Chemical Structure Drawing Packages

Dr. Don Parkin
Chemical Database Service
Daresbury Laboratory
If a picture paints a thousand words….

Valium

- **Systematic Names**
  - 7-chloro-1,3-dihydro-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one
  - 7-chloro-1,3-dihydro-1-methyl-5-phenyl-3H-1,4-benzodiazepin-2(1H)-one
  - 7-chloro-1-methyl-5-phenyl-1,3-dihydro-2H-1,4-benzodiazepin-2-one
  - 7-chloro-1-methyl-5-phenyl-1,3-dihydro-benzo[e][1.4] diazepin-2-one

- **Trade Names**
What Drawing Package Should I Use?

Windows/Macintosh/UNIX
Cost
Interface and Tools
  • Friendly User Interface
  • Drawing and Presentation tools
Information sharing
  • Stand alone or integrated into a suite
  • Input/Output data – databases; modelling software etc.
  • 2D → 3D
Extras / Add-ins – e.g. Naming, Calculation of Properties

What Do You Want To Use It For ?
# 2D Structure Drawing Packages

<table>
<thead>
<tr>
<th>2D Structure Drawing Packages</th>
<th>2D Structure Drawing Packages</th>
</tr>
</thead>
<tbody>
<tr>
<td>SciFinder (Scholar)</td>
<td>ChemSketch (ACD/Labs)</td>
</tr>
<tr>
<td>DrawIt (ChemWindow) (Bio-Rad - KnowItAll)</td>
<td>Chem 4-D Draw</td>
</tr>
<tr>
<td>MarvinSketch (ChemAxon)</td>
<td>(X)Win DrawChem</td>
</tr>
<tr>
<td>ICEdit (InfoChem) [SPRESI]</td>
<td>StrukEd</td>
</tr>
<tr>
<td>MolWorks</td>
<td>JChemPaint (SourceForge)</td>
</tr>
<tr>
<td>Beilstein Structure Editor</td>
<td>Bkchem</td>
</tr>
<tr>
<td>ConQuest Structure Editor</td>
<td>SpecSurf Structure Editor</td>
</tr>
</tbody>
</table>
Interfaces and Tools


ChemDraw Ultra V12 (net)

Windows
MAC

Commercial
Part of ChemOffice
Interfaces and Tools

http://www.symyx.com/products/software/cheminformatics/symyx-draw/index.jsp

Symyx Draw (V3.3)

Windows XP and VISTA

Free for home and academic use
Interfaces and Tools

http://www.symyx.com/micro/jdraw/

Symyx
Jdraw
DiscoveryGate

Java based
All Platforms

Free for home and academic use

Template Tools

Atom and Bond Tools

Reaction Tools
Interfaces and Tools

http://www.cas.org/products/scifindr/index.html

SciFinder Scholar (CASDraw)

Menus

Draw Tools

Selection Tool

Atom and Bond Tools

Template Tools

Windows
Mac
+ web version
Interfaces and Tools

http://www.acdlabs.com/products/draw_nom/draw/chemsketch/

For Linux users, a compatible version of ACD/ChemSketch Freeware can be run with Code Weavers’ CrossOver Office.
Interfaces and Tools

http://www.cheminnovation.com/products/chem4d.asp

Chemistry 4-D Draw
Commercial
Windows and Mac

Menus

Bond Tools

Template Tools

Drawing Aids

Demo version

Atom Tools
Interfaces and Tools

http://bkchem.zirael.org/

BKchem
Freely available open source (cross platform)
Interfaces and Tools

http://www.infochem.de/products/software/icedit.shtml

ICEdit
(InfoChem)
Stand alone and Java

Commercial but may be freely available to academics

Use with SPRESI$^{\text{web}}$

Menus

Bond Tools
Templates
Reaction Tools

Atom Tools
Interfaces and Tools

http://www.chemaxon.com/products/marvin/marvinsketch/

Marvin Sketch

- Freely available
- Cross platform
- Java - Web

Menus

Bond Tools (Dropdown Menu)

Drawing and Reaction Tools

Templates

Atom Tools
Interfaces and Tools

http://xdrawchem.sourceforge.net/

WinDrawChem
(windows)

XDrawChem
(Linux)

Freely available
Interfaces and Tools

• **Tools and Functions**
  – Tools to draw Bonds
  – Tools to draw Atoms
  – Templates
  – Drawing Aids / Presentation Tools
    – Query Tools for SubStructure Searching
    – Reaction Drawing Tools

• **Problems/Pitfalls**
Interfaces and Tools

Drawing Bonds - Pitfalls

Drawing structures without joining bonds correctly.

Zoom in

not
Interfaces and Tools

Drawing Bonds - Pitfalls

Drawing structures without joining bonds correctly.

**Symyx Draw** – Chemistry Menu *Run Chem Check* ...  

**SciFinder** (CAS Draw)  
Tools Menu -  
*Check Overlaps*  
Checks if any nodes or bonds overlap and displays a message if any do.
Interfaces and Tools

Drawing Bonds - Pitfalls

ChemDraw highlighting with red warning box

The atom is connected to two identical co-linear bonds and so may appear invisible.

Symyx Draw - highlights with Atom Symbol
Interfaces and Tools

Drawing Bonds - Pitfalls

Drawing structures without joining bonds correctly.

Most packages have set bond lengths (ChemSketch doesn’t) but you can use the **Select** key to stretch any bond to the length you want. (Symyx Draw – click, hold and drag)
Interfaces and Tools

Tools to draw Atoms

**Symyx Draw**

- Allow these atoms
- Prohibit these atoms
- Stereoconfiguration

- Any atom except H (A)
- Any atom except H or C (Q)
- Atom List...

**ChemDraw**

- C
- N
- O
- P
- S
- H
- Q
- More...
- Create abbreviation

- Periodic Table
- Set Atom Type
- Allow Selected Atoms
- Prohibit Selected Atoms

**ChemSketch**

- A = Any Atom except H
- Q = Any Heteroatom (any atom except C or H)
- HO = Any Atom but no H attached.
- L, NL = List, Not List

**Query Atom**

Can be used for searching

Example: C,S,P or C S P or C:S:P

Hydrogen is not allowed!
Interfaces and Tools

Templates

Most packages have useful templates to help draw structures. Some common ones are often available as buttons.

ISIS/Draw MDL Draw (Customisable)

Symyx Draw – Click to get more toolstrips

BKChem

MarvinSketch

ChemDraw

SciFinder

DrawIt (KnowItAll)
Interfaces and Tools

Templates

Often there is a list of a set of templates from a menu item (or button).

ConQuest

ChemDraw

Symyx Draw

ChemSketch
Interfaces and Tools

Templates

These usually expand to show the structure.

ChemDraw

Symyx Draw
Interfaces and Tools

Templates

Clicking on a bond in the drawing area will FUSE the template to it.

Clicking on an atom in the drawing area will SPROUT the template from it.
Interfaces and Tools

Templates

Care must be taken with the atom that is chosen from the template. (ISIS Draw and ChemSketch)

No choice with ChemDraw

Symyx Draw shows the point of contact
Interfaces and Tools

Hotkeys/Shortcuts

ISIS Draw

ChemDraw has 100 hot keys

Careful with upper or lower case

CAS Draw

Atom Hotkeys

<table>
<thead>
<tr>
<th>Key</th>
<th>Atom Label</th>
<th>Key</th>
<th>Atom Label</th>
<th>Key</th>
<th>Atom Label</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>A</td>
<td>f</td>
<td>F</td>
<td>R</td>
<td>4 Ph</td>
</tr>
<tr>
<td>A or 5</td>
<td>Ac</td>
<td>h</td>
<td>H</td>
<td>g</td>
<td>Q*</td>
</tr>
<tr>
<td>b</td>
<td>Br</td>
<td>i</td>
<td>I</td>
<td>r</td>
<td>R</td>
</tr>
<tr>
<td>1</td>
<td>n-Bu</td>
<td>k</td>
<td>K</td>
<td>s</td>
<td>S</td>
</tr>
<tr>
<td>2</td>
<td>s-Bu</td>
<td>m</td>
<td>Me</td>
<td>S</td>
<td>Si</td>
</tr>
<tr>
<td>3</td>
<td>t-Bu</td>
<td>n</td>
<td>N</td>
<td>t</td>
<td>TMS</td>
</tr>
<tr>
<td>c</td>
<td>C</td>
<td>N</td>
<td>Na</td>
<td>x</td>
<td>X</td>
</tr>
<tr>
<td>C or l</td>
<td>Cl</td>
<td>o</td>
<td>O</td>
<td>E</td>
<td>COOCH₃</td>
</tr>
<tr>
<td>d</td>
<td>D</td>
<td>T</td>
<td>OTs</td>
<td>6</td>
<td>CH₂OH</td>
</tr>
<tr>
<td>e</td>
<td>Et</td>
<td>p</td>
<td>P</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Bond Hotkeys

<table>
<thead>
<tr>
<th>Function</th>
<th>Key</th>
<th>Function</th>
<th>Key</th>
</tr>
</thead>
<tbody>
<tr>
<td>Change to single bond</td>
<td>1</td>
<td>Change to Dashed bond</td>
<td>d</td>
</tr>
<tr>
<td>Change to double bond</td>
<td>2</td>
<td>Change to Wavy bond</td>
<td>y</td>
</tr>
<tr>
<td>Change to triple bond</td>
<td>3</td>
<td>Position a double bond to the left</td>
<td>l</td>
</tr>
<tr>
<td>Change to quadruple bond</td>
<td>4</td>
<td>Center a double bond</td>
<td>c</td>
</tr>
<tr>
<td>Change to Bold bond</td>
<td>b</td>
<td>Position a double bond to the right</td>
<td>r</td>
</tr>
<tr>
<td>Change to Wedged bond</td>
<td>w</td>
<td>Bring bond to front</td>
<td>f</td>
</tr>
<tr>
<td>Change to Hashed bond</td>
<td>h</td>
<td>Open a bond properties text box.</td>
<td>/ (slash) or ?</td>
</tr>
<tr>
<td>Change to Hashed-wedged bond</td>
<td>H</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Interfaces and Tools

**Text Editing**

2 Types:-

1) **Structural** (atomic symbols, functional groups, atom labels)

   - Symyx Draw
   - Chem-4-D

2) **Other Text** (captions, reaction conditions, annotations etc.)

   - Symyx Draw
   - MarvinSketch
   - ChemSketch (Draw Module)
   - KnowItAll ReportIt

Some have only one tool to handle both

- KnowItAll DrawIt Label Tool
- ChemSketch Edit Atom Label Tool
- ChemDraw

**Fonts, styles, size and colour** can all be changed.
Interfaces and Tools

Text Editing

Problems

Difference between Atom tool and Text tool in handling of text such as CO$_2$Et, OAc, Ph, n-Bu etc.

Symyx Draw

--- COOEt
--- t-Bu
--- Ph
--- OEt

--- CO$_2$Et
--- n-Bu
--- OAc

---

Chem-4-D

---

e.g.

---

---

[Chemical structures and tool interfaces shown]
Text Editing

Problems

Difference between Atom tool and Text tool in handling of text such as CO$_2$Et, OAc, Ph, n-Bu etc.

ChemDraw (Structure Menu)

--------- CO$_2$Et

ChemSketch (Tools Menu)

Some can be used to search databases
Interfaces and Tools

Text Editing

Problems

With most packages you **cannot** rotate the text.

With **Symyx Draw** you can only alter the box it is in.
Interfaces and Tools

Other Tools

What do you want to use the structure drawing package for?

- As Query for searching database
- To produce a Reaction Query
- To Register in database
- For a Presentation
- To produce a Name
- To produce Physical Properties
- To produce 3D molecule
Interfaces and Tools

Pitfalls

1,2 Dipoles (two neighbouring charges of opposite sign)

Beilstein

Symyx Draw
ChemDraw
ChemSketch etc.

Hint: Use the template menu – Functional groups
Interfaces and Tools
Drawing Aids / Presentation Tools

Some have very useful templates

ChemSketch
Interfaces and Tools

Drawing Aids / Presentation Tools

Some can even have templates of lab equipment
Interfaces and Tools

Drawing Aids / Presentation Tools

Line and Arc

Symyx Draw

ChemDraw

ChemSketch (Draw Window)

Box, Polygon and Ellipse

Symyx Draw

ChemDraw

ChemSketch (Draw Window)

Click and drag to draw.
(Hold shift key to draw squares and circles)
Interfaces and Tools

Drawing Aids / Presentation Tools

Flip / Rotate

Most packages can flip BONDS horizontally or vertically or whole molecules by 180° horizontally or vertically

2D (and 3D) rotation of molecules is usually possible

Symyx Draw
ChemSketch
Chem4D

ChemDraw, ChemSketch and KnowItAll Text (2D) and Structures (Objects)

3D - ONLY Structures
Interfaces and Tools

Drawing Aids / Presentation Tools

CLEAN MOLECULE

“Improves the appearance” of one or more selected structures by giving them uniform bond lengths and angles.

Clean Molecule

ChemSketch
Symyx Draw
ISIS/Draw
ChemDraw
Interfaces and Tools
Drawing Aids / Presentation Tools

CLEAN MOLECULE

Pitfalls

ChemDraw
Symyx Draw
ChemSketch
ISIS Draw

Clean
Extras / Add-ins

Nomenclature

Structure -> Name [and Name -> Structure]

**ChemDraw** includes **Struct=Name** [and **Name=Struct**]

**Symyx Draw** has OpenEye’s **Lexichem™** structure-name converter toolkit integrated into it.

**ISIS Draw** can name structures only with **Add-ins** such as **Autonom** or one supplied by ACD Labs.

**ChemSketch** can generate a IUPAC name (or an INDEX/CAS name \((\text{ACD/Name})\) on-line but only structure from SMILES or InChI (molecules of up to 50 atoms and three rings,)

**KnowItAll** has a **IUPAC Namelt** [and **IUPAC Drawlt**] module but in the free academic version certain features are disabled (e.g. only molecules with up to 10 non-hydrogen atoms)

**Chem 4-D** has IUPAC Naming using **Nomenclator** which is fully integrated in Chemistry 4-D Draw. It is also available as an add-on for ChemDraw.

**MarvinSketch** has Preferred IUPAC Name and Traditional Name
**Common Name:** Valium, Diazepam

- **ChemDraw** IUPAC Name: 7-chloro-1-methyl-5-phenyl-1\H-benzo[e][1,4]diazepin-2(3H)-one
- **Symyx Draw** IUPAC Name: 7-chloro-1-methyl-5-phenyl-3H-1,4-benzodiazepin-2-one
- **ISIS Draw** (Autonom): 7-chloro-1-methyl-5-phenyl-1,3-dihydro-benzo[e][1,4] diazepin-2-one
- **ChemSketch**
  - IUPAC Name: 7-chloro-1-methyl-5-phenyl-1,3-dihydro-2H-1,4-benzodiazepin-2-one
  - INDEX Name: 2H-1,4-benzodiazepin-2-one, 7-chloro-1,3-dihydro-1-methyl-5-phenyl
- **MarvinSketch**
  - IUPAC Name: 7-chloro-1-methyl-5-phenyl-2,3-dihydro-1H-1,4-benzodiazepin-2-one
  - Traditional Name: 7-chloro-1-methyl-5-phenyl-3H-1,4-benzodiazepin-2-one
- **Chem 4D** IUPAC Name: 7-chloro-1-methyl-5-phenyl-3H-benzo[f]1,4-diazepin-2-one

**Web**
- 7-chloro-1-methyl-5-phenyl-1,3-dihydro-2H-1,4-benzodiazepin-2-one
  - [ChemSpider]
- 7-chloro-1-methyl-5-phenyl-3H-1,4-benzodiazepin-2-one
  - [PubChem]
- 7-chloro-1-methyl-5-phenyl-3H-1,4-benzodiazepin-2(1H)-one
  - [Aldrich]
- 7-chloro-1,3-dihydro-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one
- 7-chloro-1-methyl-5-phenol-1,3-hydro-2H-1,4-benzodiazepin-2-one
- 9-chloro-2-methyl-6-phenyl-2,5-diazabicyclo[5.4.0]undeca-5,8,10,12-tetraen-3-one
- 10-chloro-6-methyl-2-phenyl-3,6-diazabicyclo[5.4.0]undeca-2,8,10,12-tetraen-5-one
0 - not supported. No chemical name is generated

1 - Only basic naming procedures are supported - only the simplest structures

2 - All basic procedures are supported. Correct names are generated for the simple cases of this type

3 - Many procedures are supported. Correct names are generated for all simple cases and some advanced ones

4 - Most procedures are supported. Correct names are generated for the most common representatives of this class

5 - All (or almost all) naming procedures are supported. Almost any structure of this class including the complex cases

<table>
<thead>
<tr>
<th>Naming Category</th>
<th>Example of Structure</th>
<th>ACD/Name</th>
<th>ChemDraw</th>
<th>OpenEye</th>
<th>AutoNorm</th>
<th>Nomenclator</th>
</tr>
</thead>
<tbody>
<tr>
<td>Biochemical nomenclature</td>
<td><img src="image" alt="Example Structure" /></td>
<td>4</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Functional Groups</td>
<td><img src="image" alt="Example Structure" /></td>
<td>5</td>
<td>4</td>
<td>3</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>Replacement (&quot;a&quot;) nomenclature</td>
<td><img src="image" alt="Example Structure" /></td>
<td>4</td>
<td>4</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Multiplicative nomenclature</td>
<td><img src="image" alt="Example Structure" /></td>
<td>5</td>
<td>5</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Von Baeyer polycycles</td>
<td><img src="image" alt="Example Structure" /></td>
<td>5</td>
<td>3</td>
<td>1</td>
<td>4</td>
<td>5</td>
</tr>
<tr>
<td>Spiro polycycles</td>
<td><img src="image" alt="Example Structure" /></td>
<td>5</td>
<td>2</td>
<td>2</td>
<td>4</td>
<td>3</td>
</tr>
<tr>
<td>Fused and bridged fused systems</td>
<td><img src="image" alt="Example Structure" /></td>
<td>5</td>
<td>3</td>
<td>2</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>Ring assemblies</td>
<td><img src="image" alt="Example Structure" /></td>
<td>5</td>
<td>3</td>
<td>1</td>
<td>4</td>
<td>1</td>
</tr>
<tr>
<td>Multicomponent structures</td>
<td><img src="image" alt="Example Structure" /></td>
<td>5</td>
<td>5</td>
<td>4</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>Organometallic compounds</td>
<td><img src="image" alt="Example Structure" /></td>
<td>4</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
Extras / Add-ins

Nomenclature

SMILES

ChemSketch: \( \text{Clc1ccc2c(c1)C(=NCC(=O)N2C)c3ccccccc3} \)

MarvinSketch (Save File as) \( \text{CN1C(=O)CN=C(C2=CC=CC=C2)C2=CC(Cl)=CC=C12} \)

Web – ChemSpider: \( \text{Clc3cc\1c(N(C(=O)C/N=C/1c2cccccc2)C)cc3} \)

ISIS (Via Consytant/Chemeleon) \( \text{N1(c2c(cc(cc2)Cl)C(=NCC1=O)c1cccccc1)C} \)

Symyx Draw \( \text{CN1c2ccc(cc2C(=NCC1=O)c3cccccc3)Cl} \)

InChI

Symyx Draw
\( \text{1S/C16H13ClN2O/c1-19-14-8-7-12(17)9-13(14)16(18-10-15(19)20)11-5-3-2-4-6-11/h2-9H,10H2,1H3} \)

MarvinSketch and ChemSketch
\( \text{1/C16H13ClN2O/c1-19-14-8-7-12(17)9-13(14)16(18-10-15(19)20)11-5-3-2-4-6-11/h2-9H,10H2,1H3} \)

Web – ChemSpider
\( \text{1/C16H13ClN2O/c1-19-14-8-7-12(17)9-13(14)16(18-10-15(19)20)11-5-3-2-4-6-11/h2-9H,10H2,1H3} \)

Symyx Draw and ChemSketch will also convert InChI to structure
Extras / Add-ins

Import/Export

1. Export as file then Import to another package

2. Cut and Paste into another package

3. Simply generate (e.g. 3D) and view in same package
Extras / Add-ins

Import/Export

1. Export as file then Import to another package

3 Types of files:

1) Picture file (gif, tiff, png etc. – no information)

2) Sketch file – includes drawing objects (lines, text etc.)

[often program specific – ChemSketch & ChemDraw will handle ISIS/MDL/Symyx .skc files but Symyx or ChemDraw will not import ChemSketch’s .sk2 files]

3) Molecule file – includes co-ordinates

[requires filters/converters]
Extras / Add-ins

Import/Export

1. Export as file then Import to another package

Most can Export to a different file format

SciFinder

ISIS/Draw
requires Consystant/Chemeleon

ChemSketch

ChemDraw

Note: 2D formats cannot output to 3D file formats
Extras / Add-ins

Import/Export

2. Cut and Paste into another package

Pasting structures into other packages can give different results.

Most produce a structure but ISIS/Symyx Draw and ChemSketch produces tables. Use Paste Special…
### Extras / Add-ins

#### Import/Export

2. Cut and Paste into another package

<table>
<thead>
<tr>
<th></th>
<th>Microsoft Word</th>
<th>OpenOffice (Writer)</th>
<th>DS Visualise</th>
<th>Symyx Draw ISIS/Draw</th>
</tr>
</thead>
<tbody>
<tr>
<td>Symyx Draw</td>
<td>✔️</td>
<td>✔️</td>
<td>✔️</td>
<td>✔️</td>
</tr>
<tr>
<td>ChemSketch</td>
<td>✔️</td>
<td>✗</td>
<td>✔️</td>
<td>✔️</td>
</tr>
<tr>
<td>ChemDraw</td>
<td>✔️</td>
<td>✔️</td>
<td>✔️</td>
<td>✔️</td>
</tr>
<tr>
<td>DrawIt</td>
<td>✔️</td>
<td>✔️</td>
<td>✔️</td>
<td>✔️</td>
</tr>
<tr>
<td>CASDraw</td>
<td>✔️</td>
<td>✔️</td>
<td>✗</td>
<td>✔️</td>
</tr>
<tr>
<td>Chemistry 4-D</td>
<td>✔️</td>
<td>✔️</td>
<td>✗</td>
<td>✔️</td>
</tr>
<tr>
<td>BK Chem</td>
<td>✗</td>
<td>✗</td>
<td>✗</td>
<td>✗</td>
</tr>
<tr>
<td>WinDrawChem</td>
<td>✔️</td>
<td>✔️</td>
<td>✗</td>
<td>✗</td>
</tr>
</tbody>
</table>

Symyx Draw with Open Office

DS Visualise
3D Visualisation

3. Simply generate and view in same package

Most packages have modules or bundled programs/ Plug-ins/ Add-ins which are capable of some form of 2D -> 3D conversion.

- **Symyx Draw** has ‘Convert 2D to 3D’ menu option (‘push’ to Jmol or Rasmol)
- **ISIS/Draw** can use ACD/Labs 3D Viewer (Add-in) or view in Rasmol
- **ChemSketch** contains its own 3D Viewer
- **ChemDraw** requires sister program ChemBio3D (as you draw hotlink)
- **DrawIt** has bundled program 3DViewIt
- **MarvinSketch** has bundled program MarvinView and MarvinSpace
- **Chem 4-D** requires sister program ChemSite
3D Visualisation
ChemSketch – 3D View

- Rotate
- View options
- Measure Bonds, Angles
Extras / Add-ins

3D Visualisation

Pitfalls

2D packages cannot directly output to 3D

View in 3D viewer with no 3D optimisation

e.g. Rasmol

Symyx Draw – ‘Push to Jmol’ (or Rasmol)
3D Visualisation

Pitfalls

ISIS/Draw
ChemDraw
ChemSketch

MarvinSketch

Cut and Paste

DS Visualiser

not

MarvinView3D
3D Visualisation

3D Viewers with 3D optimisation

**ChemDraw** → **ChemBio3D**

**ChemSketch** →

**DrawIt** → **3DViewIt**

**Symyx Draw** → **2D to 3D Conversion**

**Pitfalls**

Only optimises to nearest energy minimum

CSE  Computational Science & Engineering Department
Extras / Add-ins

Calculation of Properties

Most packages have modules or bundled programs/Plug-ins/Add-ins which are capable of calculating simple molecular properties such as:

* Molecular Formula
* Exact Mass
* Molecular Weight
* Molecular Composition

Symyx Draw

[From View menu Show Analysis Window]

ChemDraw
Extras / Add-ins

Calculation of Properties

Some packages are capable of calculating other physical chemical properties:

- **ChemDraw** (some only with Ultra not Pro)
  MP, BP, critical temperature, pressure and volume, Gibbs energy, Logp, CLogP, molar refractivity, heat of formation.

- **ChemSketch**
  LogP, Molar Refractivity, Molar Volume, Parachor, Refractive Index, Surface Tension, Density, Dielectric Constant, Polarizability.

- **DrawIt** (optional PhysChem module)
  LogP, LogD, pKa, solubilities

- **MarvinSketch**
  pKa, Major Microspecies, Isoelectric Point, logP, logD, Charge, Polarizability, Orbital Electronegativity, Polar Surface Area (2D), Molecular Surface Area (3D), Hydrogen Bond Donor-Acceptor, Huckel Analysis, Refractivity.
Reaction Calculator

**ChemSketch** and **ChemDraw** can calculate chemical ratios (molar quantities) and percentage yields for reactions.

Symyx Draw has a Reaction Stoichiometry Calculator
Extras / Add-ins

Calculation of Properties

Spectra Calculator

ChemDraw

ChemNMR $^{13}$C Estimation

Estimation quality is indicated by color: good, medium, rough

[Graph showing NMR spectrum with peaks and chemical shifts labeled]
Extras / Add-ins

Calculation of Properties

Spectra Calculator

WinDrawChem (XDrawChem)

C16H13ClN2O

delta_C 123.8(8) +/- 14.4 in shift range 151.8-95.6, intensity 1
delta_C 125.3(10) +/- 14.3 in shift range 160.9-52.9, intensity 0
delta_C 140.4(13) +/- 17.1 in shift range 168.2-77.3, intensity 1
delta_C 158.7(2) +/- 12.1 in shift range 197.9-34.3, intensity 1
delta_C 59.1(10) +/- 14 in shift range 74.9-38.3, intensity 1
delta_C 134.4(5) +/- 13.8 in shift range 186.2-74.6, intensity 2
delta_C 156.3(8) +/- 27.9 in shift range 207.3-51.2, intensity 1
delta_C 40.1(6) +/- 14.3 in shift range 95.6-13.8, intensity 1
Extras / Add-ins

Calculation of Properties

Spectra Calculator

ChemSketch and ILab

KnowItAll – allows access to the IQ Academic Spectral Database
## Conclusions

### Draw Queries (for searching databases)

<table>
<thead>
<tr>
<th></th>
<th>Overlap Warning</th>
<th>A, Q (not) Lists</th>
<th>No. of Substituent Free Site</th>
<th>Ring/Chain Bonds</th>
<th>Link Nodes (1 - 3)</th>
<th>Create Markush</th>
<th>Atom-Atom Mapping</th>
<th>Polymers</th>
</tr>
</thead>
<tbody>
<tr>
<td>ChemDraw</td>
<td>✔</td>
<td>✔</td>
<td>?Lists</td>
<td>✔</td>
<td>✔</td>
<td></td>
<td>✔</td>
<td>✔</td>
</tr>
<tr>
<td>Symyx Draw</td>
<td>✔</td>
<td>✔</td>
<td></td>
<td>✔</td>
<td>✔</td>
<td></td>
<td>✔</td>
<td>✔</td>
</tr>
<tr>
<td>ChemSketch</td>
<td>✗</td>
<td>✔</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>✔</td>
<td>✔</td>
</tr>
<tr>
<td>MarvinSketch</td>
<td>✗</td>
<td>✗</td>
<td>✗</td>
<td>✔</td>
<td></td>
<td></td>
<td>✔</td>
<td>✔</td>
</tr>
<tr>
<td>NCEdit</td>
<td>✗</td>
<td>✗</td>
<td>✗</td>
<td>✔</td>
<td></td>
<td></td>
<td>✔</td>
<td>✔</td>
</tr>
</tbody>
</table>

### Presentations

<table>
<thead>
<tr>
<th></th>
<th>Lines, Arcs, Range</th>
<th>Templates Presentation</th>
<th>Shortcut Keys</th>
<th>Text Rotation</th>
<th>Expand Abbreviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>ChemDraw</td>
<td>✔</td>
<td>✔ Nanotubes</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
</tr>
<tr>
<td>Symyx Draw</td>
<td>✔</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ChemSketch</td>
<td>✔</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MarvinSketch</td>
<td>✗</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>NCEdit</td>
<td>✗</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Extras/Add-ins

<table>
<thead>
<tr>
<th></th>
<th>Structure -&gt; Name</th>
<th>Name-&gt; Structure</th>
<th>Structure -&gt; InChI</th>
<th>Structure -&gt; SMILES</th>
<th>2D -&gt; 3D</th>
<th>PhysChem Properties</th>
<th>Spectra</th>
</tr>
</thead>
<tbody>
<tr>
<td>ChemDraw</td>
<td>✔</td>
<td>✔</td>
<td>✗</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Symyx Draw</td>
<td>✔</td>
<td>✔</td>
<td>✗</td>
<td></td>
<td>✔</td>
<td>✗</td>
<td></td>
</tr>
<tr>
<td>ChemSketch</td>
<td>✔</td>
<td>✔</td>
<td>SMILES/InChI</td>
<td></td>
<td>✔</td>
<td>✔</td>
<td>Via IIAB</td>
</tr>
<tr>
<td>MarvinSketch</td>
<td>✔</td>
<td>✗</td>
<td>✗</td>
<td></td>
<td>✗</td>
<td>✔</td>
<td></td>
</tr>
<tr>
<td>NCEdit</td>
<td>✗</td>
<td>✗</td>
<td>✗</td>
<td></td>
<td>✗</td>
<td>✗</td>
<td></td>
</tr>
</tbody>
</table>

No one package does everything!
2D Structure Drawing Packages

<table>
<thead>
<tr>
<th>Program</th>
<th>URL</th>
</tr>
</thead>
<tbody>
<tr>
<td>Symyx Jdraw</td>
<td><a href="http://www.symyx.com/micro/jdraw/">http://www.symyx.com/micro/jdraw/</a></td>
</tr>
<tr>
<td>Chem 4-D</td>
<td><a href="http://www.cheminnovation.com/products/chem4d.asp">http://www.cheminnovation.com/products/chem4d.asp</a></td>
</tr>
<tr>
<td>ICEdit</td>
<td><a href="http://www.infochem.de/products/software/icedit.shtml">http://www.infochem.de/products/software/icedit.shtml</a></td>
</tr>
<tr>
<td>BKChem</td>
<td><a href="http://bkchem.zirael.org/">http://bkchem.zirael.org/</a></td>
</tr>
<tr>
<td>MarvinSketch</td>
<td><a href="http://www.chemaxon.com/products/marvin/marvinsketch/">http://www.chemaxon.com/products/marvin/marvinsketch/</a></td>
</tr>
<tr>
<td>XDrawChem</td>
<td><a href="http://xdrawchem.sourceforge.net/">http://xdrawchem.sourceforge.net/</a></td>
</tr>
</tbody>
</table>

Comparison of Chemical Drawing Programs
http://dragon.klte.hu/~gundat/rajzprogramok/dprog.html and …/dprog2.html
http://www.pharmainfo.net/reviews/comparative-evaluation-freely-available-chemical-structure-drawing-softwares
Chemical Database Service

Thank you for your attention….

Dr. Don Parkin
Chemical Database Service
Daresbury Laboratory