

New modules to input and edit data in SISTEMAT X. A web tool to manage databases of secondary metabolites.

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Abstract

New modules are shown to input and manage data online (web): chemical structure, species, exact mass, NMR among others.

Introdução

A simple search on the internet provides an answer; new discussion forums often provide answers that would take days or even weeks of research. Nevertheless, some information is still obtained indirectly and relatively time consuming, hence techniques of bank architecture of chemical data, query and visualization have been developed constantly. The huge volume of secondary metabolites available and related spectroscopic, biological activity, botanical and other data and their highly complex nature, efforts were directed to contribute to the successful organization and accessibility in the last 25 years [1]. SISTEMAT X WEB was developed to manage secondary metabolites and is online at: <http://www.sistemax.ufpb.br> [2].

SISTEMAT X WEB returns all compounds (secondary metabolites) that correspond to a specific query and, selecting a structure, it is possible to visualize all species where the compound has been isolated, and taxonomic classification: family, subfamily, tribe, subtribe and genus.

In this work we show new modules built in order to input data online using web interface.

Resultados e Discussão

We added to SISTEMAT X web registration modules that were developed in the last year, to input data regarding molecular structure, respective occurrence botany (species where a secondary metabolite has been isolated), biological activity, NMR data.

To input a compound in SISTEMATX web, it is necessary to draw a structure and state respective class, skeleton (both should be previously registered), and finally a common name (optional). IUPAC name, number of oxidation, exact mass, SMILES code, INCHIKEY and ID (identification number) are generated automatically as soon as a

structure is registered in the SISTEMAT X web databank by the system using API Chemaxon (www.chemmaxon.com): IUPAC name SMILES code, compound oxidation number, INCHIKEY and compound ID in the database (Figure 1).

It is also generated three-dimensional data structure from two dimensions using Chemaxon (www.chemmaxon.com) API. The structure in 3D (three dimensions) is displayed using the API developed by ChemDoodle (web.chemdoodle.com). Both kinds of structures 2D (two dimensions) as 3D can be downloaded.

The SISTEMAT X web interface is very light and friendly, suitable to use in several kinds of devices (including mobile), and works on browsers as Chrome and Mozilla.

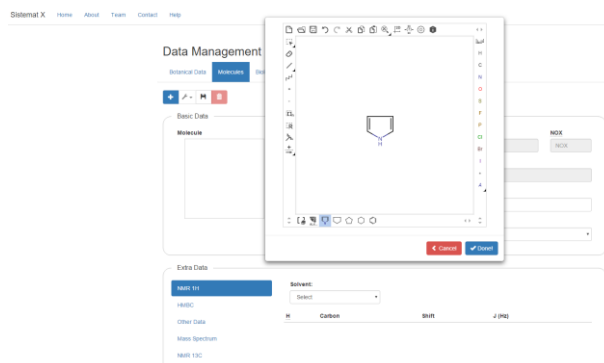


Figure 1. Screen of SISTEMAT X to input structure.

Conclusões

The site of the web tool is: www.sistemax.ufpb.br. We are developing constantly it, improving the existing features, and adding new tools too. All tools are available to the scientific community. The code is free, and it is available under on request to the authors.

Agradecimentos

CNPq

¹ Gasteiger, J. Handbook of Chemoinformatics: From Data to Knowledge, 4th ed.; Wiley-VCH. Weinheim, 2003.

² SISTEMAT X. Available online: <http://www.sistemax.ufpb.br>