

BULZ

#meetCXN

MARVIN
Chemical Drawing with ChemAxon's
Tools



Marvin
Sketch



Marvin
JS



Vision



Future

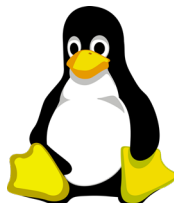


MARVINSKETCH: DRAWING ON DESKTOP



WHERE CAN YOU USE IT?

Platforms

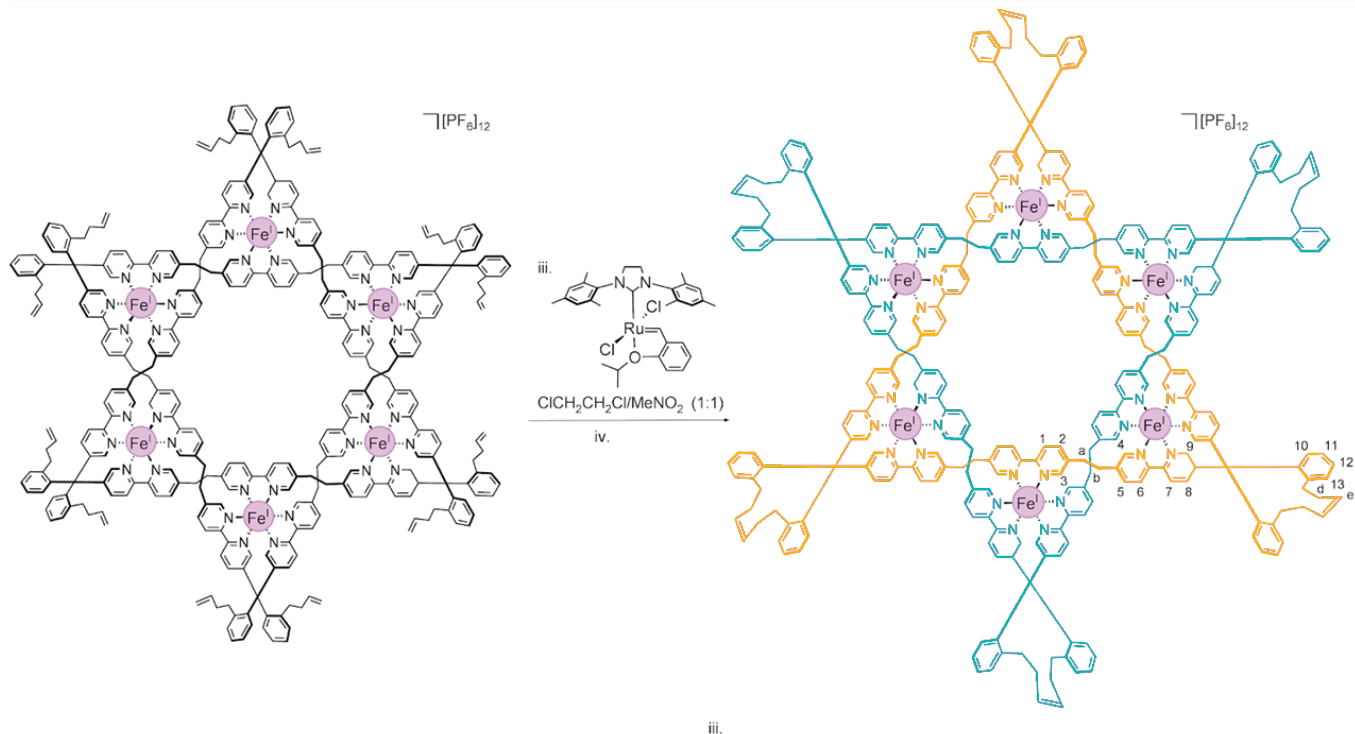


Java

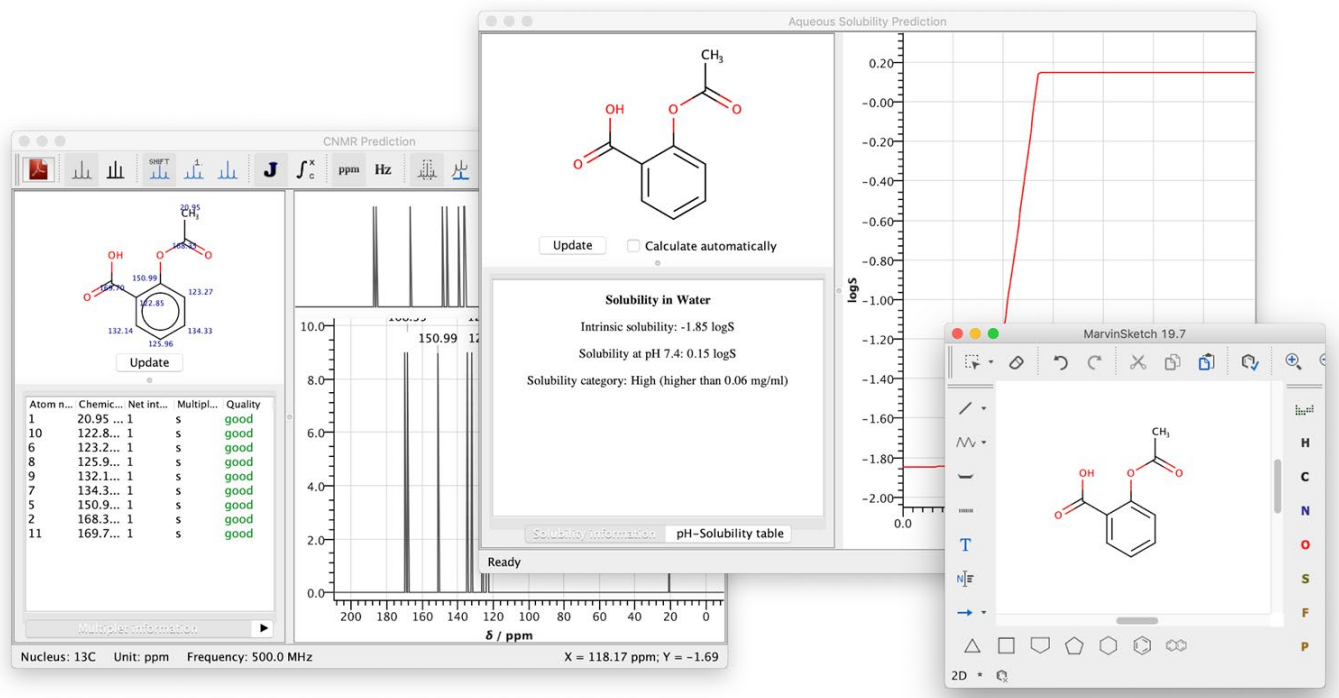


What can you use it for?

PUBLICATIONS



INTEGRATED CALCULATIONS & CHECKERS



CUSTOM SOLUTIONS

Templates
User Interface
Checkers
Naming library
Calculations

The image displays several overlapping windows from ChemAxon software:

- Terminal Window:** Shows a shell prompt `moha@northtree ~` with commands for evaluating and calculating pKa values. The output includes SMILES strings and a list of chemical structures.
- MarvinSketch 5.6.0.0beta1:** A graphical user interface for drawing and editing chemical structures. It features a toolbar and a central workspace showing a chemical structure.
- pKa (chemicalize.org):** A window for calculating pKa values. It displays the chemical structure of 5-amino-n-valeric acid, its SMILES string, and a titration curve graph showing the percentage of different ionization states as a function of pH. The pKa value is listed as 4.65.
- MMS:** A window for Molecular Modeling Simulation. It shows a chemical structure and a table of arguments for simulation, including mol, special, pka_width, and svj.



MARVINSKETCH PLANS 2019

Critical/annoying bugs will be fixed.

Minor improvements might be considered.



MARVIN JS: THE CHEMICAL DRAWING WEB COMPONENT



MARVIN JS



Major browsers supported



What can you use it for?

INTERFACE FOR CHEMICAL SEARCH & CALCULATIONS

The screenshot displays the ChemAxon software interface. At the top, a dark navigation bar contains the following menu items: CALCULATION, STRUCTURE SEARCH (highlighted), DOCUMENT SEARCH, WEB VIEWER, COMPLIANCE, BATCH, and DRAWING. A search bar on the left contains the text "norketamine". Below the search bar, the "Query structure" section shows a chemical structure of norketamine, which is a cyclohexane ring with a carbonyl group, an amino group, and a 2-chlorophenyl substituent. To the right, a panel indicates "10 results for the query." Below this, a "Draw structure" window is open, showing the same chemical structure being drawn. The drawing window includes a toolbar with various drawing tools and a vertical element palette on the right with labels H, C, N, O, S, F, P, and Br. At the bottom of the drawing window are "CANCEL" and "SEARCH" buttons. Below the main search results, there are two rows of results, each with a chemical structure icon, a count of results, and a timestamp: "10 results 2019-03-17 16:31:24" and "8 results 2019-03-17 16:29:37".

EDUCATION



Zosimos CX

Biochemistry

Score **3/18**

Exercises

- Which vitamin is depicted in the figure?
- 2** Draw the only non optically active proteinogenic amino acid!
- 3** Draw the missing product

Draw the only non optically active proteinogenic amino acid! 1/3 attempts

Marvin JS
by ChemAxon

Powered by ChemAxon

CHECK ANSWER

IDEA MANAGEMENT

DAAO: preparation 8d
Add your description...

CREATE OVERVIEW

SNAPSHOT

ADD PROPERTY

Alignment (PDB)
Reference: 3W4J - 2LD.

Calculated Properties

	Current	Pinned
▲ Mass	230.27	215.25
▼ cLogP	1.21	2.47
▲ TPSA (Å²)	76.97	49.33
▼ pKa (str. acidic)	9.12	9.6
▲ pKa (str. basic)	9.89	-4.65
FSP3	0.15	0.15
▲ Solubility (mM)	9.74	1.87
H-bond acceptors	2	2
H-bond donors	3	2

CNS MPO

	Current	Pinned
▼ MPO Score	4.23	5.27

HERG assistant
Suggestions total: 26.
Showing page 1 of 10. Prev Next

Patent search

- ✗ US4755465A
- ✗ US4775622A
- ✗ US5597797A
- ✗ US5514582A
- ✗ US4704362A

Enamine Real
Showing page 1 of 5. Prev Next

Pubchem analogs
Matches: N/A

Molport
Matches: N/A

Chemical structure: Nc1ccc(cc1)CC(=O)c2cc(O)nc2

Alignment (PDB) visualization showing protein structure and ligand fit.

Calculated Properties visualization showing a 3D plot of various properties.

HERG assistant visualization showing a chemical reaction scheme.

Enamine Real visualization showing a chemical reaction scheme.

Pubchem analogs and Molport visualization showing chemical structures.

Conformers visualization showing multiple conformations of the molecule.

Chemical structure details: Last edited by Andris just now

ELN, REGISTRATION, INVENTORY



Registration Upload Staging Search Quick search: type here any ID... rknispel@chemaxon.com

Submission 4474

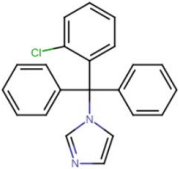
Using source REGISTRAR - Created on 2019-03-11 12:22:12

Created by rknispel@chemaxon... Molecular formula C22H17ClN2 Calculated molweight 344.84 Submitter kszabo@chemaxon... Library --

Register **More actions**

✓ Ready For Registration - No issues found

< Apply Cancel



Structure Checker Stereo Analyzer

Wiggly Bond Checker Crossed Double-Bond Checker
 Straight Double Bond Checker

Structure checker is **ON**

✓ No structural errors were found.

LnbRef	Molweight	Restriction
K546789823	0	0

Additional Data

Project	Lot Molecule Formula	Test 3
	C22H17ClN2	
IUPAC name	logP	logD (pH:7.4)
1-[(2-chlorophenyl)di(phenyl)methyl]-1H-imidazole	5.8394516706666675	5.816906190602557
Shipped	test2 (positive int)	PSA
<input type="checkbox"/>		17.82
Testing	Data (valid JSON)	Stereochemistry
Geometric isomerism	Comment	



MARVIN JS PLANS 2019

Accessibility improvements

Structure Checker integration

Oligopeptides support, more S-groups

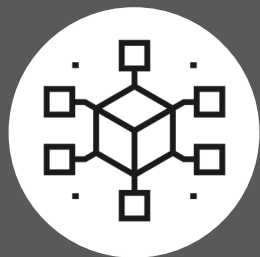


THE FUTURE OF MARVIN

Web-based chemical editor component which is capable of drawing **big** syntheses **schemes**, can be **easily extended** with other modules and can be **seamlessly integrated** to ChemAxon's and other vendors' products.

MARVIN_NG PROJECT

Q1



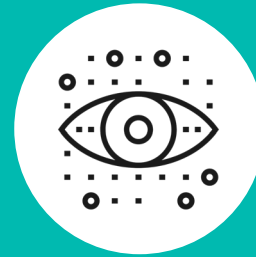
Architectural
Concept

Q2



Chemical
Model

Q3-Q4



Graphical
Concept



Objective

Review of structure drawing concept



High-risk factors to consider feasibility

Movable charge/map

Handling separate molecules on canvas
(formula/absolute label)

Intuitive drawing

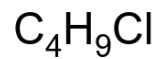
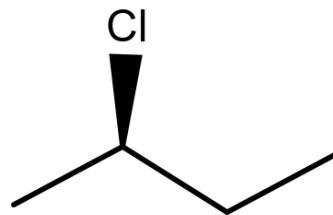
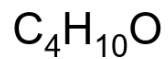
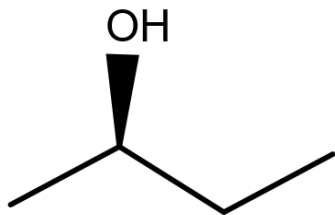
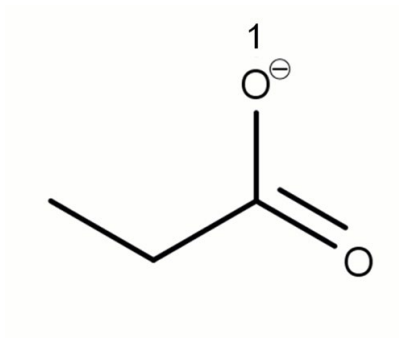


Outcome

Chemical Model Concept

Q2

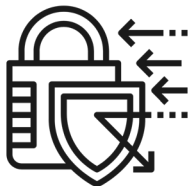
EXAMPLE





Objective

Publication quality elements



High-risk factors to consider feasibility

Picture on canvas

Graphical objects

Chemical structure formatting:

Coloring atoms, bonds

Setting atom fonts, bond properties

Page settings

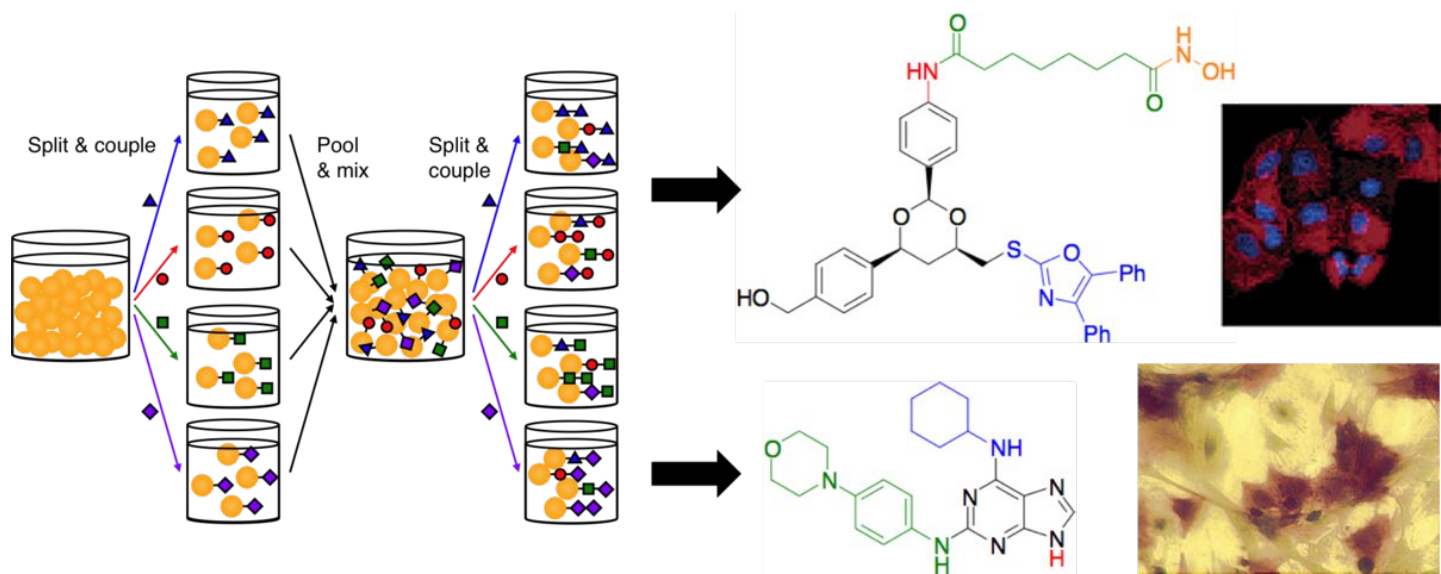


Outcome

Graphical Model Concept

Q3

EXAMPLE





Objective

Reaction scheme drawing



High-risk factors to consider feasibility

Graphical grouping

Structure-Image grouping

Scale, move, align groups together

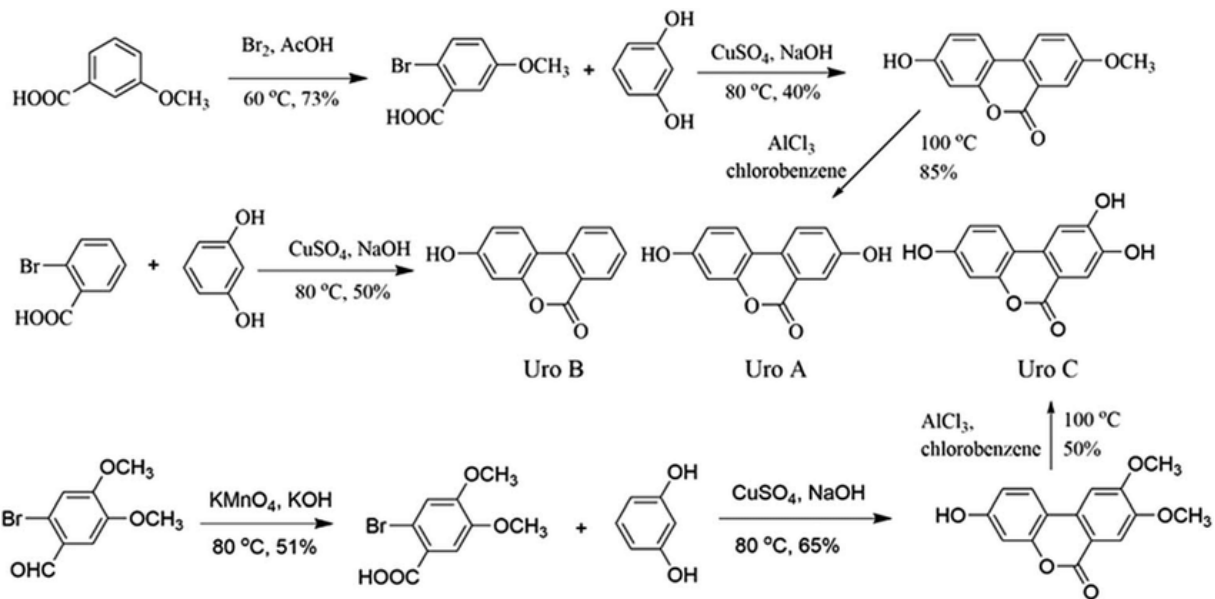
Performance



Outcome

Graphical Model Concept

EXAMPLE





User interviews

Usability test

Workshops

“Coming together is a beginning.
Keeping together is progress.
Working together is success.”

[Henry Ford]



Thank you