PSC-db: A Structured and Searchable 3D-Database for Plant Secondary Compounds

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Abstract
Plants synthesize a large number of natural products, many of which are bioactive and have practical values as well as commercial potential. To explore this vast structural diversity, we present PSC-db, a unique plant metabolite database aimed to categorize the diverse phytochemical space by providing 3D-structural information along with physicochemical and pharmaceutical properties of the most relevant natural products. PSC-db may be utilized, for example, in qualitative estimation of biological activities (Quantitative Structure-Activity Relationship, QSAR) or massive docking campaigns to identify new bioactive compounds, as well as potential binding sites in target proteins. PSC-db has been implemented using the open-source PostgreSQL database platform where all compounds with their complementary and calculated information (classification, redundant names, unique IDs, physicochemical properties, etc.) were hierarchically organized. The source organism for each compound, as well as its biological activities against protein targets, cell lines and different organism were also included. PSC-db is freely available for public use and is hosted at the Universidad de Talca.

Author keywords
3D-structures
chemical and structural properties
database
natural products
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plant secondary metabolites