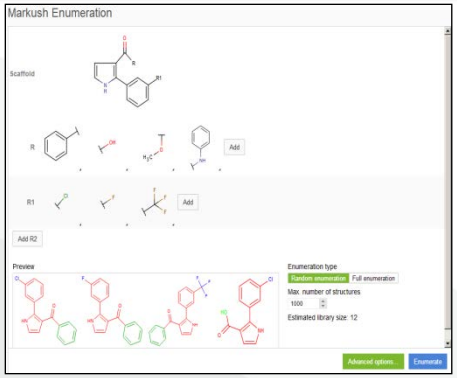
The Power of Plexus Provided by OIDD

An exciting and user-friendly platform for chemical structure exploration

Library Enumeration

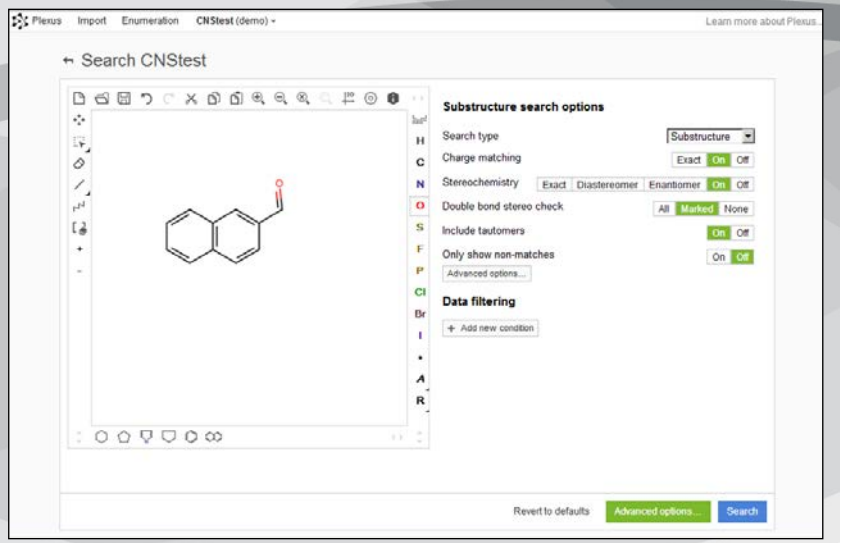
Plexus supports the handling of generic Markush structures, using a user-friendly approach that allows conversion of enumerated libraries into lists of exemplified chemical structures. This functionality also enables patent application searches and stores results in table format.



Chemical Structure Searching

In alignment with the early-discovery focus of the **OIDD** program, **Plexus** relies on well-known sources to provide compound structures and associated chemical information. These sources are the Chemical Entities of Biological Interest (ChEBI) and Drugbank databases.

Users are presented with the option to either query a given structure or perform diverse structural searches (i.e. substructure, similarity, duplicate, full fragment, full structure and superstructure). Other functionalities such as advanced searching and use of sequential hit list filtering are also available.



OPEN INNOVATION DRUG DISCOVERY | Lilly

OPEN INNOVATION DRUG DISCOVERY PROGRAM

A Platform for Collaboration

Now offering

Plexus

In collaboration with ChemAxon

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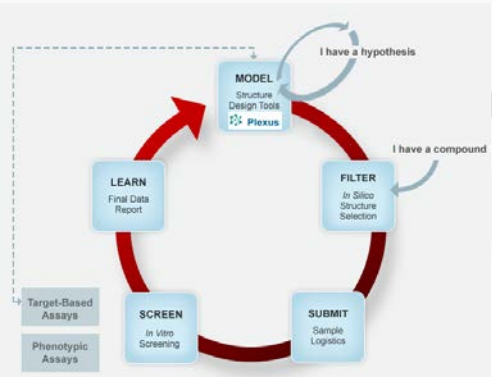
What is Plexus?

Plexus is a brand-new chemistry application by **ChemAxon** which provides simple, yet powerful workflows for handling chemical structure processes commonly used by discovery chemists. The application is under active development in collaboration with the **Lilly OIDD** chemoinformatics team.

Plexus provides users interactive capabilities to import all standard data source types, handle large datasets, and display screening and clustering results using different visualization techniques (heat maps, tables, histograms).

Through **Plexus**, **OIDD** will offer participants with a state-of-the-art computational tool panel which will continuously evolve to reflect Lilly 's strategic interests.



Plexus for OIDD Participants

The incorporation of **Plexus** within the **OIDD** platform will allow users to greatly enhance their structure design capabilities, backed by the combination of **ChemAxon**'s cheminformatics capabilities and **Lilly**'s drug design expertise .

Plexus facilitates the parallel incorporation of desirable drug-like properties and optimization of target-based activity to virtually design and evaluate new chemical entities.

Plexus combines an intuitive, user-friendly platform with powerful cheminformatics capabilities, advanced visualization technology and analytics tools.

SPR and/or SAR Exploration

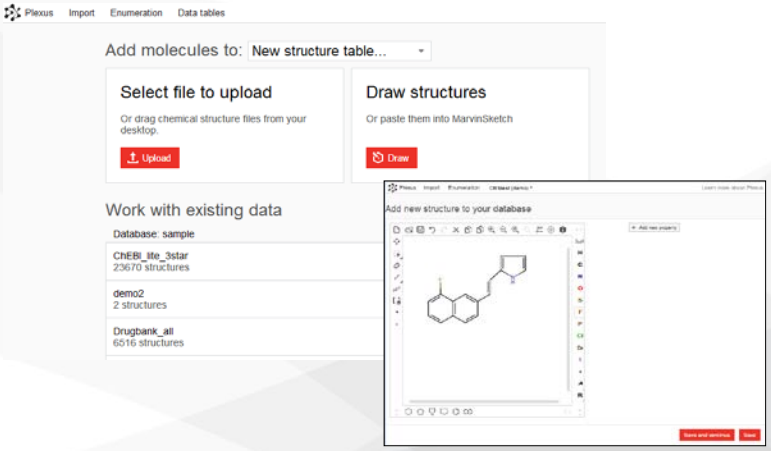
Structure-Property Relationship tools: include physical property calculators (i.e. cLogP, PSA, MW, etc) as well as multi-parameter tools for use in molecular design. Additionally, **Plexus** provides easy-to-interpret guidance on the crucial influence of selected properties on overall ADME/Tox molecular profile.

Structure-Activity Relationship tools: include customized models to maximize activity at a given biological target (i.e. activity or pharmacophore models, etc). The corresponding *in vitro* assays are also available via the **OIDD screening panel**.

Workflows already supported by Plexus

Drawing Chemical Structures

Plexus features Marvin JavaScript standalone chemical editor for drawing structures. Structural and non-structural chemical data fields can be imported and exported from databases using a simple interface, which allows users to drag and drop while supporting the major file formats.



One of the key features of **Plexus is** the integration of **ChemAxon** structure-based property calculations displayed in a detailed view.