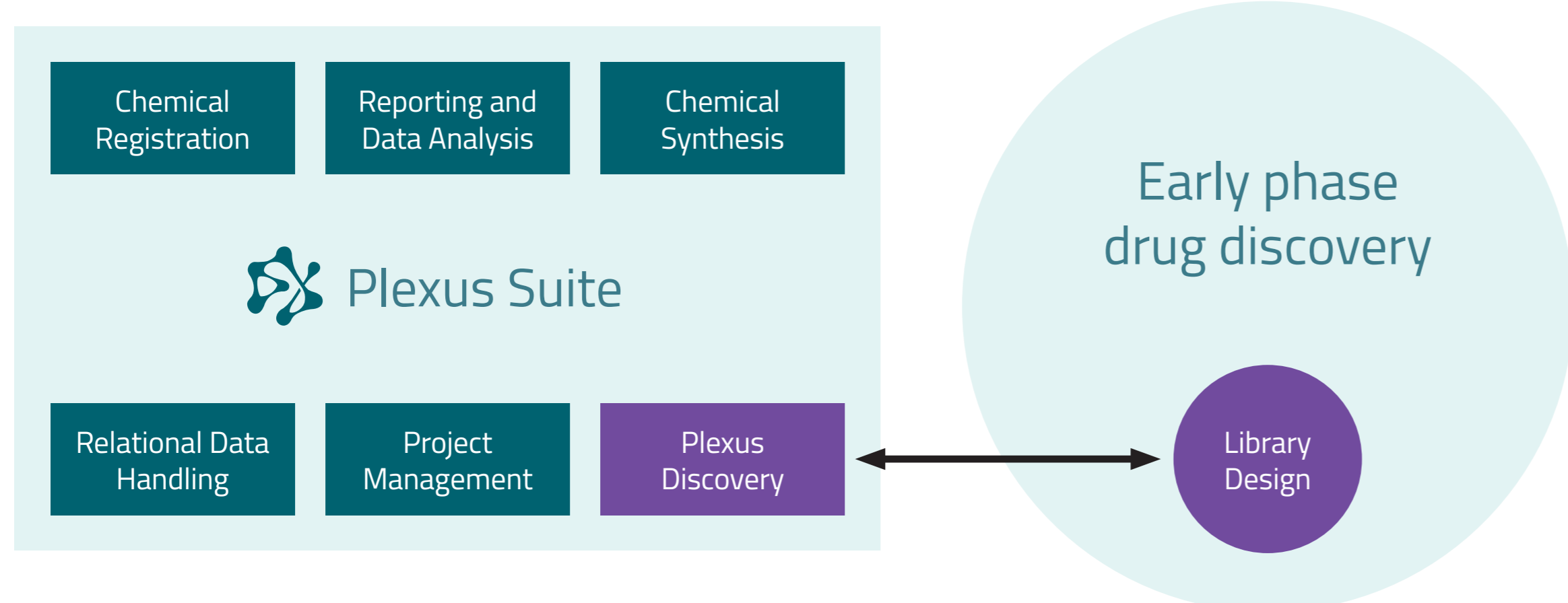


Plexus – Design & Discovery

KRISZTIAN NIESZ, IVAN SOLT AND ANDRAS STRACZ

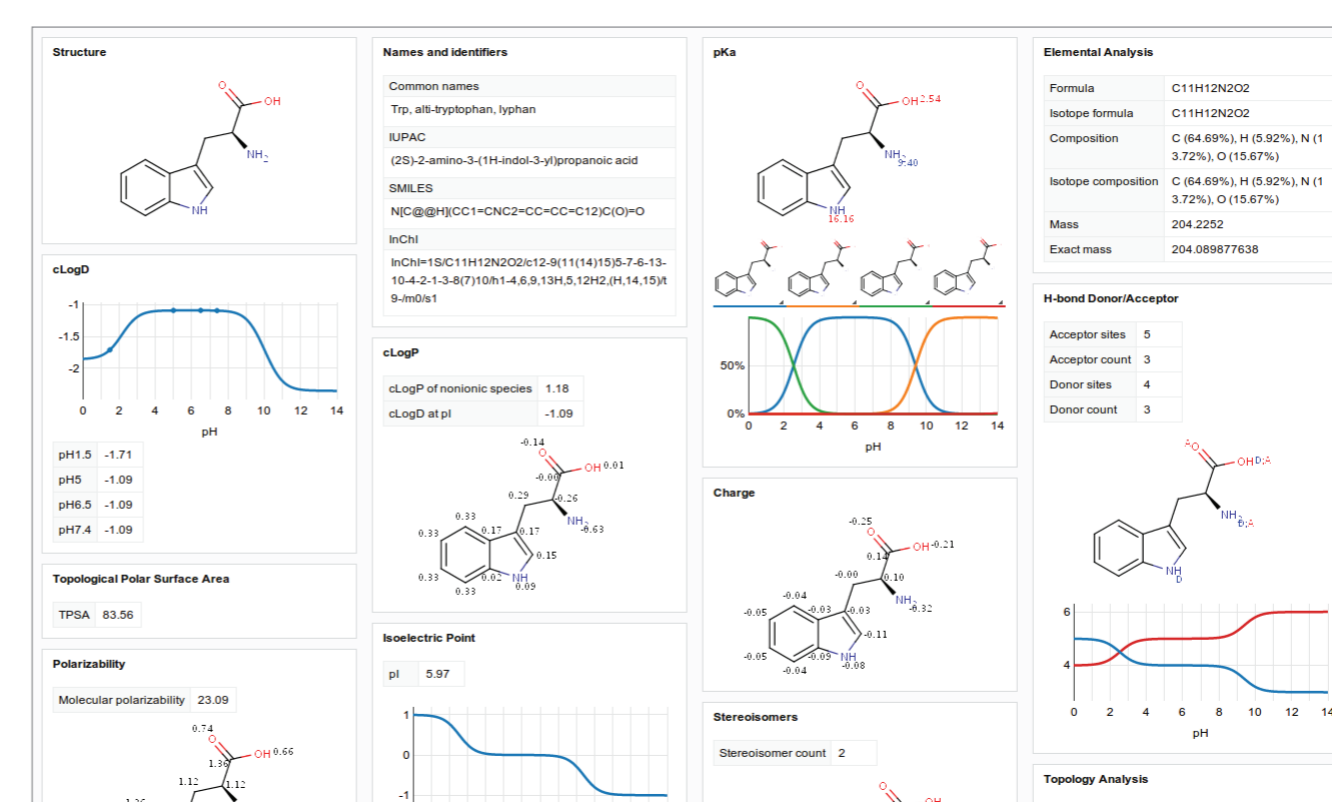
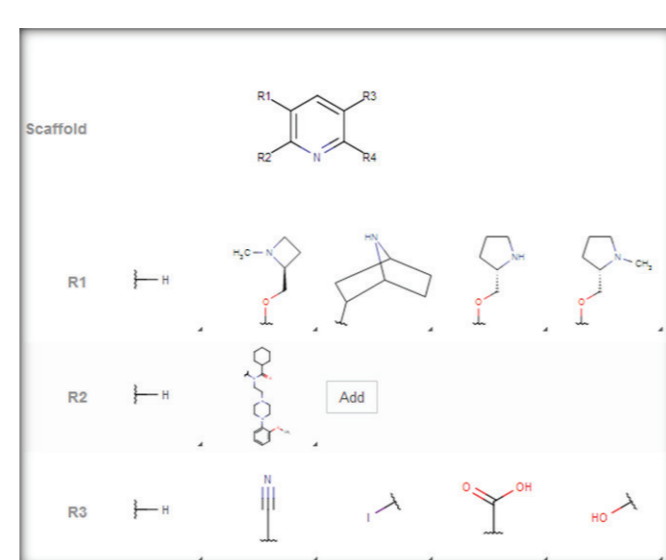
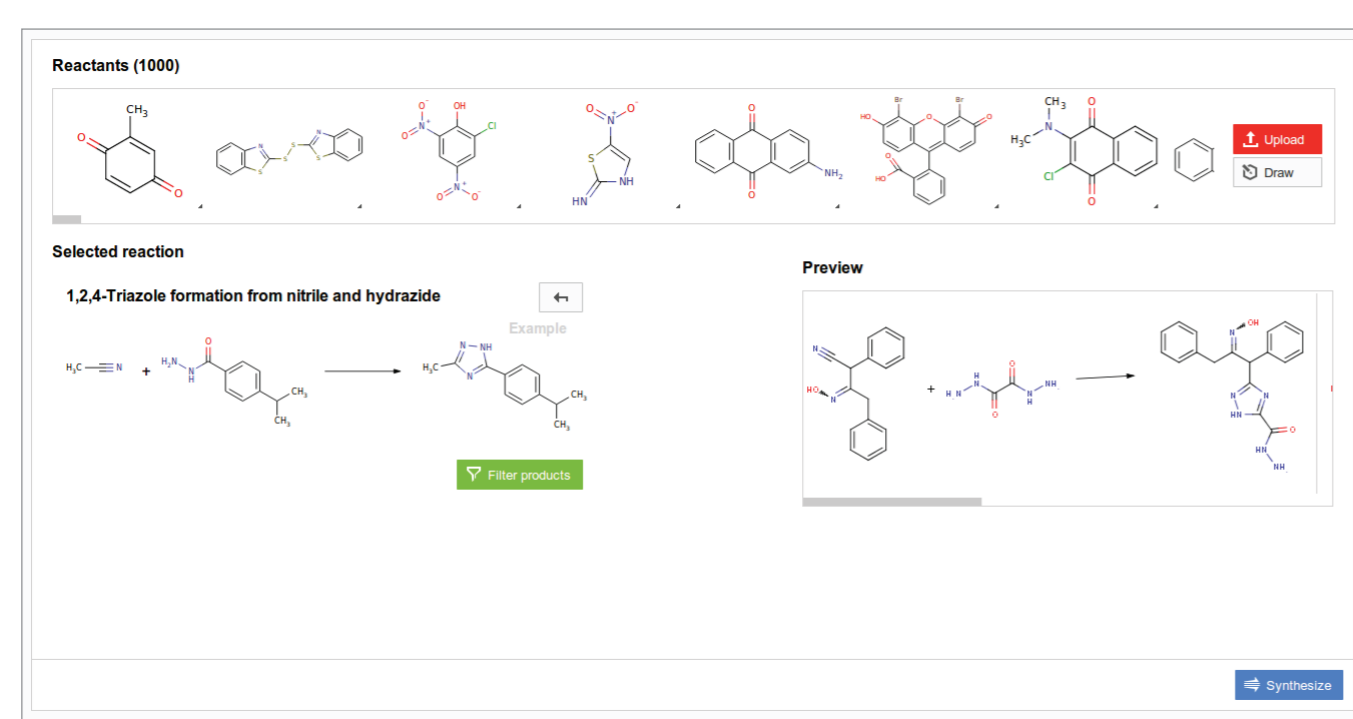


In a nutshell:

- Plexus Discovery is a full drug discovery platform that allows chemists to easily get on the most common virtual library design processes.
- It aims to give chemists powerful cheminformatics capabilities, advanced visualization and analytics tools within a series of intuitive interfaces which simplify and speed up their everyday research.
- It is wiring all of ChemAxon's extensive and industry leading cheminformatics capabilities to let researchers more quickly and easily design, evaluate and take action on new chemical entities.
- It is a desktop/web application, which not only can be installed for individual users on all major devices and operating systems, but can also be centrally deployed as a collaborative research environment.

Featuring:

- Marvin for JavaScript for drawing
- JChem backend serving any RDBMS
- Document to Structure technology
- Scaffold-based compound enumeration
- Reaction based combinatorial enumeration
- Phys-chem property based filtering
- A variety of similarity searching methods
- Similarity-based clustering
- All the useful exporting functions



Structure Source

multi structure file, office documents, online database

Data Storage

chemical structure database

enumeration

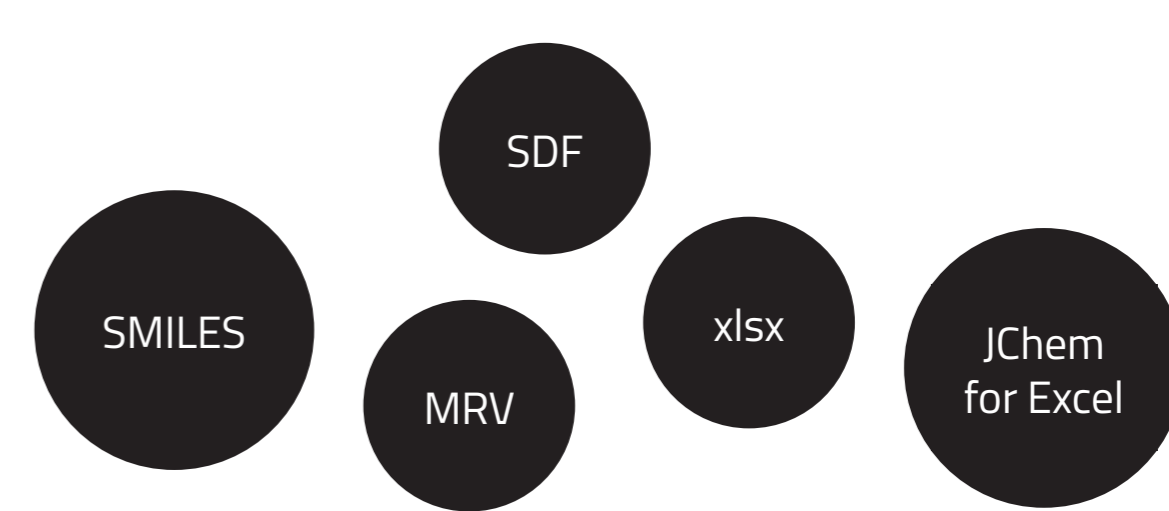
phys-chem properties

str. search, property filter, virtual screen

clustering

analyze

reports



ID	Structure	Cluster ID	Represent.	Formula
14		14	1	C8H14N2O2
19		14	0	C5H12N2O2
2971		14	0	C8H14N2O2
4145		14	0	C8H18N2O2
15		15	1	C8H14N4O2

Future prospectives

- Plexus Discovery is the first available module of Plexus Suite (PS), a single integrated framework designed to manage your scientific data.
- PS is built on industry-leading JChem Base & ChemAxon Web Services.
- PS is initially aimed at solving Medicinal Chemistry related issues, extending to other disciplines in future.
- PS is a modular system to serve specific, user-defined use cases (e.g. chemical library design)
- PS will feature a single, very intuitive User Interface to access all requested and supported scientific data and support multiple workflows
- Check back on us for updates!



References

<http://www.chemaxon.com/products/plexus/>