
Re-imagining Marvin

Eufrozina Hoffmann



ChemAxon

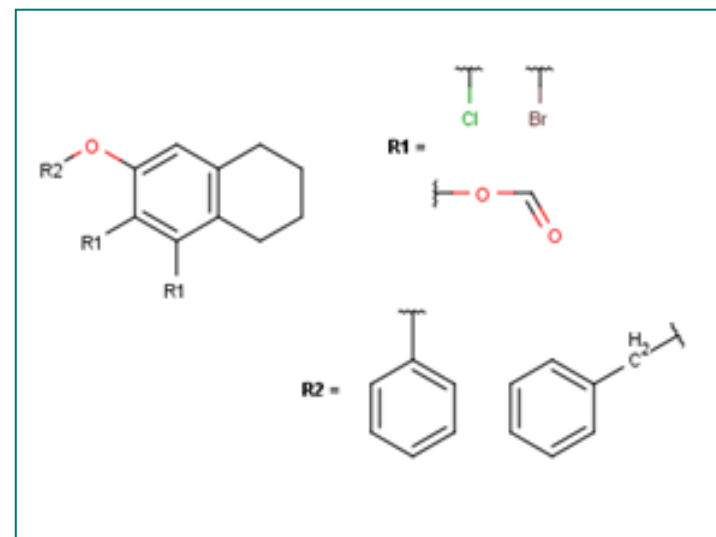
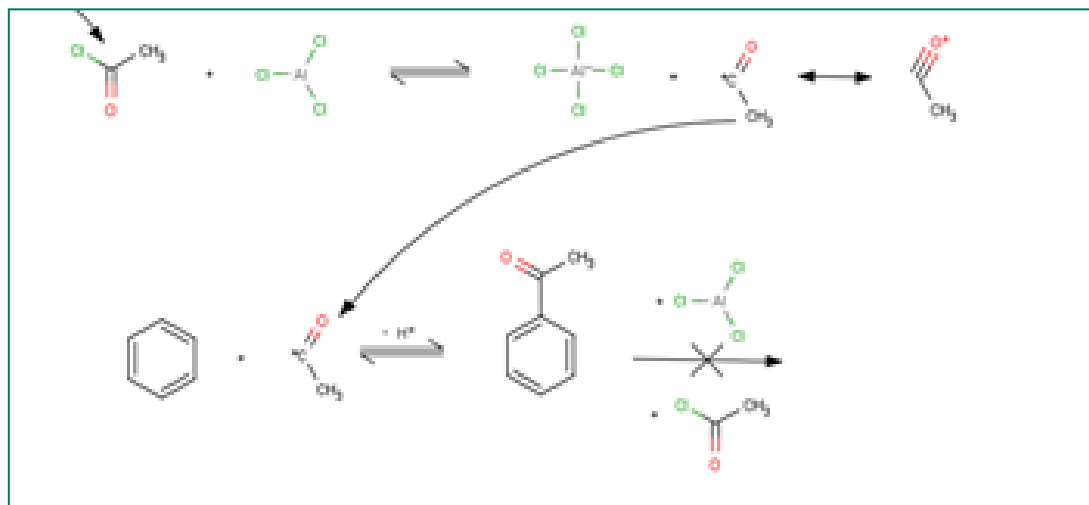
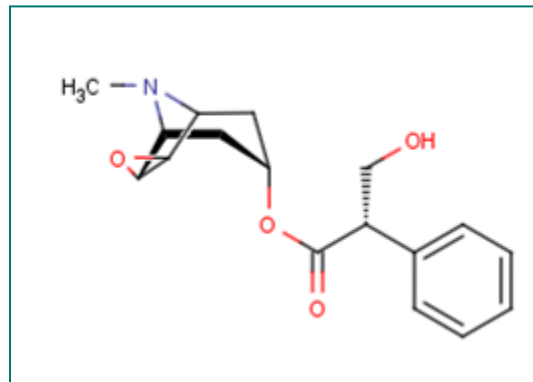
Solutions for Cheminformatics



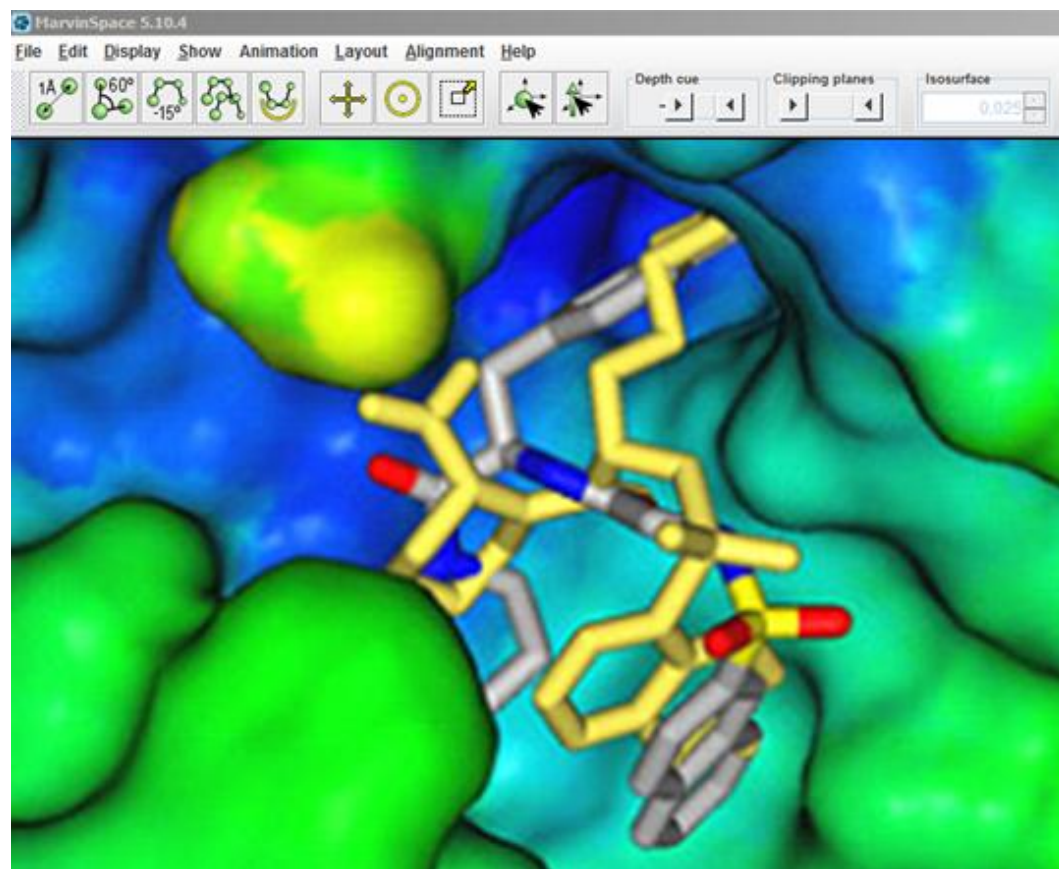
Marvin-JS

Marvin news

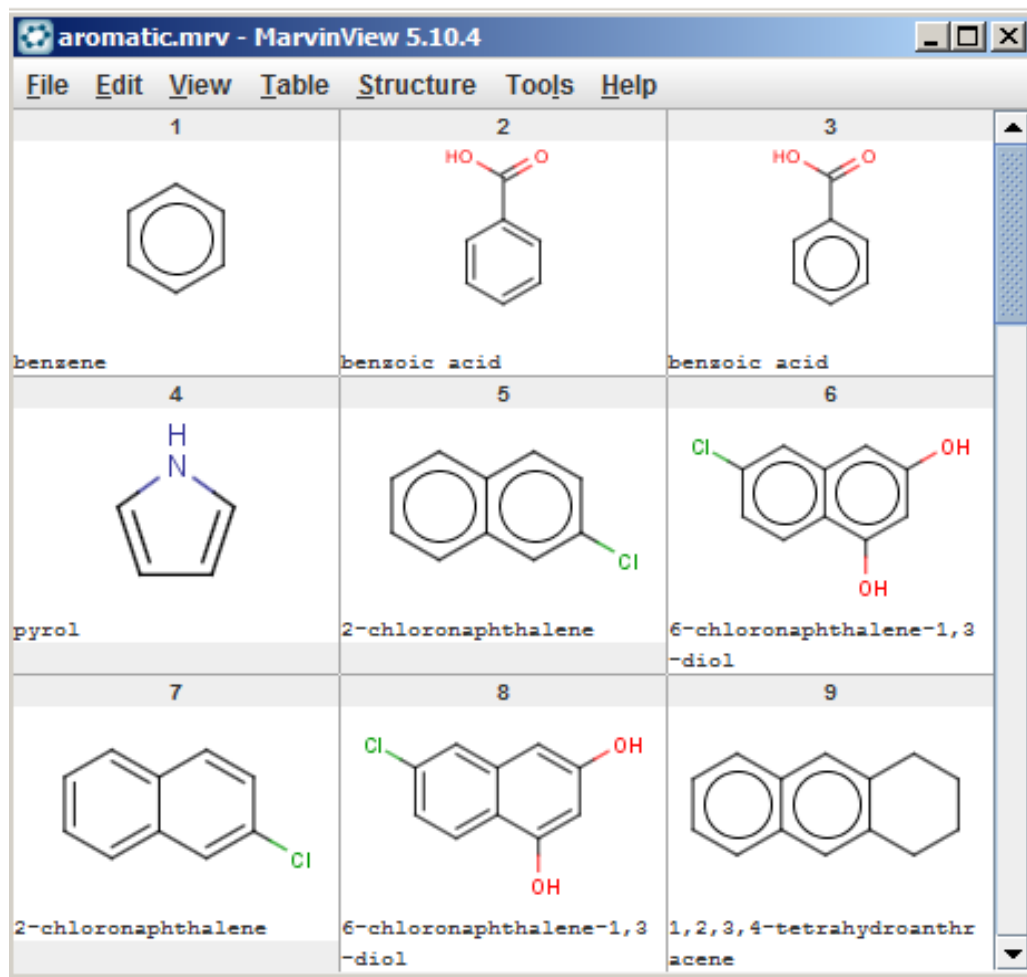
Marvin Sketch



Marvin Space



Marvin View



Marvin web solution

Marvin Sketch

Marvin Space

Marvin View



Marvin Applet

New frontiers

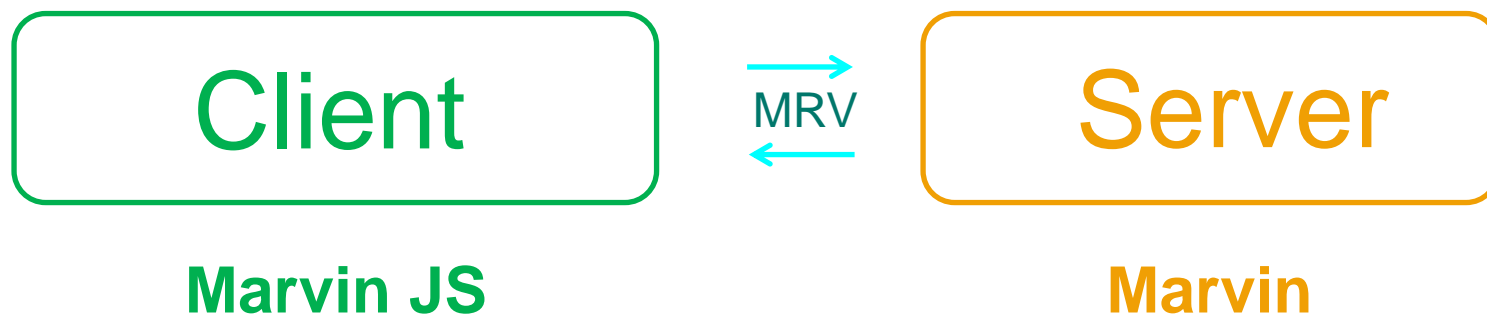
- Tablets, Touch screen devices
- New set of standards and developing techniques:
 - HTML5
 - JavaScript
 - CSS3
- New, effective web applications

Need for speed – “instantly available”

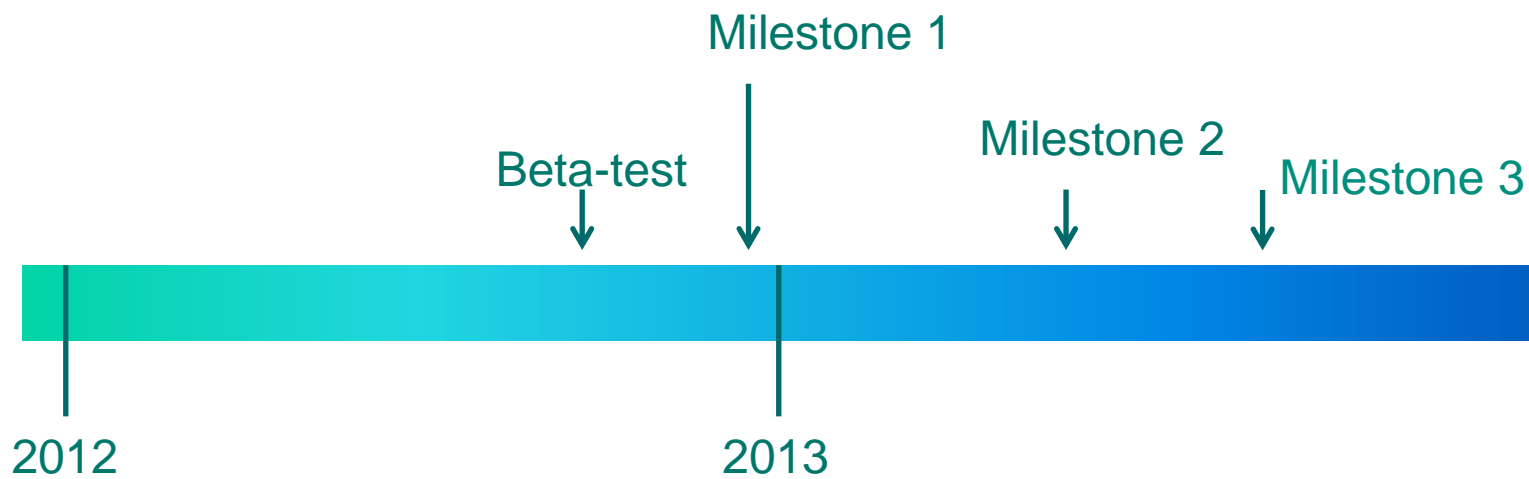
Why JavaScript

- The leading web application technology
- Platform independent: main browsers support it, no extra tool required
- Extended functionality to web pages
- Lightweight (but frequent server-client communication)
- Original java code can be “reused” (GWT)

Architecture of Marvin-JS



Timeline



Milestone I.

- Basic Drawing and Editing Features ✓
- Basic Displaying Features ✓
- Atom properties ✓
- Query atoms and bonds ✓
- Valance check ✓
- File Import/Export ✓
- Abbreviated Groups, S-groups
- Displaying biomolecules
- Basic Server Side Calculations ✓

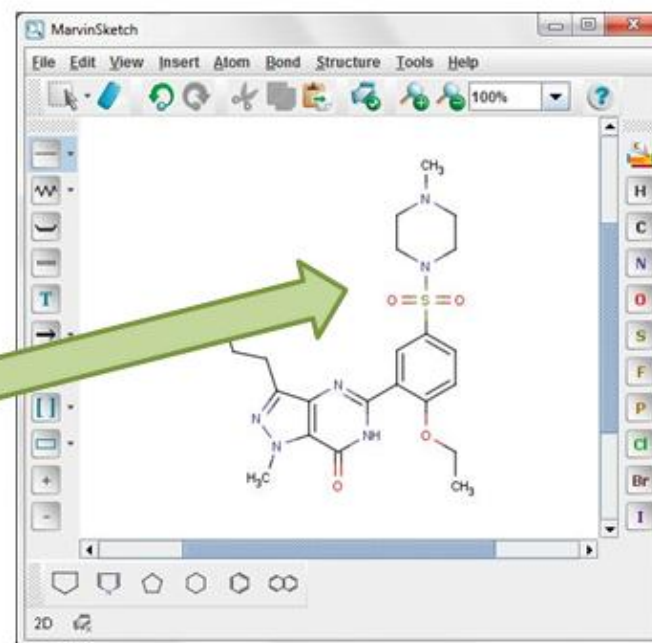
More planned features

- Reaction drawing
- Reaction query features
- Text box
- User defined templates
- Calculators on server side (logP, logD, pKa...)
- All query features
- Complex S-groups
- Graphical objects
- 3D display

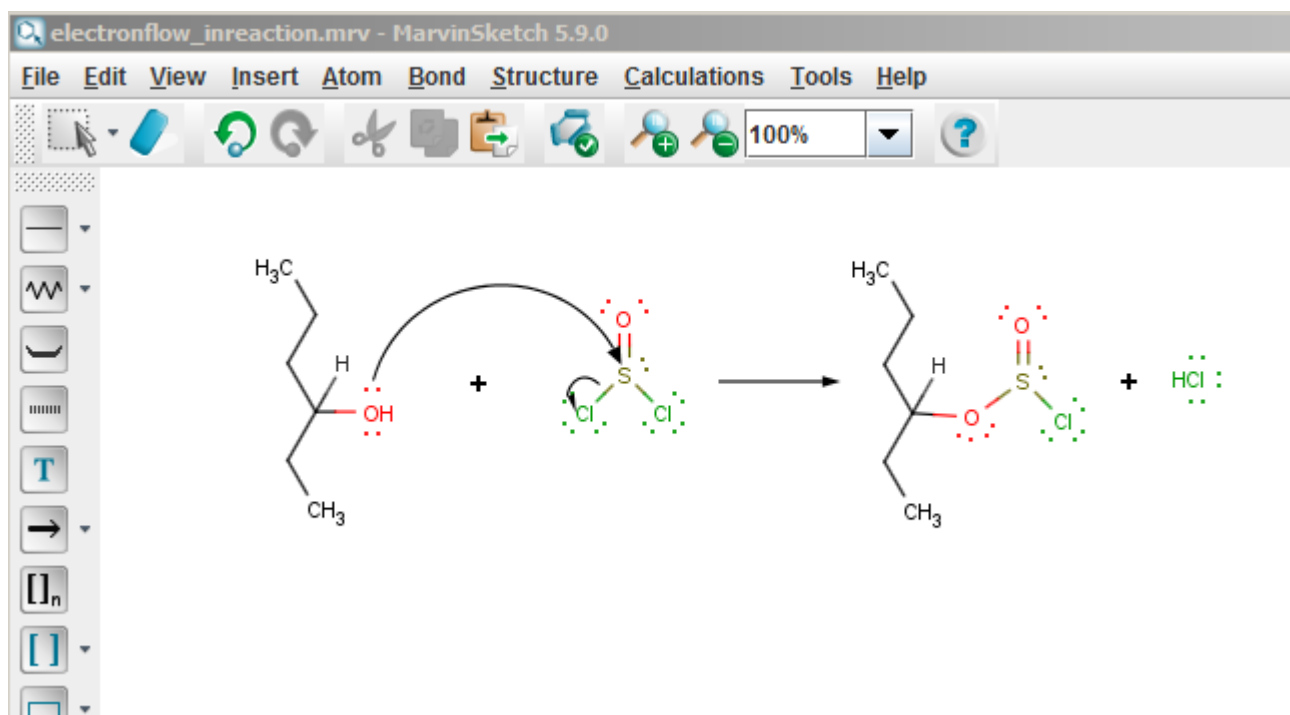
News in Marvin

Marvin 5.8

Native PDF format as the default image
pasteboard format is used on MAC systems.



Drawing electron flow arrow in a reaction



Marvin 5.10

Exporting disconnected molecules separately

The screenshot displays the MarvinSketch 5.10.0 software interface. The main window, titled 'naphtalane_deriv.mrv', shows three disconnected naphthalene derivatives: 1-bromonaphthalene, 1-methylnaphthalene, and 1-oligonaphthalene. The right-hand pane, titled 'The Source - MDL SDFfile', shows a list of source information with the 'View' menu open, highlighting 'View as multiple molecules'. A dialog box titled 'Saving multiple fragments...' is overlaid on the bottom, asking the user to select how to handle the multiple fragments. The dialog box contains the following text and options:

Saving multiple fragments...

? The canvas contains multiple fragments, please select how to handle them.

- Save as one file containing all molecules in one
- Save as one file containing multiple molecules separately
- Save molecules as separate files (if filename_idx.format exists this option will overwrite it)

OK Cancel

Marvin 5.10

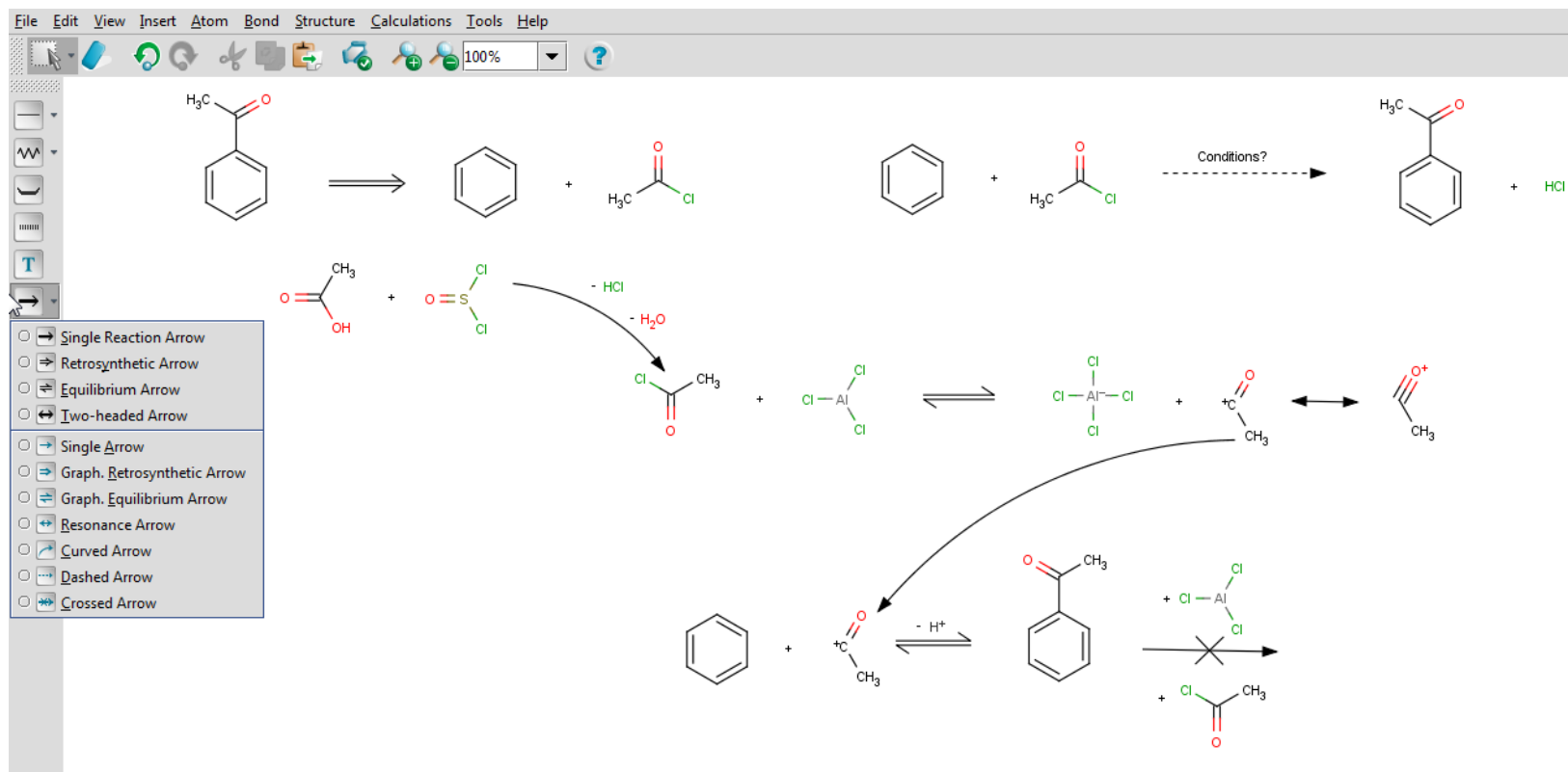
Easily extendable abbreviated group list

The screenshot displays the MarvinSketch 5.10.0 interface. The main workspace shows three chemical structures: 1) A benzene ring with a hydroxymethyl group (-CH₂OH) and a methyl group (-CH₃). 2) A central carbon atom bonded to a methyl group (-CH₃), another methyl group (-CH₃), and a CBr₃ group. The label 'AromaticRing1' is highlighted in pink. 3) A cyclohexane ring with two isopropyl groups (-C₃H₇) and two CBr₃ groups. The labels 'i-C₃H₇' and 'CBr₃' are highlighted in green.

A 'user.abbrevgroup' dialog box is open, showing the following table:

Abbreviation	SMILES	Ring Count	Left Name	Right Name
ring6	(c1ccccc1)CO	4		
AromaticRing1	c1ccccc1Br	2		
C5F	CCCCCF	1	leftName=F5C	
CBr3	BrC(Br)Br	2		rightName=CBr3

New Graphical Arrows



Marvin 5.10

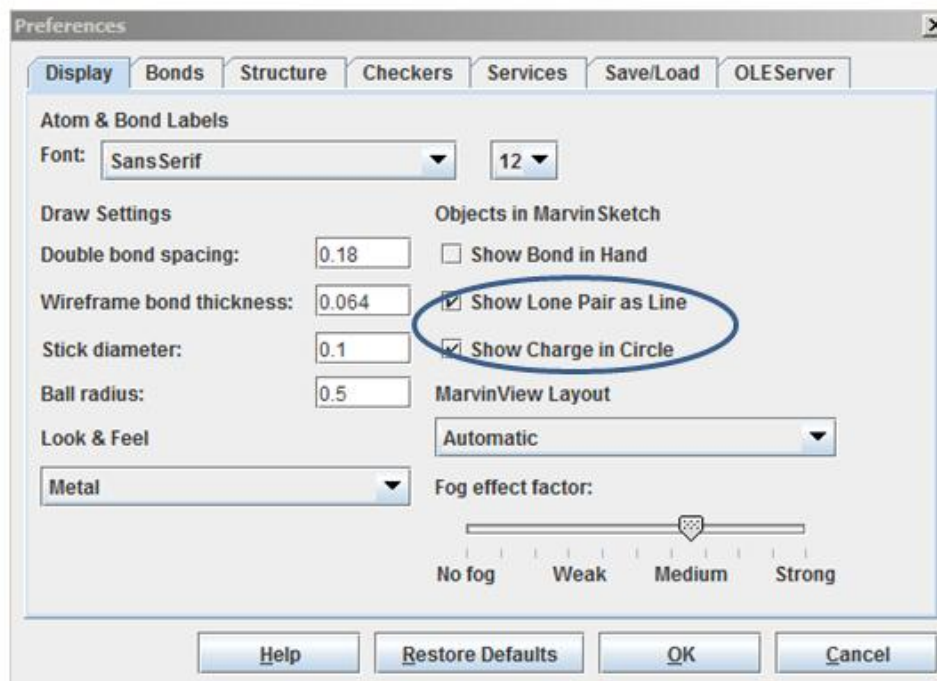
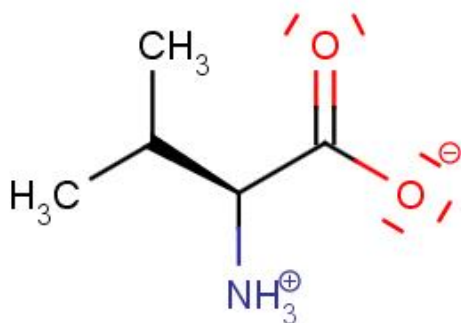
Visualize peptide sequence using 1-letter abbreviations

The screenshot shows the Marvin 5.10 software interface. The 'View' menu is open, and the 'Peptide Display' option is selected. A sub-menu is visible, showing two options: '1-letter' (selected) and '3-letter'. The peptide sequence H-M-A-R-V-I-N-OH is displayed below the menu. The letters M, A, R, V, I, and N are in black, while H and OH are in red. The sequence is connected by horizontal lines.

H — M — A — R — V — I — N — OH

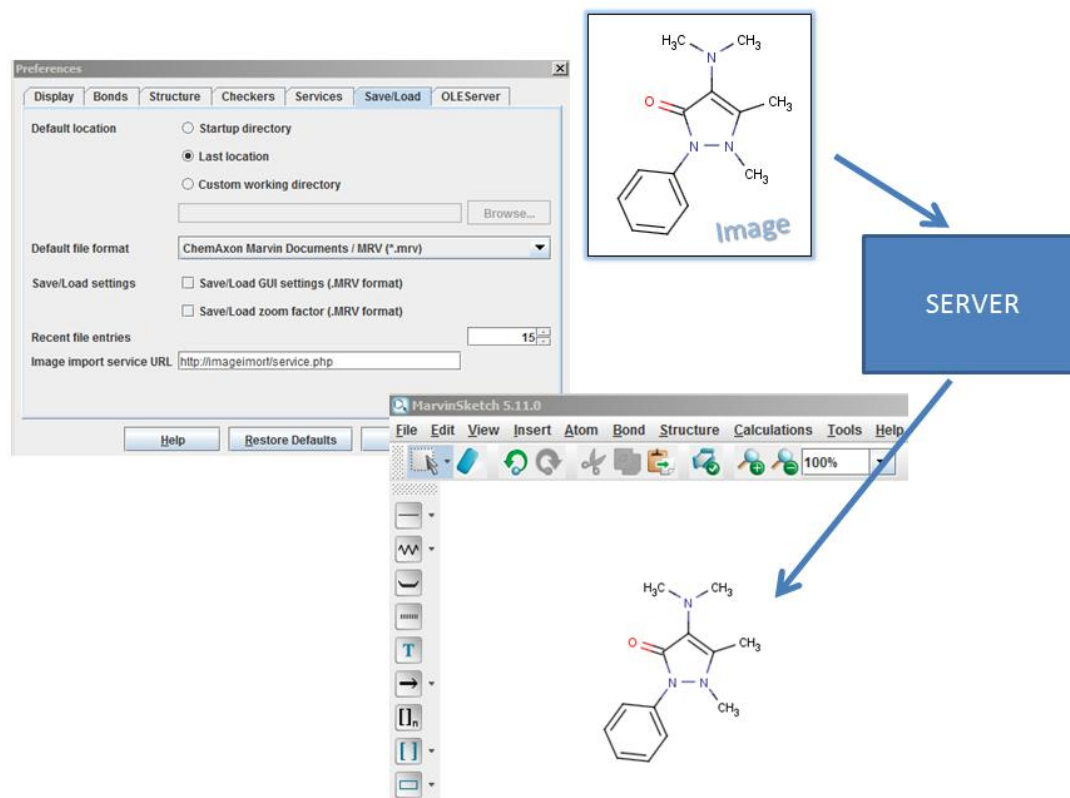
Marvin 5.11

New display options: lone pairs can be displayed as lines and charge can be displayed in a circle.




Marvin 5.11

Central server solution for image import





Coming soon....



ChemAxon



H

C

N

O

S

F

P

Cl

Br

I

A





[https://marvinjs.chemaxon.com/demo/
gui-1.0-SNAPSHOT/index.html](https://marvinjs.chemaxon.com/demo/gui-1.0-SNAPSHOT/index.html)

username: demo

password: USUGM12

ehoffmann@chemaxon.com



H

C

N

O

S

L

P

Cl

Br

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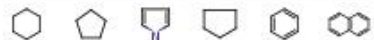
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