings to web-based platforms; (e) computational tools for sequence and structure evaluation, a primary interest in bioinformatics. The recent introduction of genetically modified foods has pushed a lot the use of such tools to predict the potential allergenicity of proteins newly introduced in largely consumed foods [7–9]. Not all the databases have been designed to deal with all the aspects reported above. They all contains at least a list of allergens, computational tools for sequence search and comparison working on

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