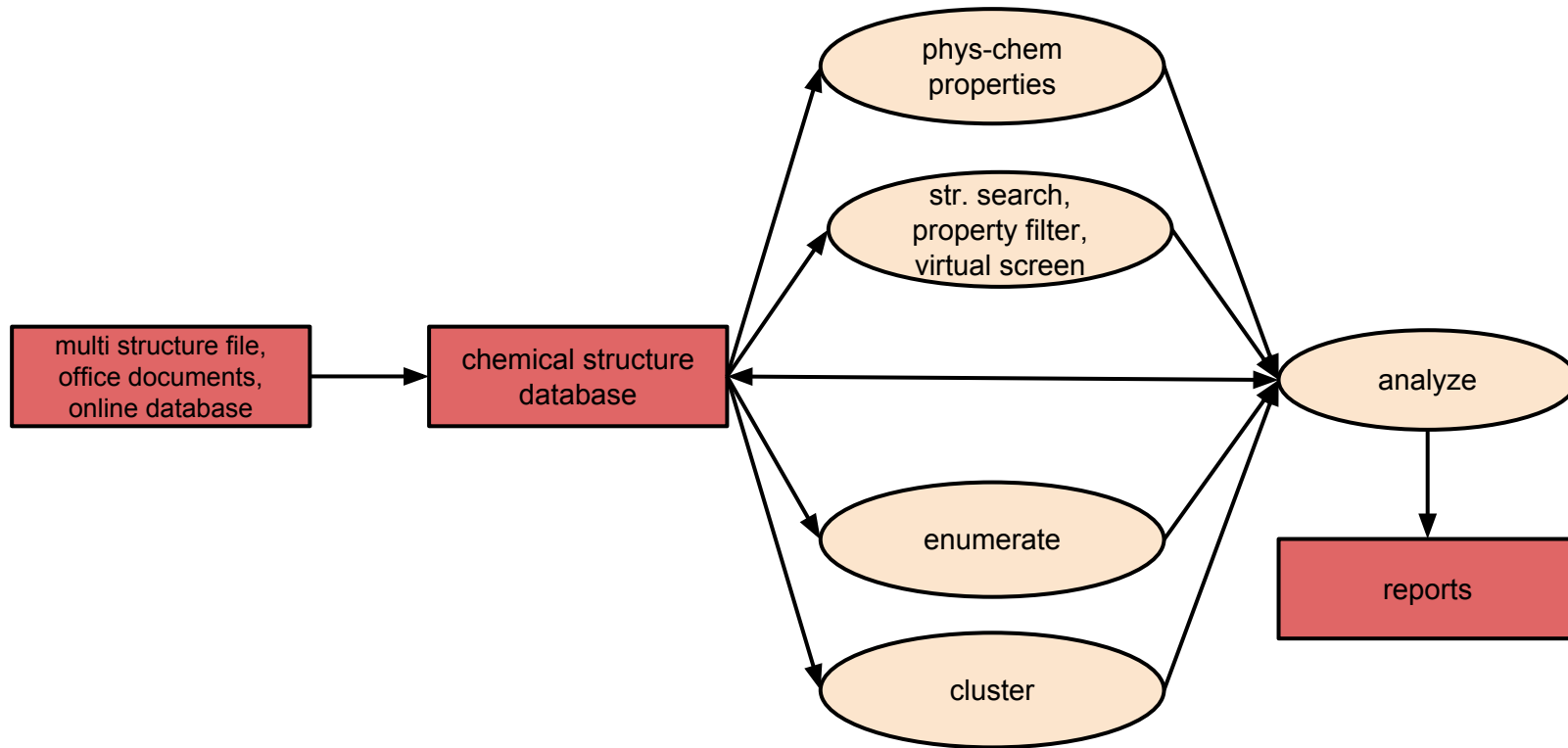


# Introducing Plexus

Andras Stracz

# Early phase drug discovery

## library design



# Versatile

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

# 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







Sheet 1 of EP2377850A1.pdf completed - Searching

Search

Displaying items 1 to 6 of 120 words

Add new row


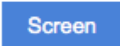

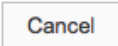


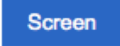

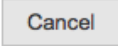
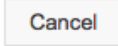





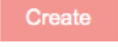
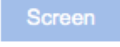



Export

ID	Structure	Formula	Molecular Weight	SMILES	Category	Description	Type
1		C18H35O2	281.519	CCCCCCCCCCCCCCCC(O)C	Alkanol	is chemical structure including caproic acid and hydroxy	organic
2		C17H34O2	270.491	CCCCCCCC(C)CCCC(O)C	Alkanol	branched including caproic acid and hydroxy	organic
3		C18H35O2	281.519	CCCCCCCCCCCCCCCC(O)C	Alkanol	including caproic acid and hydroxy	organic
4		C17H34O2	270.491	CCCCCCCC(C)CCCC(O)C	Alkanol	is chemical structure including caproic acid and hydroxy	organic
5		C18H35O2	281.519	CCCCCCCCCCCCCCCC(O)C	Alkanol	but DAPI is available in formula Caproic acid	organic
6		C18H35O2	281.519	CCCCCCCCCCCCCCCC(O)C	Alkanol	but DAPI is available in formula Caproic acid	organic

# 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

	CREATE BUTTON	PROCESS BUTTON	MODIFY BUTTON	SECONDARY BUTTON	REVERT BUTTON
DEFAULT					
HOVER					
ACTIVE					
DISABLED					

color: #363636

SECONDARY BUTTON

REVERT BUTTON

DEFAULT

Create

Screen

Advanced

Cancel

Cancel

HOVER

Create

Screen

Advanced

Cancel

Cancel

ACTIVE

Create

Screen

Advanced

Cancel

Cancel

DISABLED

Create

Screen

Advanced

Cancel

Cancel



# Plexus - style guide / settings elements

E-mail address

E-mail address

Option A

Option B

Option C

## Message

This is Arial 12px text with 18px line height.  
Phosfluorescently aggregate 24/365 imperatives rather than user-centric best practices. Seamlessly negotiate frictionless testing procedures with equity invested synergy. Quickly maximize client-focused web-readiness without tactical manufactured products.

Enthusiastically envisioneer interdependent portals via

Exact On Ignore

Radical matching

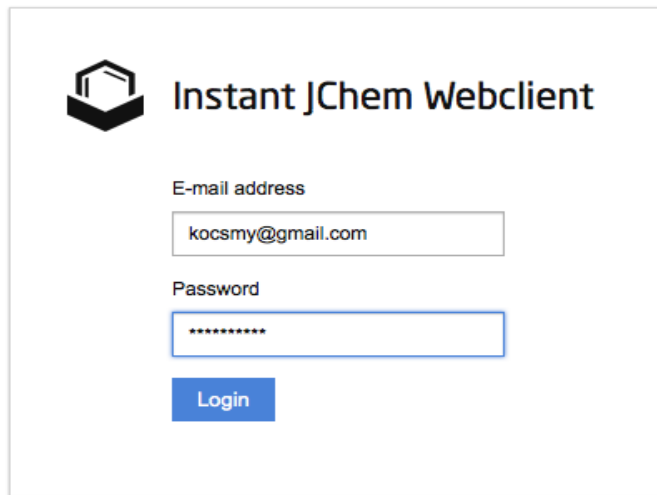
Sp-Hybridization state checking

Radical matching

Exact On Ignore



# Plexus - style guide / login page

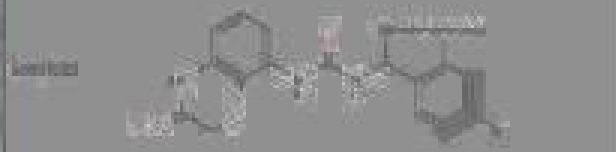


The image shows a login form for 'Instant JChem Webclient'. It features a logo on the left consisting of three stacked hexagons. The title 'Instant JChem Webclient' is positioned to the right of the logo. Below the title, there are two input fields: one for 'E-mail address' containing 'kocsm@gmail.com' and one for 'Password' containing a series of dots. A blue 'Login' button is located below the password field.

# 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 Enumeration Results

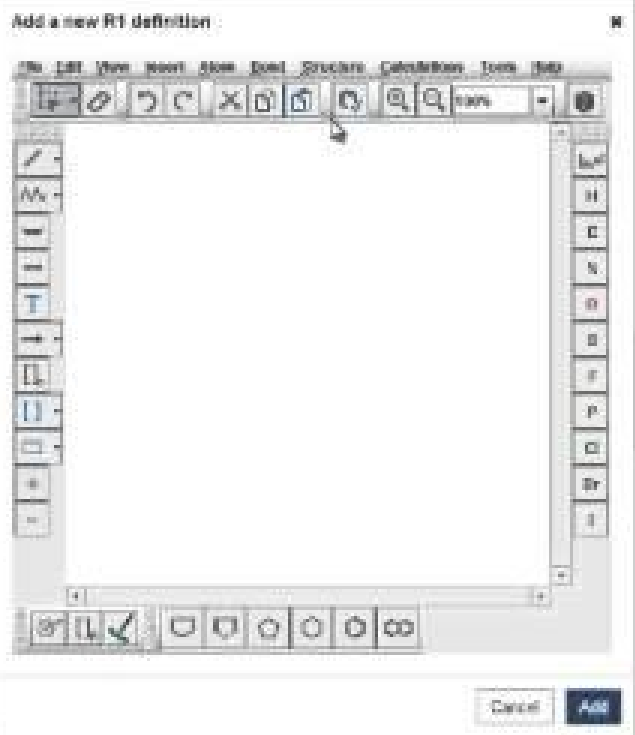


SMILES



#### Add a new R1 definition

File Edit View Insert Draw Tools Structure Calculation Tools Help



# 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

The search interface features a central window displaying a chemical structure of a hexagon. To the left of this window is a vertical legend with icons labeled A through Q. Above the window is a horizontal toolbar with icons for zooming and other actions. Below the window is a row of five circular icons.

#### Substructure search options

Search type:

Charge matching:   On  Off

Sanctuary:   Database  Explorer  On  Off

Double bond stereo check:   None  None

Include isotomers:  On  Off

Only show non-matches:  On  Off

#### Data filtering

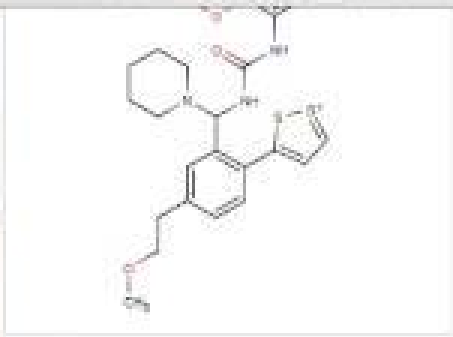
# Plexus - details view

- 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

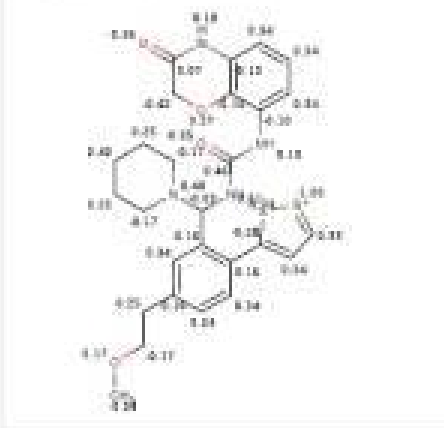




SMILES: CCCC1CCCC(NC(=O)NC1Cc2ccc(cc2)CCc3ccncc3)C(=O)O  
 InChI: InChI=1=CC1=NC(=O)NC1Cc2ccc(cc2)CCc3ccncc3  
 3-11-15-35-27-23(28)(16-20)2(1-12-3-4-13-31)  
 30-27(23)29(25-7-5-6-21-25)2(25-17-3-4)2(29-21-5-6-11-15-16-28)2(4-10-10)14,17H2,1-9,13H2,29  
 29,30,32,33H+1

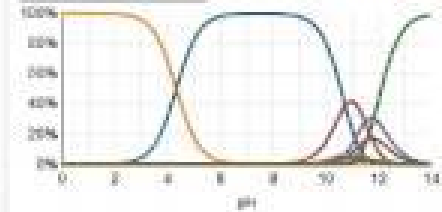
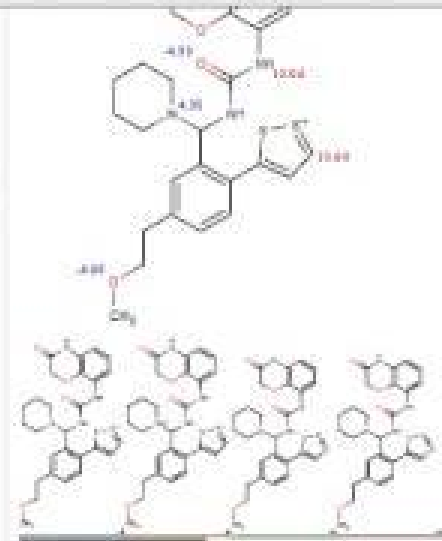
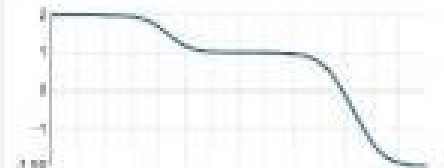
LogP

LogP of ionized species: 2.75



Number of Polar

13.27



H-bond Donor/Acceptor

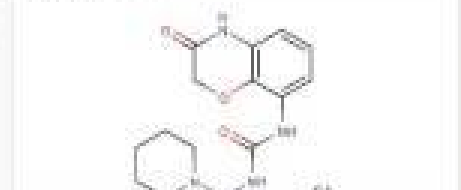
Acceptor sites: 5  
 Acceptor count: 5  
 Donor sites: 3  
 Donor count: 3

Isotope composition: C (99.89%), H (9.99%), N (99.96%), O (99.96%), S (99.96%)  
 Mass: 338.603  
 Exact mass: 338.17607188

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	18	
Chain bond count	18	
Cyclic center count	1	
Cyclic number	5	
Ring atom count	27	
Ring bond count	25	
Rotatable bond count	8	
Double double bond count	0	

Major Microspecies



Topological Polar Surface Area

TPSA: 81.93

Polarity

Molecular polarity: 57.89



# Plexus - current coverage

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

# Future additions to LD

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

## Virtual Synthesis

### Reactants

Four empty boxes for reactants, each with a diagonal line through it. Below the boxes is a red button labeled "Add extra reactants".

### Reactions

Q search 255 reactions

Coupling, Alkylation, Acylation, Oxidation, Reduction, Hydrolysis, Nitration, Synthesis of heterocycles, Halogenation, Synthesis of acid halides

Add reaction

Run reaction

Clustering configuration

Descriptor: Topological similarity

Cluster distance: 0.2

Cluster count: 5, 15

Cancel Cluster

# 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>