

## ***Screening Assistant: a Free Platform for Managing Huge Chemical Databases and Selecting Compounds for Screening***

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Managing a database of screening compounds is a tedious task. *Screening Assistant* is a platform dedicated to make this operation easier. It can use the SDF libraries provided by the suppliers to create a screening database. The software is designed to insert only new chemical structures, keeping all the references of all the providers for a given compound. Analyses of the libraries, using molecular frameworks, scaffolds, diversity, and several physicochemical properties are available. Furthermore, the compounds can be represented in a 2D chemical space.

“Progressive Drug-Like” (PDL) and “Progressive Lead-Like” (PLL) scores based on progressive limits on physicochemical properties (molecular weight, logP, H bond acceptors, H bond donors, rotatable bonds, SSSR, maximum ring size and halogens) are computed for all the compounds. On the basis of these scores, a new personalized score, “Cleaning For My Screening” (CFMS), can be computed. Depending on the choice of the user, reactive functions, warheads agents, promiscuous aggregating inhibitors, single chains, perfluorinated chain, absence of N or O, can be used to add additional penalties to the compounds. CFMS can be used, in combination with filters for any other descriptors computed by *Screening Assistant*, to select compounds for real or virtual screenings.

Technically, this platform is based on free tools allowing any research team to use it. Furthermore, the software is provided with source code under the LGPL license, allowing to be improved by other developers. However, interface to some commercial softwares is provided, allowing *Screening Assistant* to access to other functionalities such as improved molecular display (Marvin), 2D to 3D conversion (Corina), and conformers generations (Omega).