

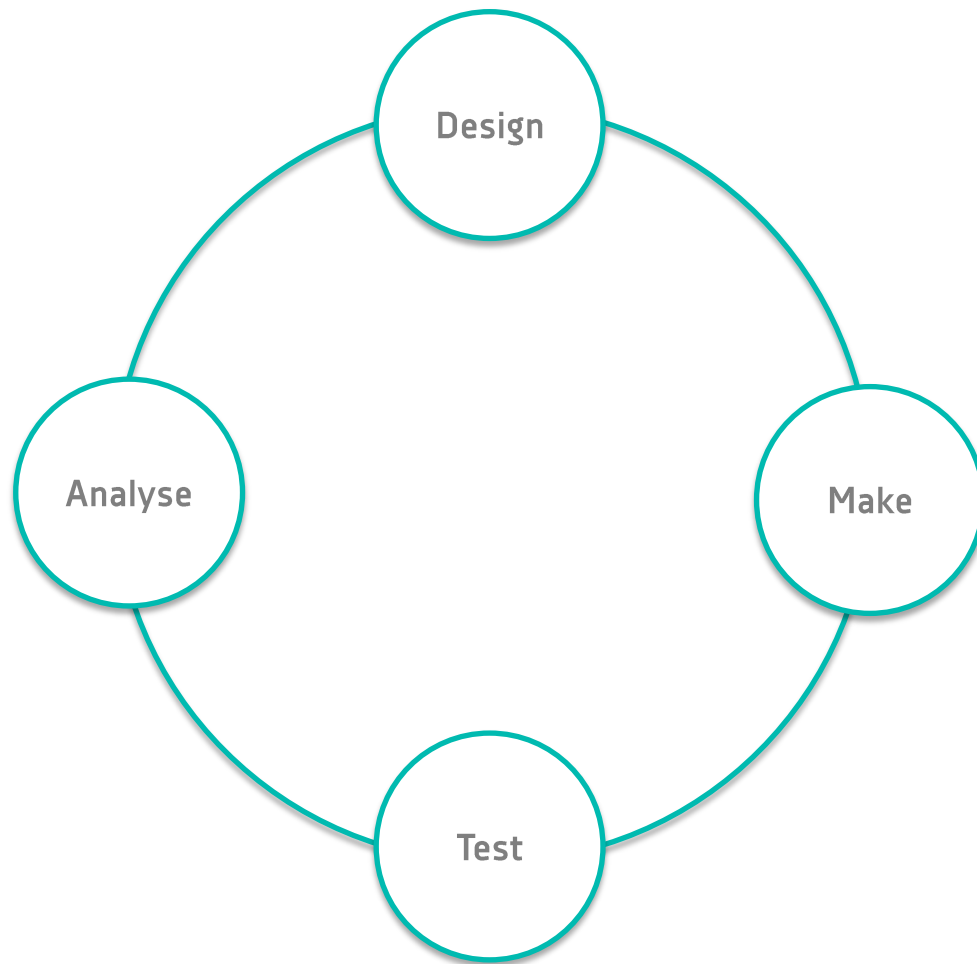
20th

anniversary

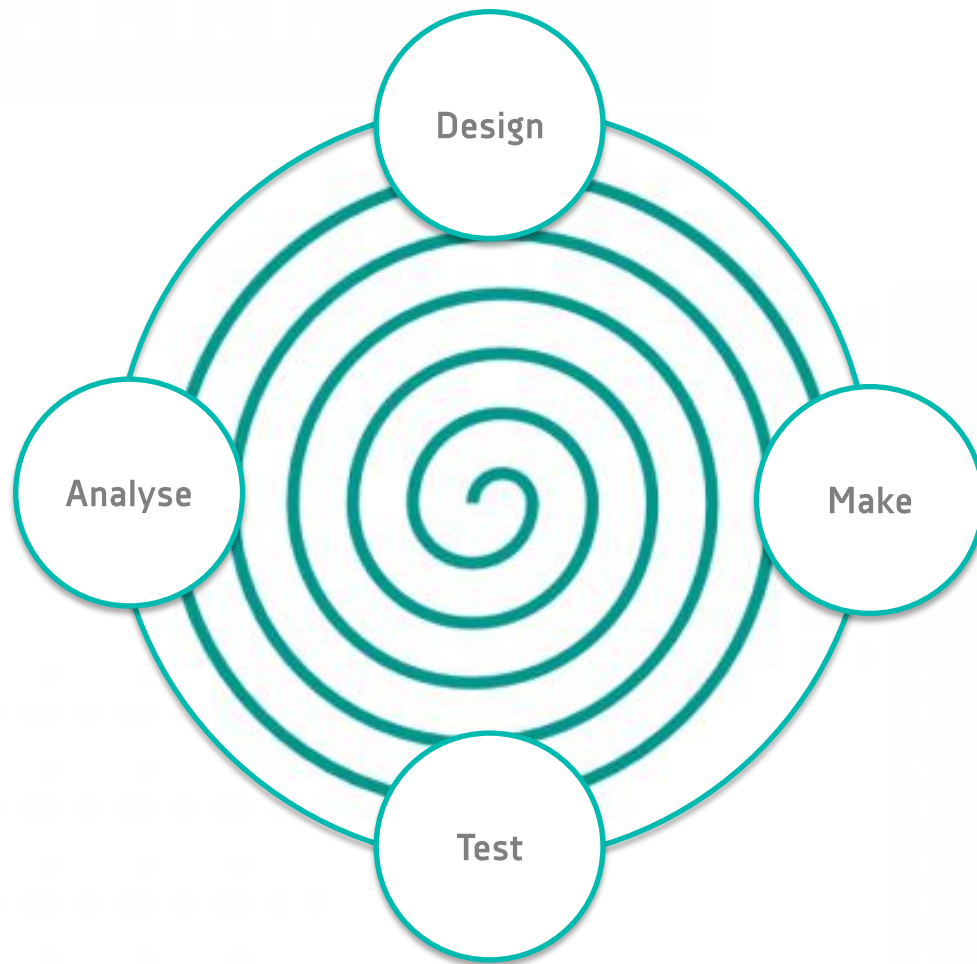
Serving drug discovery with
cutting-edge software

Certara-ChemAxon synchrony for seamless analysis and design

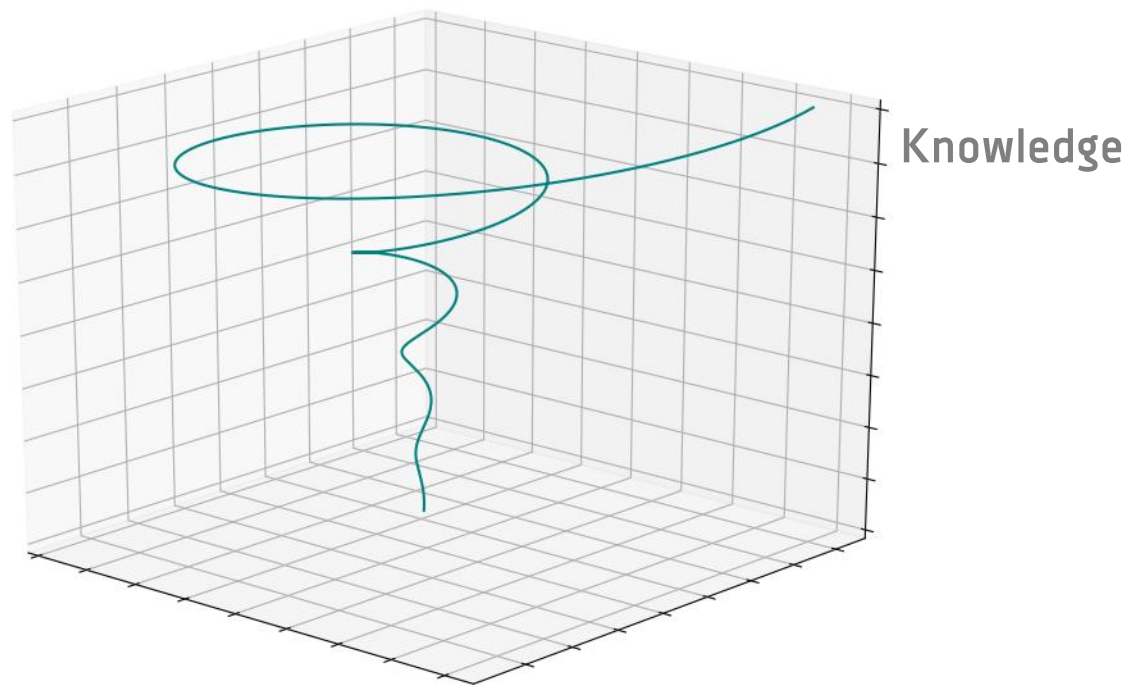
Drug discovery



Drug discovery



Drug discovery



nature

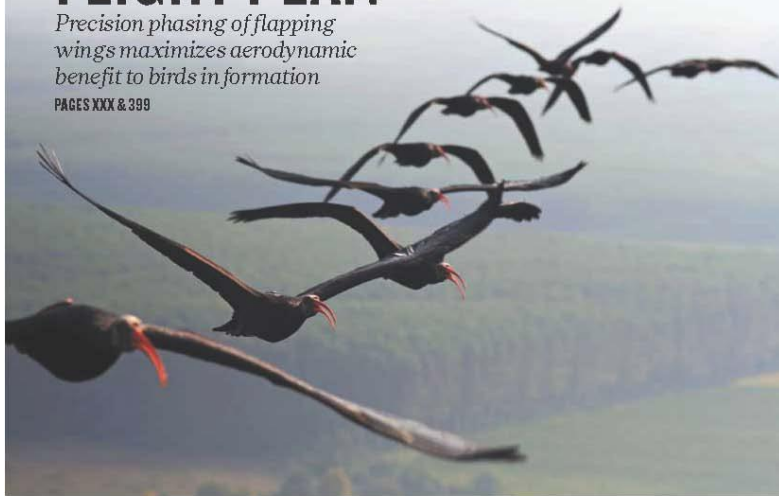
THE INTERNATIONAL WEEKLY JOURNAL OF SCIENCE

INSIGHT
Frontiers in
Biology

FLIGHT PLAN

Precision phasing of flapping wings maximizes aerodynamic benefit to birds in formation

PAGES XXX & 399



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 283



PUBLIC HEALTH

GENE TESTING FOR ALL

Too-cautious regulation will stifle progress

PAGE 288

NATURE.COM/NATURE

16 January 2014 £10

Vol. 505, No. 7483



28

 ChemAxon

ChemAxon for eDesign landscape

ChemAxon for eDesign landscape

2D Design

Marvin Live

Seamless design

Service integration (CCFW)

Idea management

eDesign registration

ChemAxon for eDesign landscape

2D Design

Marvin Live

Virtual Reg.

eDesign DB

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ChemAxon for eDesign landscape

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Analysis

D360

Seamless design

Service integration (CCFW)
Idea management
eDesign registration

Consistent chemical backend

Standardization (Standardizer)
Structure check (Structure Checker)
Search (JChem Oracle Cartridge)

ChemAxon for eDesign landscape

2D Design

Marvin Live

Virtual Reg.

eDesign DB

Analysis

D360

Report

JChem4Office

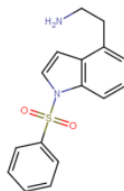
Seamless design

Service integration (CCFW)
Idea management
eDesign registration

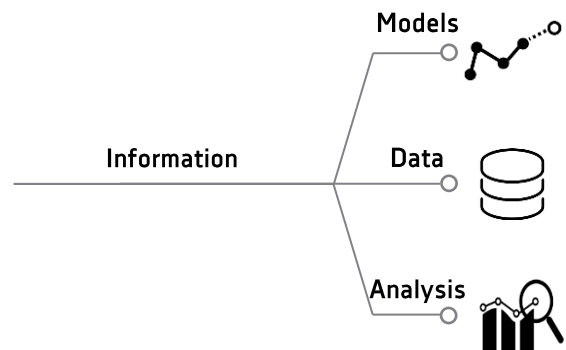
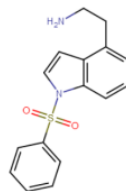
Consistent chemical backend

Standardization (Standardizer)
Structure check (Structure Checker)
Search (JChem Oracle Cartridge)

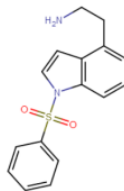
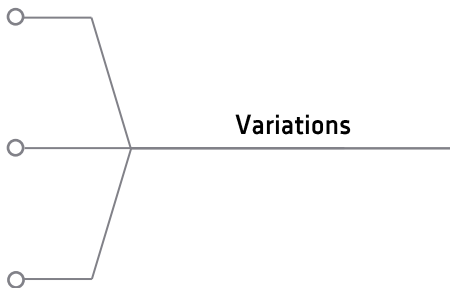
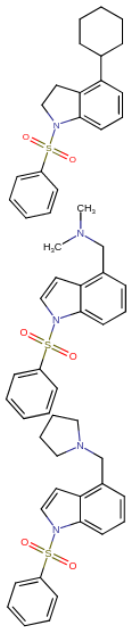
Live structures in documents



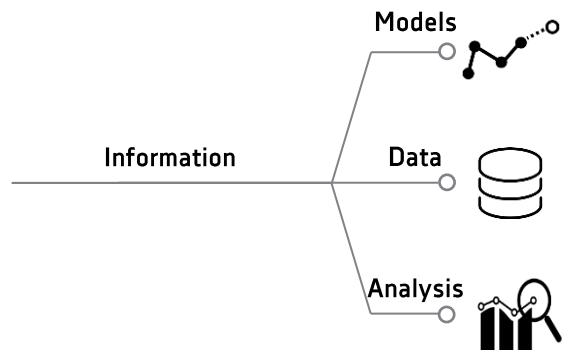
Brainstorming
space

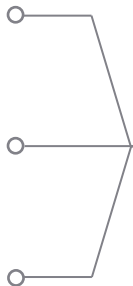
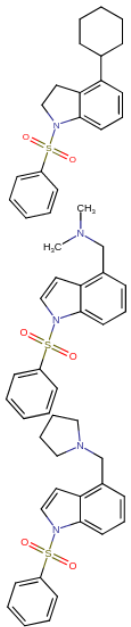


Brainstorming
space

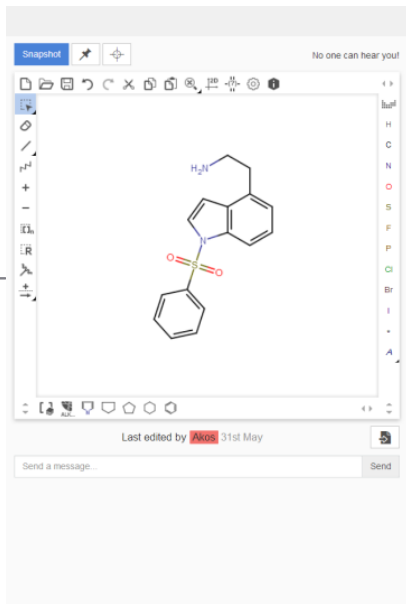


Brainstorming
space





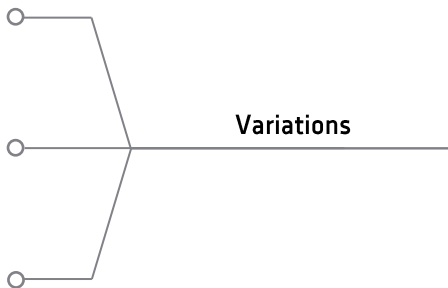
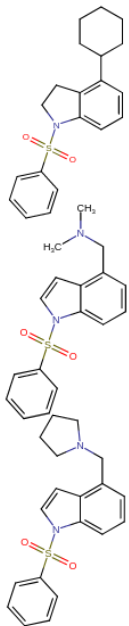
Variations



Information



Brainstorming
space



Variations

The screenshot displays the ChemAxon software interface. The central window shows a chemical structure of a benzimidazole derivative with a phenylsulfonyl group and a piperidine ring. The interface includes a toolbar at the top with various editing tools. Below the structure editor, there are several panels:

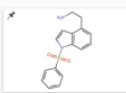
- Calculated Properties:** A table showing various molecular descriptors for the current and pinned structures.
- CNS MPO:** A section showing the MPO score and a radar chart comparing different scores.
- Sweet Spot:** A heatmap showing the relationship between various molecular descriptors.
- SureChEMBL:** A section showing search results for similar compounds, including their IDs and similarity scores.
- CHEMBL Activity:** A section showing matches for the structure, including their IDs and activity data.

Brainstorming
space

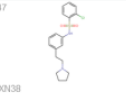
Plugin
results

HTR6 H2L Internal 18d Save report Akos

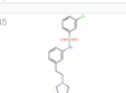
Import Overview



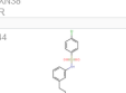
#47
CXN38
ER



#45
CXN38
ER



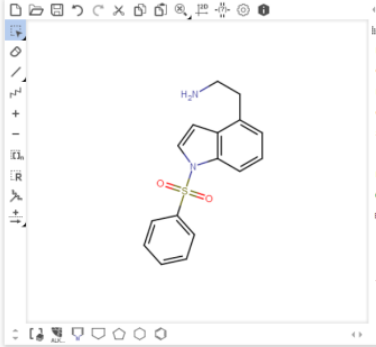
#44
CXN38
ER



#43
CXN38
ER

Snapshot

No one can hear you!



Last edited by Akos 31st May

Send a message... Send

Add property

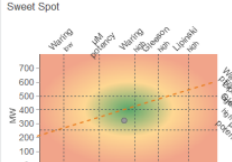
Calculated Properties	Current	Pinned
Mass	300.38	300.38
cLogP	2.75	2.75
TPSA (Å²)	66.71	66.71
pKa (str. acidic)		
pKa (str. basic)	9.73	9.73
FSP3	0.13	0.13
Solubility (mM)	0.58	0.58
H-bond acceptors	3	3
H-bond donors	1	1

CNS MPO

MPO Score	Current	Pinned
MPO Score	4.96	4.96


H-bond donor score: 1
 Mass score: 1
 pKa (str. basic) score: 0.25
 cLogP score: 1
 TPSA score: 0.5
 cLogD score: 1

Sweet Spot




SureChEMBL


Showing page 1 of 5 [Prev](#) [Next](#)




SCHEMBL739877 (1)



SCHEMBL7245193 (0.951)



SCHEMBL7433685 (0.944)



SCHEMBL4019041 (0.914)

CHEMBL Activity

Matches: 134

Showing page 1 of 10 [Prev](#) [Next](#)

CHEMBL125745 Sim: 1.00

- Ki = 2.4nM (Serotonin 6 (5-HT6) receptor)
- Ki = 4.5nM (Serotonin 1d (5-HT1d) receptor)
- Ki = 4.8nM (Serotonin 2a (5-HT2a) receptor)
- Ki = 6.5nM (Serotonin 1b (5-HT1b) receptor)
- Ki = 22nM (Serotonin 7 (5-HT7) receptor)
- Ki = 47nM (Serotonin 1f (5-HT1f) receptor)

CHEMBL363275 Sim: 0.93

- Ki = 10nM (Serotonin 6 (5-HT6) receptor)
- Ki = 10.3nM (Serotonin 6 (5-HT6) receptor)

Idea
repository

Brainstorming
space

Plugin
results

Plugin system



Service-agnostic

Easy to extend
(REST, SQL, CLI)

Plugin system



Service-agnostic

Easy to extend
(REST, SQL, CLI)



Real-time

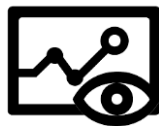
As you draw

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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Corporate assay DB

Legislations

Registration

Exploring

Med. chem. descriptors

Predictive models

Conformations

Overlays

Similarities

Charts

KNIME workflows

PP protocols

Ligand preparation

Real-time plugins

Mining

SciFinder
Reaxys
ChEMBL
SureChEMBL
Corporate assay DB
Legislations
Registration

Exploring

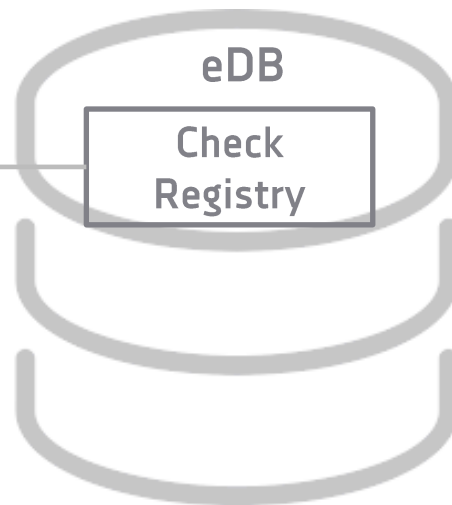
Med. chem. descriptors
Predictive models
Conformations
Overlays
Similarities
Charts
KNIME workflows
PP protocols
Ligand preparation

Planning

Reactions
Inventory
Supplier catalogs

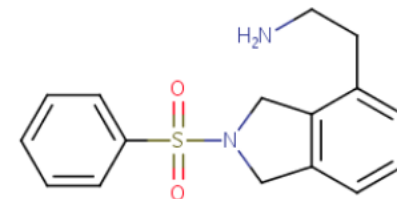
Sketch

Sketch

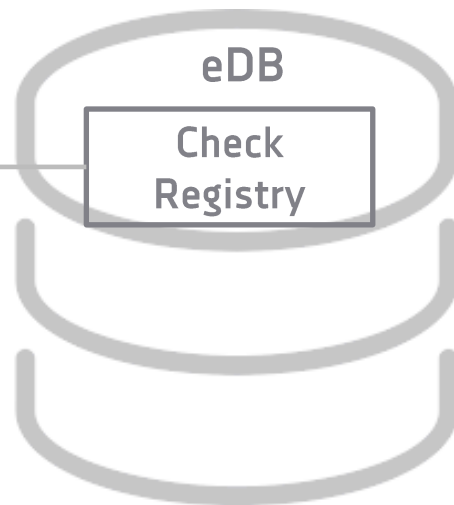
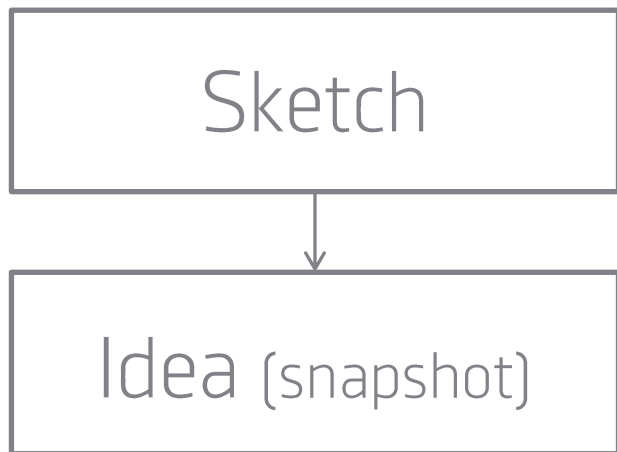


Matches: 20

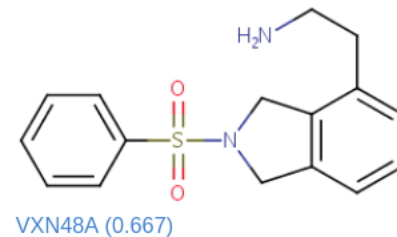
Showing page 1 of 5. [Prev](#) [Next](#)

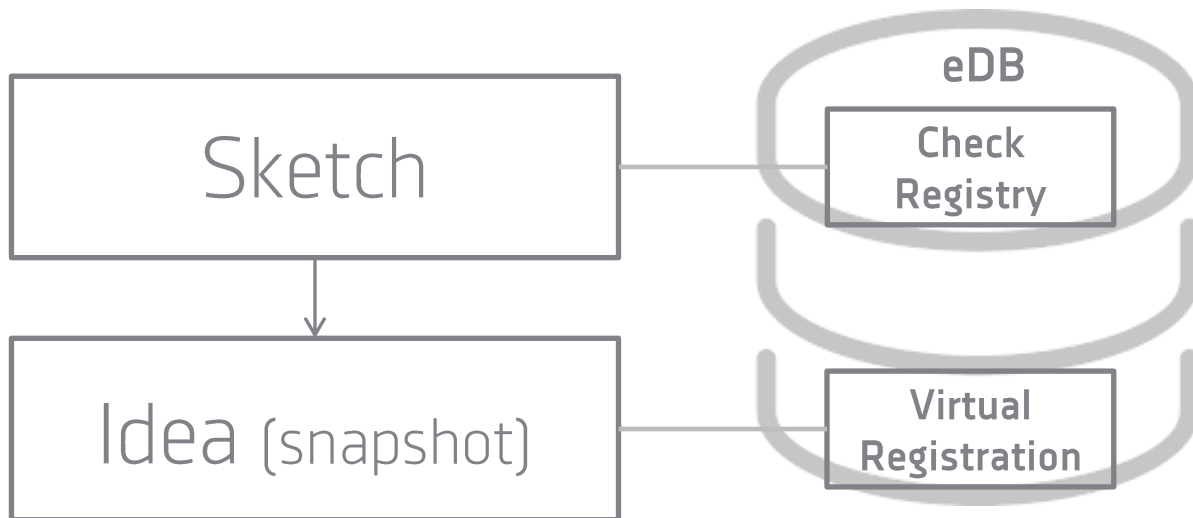


VXN48A (0.667)



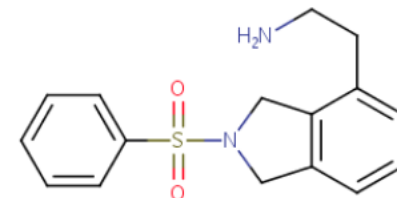
Matches: 20
Showing page 1 of 5. [Prev](#) [Next](#)





Matches: 20

Showing page 1 of 5. [Prev](#) [Next](#)



VXN48A (0.667)

A

Chemical structure of VXN83 #2, a complex heterocyclic molecule with multiple rings, including a benzothiazine core, and various substituents including a methoxy group, a methyl group, and a hydroxyl group.

COC1=CC=C2N3C(=C1)N(C)C(=O)N3C2=O

VXN83 #2

Activity

Hypothesis

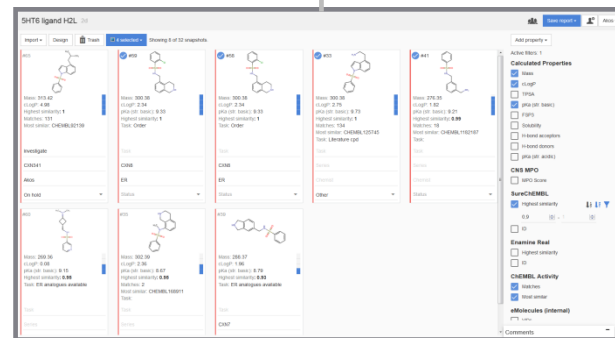
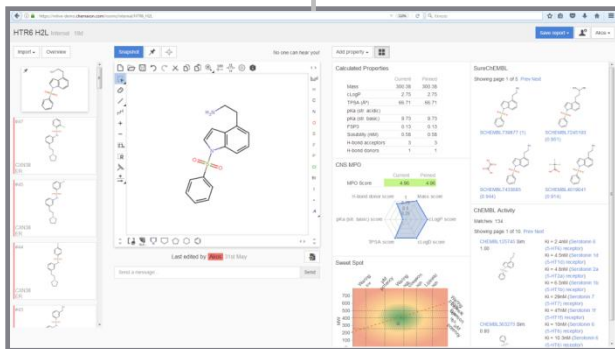
Required assay

Medium

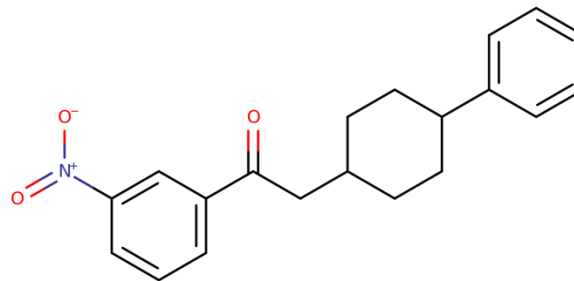
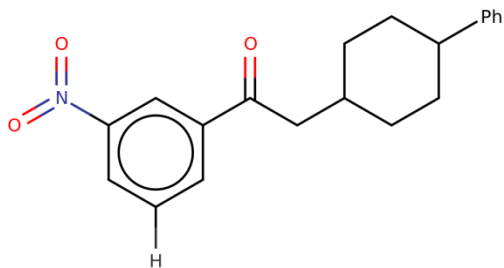
Marvin Live

Create
(design mode)

Manage
(overview mode)



Standardizer for consistency



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

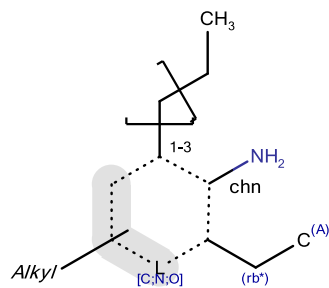
*stereo specific
structure and
reaction
specifications*

structure
canonicalization

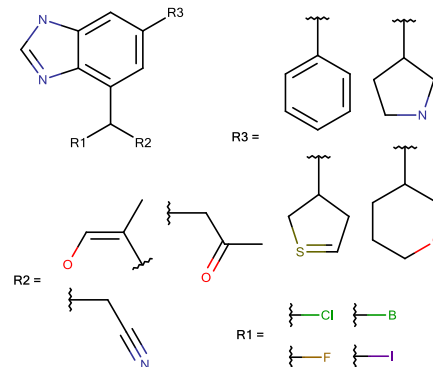
chemical terms
support

different types of
tautomer search

JChem: database engine for chemistry



a query structure



a Markush structure

ChemAxon for eDesign landscape

2D Design

MarvinLive

Virtual Reg.

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eDesign registration

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Search (JChem Oracle cartridge)

Live structures in documents





THANK YOU