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SISTEMAT X - A WEB TOOL FOR DATABASES MANAGEMENT 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 [1]. 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 [2]. 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.sistematx.ufpb.br. We are developing constantly it, improving existing features such as adding new. All tools are available to the scientific community.

References:

[1] Gasteiger, J. 2003. Handbook of Chemoinformatics: From Data to Knowledge, Ed. 4 v. Wiley-VCH. Weinheim.
[2] www.sistematx.ufpb.br