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Exploring pharmacological potential of Brazilian plants: SAM database - A tool for recording and comparison of molecules isolated from plants of the Brazilian semiarid

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Databases of molecules have become a great tool for scientists and researchers working in drug development because they provide information of various types of molecules, which becomes crucial when trying to find a structure with pharmaceutical activity. Several plants of semi-arid of Bahia, Brazil, have been studied in recent years in an attempt to find new therapeutic targets for a variety of pathologies. However, despite several efforts our knowledge is still very small about its mechanism of action of these natural compounds. Then, we developed a database which allow the storage of information and comparison of molecules isolated from plants of Brazilian semiarid region, because of its great diversity of plant species, and compounds that can be useful for applied drug development against human diseases. Some of the functionalities of this tool include recording molecule structures, using SMILES code, evaluation of similarity between molecule structures (including Tanimoto coefficient), comparison of molecules with external databases like ChEMBL and ZINC, as well as the calculation of chemical proprieties such as molecular weight, HbA, HbD and ClogP that satisfy or not the Lipinski's rule. The construction of this database is based on Java technology used for the internet and intranet. Some features, such as creating the structure of molecules, calculating the similarity between molecules and MOL files generation were obtained from the Open Source library Indigo, developed by GGA Software Services. The generated data is stored in a relational database, used as System Manager Database (DBMS) MySQL Server 5.5.28.

Biography

Bruno Andrade has completed his PhD from the State University of Feira de Santana, Brazil, in 2011. He has experience in Biotechnology with emphasis on structural and functional analysis molecules isolated from microorganisms, animals and plants with pharmacological potential, and working on the following topics: Homology Molecular Modeling, Docking and Virtual Screening. He is currently adjunct professor at the State University of Southwest Bahia, Brazil, School of Medicine. He has published over 25 works (including 6 papers) in reputed journals and international meetings.

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