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Application Note

AMDD: Antimicrobial Drug Database

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Abstract

Drug resistance is one of the major concerns for antimicrobial chemotherapy against any particular target. Knowledge of the primary structure of antimicrobial agents and their activities is essential for rational drug design. Thus, we developed a comprehensive database, anti microbial drug database (AMDD), of known synthetic antibacterial and antifungal compounds that were extracted from the available literature and other chemical databases, *e.g.*, PubChem, PubChem BioAssay and ZINC, *etc.* The current version of AMDD contains ~2900 antibacterial and ~1200 antifungal compounds. The molecules are annotated with properties such as description, target, format, bioassay, molecular weight, hydrogen bond donor, hydrogen bond acceptor and rotatable bond. The availability of these antimicrobial agents on common platform not only provides useful information but also facilitate the virtual screening process, thus saving time and overcoming difficulties in selecting specific type of inhibitors for the specific targets. AMDD may provide a more effective and efficient way of accessing antimicrobial compounds based on their properties along with the links to their structure and bioassay. All the compounds are freely available at the advanced web-based search interface http://www.amddatabase.info.

Keywords: Antimicrobial agents; Drug resistance; Database

Introduction

Bacterial and fungal infections lead to an enormous disease and social burden. There are millions of people affected by infectious diseases attributed to bacteria and fungi worldwide. Therefore, there is a large market of antimicrobial drugs, increasing day by day, which are important in the control of infection. However, despite the discovery of new drug molecules, the worldwide spread of drug resistant microorganism has become a major problem [1,2]. There is a need to design novel agents with specific and enhanced antimicrobial activities, which requires the proper understanding of existing compounds and their associated properties. There are a number of databases, *e.g.*, CAMP [3], APD2 [4], PhytAMP [5] and ANTIMIC [6], of natural antimicrobial peptides which are used for treating bacterial and fungal infections. Moreover these peptides are effective against resistant microorganisms [7]. Currently, data related to antimicrobial drugs can be found scattered across different repositories at different locations and there is no common platform or resource that enables easy access to systematic information about synthetic antimicrobial agents. Thus, collection of these scattered data onto one platform will be helpful for the scientist to understand the properties of these antimicrobial agents and to develop methods for narrowing down candidate compounds. To fill this gap, we have made a comprehensive effort to collect and analyze antimicrobial agents and to organize them into the antimicrobial drug database (AMDD). This database could benefit not only understanding available antimicrobial agents but also might help in the development of new candidates to overcome drug resistance.

Implementation

Construction and content

Data of AMDD were collected from PubChem (http://pubchem.ncbi.nlm.nih.gov/), PubChem BioAssay and

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other chemical databases available including ZINC database, ChemDB and DrugBank, *etc* [7–9]. Only compounds that are active in antibacterial and antifungal bioassays were extracted. The current version of AMDD contains ~2900 antibacterial and ~1200 antifungal compounds. The data was organized as AMDD ID, compound name, description, mechanism of action, target, molecular weight, molecular formula, XLogP (ratio of concentrations of un-ionized compound between the two solutions), hydrogen bond donor, hydrogen bond acceptor, rotatable bond, canonical SMILES, isomeric SMILES, structure, ChemDB ID and ZINC ID (**Figure 1**).

Database architecture and interface

AMDD is built on Apache server 2.2.11 (http://www.apache.org/) with Hypertext preprocessor program PHP (http://www.php.net/). The database tables are stored in MySQL Server 5.0 relational database. MySQL and PHP technology were preferred as they are open source software and platform-independent. Interfaces in AMDD are designed in a user friendly manner that allows for easy navigation. The database interfaces include: HOME, DATABASE, DOWNLOADS, CONTACT US, FEEDBACK and HELP (**Figure 2**). A brief description of the interfaces is given below.

HOME: The AMDD database along with its various features is described in this section.

DATABASE: This section is further classified into two subclasses: antibacterial and antifungal. The user can easily fetch the data in this section by searching either by name or by five specific properties. The user can download 3D structure, structure data file (SDF) and MOL2 data for any particular compound in this section.

DOWNLOADS: In this section the user can download SDF, 3D structure and MOL2 data for all antibacterial and all antifungal molecules.

CONTACT US: In this section contact details of authors are provided.

FEED BACK: The user can submit their suggestions, comments and questions using this feature.

HELP: A detailed description on the use of the various features incorporated in AMDD is provided in this section for the benefit of users.

Data access

The purpose of the database is to provide a user-friendly interface. The interface provides simple, advanced search options (**Figure 3**). We classified the database into two categories: antibacterial and antifungal. An individual AMDD ID (*e.g.*, AB_0001 for antibacterial and AF_00001 for antifungal) is assigned to each compound. Users can use these unique codes to search a compound of interest (Figure 3A). We also provide the name of some compounds (according to literature and chemical databases available) which can be used as an option to search the compound of interest. The database interface allows the user to employ flexible search filters by specifying thresholds for any combination of molecular descriptors, *i.e.*, molecular weight, rotatable bonds, octanol/water partition coefficient log P, number of hydrogen-bond acceptors and number of hydrogen-bond donors (Figure 3B). Molecular substructures may be drawn using the Java Molecular

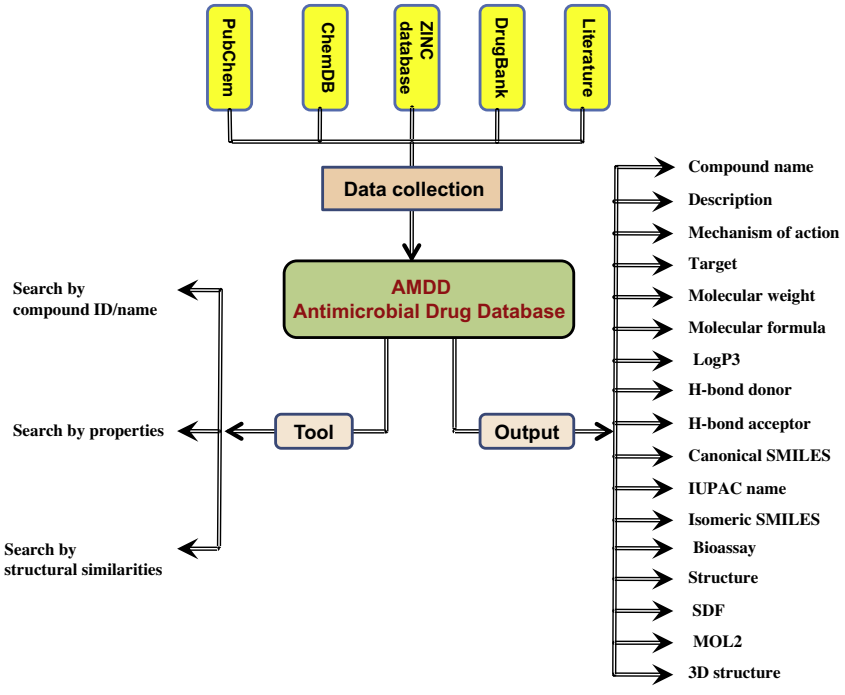

Figure 1 A schematic representation of architecture of database AMDD

Figure 2 Homepage of AMDD

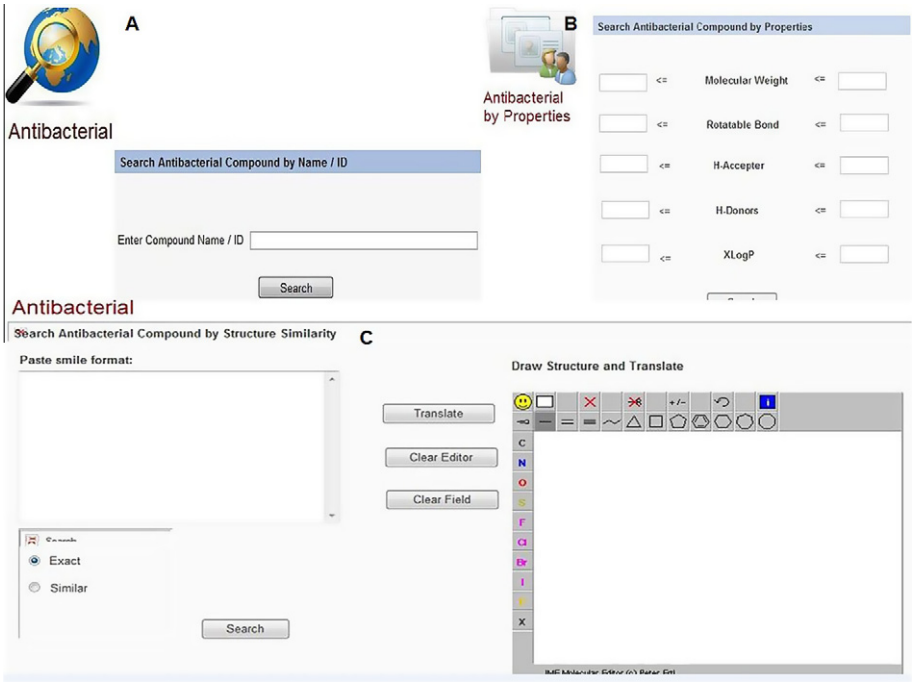

Figure 3 Composite screenshot example of an integrated search
A. Search by AMDD IDs or name. **B**. Search by properties. **C**. Search by structure similarity.

Editor (JME) [10] to search the related substructure (Figure 3C). The compounds are provided in three formats, *i.e.*, SDF, MOL2 and 3D. These files can be downloaded from the database option provided on the home page.

Conclusion

AMDD is a database that has been built aiming to make a comprehensive repository of synthetic antibacterial and antifungal compounds. The web interface of AMDD consists of unique tools which allow formulation of queries for retrieval of basic information and properties of each compound. Furthermore, the compounds are provided in three formats: SDF, Mol2 and 3D. The users can download the compounds in their choice of format from the download options of AMDD. The important aspect of this database is that all the data are readily available for open access through a publically accessible web site. These data

constitute an important resource for researchers working on antimicrobial agents and drug resistance that may eventually lead to the development of novel therapeutic leads against multi drug resistant bacteria and fungi.

The database will continue to be updated on the discovery of upcoming antimicrobial agents. We will provide all support for the users of this database in order to update their knowledge. Any further queries and comments are most welcome from the readers and users of this database.

Authors' contributions

AUK conceived and designed the project. MD, LK and MH collected the data and MD developed the website. MD and LK wrote the manuscript. All authors read and approved the final manuscript.

Competing interests

The authors have no competing interests to declare.

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