ChemAxon

20th anniversary

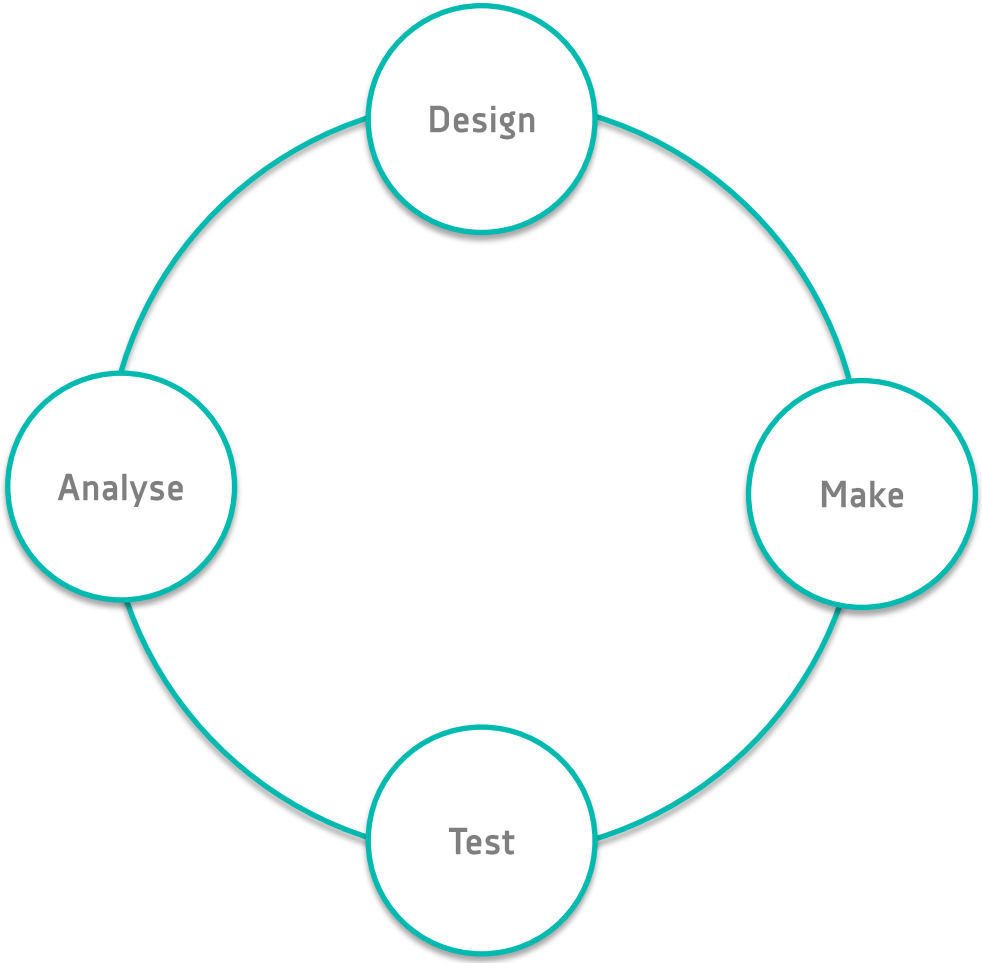
Serving drug discovery with cutting-edge software

ChemAxon

Akos Tarcsay
Senior Application Scientist
10-10-2018

Certara-ChemAxon synchrony for seamless analysis and design

Drug discovery



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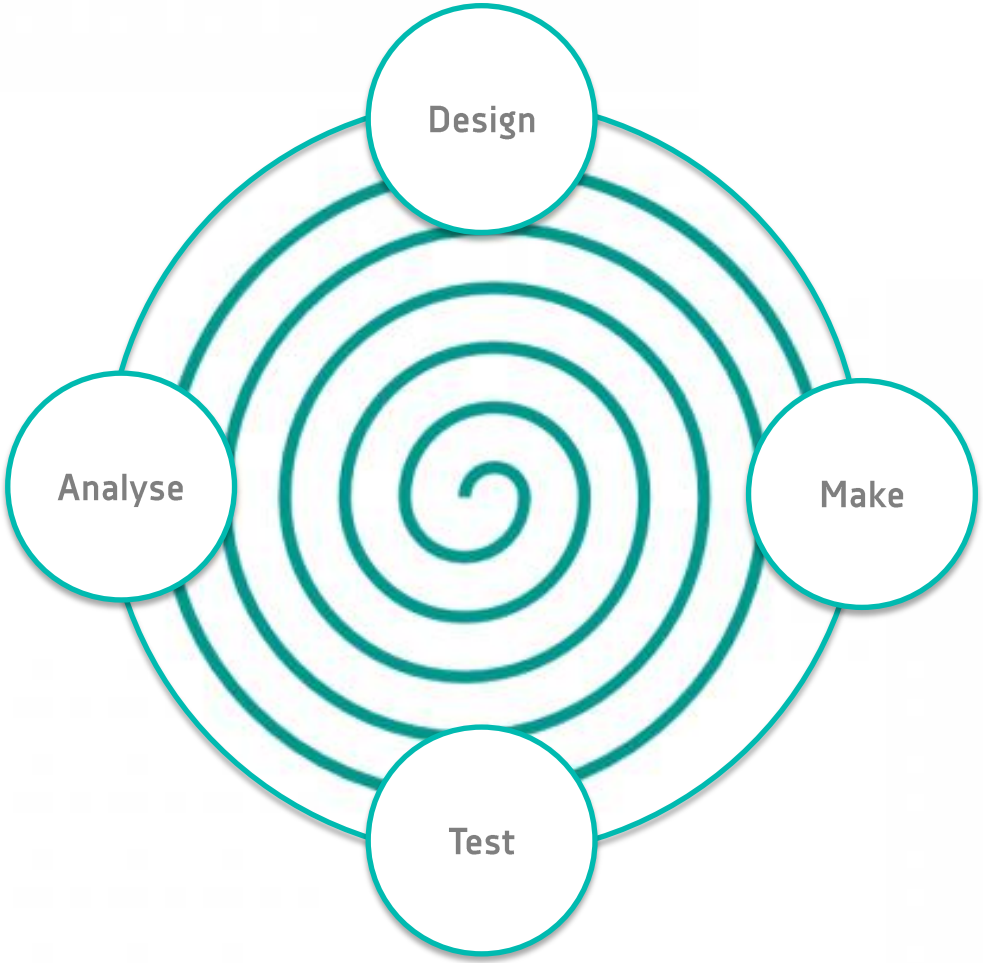
Drug discovery



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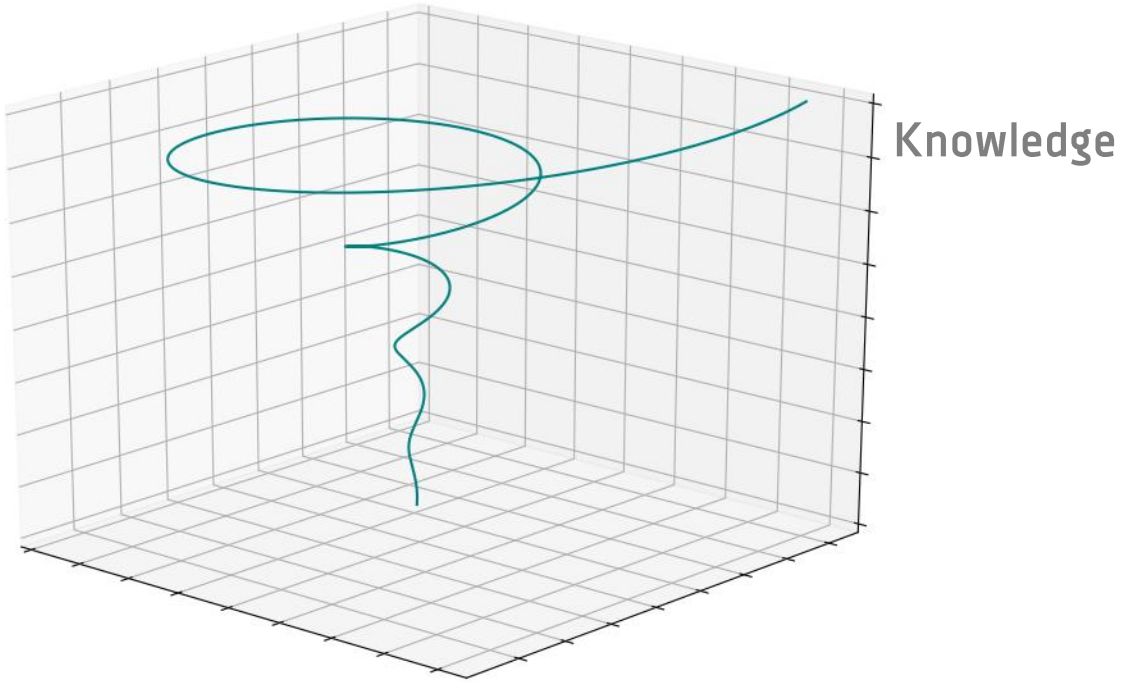
Drug discovery



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CLIMATE

SEARCH FOR HIDDEN HEAT

Pacific holds key to global-warming hiatus

PAGE 276

SUSTAINABILITY

TIME TO DITCH THE GDP

Future depends on better measures of national wealth

PAGE 293

PUBLIC HEALTH

GENE TESTING FOR ALL

Too-cautious regulation will stifle progress

PAGE 286

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9 770028 083095 28

ChemAxon for eDesign landscape

ChemAxon for eDesign landscape

2D Design
Marvin Live

Seamless design
Service integration (CCFW)
Idea management
eDesign registration

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ChemAxon for eDesign landscape

2D Design
Marvin Live

Virtual Reg.
eDesign DB

Seamless design
Service integration (CCFW)
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ChemAxon for eDesign landscape

2D Design	Virtual Reg.	Analysis
Marvin Live	eDesign DB	D360

Seamless design
Service integration (CCFW)
Idea management
eDesign registration

Consistent chemical backend
Standardization (Standardizer)
Structure check (Structure Checker)
Search (JChem Oracle Cartrdige)

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ChemAxon for eDesign landscape

2D Design	Virtual Reg.	Analysis	Report
Marvin Live	eDesign DB	D360	JChem4Office

Seamless design
Service integration (CCFW)
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Live structures in documents

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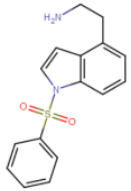

Brainstorming
space

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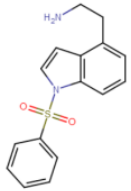
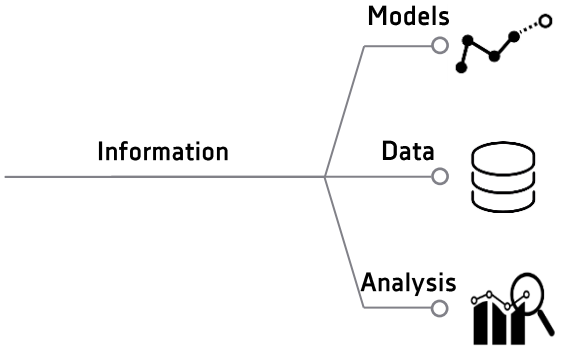
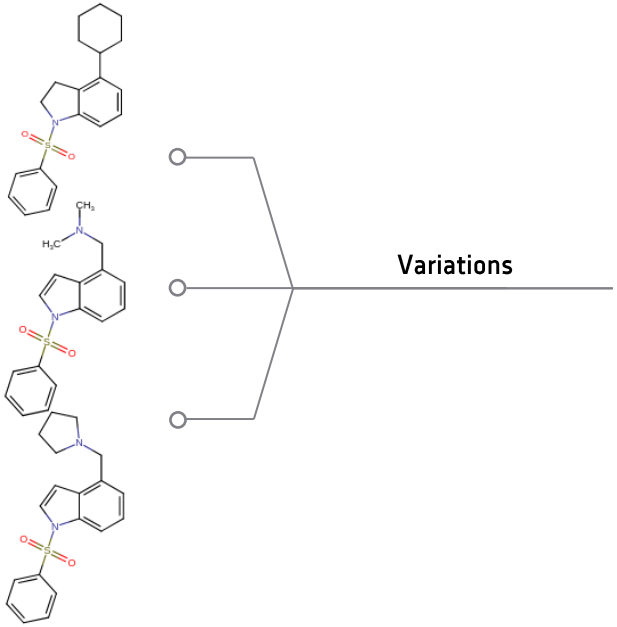
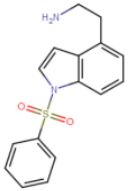


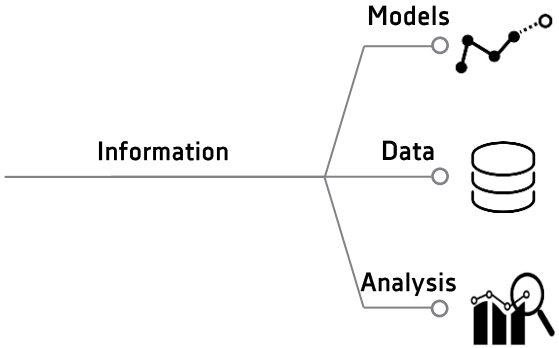


Brainstorming
space

ChemAxon

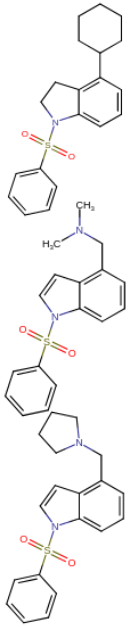




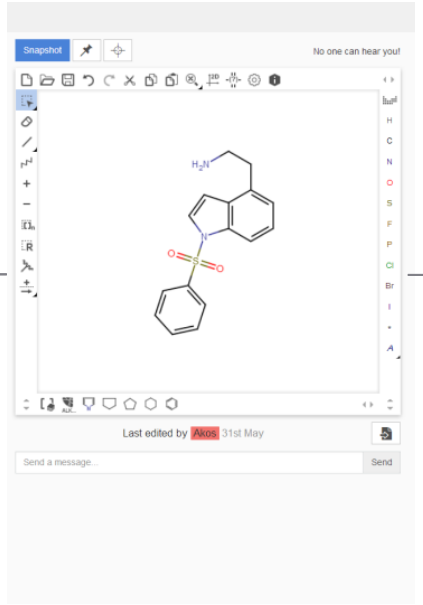


Brainstorming
space

ChemAxon



Variations



Information

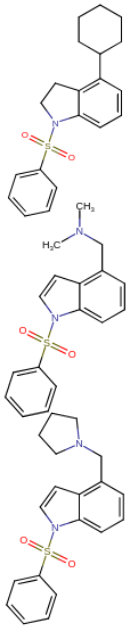
Models

Data

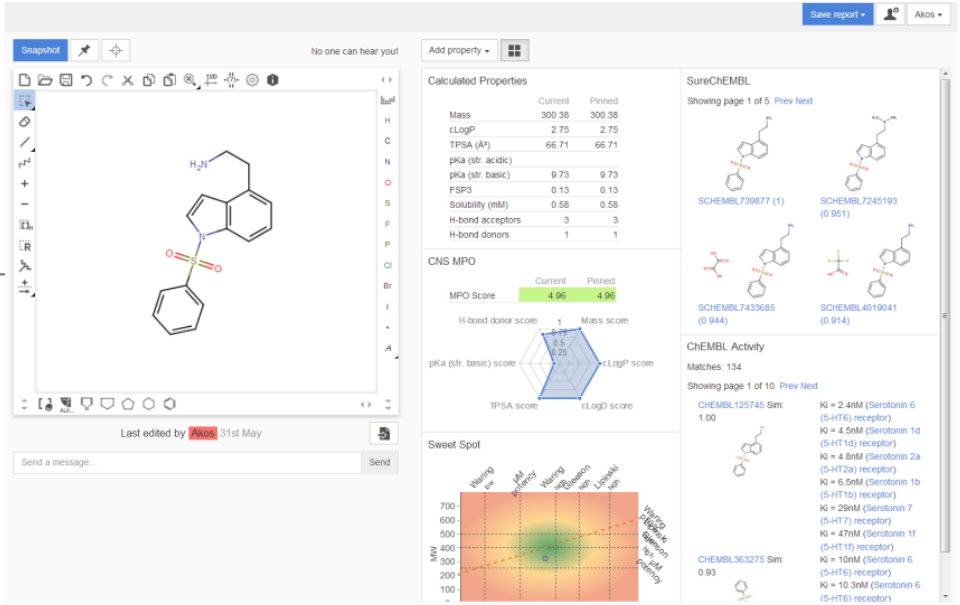
Analysis

Brainstorming
space

ChemAxon



Variations



Brainstorming space

Plugin results

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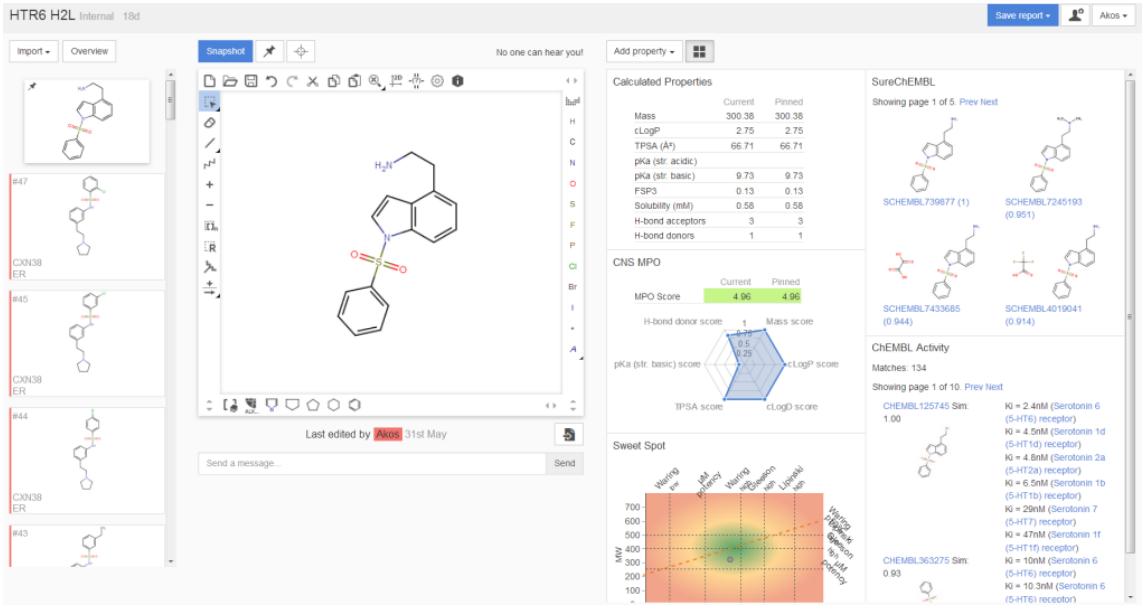

Idea
repository

Brainstorming
space

Plugin
results

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Plugin system

Service-agnostic

Easy to extend
(REST, SQL, CLI)

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Plugin system

Service-agnostic

Easy to extend
(REST, SQL, CLI)

Real-time

As you draw

Plugin system

Service-agnostic

Easy to extend
(REST, SQL, CLI)

Real-time

As you draw

Dynamic

Right amount of information

Real-time plugins

Mining

SciFinder
Reaxys
ChEMBL
SureChEMBL
Corporate assay DB
Legislations
Registration

Real-time plugins

Mining

SciFinder
Reaxys
ChEMBL
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Legislations
Registration

Exploring

Med. chem. descriptors
Predictive models
Conformations
Overlays
Similarities
Charts
KNIME workflows
PP protocols
Ligand preparation

Real-time plugins

Mining

SciFinder
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Med. chem. descriptors
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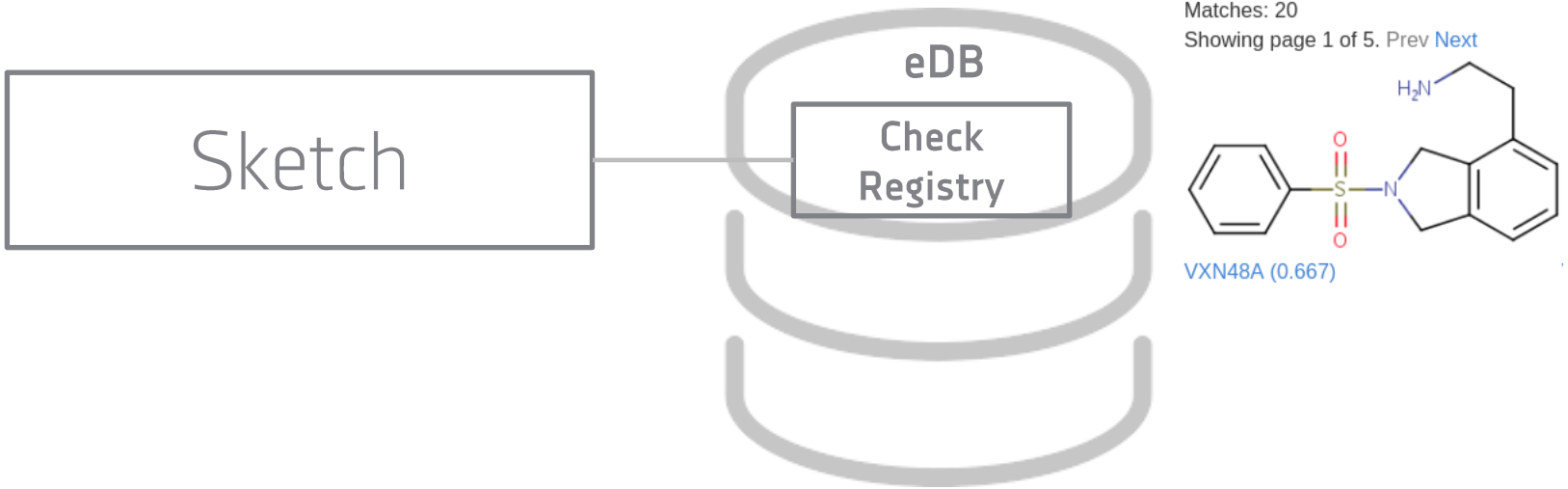
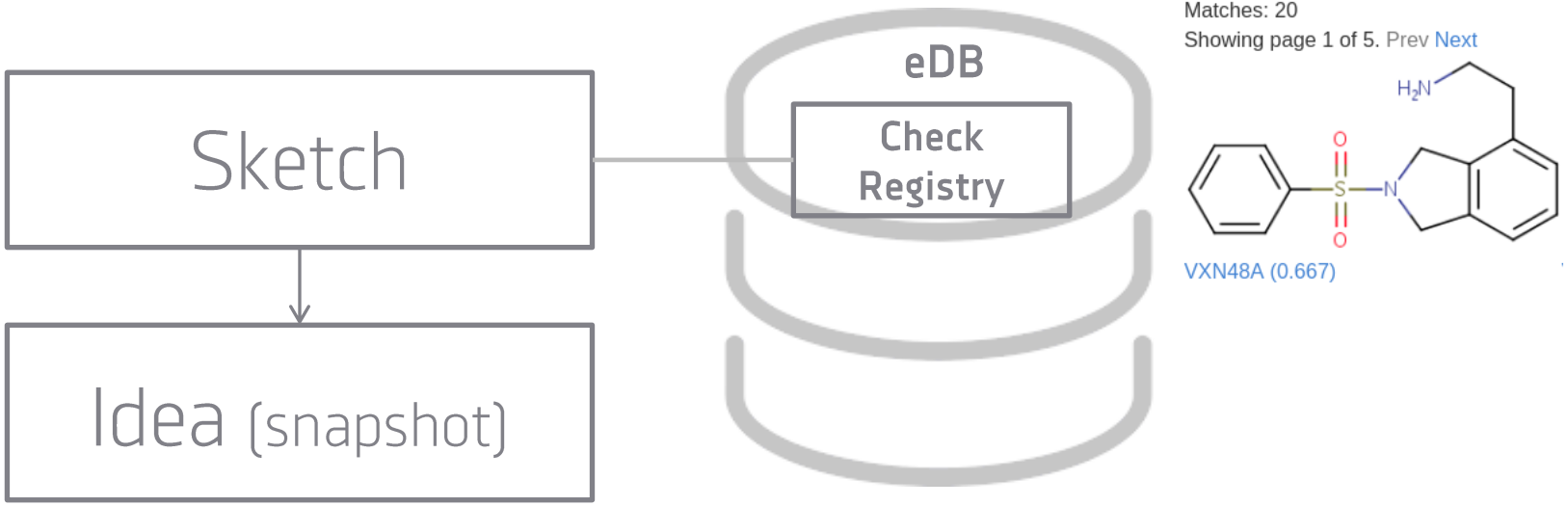
PP protocols
Ligand preparation

Planning

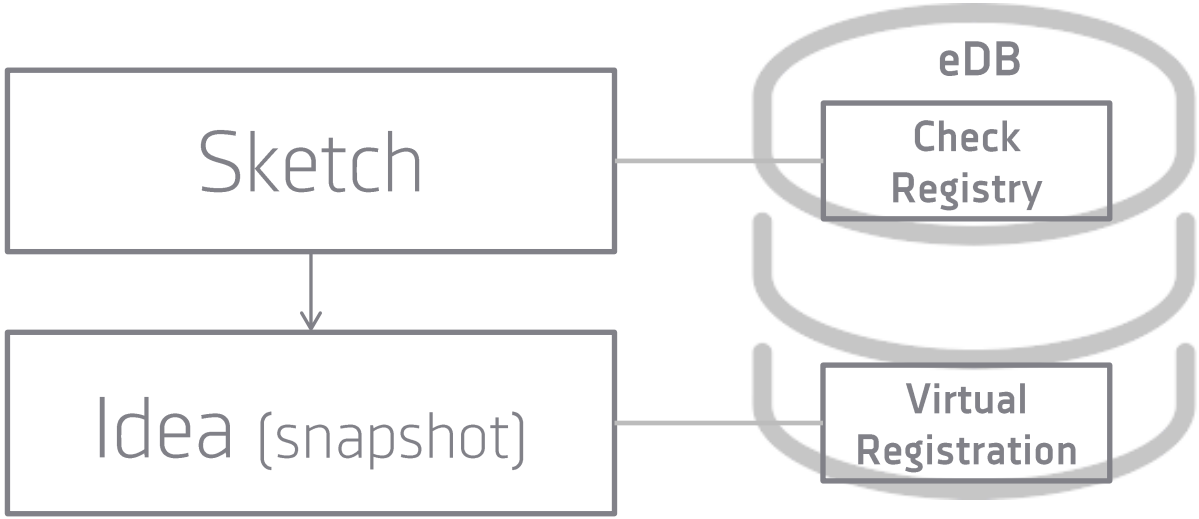
Reactions
Inventory
Supplier catalogs

Sketch


Sketch
eDB
Check
Registry
Matches: 20
Showing page 1 of 5. Prev Next
VXN48A (0.667)


Sketch
Idea (snapshot)
eDB
Check Registry
Matches: 20
Showing page 1 of 5. Prev Next
VXN48A (0.667)

ChemAxon



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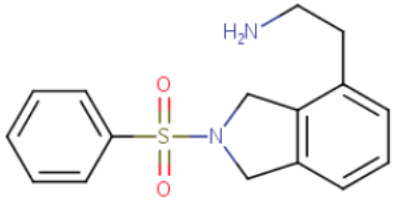
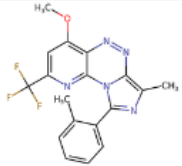


VXN48A (0.667)

A



VXN83 #2

Activity

Hypothesis

Required assay

Medium

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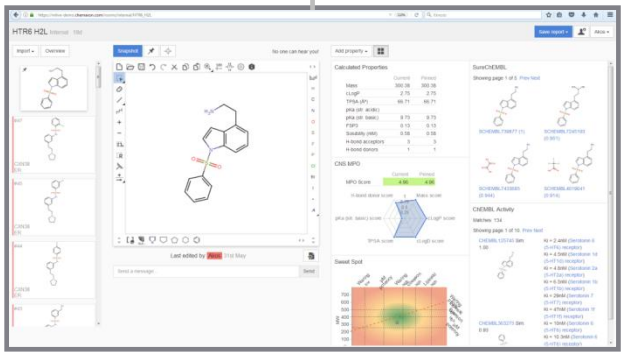
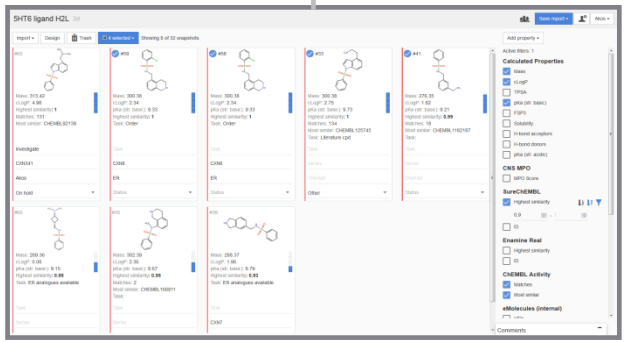
Marvin Live

Create (design mode)



Manage (overview mode)



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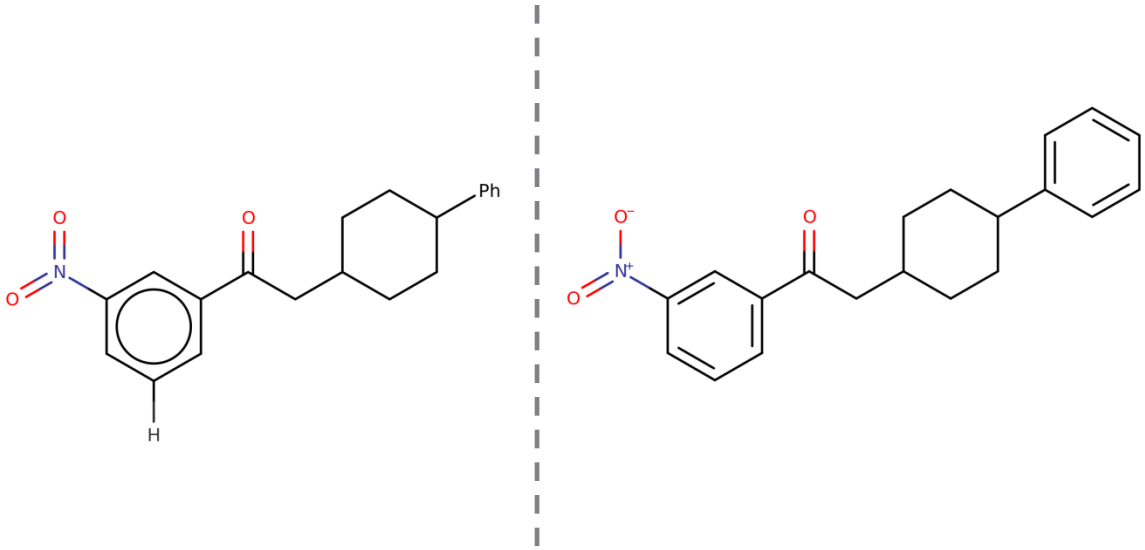
Standardizer for consistency



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JChem: database engine for chemistry

Manage chemical information without compromise

- full structure, substructure, superstructure and duplicate matching
- variable similarity searching including reaction similarity
- registration and searching of polymers, mixtures and formulations
- generic query atoms
- various query properties supported
- full SMARTS support including recursive SMARTS
- R-group query expressions
- reaction queries, including reaction mapping, reaction query features
- stereo specific structure and reaction specifications
- structure canonicalization
- chemical terms support
- different types of tautomer search

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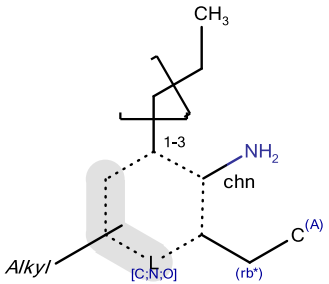
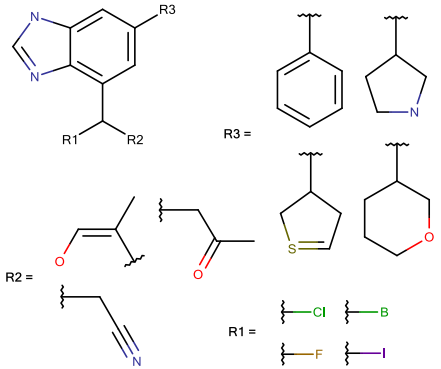
JChem: database engine for chemistry



a query structure



a Markush structure

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THANK YOU

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