



SISTEMAT X - A Web Tool to Manage Databases of Secondary Metabolites

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Abstract: The internet aids to promote a new process of data/information transmission that two decades ago simply did not exist. 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 chemical data, query and visualization have been developed constantly. We can find several internet applications to search and predict spectroscopic data, biological activity of ligands, or to predict toxicity of new compounds or pesticides. Our research group is developing SISTEMAT X web, [2] a tool that manages databases of natural products. Currently, our database has more than 1,100 sesquiterpene lactones and 800 flavonoids with more than four thousand botanical occurrences of the Asteraceae family and approximately 400 alkaloids which represents more than 750 botanical occurrences of the Apocynaceae family and several terpenes of Annonaceae that correspond more than 800 botanical occurrences. SISTEMAT X is a set of integrated programs and tools that perform cheminformatics tasks that include database management, chemical structure editor, visualization of chemical structures, and prediction of physicochemical properties among others. Most of the components are intuitive and friendly using a graphical interface. In the last year we have migrated applications that use Java interface for JavaScript, since the last is geared to web pages. This software has already been registered by our research group, through UFPB, in “Instituto Nacional de Propriedade Industrial” with number BR 51 2015 000073. The site is running at the address: www.sistemax.ufpb.br. We are developing constantly it, improving existing features such as adding new. All tools are available to the scientific community.

Keywords: web tools, secondary metabolites, databank, cheminformatics.

Mol2Net YouTube channel: <http://bit.do/mol2net-tube>

1. Introduction

The internet aids to promote a new process of data/information transmission that two decades ago simply did not exist. 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 chemical data, query and visualization have been developed constantly. We can find several internet applications to search and predict spectroscopic data, biological activity of ligands, or to predict toxicity of new compounds or pesticides [1].

Studies of publications on modern chemistry dating from the eighteenth century and its volume has increased steeply since the First World War. Being the huge volume of current data and highly complex nature, efforts were directed to contribute to the successful organization and accessibility in the last 25 years [1].

2. Results and Discussion

The SISTEMATX WEB has the function of producing and designing Web pages, objects such as images, headings, tables, among others. It was developed the system of management of chemicals that is in operation at: <http://www.sistemax.ufpb.br> [2]. The contact modules were created by the chemical name for SMILES (Simplified Molecular Input Line Entry Specification) and substructure. Also created by the query returns all species compounds (secondary metabolites) that have been isolated

in this (Figure 1), and all the species in the taxonomic classification family. SISTEMAT X added to the web registration system that was developed in the last year, data from the molecular structure and its occurrence botany from the literature review. To draw a molecule associate with a class, skeleton, both previously registered, and finally a name. It can be in the query screens besides the registered data, information generated automatically by the system using Application Programming Interface (API) Chemaxon (www.chemmaxon.com): IUPAC name, SMILES code, compound oxidation number, INCHIKEY and compound ID in the database (figure 2).

SISTEMATX WEB has functions to produce and design Web pages, objects such as images, headings, tables, among others. It was developed to manage secondary metabolites and is online at: <http://www.sistemax.ufpb.br>. Modules in order to perform searches using a chemical name (IUPAC or common), SMILES (Simplified Molecular Input Line Entry Specification) and substructure (Figure 1). It is possible to perform selecting a specific genus and species (Figure 1). The query returns all compounds (secondary metabolites) that correspond the performed query and selecting a structure, it is possible to visualize all species where the compound has been isolated (Figure 2), and all the species and their taxonomic classification: family, subfamily, tribe, subtribe, genus and specie. We added to SISTEMATX web registration modules that were developed in the last year, data from the molecular structure and its occurrence botany (species where a secondary metabolite has been

isolated), data that is being collected from the literature review.

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, SMILES code, INCHIKEY and ID (identification number) are generated automatically as soon as a structure is registered in the SISTEMATX 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 2).

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 in figure 3 using the API developed by ChemDoodle (web.chemdoodle.com). Both kind of structures 2D (two dimensions) as 3D can be downloaded.

The SISTEMATX web interface is very light and friendly, suitable to use in several kinds of devices (including the mobile), and works on browsers as Chrome and Mozilla and it does not require JAVA installed on the device.

Currently, our database has more than 1,100 sesquiterpene lactones and 800 flavonoids with more than four thousand botanical occurrences of the Asteraceae family and approximately 400 alkaloids which represents more than 750 botanical occurrences of the Apocynaceae family and several terpenes of Annonaceae that correspond more than 800 botanical occurrences

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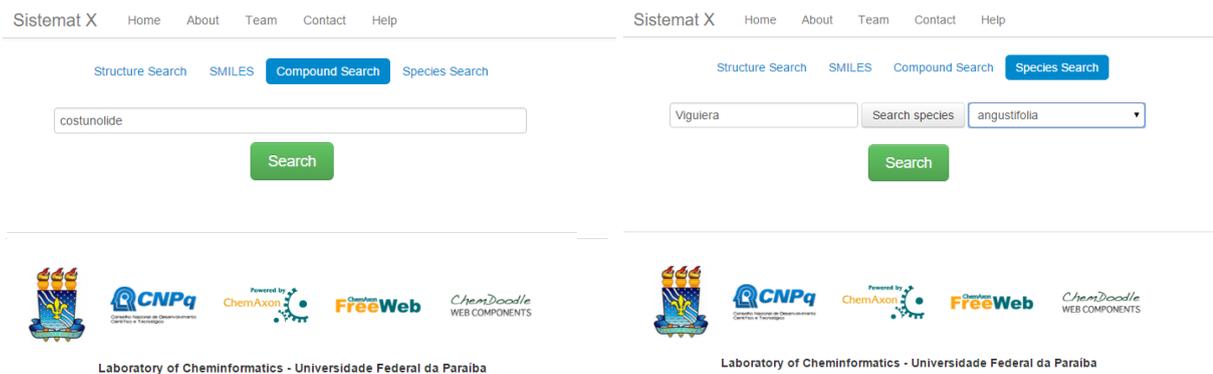


Figure 1. Screens of search for substructure, for SMILES code, for compound name, and for species name.

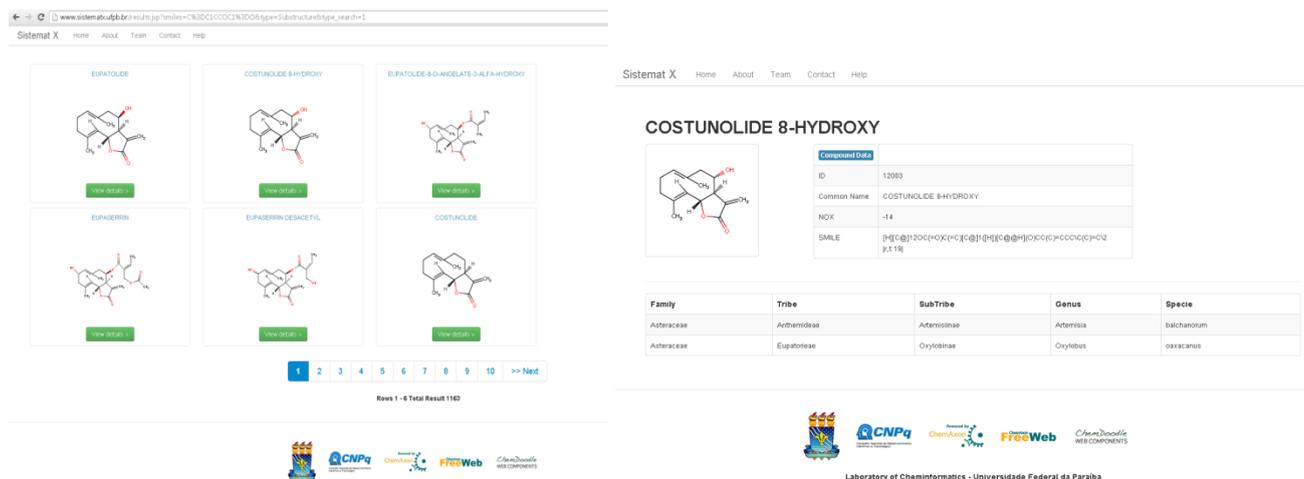


Figure 2. Screen with the result of a search for lactone substructure and some data of costunolide 8-hydroxy available.



Figure 3. Screen of a structure in 3D of SISTEMATX web.

3. Materials and Methods

To build all tools and develop interfaces that is able to be used in several kinds of mobile devices and computers without the need for Java installed in the machine, we use technologies such as HTML 5, CSS3, JavaScript, PHP, AJAX (Asynchronous JavaScript XML together), JSF (JavaServer Faces).

The database was developed using MySQL and various security tools based on OWASP (Open Web Application Security Project - https://www.owasp.org/index.php/Main_Page) were implemented.

APIs the CHEMAXON were used for the generation of auxiliary data related to the structure and to make the search tool. The API ChemDoodle was used for visualizing the 3D structures.

4. Conclusions

The site of the web tool is: www.sistemax.ufpb.br. We are developing constantly it, improving existing features such as adding new. All tools are available to the scientific community.

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Author Contributions

Marcus Tullius Scotti is the coordinator of this work, and idealize the web tool. Selected the IDE and API that are used. **Roberto Oliveira da Silva Junior aid to develop the database and the integration APIs, working mainly in the background of the web tool configuring the server and improving its security. Silas Yudi Konno De Oliveira Santos has worked mainly in the front end of the web tool, aid to planning the screen and building it. He aids in the integration of some APIs too. Luciana Scotti aids to design some functionalities of the web tool and testing some implemented functionalities.**

Conflicts of Interest

The authors declare no conflict of interest.

References and Notes

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

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