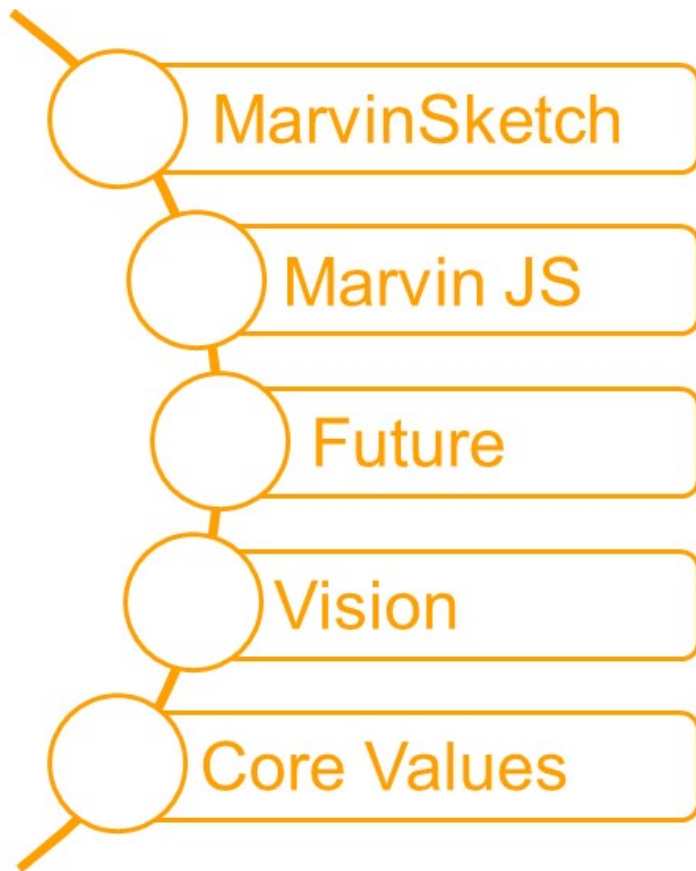


Marvin

Chemical drawing with ChemAxon's Tools

Objective







MarvinSketch

Drawing on desktop

Where can you use it?

Platforms



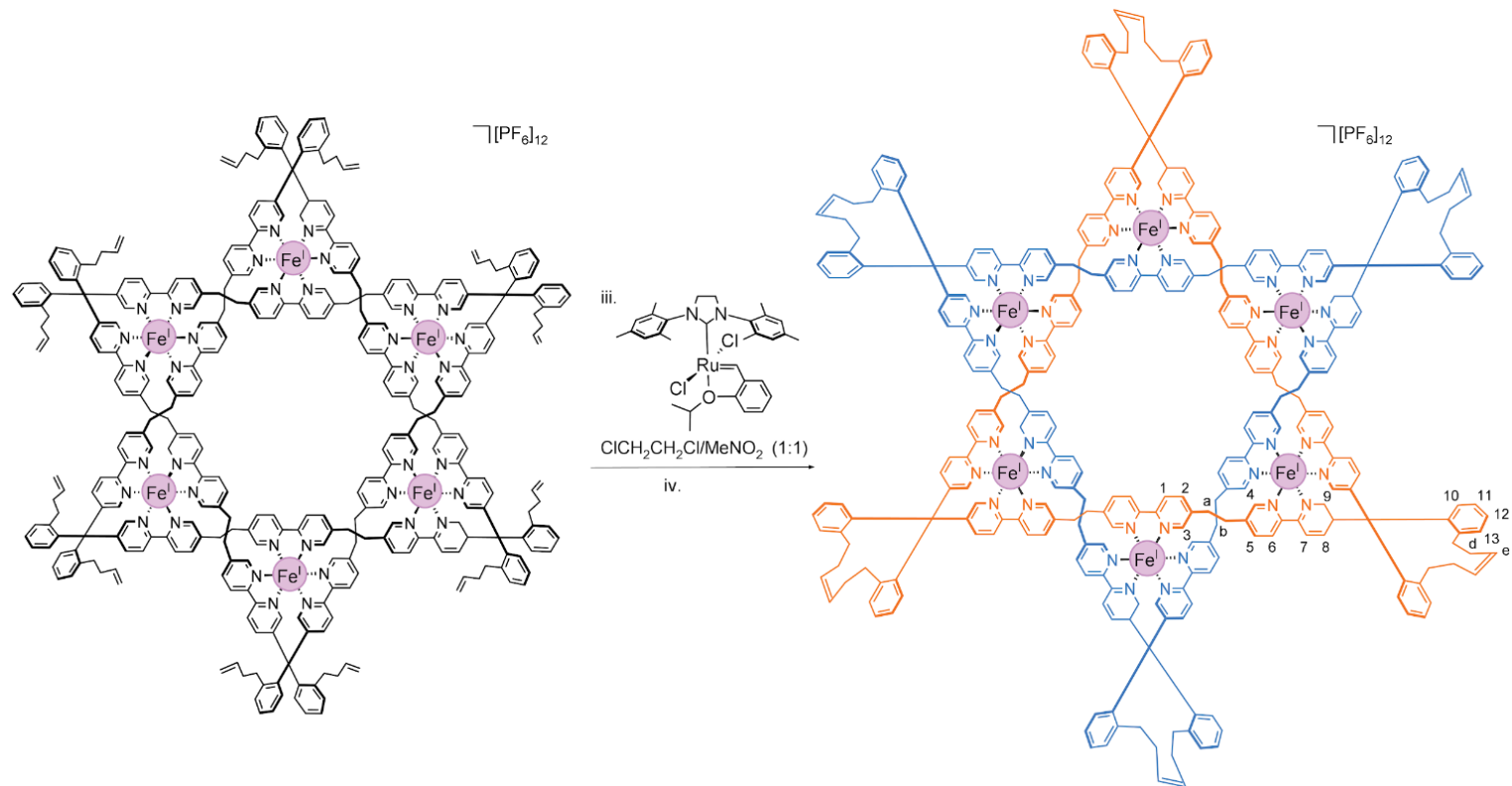
Java



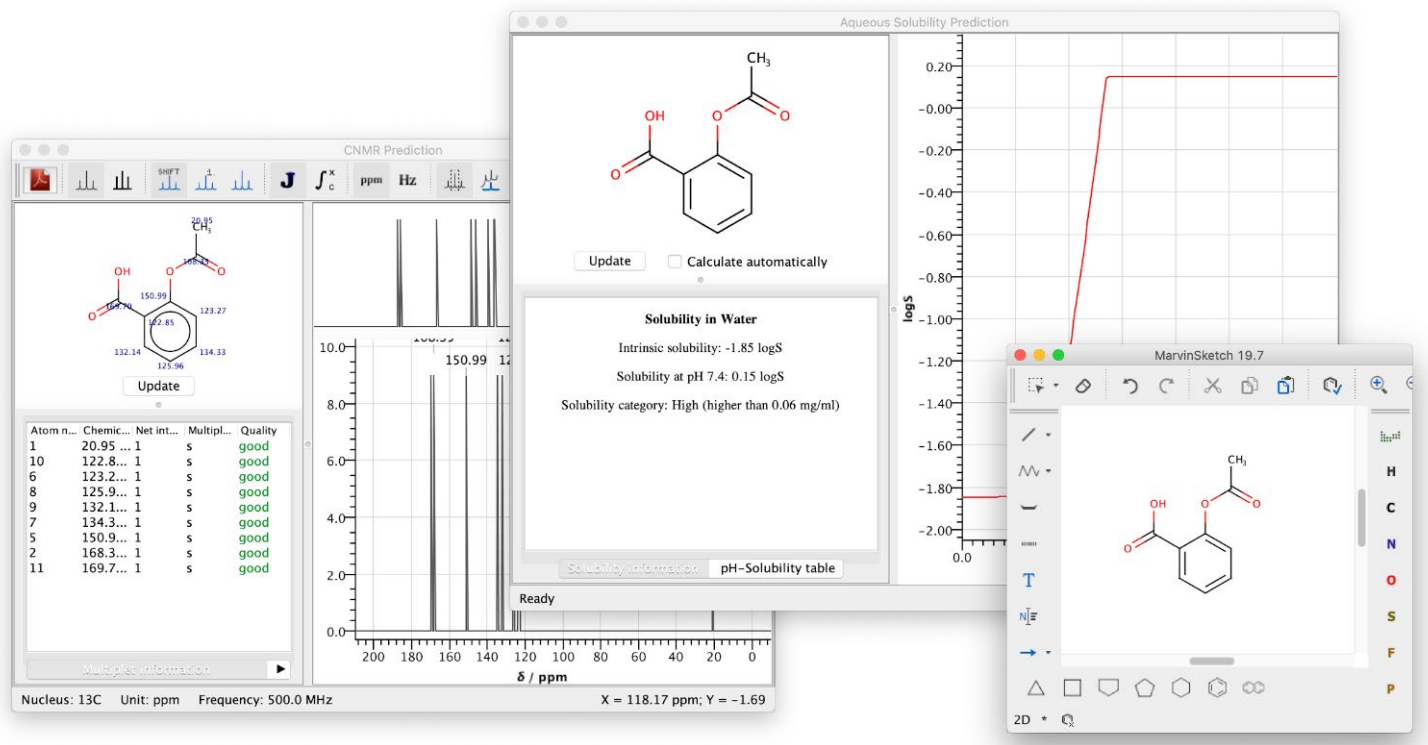
.NET

What can you use it for?

Publications



Integrated calculations



Custom calculation via Marvin Services

The image illustrates a workflow for custom calculations using Marvin Services. It features three main components:

- Terminal Window:** Shows the execution of a custom calculation. The user runs `cxcalc mms --ph 7.4 mols/nc110.sdf`, which outputs a list of molecules with their IDs and SMILES strings.
- MarvinSketch 5.0.0.0beta1:** A chemical structure editor displaying the structure of 5-amino-n-valeric acid, which was generated from the terminal output.
- Web-based pKa Calculation Windows:** Two overlapping windows from chemicalize.org. The top window shows the input structure and arguments (mol, special, pka_width, svg). The bottom window shows the results, including the calculated pKa value of 4.65 and a titration curve graph showing the percentage of ionized and non-ionized forms as a function of pH.

The titration curve graph in the bottom window shows the percentage of ionized and non-ionized forms as a function of pH. The x-axis is pH (0 to 14) and the y-axis is % (0% to 100%). The curve shows a sharp increase in ionization around pH 4.65, which is the pKa value.

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



JChem/Marvin webservice needed

What can you use it for?

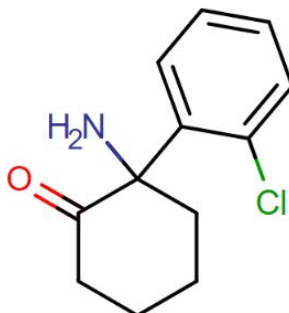
Interface for chemical search and calculations

CALCULATION **STRUCTURE SEARCH** DOCUMENT SEARCH WEB VIEWER COMPLIANCE BATCH DRAWING

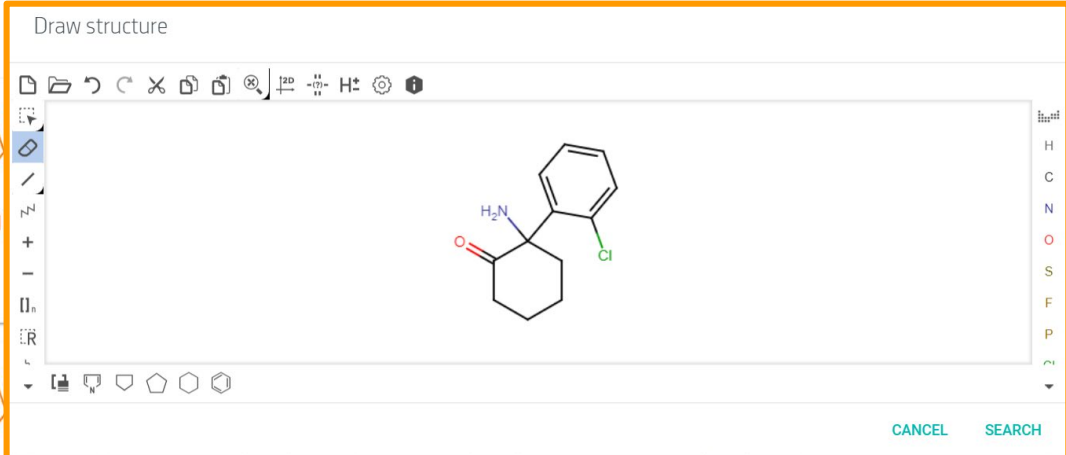
CREDITS: 100 EUFROZINA

norketamine DRAW SEARCH

Query structure


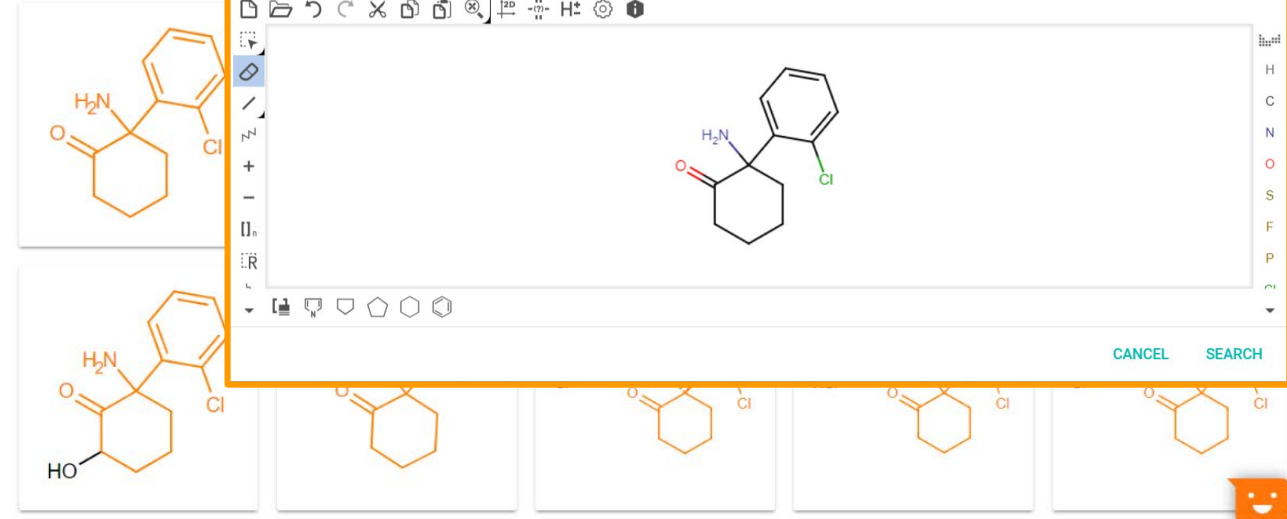


10 results for the query. Draw structure



10 results
2019-03-17 16:31:24

8 results
2019-03-17 16:29:37



Chemical Catalogs



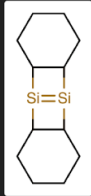
Education



Zosimos

Adding answer structure

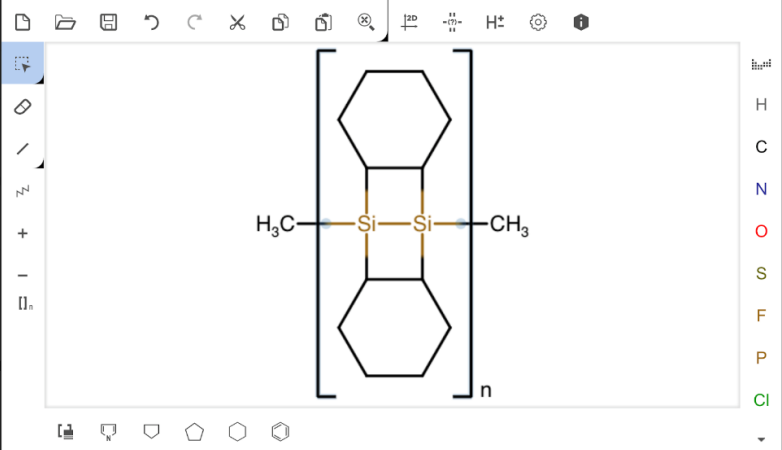
Draw the silicone that can be made from this monomer:



Structure A

Correct answer

CANCEL SAVE



The screenshot shows a chemistry drawing tool interface. The main canvas displays the correct answer: a polydimethylsiloxane (PDMS) chain. It consists of two silicon atoms (Si) connected by a single bond, with two methyl groups (CH₃) attached to each silicon atom. Two cyclohexane rings are attached to the silicon atoms, one on each side. The entire structure is enclosed in large square brackets with a subscript 'n' at the bottom right. The interface includes a toolbar at the top with various drawing tools and a vertical legend on the right side listing elements: H, C, N, O, S, F, P, Cl.

ELN, Registration, Inventory



Registration Upload Staging Search 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

LnRef	Molweight	Restriction
K546789823	0	0

Additional Data

Project	Lot Molecule Formula	Test 3
	C22H17ClN2	
IUPAC name	logP	logD (pH7.4)
1-(2-chlorophenyl)diphenylmethylethyl-1H-imidazole	5.8394516706666675	5.816906190602557
Shipped	test2 (positive int)	PSA
OFF		17.82
Testing	Data (valid JSON)	Stereochemistry
Geometric isomerism	Comment	

Idea management

DAAO: preparation 8d CREATE OVERVIEW

Add your description...

SNAPSHOT

#18

#17

#16

#15

ADD PROPERTY

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

Calculated Properties

Property	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

Property	Current	Pinned
MPO Score	4.23	5.27

Sweet Spot

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](#)

Enamine Reaction

Enamine Real

Z2634176173 (0.626) Z2634177815 (0.602)

Z2633956090 (0.602) Z2226576739 (0.592)

Conformers

Chemical Structure

SMILES: CC(=O)Nc1ccc(O)c(CCN1Cc2ccccc2)c1

Last edited by **Andris** just now

Marvin JS Plans 2019



Accessibility improvements

Structure Checker Integration

Oligopeptides support, more S-groups

217

217

Marvin JS Integrators

7

7
years
of
development



The future of Marvin

Vision



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.

Core values

- Great UX
- Browser component
- Seamless integration
- Perfect clipboard event handling
- Modular and pluggable (structure checker, calculations)
- Rendering of image = drawing(WYSIWYG)
- Can create nice drawings (publication quality)
- Chemically intelligent
- Easy deployment, install, update, public API
- Runs on Touch devices
- Runs on desktop





Questions?



THANK YOU