

CDAC - Development of a curated database of anticancer compounds from marine resources

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Abstract:

Anticancer compounds from marine source find application in cancer treatment. Several such compounds have been identified and documented. Here, we describe the development of CDAC, a curated database on anticancer compounds from marine sources.

Keywords: anticancer; drugs; curated database; marine

Background:

The marine source is a rich reserve for many important small molecule compounds. [1] It serves as a diversity pool for anticancer compounds. Numerous drugs from marine sources are traditionally used for treating ailments. In modern drug discovery, many compounds identified to have anticancer activity do not enter the pharmaceutical market due to competition and stringent Food and Drug Administration (FDA) policies. [2, 3] However, computational analyses have accelerated the discovery process. Such analysis can be further improved using data collected on compounds from different natural sources in the form of a comprehensive database. A database of anticancer compounds from marine sources is not available. Here, we describe the development of a database containing data on anticancer compounds from marine sources.

Database Model:

Data mining

Published articles containing data on anticancer compounds from marine sources were collected from PUBMED [6] and PUBMED CENTRAL [7] using KEYWORD search. Data on molecular weight, molecular formula and SMILES notation are retrieved from PUBCHEM.

Database development

The server used in this application is Apache Tomcat and the database is MySQL. A web based application is developed for the database using JSP (Java Server Pages). The demo database is made available for free at <http://demo.cheapchess.com/hpcancer/>

Future development:

The manual mining process is laborious, time consuming and error prone. The future plan is to replace manual creation by automated methods.

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