Chemoinformatics module for CMKb, a Customary Medicinal Database

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Indigenous medicinal plants are a major resource for safe alternative medicines and the discovery of new drugs. Approximately 80% of all plant-derived drugs that are in current use globally were discovered as a direct result of the study of plants used by humans as medicines (ethnomedical use) and are used for the same or related ailments as the original medicinal plant [1]. Australian Aboriginal people have used plants as medicines for thousands of years and have a vast knowledge of Australia's unique flora. However, only a limited number of studies on this knowledge have been undertaken and much of this knowledge is poorly documented.

We are developing the Customary Medicinal Knowledgebase (CMKb), containing medicinal plant data present in public domain and from Australian Aboriginal communities. Besides ethnobotanical information, customary use, mode of preparation and results from biochemical or microbial assays, we have included details of bioactives identified, in the chemoinformatics module (CM). The design of this module and its features are presented here.

CM gathers information about the bioactive compound in terms of chemical name, chemical structure in SMILES format and chemical properties (logP, molecular mass etc.). Implemented on a relational database format, CM can be queried through the CMKb search page, by 1D whole molecule descriptors (chemical name, IUPAC name and CAS number). Visualization of structural data is enabled through MarvinViewer (http://www.chemaxon.com/). 2D and 3D searching [2] are in the pipeline.

References

1. D.S. Fabricant, N.R. Farnsworth, The Value of Plants Used in Traditional Medicine for Drug Discovery, *Environmental Health Perspectives*, **2001**, *109*, 69-75.
2. P. Willet, Similarity methods in chemoinformatics, *Annual Review of Information*

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