

Marvin Features and News

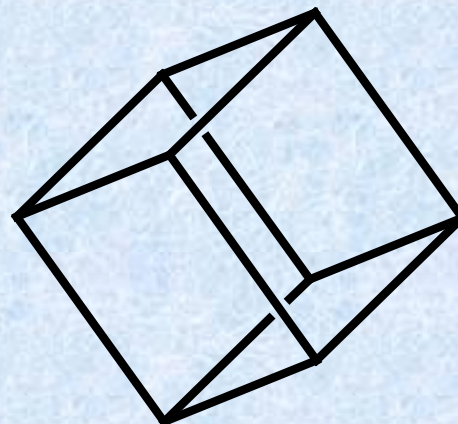
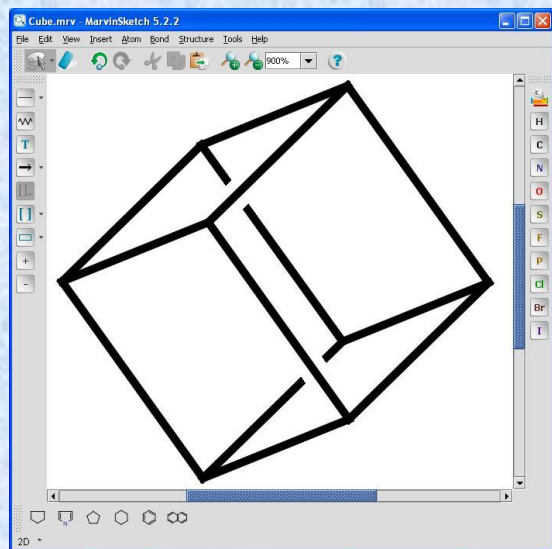
Akos Papp

- Live demonstration
 - New features in 5.2.x versions
 - Features planned in 5.3
 - Future features
 - Tips and tricks for faster sketching

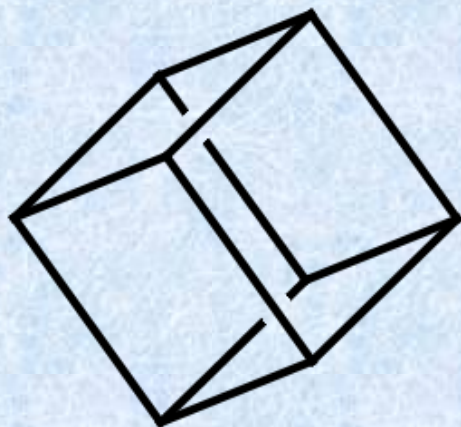
Main new features in 5.2.x

- Transparent structure painting
 - Transparent background images (EMF, SVG, PNG)
 - Transparent OLE object
- MView spreadsheet view speedup
- Marvin initialization speedup in applet version
- Charges can be displayed on brackets
- OLE object improvements
 - Image properties (colors, implicit H, etc.)
 - Speed (memory resident OLE server)
- Periodic system coloring schemes
- Reaxys Generics atoms and groups

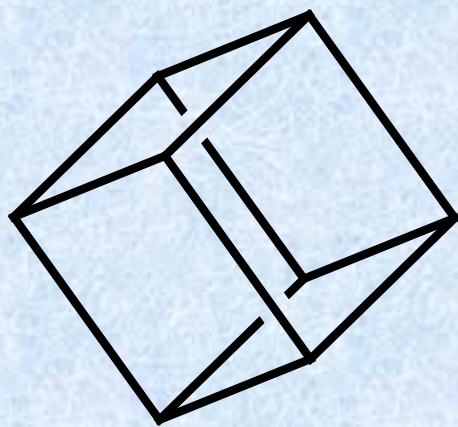
Transparent drawing and images



OLE Object

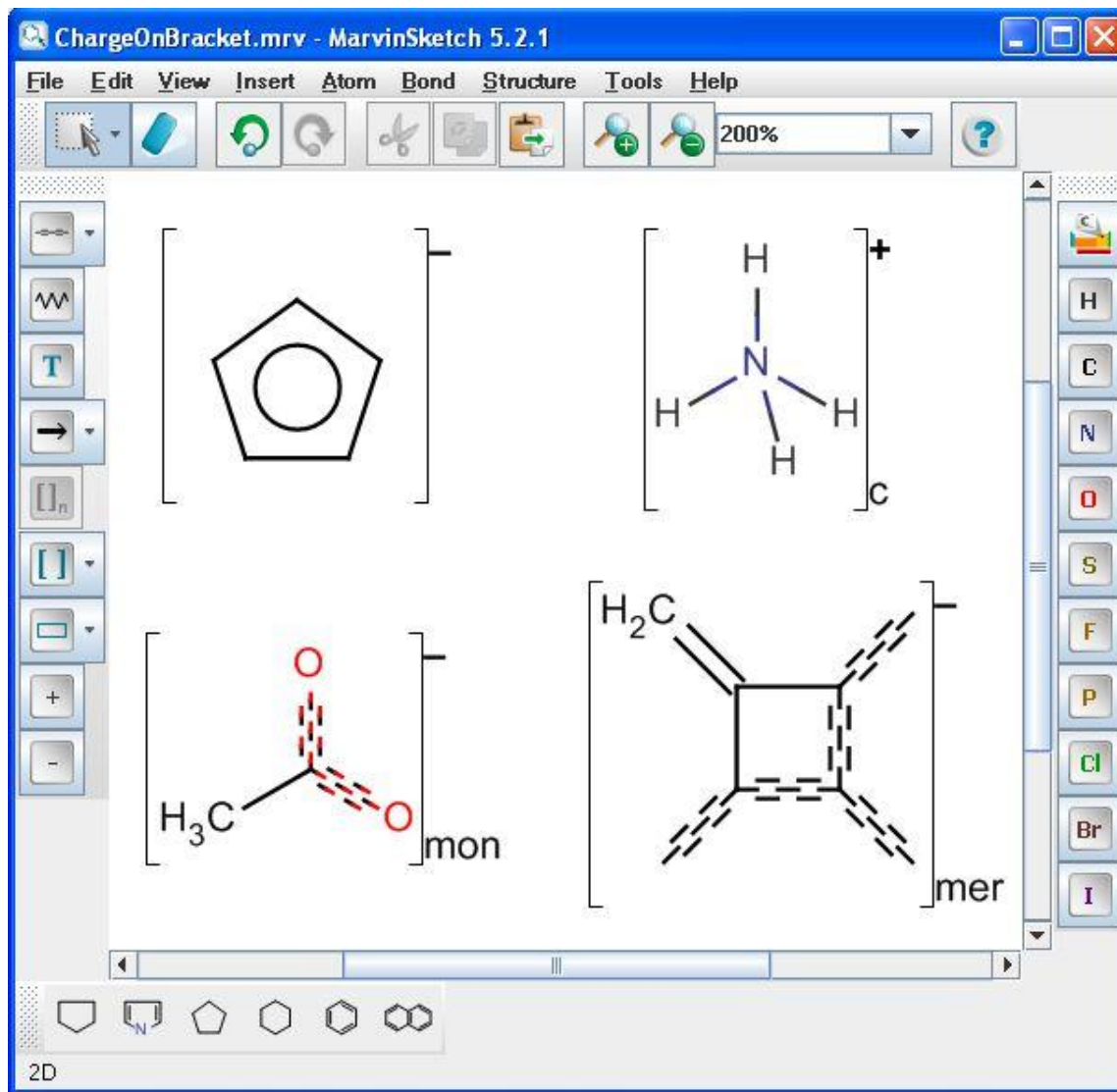


PNG



EMF

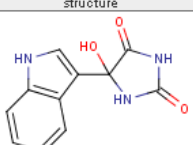
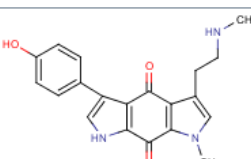
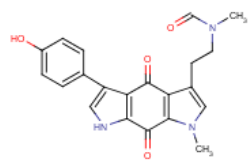
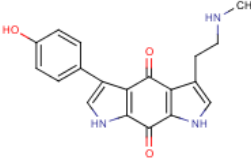
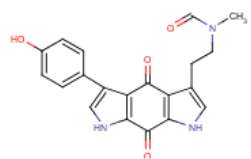
Charges on brackets



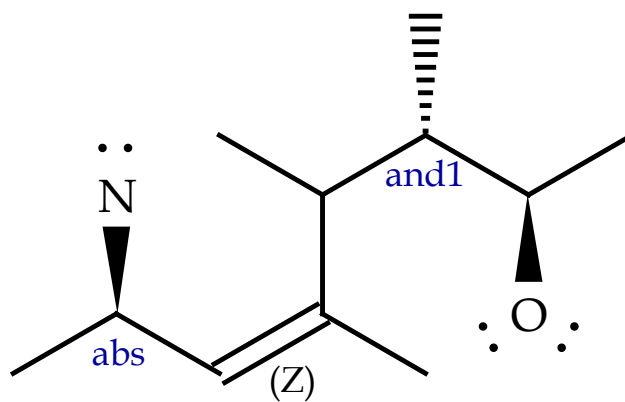
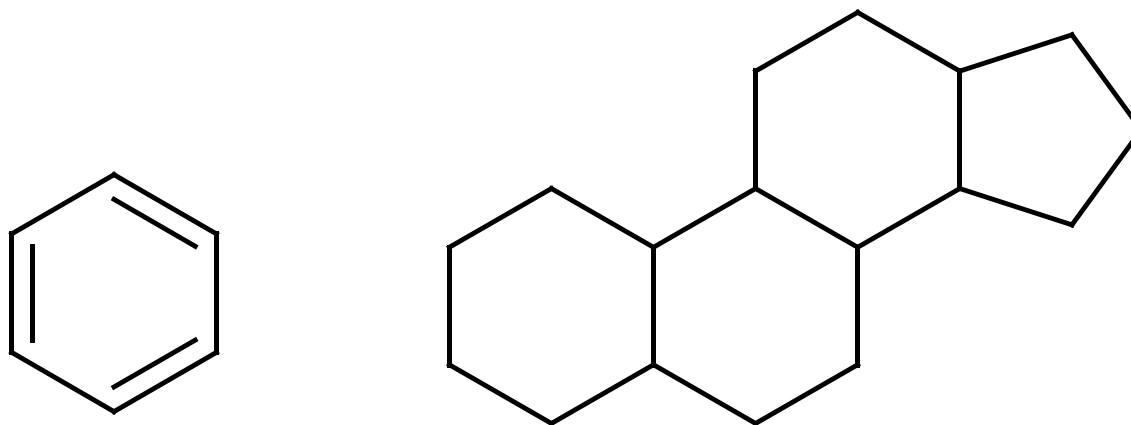
MarvinView spreadsheet view speedup

TandFnewest.sdf - MarvinView 5.2.4

File Edit View Table Tools Help

#	structure	EXNO	UKEY	NAME	CTFL	VARD	DERD
538524		MTX25	00016302-005	Zyzzin	N		5-Oxo analogue, 3,4-dihydro, 4-hydroxy
538525		OHD44	00249871-000	Zyzzyanone A	N		
538526		OOK54	00249871-001	Zyzzyanone A	N		<h1>N<h0><p1>2_p<p0>-Formyl
538527		OOK55	00249871-002	Zyzzyanone A	N		<h1>N<h0><p1>1<p0>De-Me
538528		OOK56	00249871-003	Zyzzyanone A	N		<h1>N<h0><p1>1<p0>De-Me, <h1>N<h0><p1>2_p<p0>-formyl

OLE object improvements



Periodic system coloring schemes

Periodic System

Periodic Table | Advanced

Name: Iodine (I)
Atomic number: 53
Mass: 126.90447
Electronegativity: 2.5
Ox. state(s): -1,1,3,5,7

1	H	2											13	B	14	C	15	N	16	O	17	F	18	He
2	Li	Be											Al	Si	P	S	Cl	Ar						
3	Na	Mg	3	4	5	6	7	8	9	10	11	12	Ga	Ge	As	Se	Br	Kr						
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	In	Sn	Sb	Te	I	Xe						
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	Tl	Pb	Bi	Po	At	Rn						
6	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn						
7	Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt															
Atom list			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu								
NOT list			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr								
Clear list																								

Color schema:

CPK Standard state Blocks Metals/Nonmetals

Color legend:

Alkali metal Metalloid Other metal
Alkaline earth metal Transition metal Nonmetal

Close

Reaxys Generics

The image shows the MarvinSketch 5.2.1 software interface. A context menu is open over a hexagonal structure, with the 'Reaxys Generics...' option selected. A red arrow points from the 'R' button in the right-hand toolbar to this option. Another red arrow points from the 'Reaxys Generics...' option to the 'Reaxys Generics' dialog box.

The 'Reaxys Generics' dialog box contains the following sections:

- Atom Generics:** A, AH, Q, QH, M, MH, X, XH
- Group Generics:** G, GH, G*, GH*
- Acyclic:**
 - Carbaacyclic: ABC, ABH
 - Hetero acyclic: AHC, AHH
 - Alkynyl: AYL, AYH
 - Alkyl: ALK, ALH
 - Alkenyl: AEL, AEH
- Cyclic:**
 - Carbocyclic: CBC, CBH
 - Aryl: ARY, ARH
 - Cycloalkyl: CAL, CAH
 - Cycloalkenyl: CEL, CEH
 - Heterocyclic: CHC, CHH
 - Hetero aryl: HAR, HAH
 - No carbon: CXX, CXH

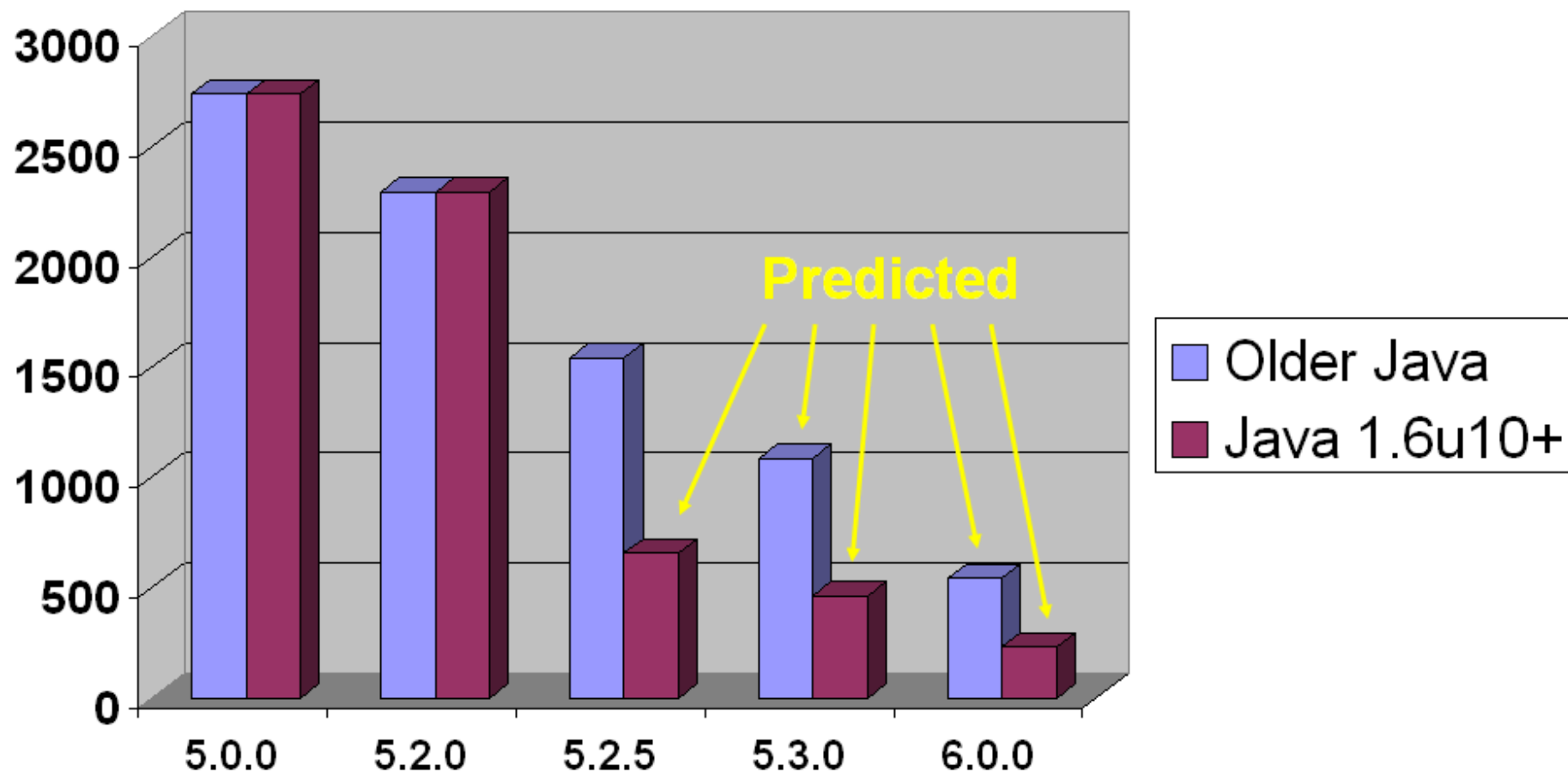
Buttons for 'Close' and '* Attachment Point' are also visible.

Features planned in 5.3

- MarvinSketch initialization speedup
 - **Two** (with java 1.6u10+ **five**) times faster loading is expected in version 5.3 vs. 5.2.0
- MarvinSketch.Net and MarvinView.Net
- Sprout drawing
- Brackets as graphical objects
 - Bracket tool: creating groups by framing them
 - Automatic bracket coordinates, but can be moved
 - Data can be attached to the bracket
- Ellipses/circle, rounded rectangle/square
- SKC file import and export, CDX file export

MarvinSketch applet initialization speedup

Total size of files for initialization (kB)



MarvinSketch.Net and MarvinView.Net

MarvinSketch 5.2.4 Snapshot for .NET

File Edit View Insert Atom Bond Structure Tools Help

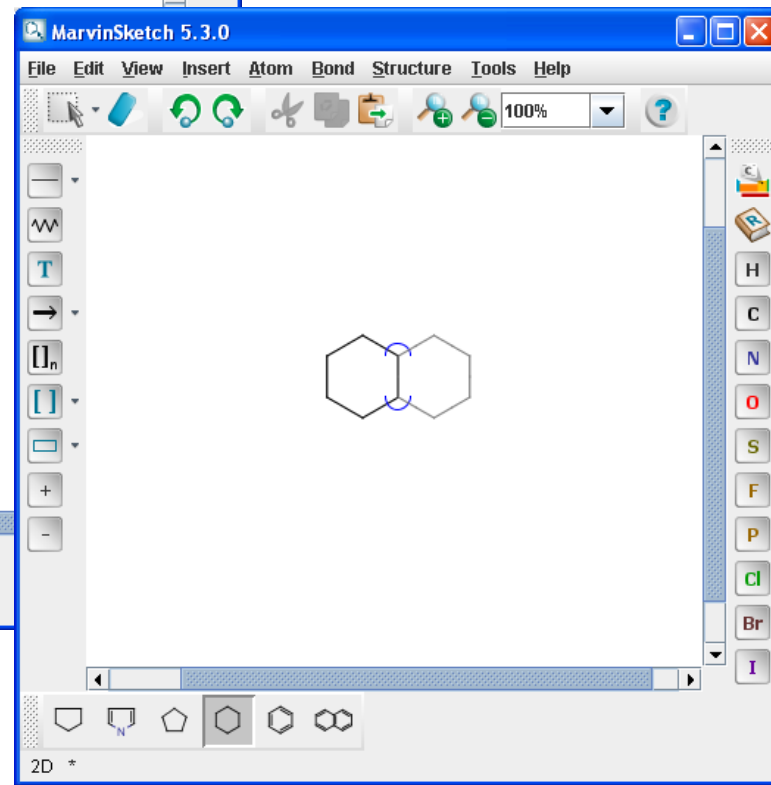
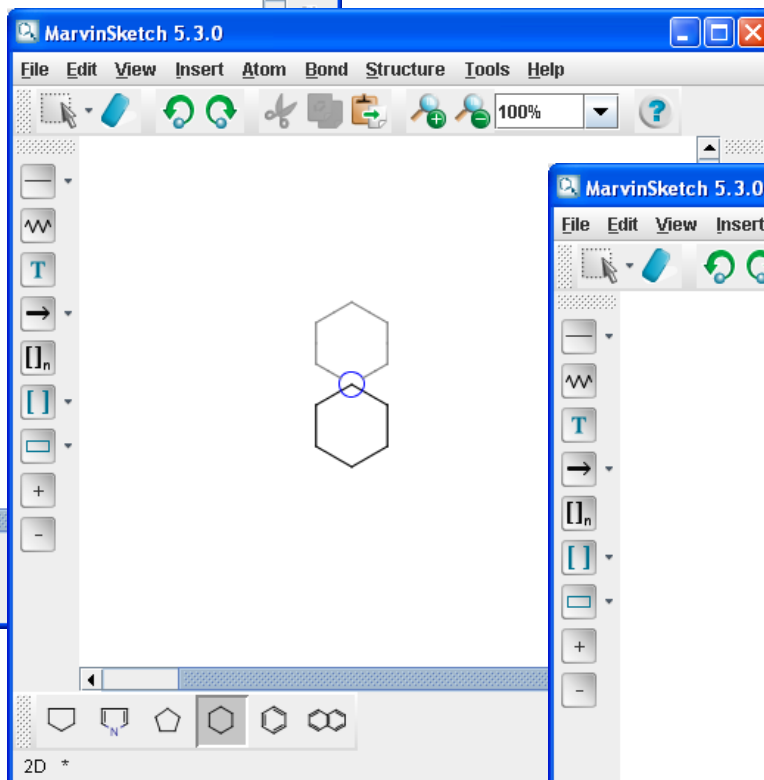
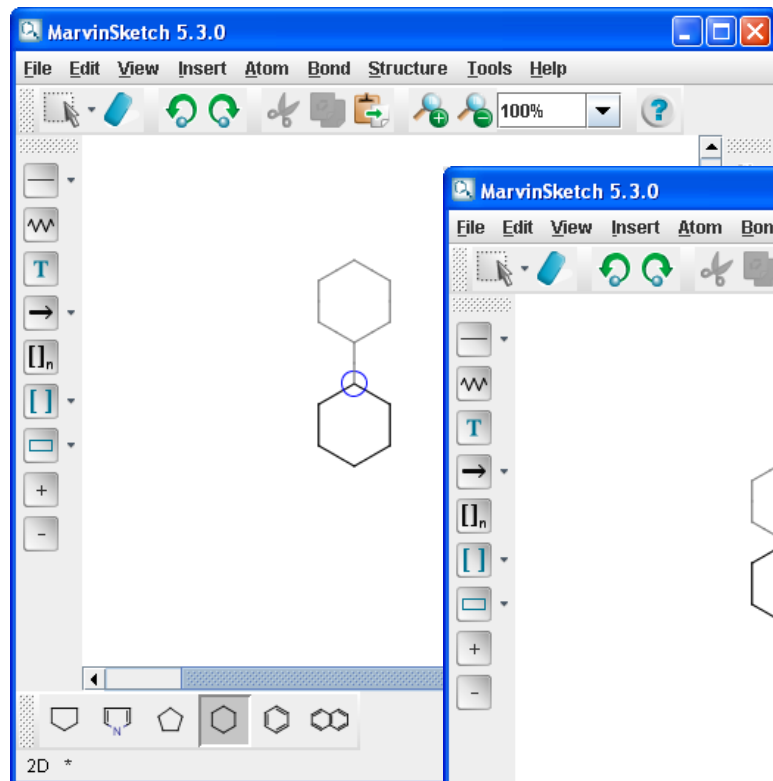
MarvinView 5.2.4 Snapshot for .NET

File Edit View Table Tools Help

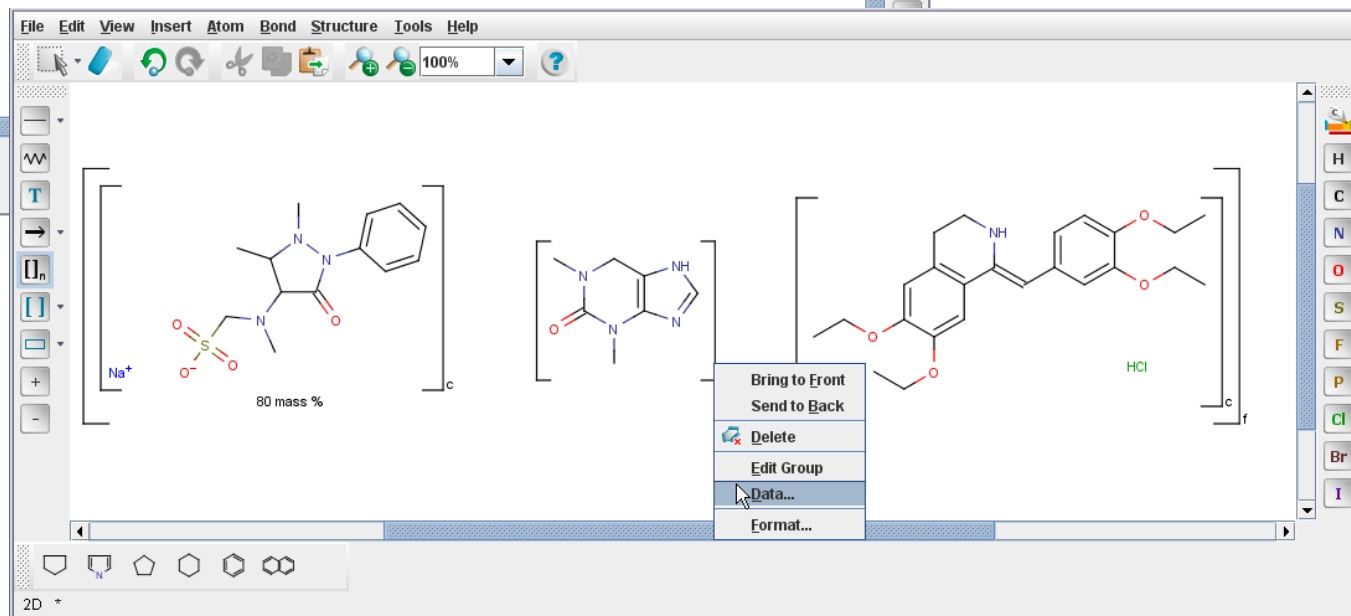
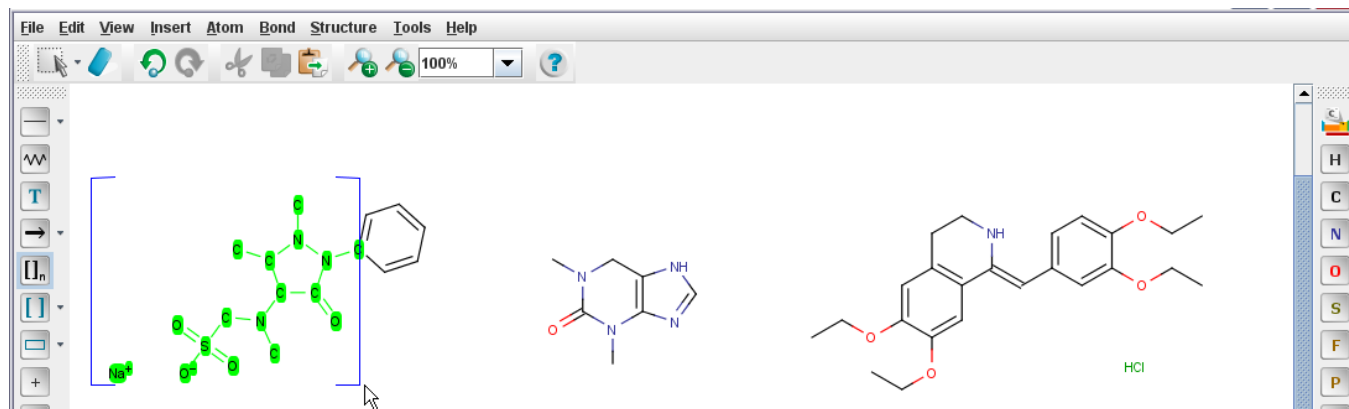
#	structure	EXNO	UKEY	NAME	CTFL	VARD	DERD
						AAL Toxin TA<p2>1<p0>	4,5-Dideoxy
						AAL Toxin TA<p2>1<p0>	4,5-Dideoxy, <h1>N<h0>-Ac
						AAL Toxin TA<p2>2<p0>	
						AAL Toxin TA<p2>2<p0>	5-Deoxy
						AAL Toxin TA<p2>2<p0>	5-Deoxy, <h1>N<h0>-Ac

MarvinSketch version 5.2
Copyright 2009, ChemAxon

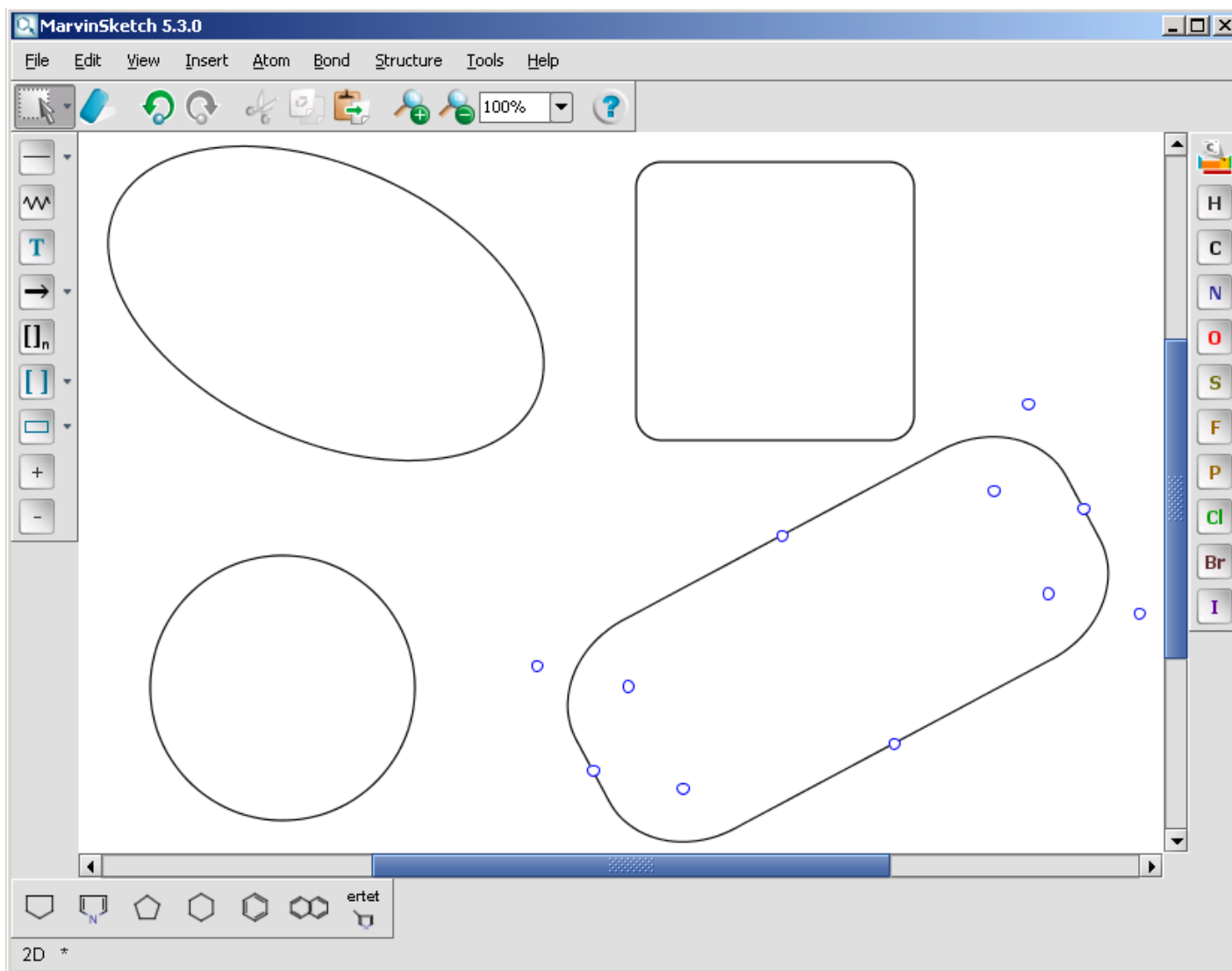
Sprout Drawing



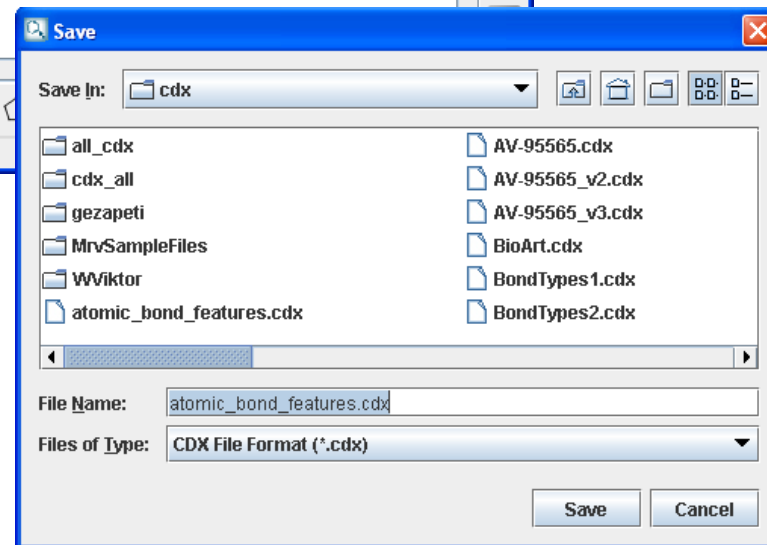
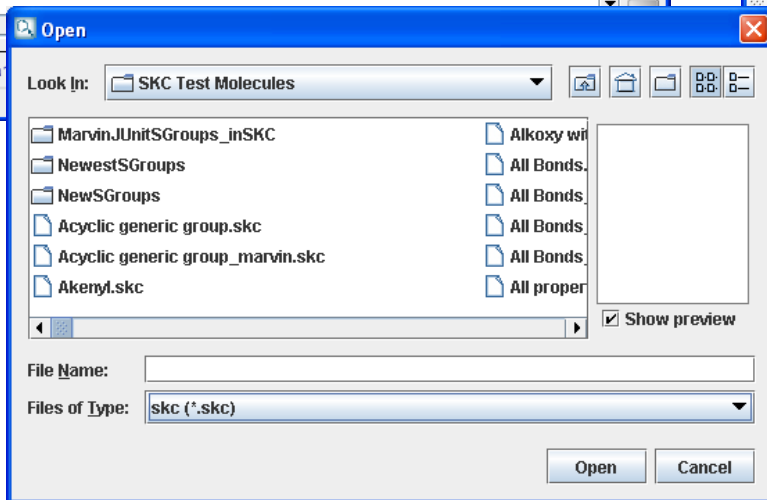
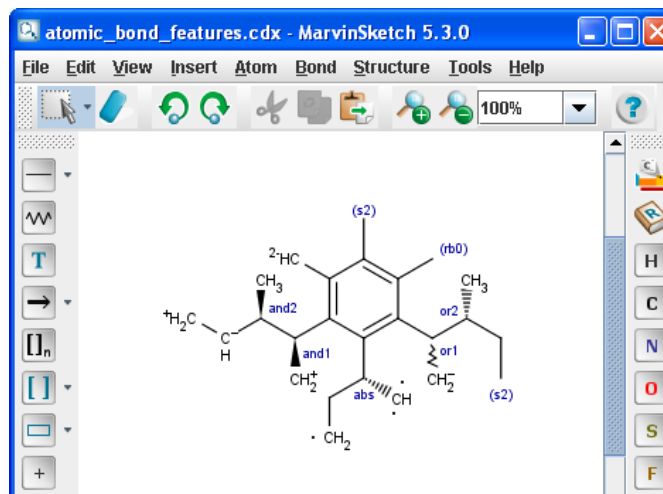
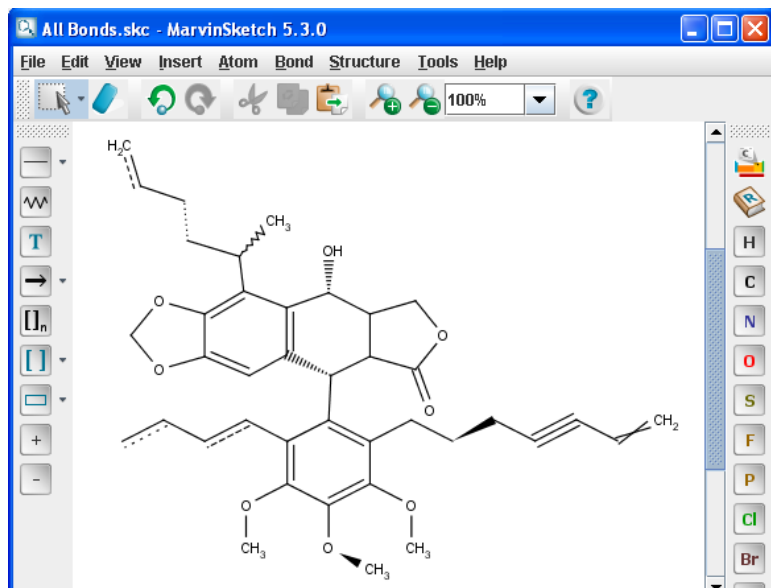
Brackets as graphical objects



Ellipse/circle, rounded rectangle/square



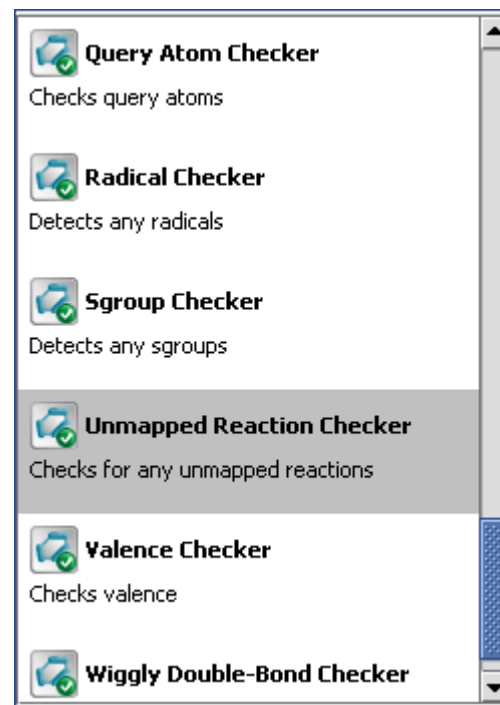
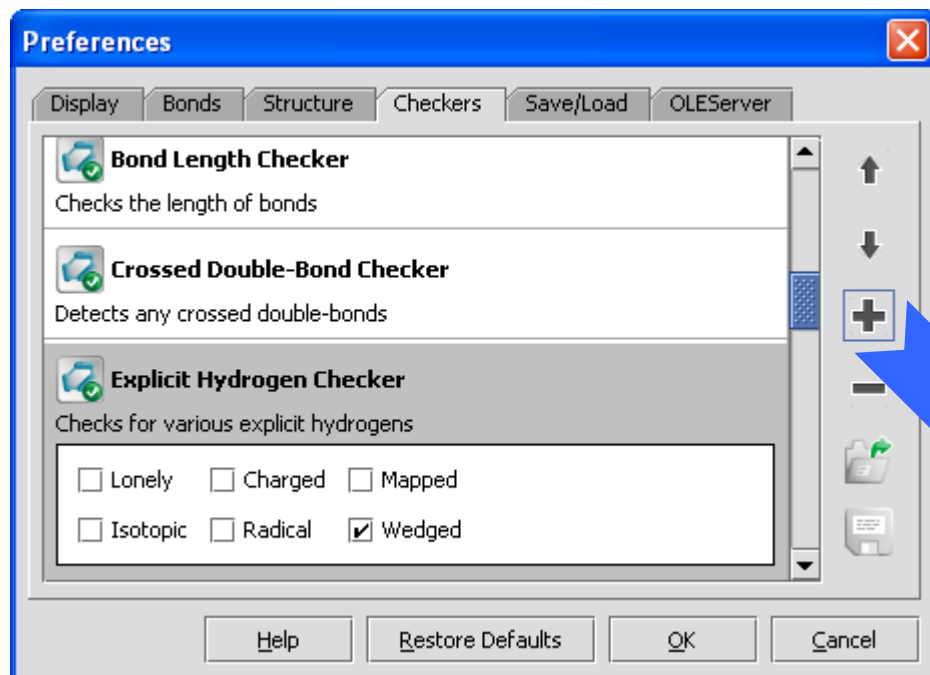
SKC import/export, CDX export



Features planned in 5.3

- Structure checker component in MarvinSketch GUI
- Chemical terms editor in GUI
- Template handling redesign
 - Load templates from specified directories
- Projected drawing
 - Bold bonds, ellipses in aromatic rings
 - Turning structures into projection
- Multirecord file (SDFFile) import to the same canvas
- Spreadsheet view mode for MView applet

Structure checker in MarvinSketch GUI

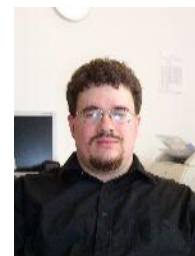


Future features

- Marvin Lite (Modular system)
 - **Four** (with java 1.6u10+ **ten**) times faster loading is expected in version 5.3 vs. 5.2.0
- Enhanced handling of group attachment points
 - Leaving group definition
- Multistep reaction support
 - Real arrows with automatic assignment of reactants
- MarvinView GUI redesign

- Menus and Toolbars
 - Customization
 - Configurations
 - Popup menus
- Preferences
- Drag and drop to MyTemplates
- Keyboard Usage
 - Shortcuts
 - Abbreviated groups
 - Markush drawing
 - SHIFT button

Acknowledgements



Thank you for your attention!

Find out more

- **Product descriptions & links**
www.chemaxon.com/products.html
- **Forum**
www.chemaxon.com/forum
- **Presentations and posters**
www.chemaxon.com/conf
- **Download**
www.chemaxon.com/download.html

The screenshots illustrate various aspects of ChemAxon's offerings: product news, software updates (Insta 5.0), a demo of the Marvin editor, and a technical support forum. The forum table is as follows:

Support	Topics	Posts	Last Post
Structure editing, viewing and file formats	827	4081	Fri Feb 01, 2008 1:00 pm Closed
Support for MarvinSketch, MarvinView and MarvinCenter	60	306	Thu Jan 31, 2008 9:16 pm Closed
MarvinSpace	60	374	Fri Feb 01, 2008 10:02 am Closed
Development discussion area for OpenEye, 3D rendering, Marvin and MarvinView	351	174	Fri Feb 01, 2008 10:02 am Closed
Structure based prediction and Chemical Terms	426	1982	Fri Feb 01, 2008 10:43 am Closed
Support for Calculator Plugin operation through cracks, API, Marvin, Insta2Chem and Chemical Terms	179	416	Wed Jan 30, 2008 9:10 pm Closed
Structure search and chemical database	76	345	Wed Jan 30, 2008 9:10 pm Closed
Support for Insta2Chem, Structure database GUI, both Calculator Plugin processor etc)	116	577	Thu Jan 30, 2008 9:10 pm Closed
Structure visualization / standardization	116	577	Thu Jan 30, 2008 9:10 pm Closed
Library enumeration, virtual synthesis and metabolite generation	308	471	Thu Jan 30, 2008 1:00 am Closed
Support for Reactor and Fragmenter	4	7	Tue Jan 29, 2008 10:32 am Closed
Virtual screening, clustering and molecular descriptors			
Support for Inven and Shutter			
License Issues			
Support for the technical questions related to license handling			