Introducing Plexus

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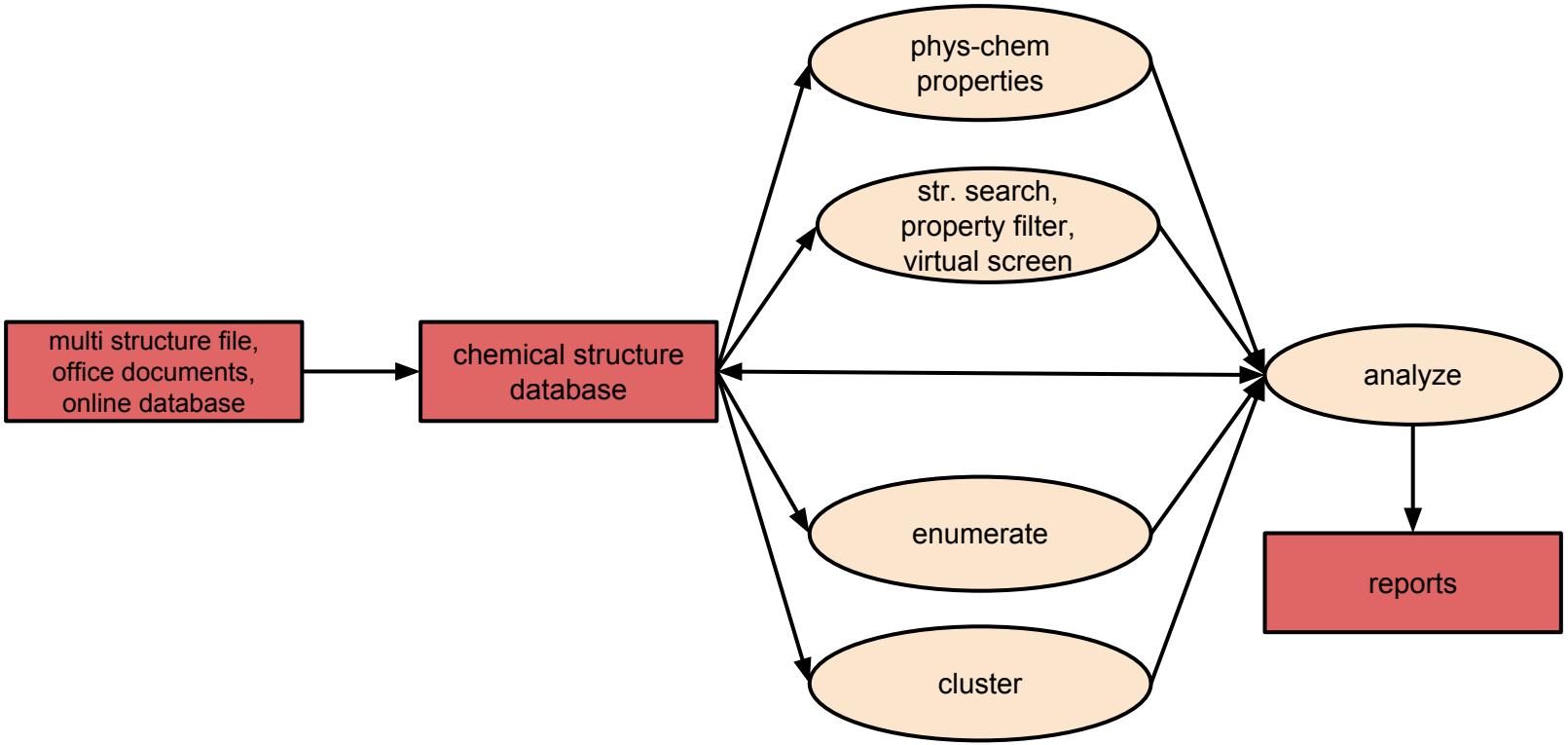
UGM

Early phase drug discovery

library design

ChemAxon


multi structure file,
office documents,
online database
chemical structure
database
phys-chem
properties
str. search,
property filter,
virtual screen
enumerate
cluster
analyze
reports

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Versatile

- Thin client, web app
- Deployable in all scenarios
  - PC/Mac
  - internal network
  - external partners
  - cloud

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Plexus - data table

- spreadsheet view for your data, expected features
- import office documents
- export JChem for Excel workbook
- fast, looks great
- easily add phys-chem properties, filters

EP2377850A1 - Plexus

192.168.1.7:8080/plexus/table/sample/EP2377850A1

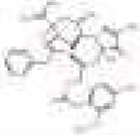
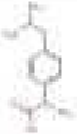
Plexus Import Enumeration Data table: EP2377850A1

Import of EP2377850A1 pdf completed.

Searching

Search Displaying from 1 to 6 of 1230 records

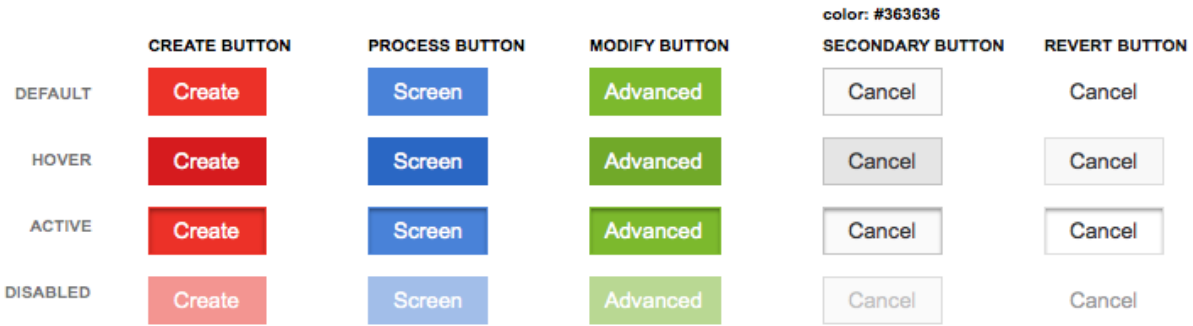
Add new row Export

ID	Structure	Formula	Molweight	Text	Page	Context	Type
1		C18H27NO3	305.2119	capsaicin	3	[illegible]	compound
2		C37H40O9	628.2697	resiniferatoxin	3	[illegible]	compound
3		C18H27NO3	305.2119	capsaicin	3	[illegible]	compound
4		C13H10O2	200.2026	[illegible]	3	[illegible]	compound
5		C18H27NO3	305.2119	Capsaicin	3	[illegible]	compound
6		C18H27NO3	305.2119	capsaicin	3	[illegible]	compound

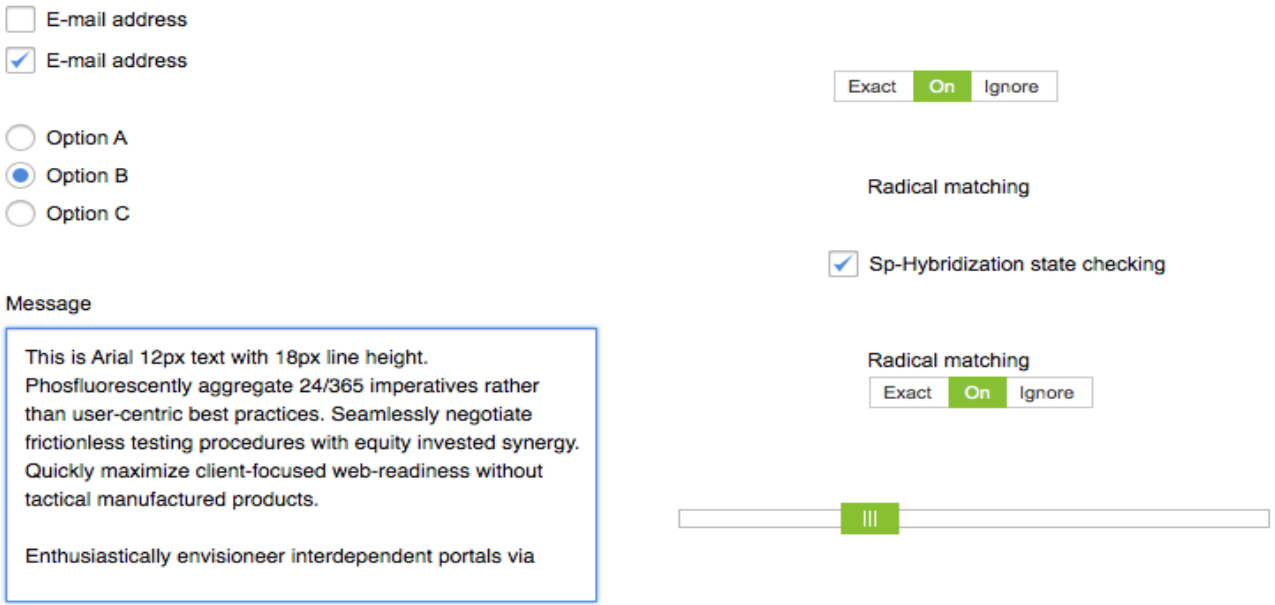
User experience

- design - consistent web app look & feel
- high visibility of important actions
- layout - clear and structured, fluid design
- user experience - fast, streamlined, intuitive solutions
- Marvin for JavaScript fits perfectly

Plexus - style guide / buttons



Plexus - style guide / settings elements



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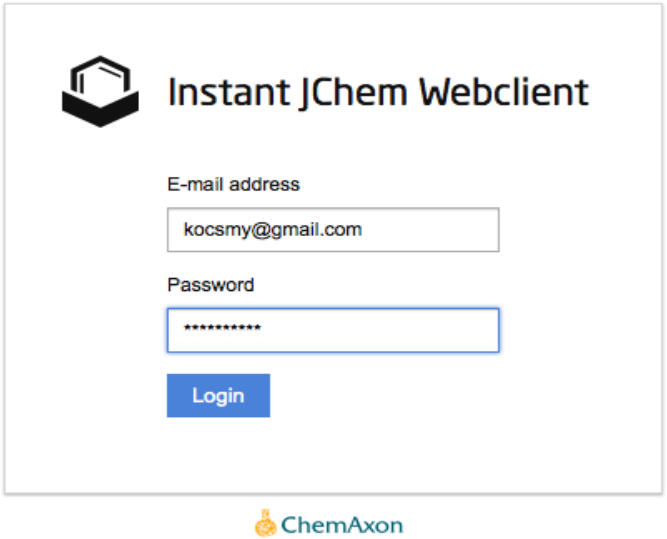
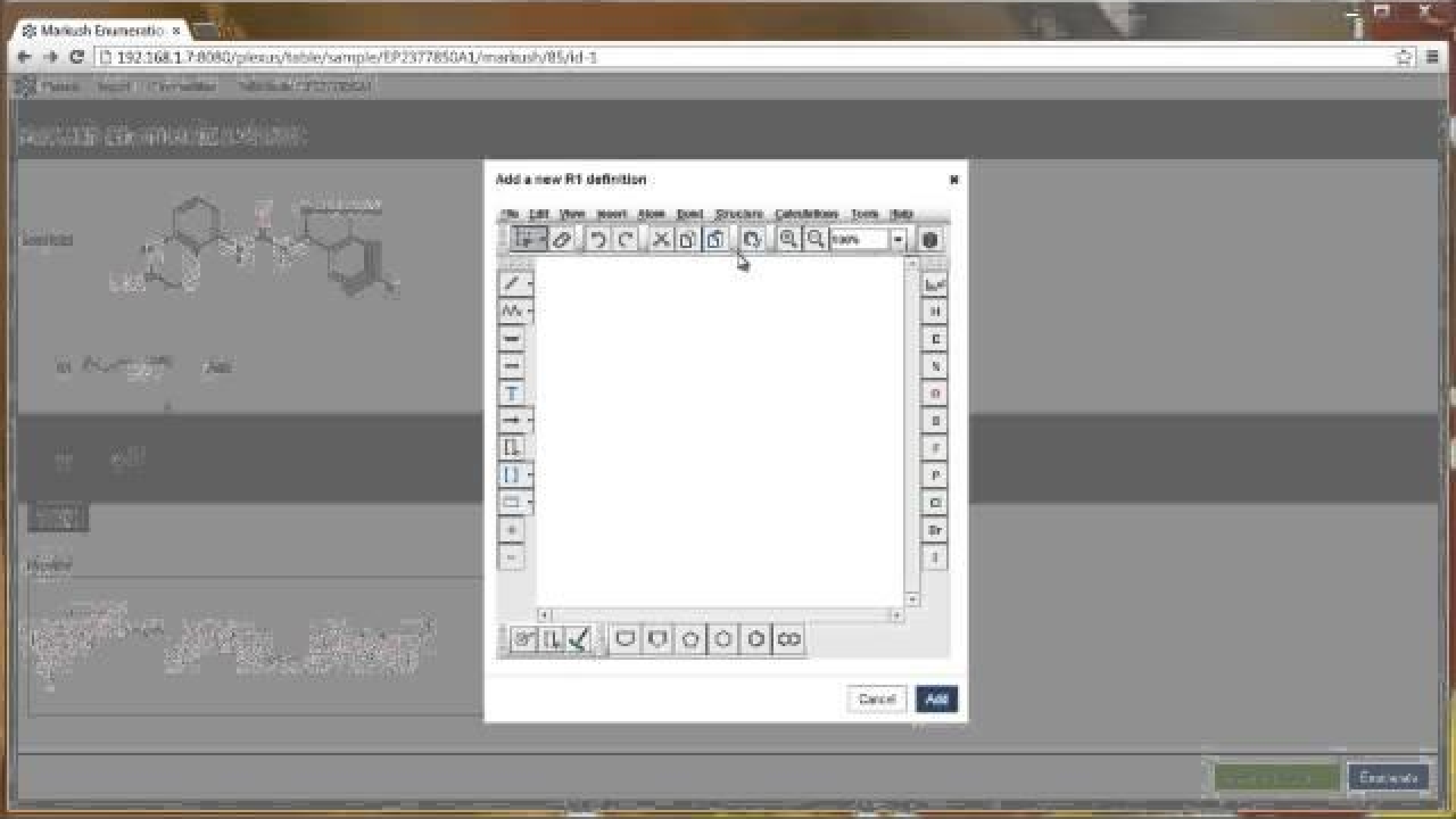
Plexus - style guide / login page



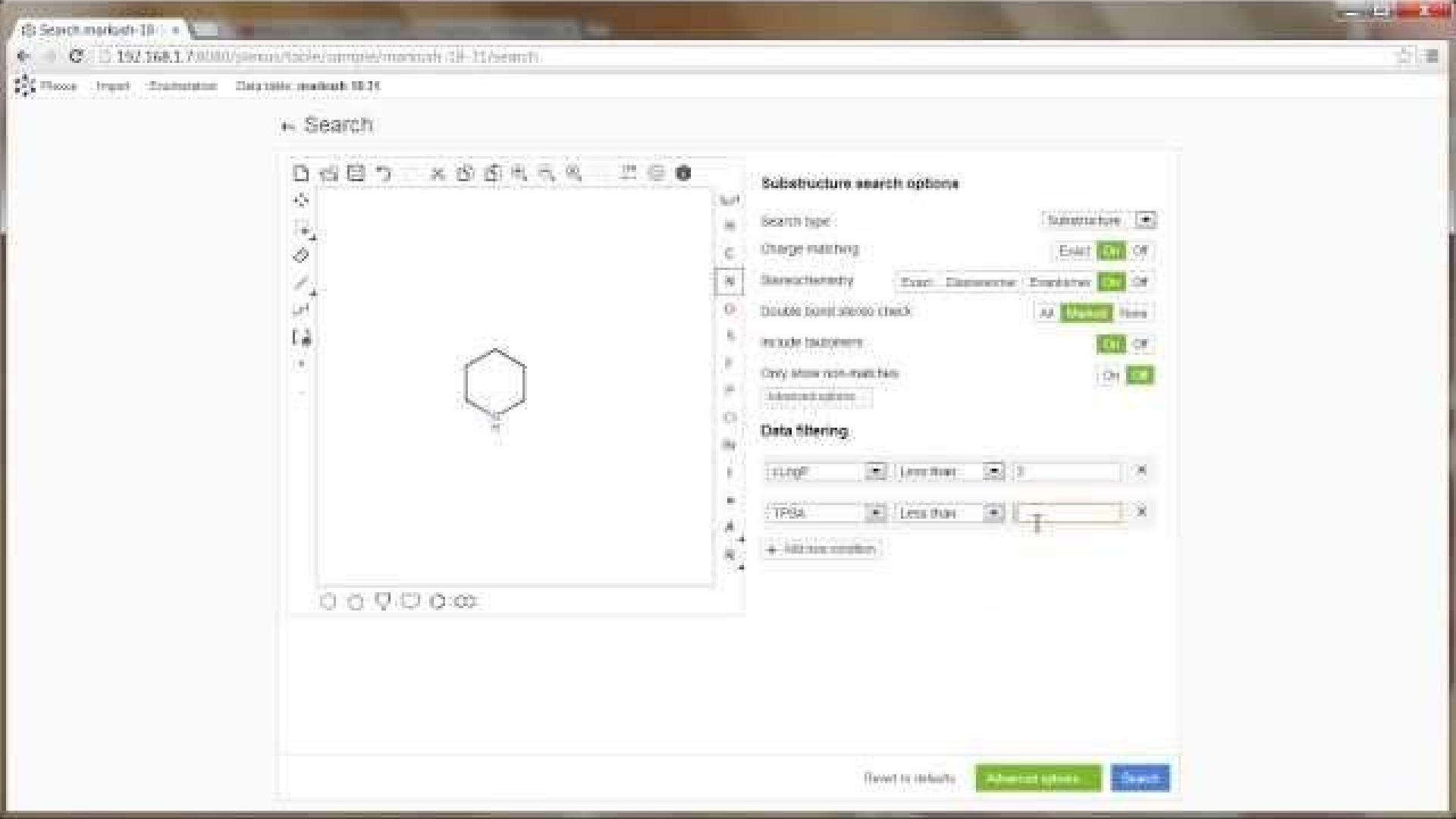
Plexus - library enumeration

- innovative editor
  - view/edit parts of the Markush structure separately
  - structure issues can be isolated to pieces
  - works well with small and large libraries
- library analyzer
  - interactive preview of enumerated structures
  - preview selected parts of the library


Markush Enumeratio
192.168.1.7:8080/plexus/table/sample/EP2377850A1/markush/85/id-1
Add a new R1 definition
Cancel
Add

Plexus - structure search

- JChem search, with
  - common and rarely used options separate
  - default Standardizer config included
- includes Marvin for JavaScript, our new lightweight editor


Search
Substructure search options
Search type
Substructure
Charge matching
Exact
On
Off
Stereochemistry
Exact
Ignore
On
Off
Double bond stereo check
All
Marked
None
Include tautomers
On
Off
Only show non-matches
On
Off
Data filtering
TPSA
Less than
Reset to defaults
Search

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Plexus - details view

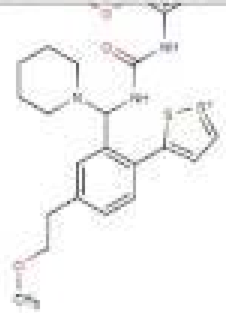
- form view showing everything about a structure
- database contents
- Calculator Plugins (phys-chem predictors, structural prop. calculators, ADME descriptors)
  - structures with atomic calculation results
  - property lists
  - charts
  - all the options you know & love

Plexus - structure search #2

- virtual screening seamlessly integrated into JChem search
- easy access to:
  - structural similarity
  - 2D pharmacophore similarity
  - close analog searching and scaffold hopping

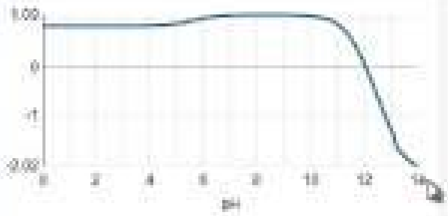
Details of #113 - Pl...

192.168.1.7:8080/plexus/table/sample/markush-18-31/details/113



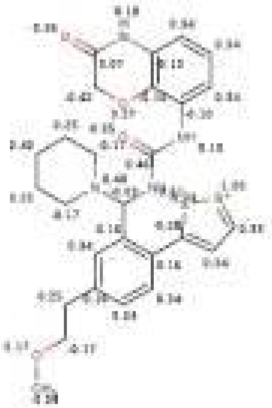
SMILES	[illegible]
InChI	[illegible]

cLogD



cLogP

cLogP of nonionic species 2.75

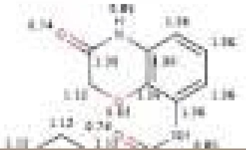


Topological Polar Surface Area

TPSA 91.93

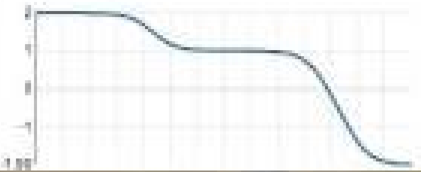
Polarizability

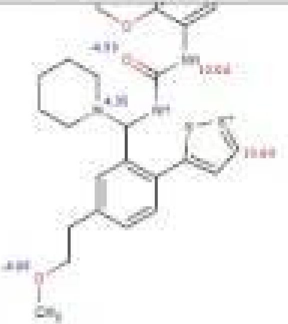
Molecular polarizability 57.99

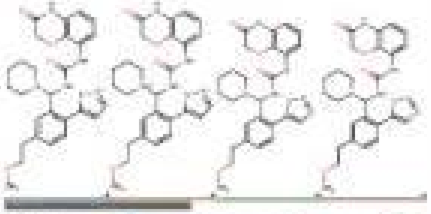


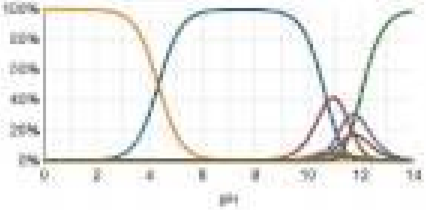
Isoelectric Point

pI 10.27









H-bond Donor/Acceptor

Acceptor sites	5
Acceptor count	5
Donor sites	3
Donor count	3

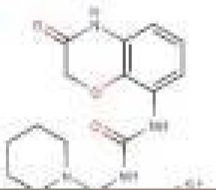
	11.88%), S (11.88%)
Isotope composition	C (65.89%), H (5.79%), N (10.38%), O (11.88%), S (11.88%)
Mass	539.669
Exact mass	539.17957108

Topology Analysis

Atom and bond | Ring | Path and distance

Aliphatic atom count	20
Aliphatic bond count	24
Aromatic atom count	17
Aromatic bond count	17
Asymmetric atom count	1
Atom count	37
Bond count	72
Chain atom count	10
Chain bond count	10
Chiral center count	1
Cyclomatic number	5
Ring atom count	27
Ring bond count	29
Rotatable bond count	8
Stereo double bond count	0

Major Microspecies



Plexus - current coverage

- Document to Structure
- JChem Base
- Standardizer
- Markush Enumeration
- Calculator Plugins
- Screen
- Marvin Applet, Marvin for JavaScript

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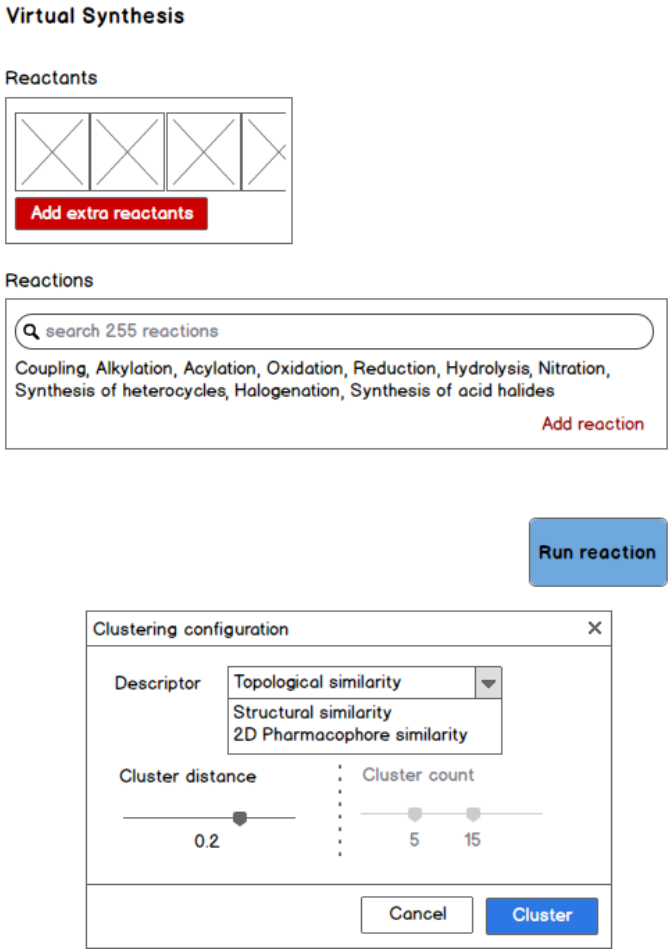
Future additions to LD

- virtual synthesis with Reactor
- clustering with JKlustor
- incremental upgrades throughout
  - predefined R groups
  - comparing similarity searches



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Strategy

- integrate and rethink features
  - user friendly, common design, attention to detail
  - Marvin for JavaScript
- next version
  - extend scope beyond early phase drug discovery
  - reporting, assay management, lead optimization, more…
  - Plexus Suite

Thanks!

Today 2:45pm - the backend

JChem Web Services - The New Story

Today 4:40pm - the strategy

New Product Developments, Tim Aitken

http://plexus.chemaxon.com/
http://www.chemaxon.com/download