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Drug Discovery

DABP: Database of antibacterial peptides

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General Note
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ABSTRACT

Antibacterial peptides are the effector's molecules of innate immunity and act as the first line of host defense against pathogenic infections. Over the last few decades, the search for new drugs and drug targets has prompted an interest in these antibacterial peptides. Antibacterial peptides have been identified in various species ranging from bacteria, frogs to mammals, including humans. Generally they are having 15 to 45 amino acid residues and the net charge is positive. This paper describes a curated database DABP, an integrated online repository that provides access to information relevant to antibacterial peptides where information is collected from published literature and web resources. Peptide information can be searched using keywords such as peptide name, sequence, source and activity. Each entry of the DABP is referred by a peptide name, family, function, activity, site of expression, peptide sequence, sub cellular localization, gene name and taxonomy. Additional annotation includes cross-references to databases like Swissprot, PIR and PubMed. DABP is a useful for studying the structure–function relationship of antibacterial peptides. DABP was publicly available at the URL http://scbt.sastra.edu/DABP.

Keywords: Antibacterial peptides, Subcellular localization, Web server, MySQL, Internal hyperlink.

INTRODUCTION

In the past few decades, a large number of bacterial strains have evolved ways to adapt or become resistant to the currently available antibiotics (Hancock et al. 2001). Researchers are focusing on alternative drugs based on antibacterial peptides, which play an important role in innate immunity. As part of innate immune system, antibacterial peptides provide protection against a wide variety of microorganisms in both vertebrates and invertebrates (Ganz, 2003, Hancock et al. 2000, Nicolas et al., 1995, Van't Hof et al. 2001). These peptides are very diverse with respect to amino acid sequence and secondary structure but share certain properties, such as affinity for the negatively charged phospholipids that are present on the outer surfaces of the cytoplasmic membrane of many microbial species. These peptides are ubiquitous, simple and effective factors acting within the innate immune system. Their short length and fast & efficient action against microbes has made them potential candidates as peptides (Ganz, 2003, Loffet, 2002, Van't Hof et al. 2001). Several peptides and their derivatives have already passed clinical trials successfully and several others are considered as potential therapeutics (Hancock et al. 2002). Antibacterial peptides have a broad spectrum of activity, including activity against bacteria, fungi, viruses, and even cancer cells (Hancock et al. 2000). Other than having pathogen-lytic activities, these peptides have other properties like anti-tumor activity, mitogen activity, or act as signaling molecules. In addition, they have a number of biotechnological applications, e.g. in transgenic plants, in aquaculture, and as aerosol spray for patients of cystic fibrosis (Baker et al. 1997, Osusky et al. 2000), (http://www.nce.gc.ca/pubs/reports/9697/ann96-97-7l_e.htm). Over the last few decades, the search for new drugs and drug targets has prompted an interest in these antibacterial peptides. In the past extensive work has been done in the field of antibacterial peptides, describing their identification, characterization, mechanism of action etc. The information about these peptides has been collected and compiled and organized as a database named as DABP. The antibacterial peptides have little sequence homology, despite common properties. Thus it is difficult to develop method for predicting the antibacterial peptides based on similarity. Moreover, experimental methods for identification and designing of antibacterial peptides are costly, time consuming and resource intensive. Thus there is a need to develop a comprehensive database for easy access of antibacterial peptides, which could be used to design potent peptides against bacterial pathogens. In the present study, a systematic attempt has been made to understand this important class of peptides and to develop a database for identification of antibacterial peptides (DABP) with high accuracy. The database was updated regularly to provide comprehensive information about the peptides. We collected and analyzed antibacterial peptides in order to understand their function and therapeutic activity.

MATERIALS AND METHODS

Database construction and content

Antibacterial peptides were collected from the literature by PubMed search using keywords such as 'antibacterial peptide'. The peptides collected in this version of DABP are mainly from natural sources. Each entry was checked in PDB or Swiss-Prot. If the peptide exists in the established databases, a web link was created in DABP for that entry to facilitate consultation of the original databases. In addition, each entry also contains peptide name, sequence, structure (such as α-helix or β-strand), sub cellular location, sites of expression, and taxonomic classification, biological activity (gram+, gram-, fungi, etc). A web link for Swiss-prot, Interpro, and PIR are created in DABP for each peptide entry to provide more useful information's regarding peptides. DABP was hosted on the Windows operating system using the IIS web server. The collected peptide information was organized using the freely available relational database management system MySQL (http://ww w.mysql.com). For the purpose of database bookkeeping, a unique five-digit identification number (ID) starting with AP was assigned to each peptide. A web-based graphical user interface was implemented using server-side scripting language PHP (http://www. php.net), (http://www.mysql.com). The schema diagram of DABP database is shown in (Fig.1).

DABP Search and retrieval

The homepage of DABP (Fig.2A) provides variety of web interface for the search and retrieval of peptide information. Data stored in DABP can be queried using the following ways

1. Search: The DABP web interface allows user to query the database using the attributes: Accession IDs -such as the Swiss-Prot ID, PubMed ID, Interpro ID and also using Keywords (peptide name, gene name, source, activity). Fig.2C shows the table of entries satisfying the user query. An internal hyperlink is made for each entry to get the detailed view of peptide information.

2. Browse: The user can browse the DABP database by using the initial letter of peptide name. Advanced search option is available which allows users to make complex queries by using different combinations of data.

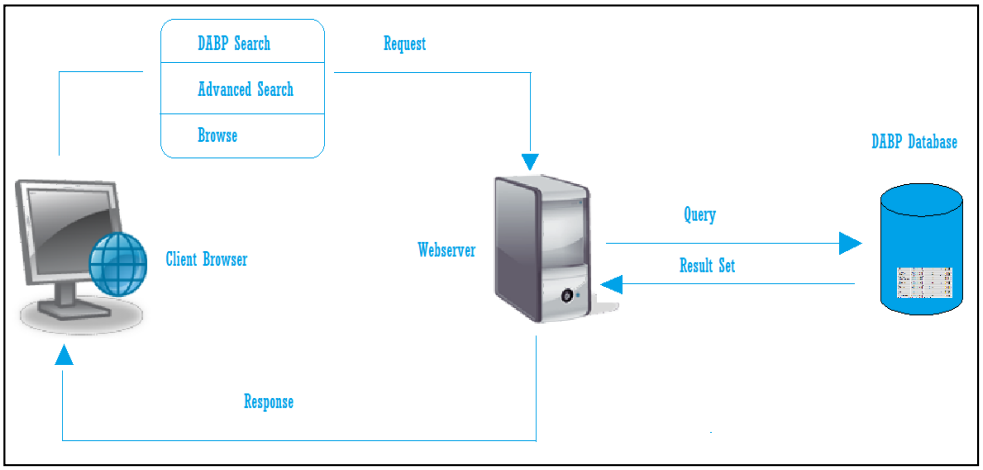

Figure 1
Schema diagram of DABP database

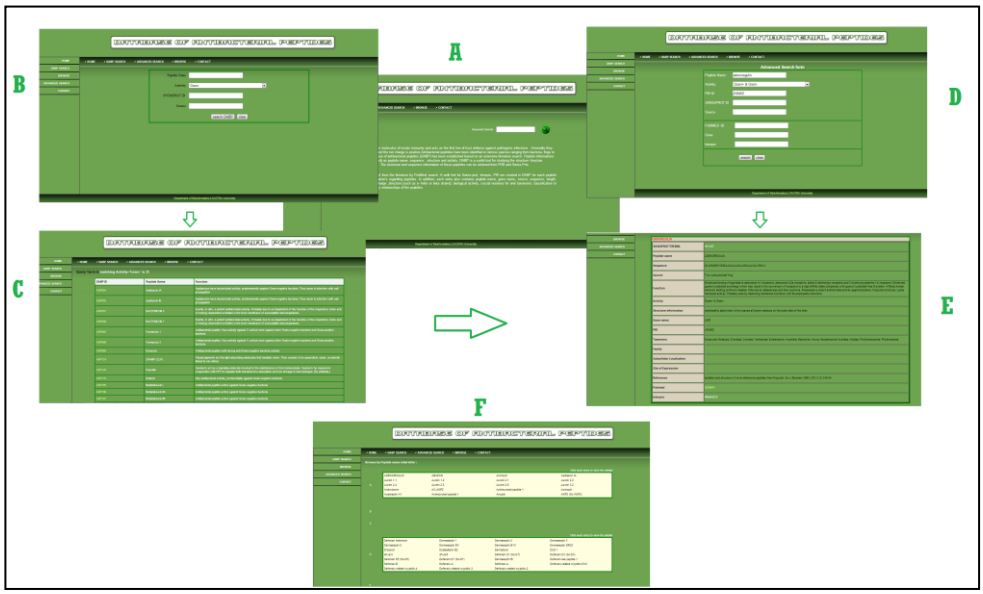

Figure 2
A screen shot of [A] DABP home page. [B] DABP search page which displays the search made for 'Gram+ & Gram-'. [C] Displays the Hits matching the query term ''Gram+ & Gram-'. [D] Advanced Search Page in DABP using complex search terms.[E].DABP detailed view of each entry. [F] Browse page which user browses the DABP by using the initial letter of Peptide Name

CONCLUSION

DABP is a unique database which gives complete information about antibacterial peptides. Using DABP the user can get complete knowledge about the peptide sequence information. The data got through DABP are taken from curated databases and hence it can be used for various research and analysis work done by molecular biologists.

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Conflict of Interest:

The authors declare that there are no conflicts of interests.

Data and materials availability:

All data associated with this study are present in the paper.

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