D-Tools: An Open Platform for Research and education in Chemoinformatics

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DIFACQUIM Tools for Cheminformatics (D-Tools) is a suite of open-access resources to foster education in chemoinformatics and support research. Current tools include the Platform for Unified Molecular Analysis (PUMA), Activity Landscape Plotter, D-Peptide Builder, and Epigenetic Target Profiler. Such resources facilitate the automated diversity analysis of compound data sets, analysis of activity landscapes, enumeration of peptide libraries, and prediction of epigenetic activity of small molecules, respectively. All the tools are freely available and can be accessed through the site: https://www.difacquim.com/d-tools/. Herein, we will discuss three of the most recent additions to D-Tools, namely, 1) a Chemoinformatics GitBook for Chemical Data Retrieval and Analysis Using Python Programming, 2) BIOMX-DB, a website that enables the navigation of a curated database of natural products from Mexico, and 3) MAYA, (Multiple Activity Analyzer) a tool designed to automatically construct a chemical multiverse, generating multiple visualizations of chemical spaces of a compound data set described by structural descriptors of different nature.