ChemBioDraw
Today & Tomorrow

Desktop Software
Enterprise Solutions

Chemical & Biological
Research Informatics

Laboratory, Development &
Manufacturing Informatics

Knowledge Management
Scientific Databases

Mark L. Olson, PhD
Vice-President, Software Development
ChemBioOffice Ultra

Core Components

- ChemBioDraw Ultra
- ChemBio3D Ultra
- ChemBioFinder/ChemBioViz Ultra

Additional Components

- E-Notebook Ultra
- Inventory Ultra
- BioAssay Ultra

Workgroup and Enterprise Software

- ChemBioViz Ultra Desktop Suite

Partner Software

- ChemDraw and Chem3D Active X Pro Plugins & Controls
- ChemiINDEX (Index, RXN, NCI & AIDS)
- 1-year subscription to ChemACX and Drugs: Synonyms and Properties

CambridgeSoft

Life Science Enterprise Solutions
• What’s new in version 11 & version 12
• Differences between ChemDraw Pro & Ultra
• Productivity features vs. ActiveX version
ChemBioDraw Product Milestones

- 1985: Chemistry Drawing on Macintosh
- 1990: Chemistry Drawing on Windows
- 1995: Browser Plugin / ActiveX Control
- 2000: Chemistry Intelligence
- 2005: Biology Drawing
- 2010: Biology Intelligence
- 2015:
ChemDraw Hotkeys
- Speed Up Your Drawing -

Customizable Hotkeys

<table>
<thead>
<tr>
<th>Hotkey</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Change to single bond.</td>
</tr>
<tr>
<td>2</td>
<td>Change to double bond.</td>
</tr>
<tr>
<td>3</td>
<td>Change to triple bond.</td>
</tr>
<tr>
<td>4</td>
<td>Change to quadruple bond.</td>
</tr>
<tr>
<td>c</td>
<td>Center a double bond.</td>
</tr>
<tr>
<td>l</td>
<td>Position a double bond to the left.</td>
</tr>
<tr>
<td>r</td>
<td>Position a double bond to the right.</td>
</tr>
<tr>
<td>f</td>
<td>Bring a bond to the front.</td>
</tr>
<tr>
<td>a</td>
<td>A</td>
</tr>
<tr>
<td>A or 5</td>
<td>Ac</td>
</tr>
<tr>
<td>b</td>
<td>Br</td>
</tr>
</tbody>
</table>

- Use Hotkeys to draw chemical structures
- Avoid going back to the Tools Palette to change tools
- Share Hotkey customizations with colleagues
- ChemBioDraw
  - Reduce Drawing Time via Templates

- Save hours by using predefined rings, templates and drawings
- Create custom templates, reducing time for repeated experiments
- Include items from BioDraw and ChemDraw, reactions and drawings

Make your own templates and save them for future use

Customizable in ChemDraw but not in ActiveX
Mass Spec and Rapid Drawing of Syntheses
- Increase Your Efficiency -

Chemical Formula: \( C_4H_7^+ \)
Exact Mass: 55.05

Chemical Formula: \( C_3H_7O^+ \)
Exact Mass: 59.05
ChemDraw Calculates Reaction Stoichiometry  - Do More Lab Work and Less Math -

Stoichiometry Grid Tool

- Menu Structure → Analyze Stoichiometry
- Auto-calculates values where possible
- Data stays synchronized with reaction components
- Ability to hide fields you don’t need
- Full control over text properties

### Stoichiometry Grid

**Reactants**

<table>
<thead>
<tr>
<th>Formula</th>
<th>C₈H₇N</th>
<th>MW</th>
<th>93.13</th>
</tr>
</thead>
<tbody>
<tr>
<td>Limiting?</td>
<td>Yes</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Equivalents</td>
<td>0.84</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sample Mass</td>
<td>34.00g</td>
<td></td>
<td></td>
</tr>
<tr>
<td>%Weight</td>
<td>93.00%</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Products</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula</td>
</tr>
</tbody>
</table>

| Reactant Moles | 339.54mmol |
| Reactant Mass | 31.62g |

| H₂ | MW | 2.02 |
| No |

| Equivalents | 814.84mg |
| Expected Mass | 40.09g |
| Expected Moles | 404.21mmol |
| Measured Mass | 814.84mg |
| Purity |
| Product Mass |
| Product Moles |
| %Yield |
Customizable Nicknames
- Name Your Functional Groups -

- Simplify and speed up chemical drawings using Nicknames.
- Draw structures where parts of the molecule aren’t shown in full detail, but instead are represented by a chemically intelligent label that can be expanded and contracted.
- Define new nicknames in ChemDraw to fit your research.

Customizable in ChemDraw but not in ActiveX.
ChemBioDraw
- Document Settings -

In ChemDraw but not in ActiveX

Available Style Sheets

Document Settings for Untitled Document-1

- Layout
- Hdr/Ftr
- Drawing
- Auto-update
- Captions
- Atom Labels
- Colors

- Chain Angle:
  - 120 degrees
  - Bond Spacing:
    - 12 % of length
    - 0.05 in absolute

- Fixed Length:
  - 0.4167 in
  - Bold Width:
    - 0.0556 in
  - Line Width:
    - 0.0139 in

- Margin Width:
  - 0.0278 in
  - Hash Spacing:
    - 0.0375 in

- Atom Indicators:
  - Show Query Indicators
  - Show Stereochemistry
  - Show Enhanced Stereochemistry
  - Show Reaction Indicators
  - Show Atom Numbers

- Bond Indicators:
  - Show Query Indicators
  - Show Reaction Indicators

Units: Inches

CambridgeSoft
Life Science Enterprise Solutions
I/Draw mode allows the user to work as though he or she is working within ISIS/draw.

In ChemDraw but not in ActiveX.
### ChemDraw Interface with Other Applications

- **Save or Migrate**

<table>
<thead>
<tr>
<th>ChemDraw (CDX)</th>
<th>ISIS Sketch (SKC)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ChemDraw XML (CDXML)</td>
<td>ISIS Reaction Files (RXN)</td>
</tr>
<tr>
<td>Old versions of ChemDraw (CHM)</td>
<td>ISIS RXN V3000 (RXN)</td>
</tr>
<tr>
<td>ChemDraw Template (CTP)</td>
<td>MDL MolFile (MOL)</td>
</tr>
<tr>
<td>ChemDraw Template Style Sheet (CTS)</td>
<td>MDL MolFile V3000 (MOL)</td>
</tr>
<tr>
<td>ChemDraw Stationery/Style Sheet (CDS)</td>
<td>MDL RGFile (RGF)</td>
</tr>
<tr>
<td>Connection Table (CT)</td>
<td>Molecular Simulations MolFile (MSM)</td>
</tr>
<tr>
<td>Chemical Markup Language (CML)</td>
<td>PICT (Macintosh)</td>
</tr>
<tr>
<td>Bitmap (BMP)</td>
<td>Portable Network Graphics (PNG)</td>
</tr>
<tr>
<td>Graphic Image Format (GIF)</td>
<td>Standard Molecular Data (SMD)</td>
</tr>
<tr>
<td>Encapsulated PostScript (Mac)</td>
<td>Windows Metafile (EMF, WMF)</td>
</tr>
<tr>
<td>PostScript (EPS)</td>
<td>TIFF file (TIF)</td>
</tr>
<tr>
<td>ISIS Transportable Graphics File (TGF)</td>
<td>InChI</td>
</tr>
<tr>
<td>SMILES</td>
<td>InChIKey</td>
</tr>
<tr>
<td>SYBYL Line Notation (SLN)</td>
<td></td>
</tr>
</tbody>
</table>

- **ChemDraw ActiveX** can be incorporated in HTML pages or custom applications
- **V3000** supports MDL-style relative stereochemistry
- **V3000** supports files containing > 999 atoms
- **EPS, TIFF** support for stellar printed output
- **Supports InChI** file formats
Highest Presentation Quality Graphics
- Instant Structure and Reaction Clean-up -

- One click with *Structure or Reaction Cleanup* provides neater, more accurate drawings
- Fixed Lengths and Fixed Angles options
- Supports a wide spectrum of structure types

Removal of overlap: Bridged rings

Selection of base ring in cyclic system

Vertically oriented carbonyls

Positioning of hashed and wedged bonds

[Chemical diagrams showing examples of overlaps and their corrections]
Advanced Drawing Conventions
- Stereochemistry Enhancements -

- Recognize the common drawing styles that represent tetrahedral stereochemistry without using stereo bonds in their usual sense
- Changes are consistent with the latest IUPAC recommendations for the depiction of stereochemistry

\[ \text{Chemical Structures} \]
ChemDraw Predicts Chemical Properties

– Make sure you are drawing what you expect -

- **Structural Analyses** *(Updated real-time)*
  - Formula
  - Exact mass
  - Molecular Weight
  - Isotope distribution patterns
  - Elemental Analysis

- **Physical Properties**
  - Boiling Point
  - Melting Point
  - Critical Temp, Pres, Vol
  - Gibbs Energy
  - LogP
  - MR
  - Henry’s Law
  - Heat of Formation
  - CLogP
  - CMR

*Topological Polar Surface, tPSA

CLoP and CMR are Ultra feature (not in ChemDraw Pro)
“View 3D Preview” is a new menu item under the View menu.

A separate floating window shows a 3D model of the current structure as generated by Chem3D.

A current version of Chem3D must be installed.

ChemDraw Ultra only (not in ChemDraw Pro or ActiveX).
ChemBioFinder Hotlink
- Search Databases In Real Time -

- Real-time search
  - Search as you draw
  - Search all CS databases
  - Search internal databases

- Drill-down results
  - Click on data source name to see results from that source
  - Links open in external browser window so work in ChemDraw can continue

*ChemDraw Ultra only (not in ChemDraw Pro and not in ActiveX)*
Structures from Names - And Vice Versa -

- Name → Struct handles more structure types and has a typo recognition feature
- Struct → Name can successfully name 95% of examples in test databases, successfully naming:
  - Ring systems
  - Most salts
  - Structures with a net charge
  - Simple mixtures and multi-component systems
  - Heterochains
  - Bicyclics
  - Simple Inorganics

Isotopes in ver.11; Bridged rings in ver.12; Ultra feature only

Inner salts

- 9,10-epidiazenoanthracene
- N-(1H-1λ4,2,3-Thiadiazol-1-ylidene)carbamic acid
- 2-Methyl-1-(3-sulfopropyl)naphtho(1,2-d)thiazolium inner salt
**ChemBioDraw**

- New Name → Struct Features -

**Name → Struct Improvements**

- Provides reports when structures are generated from misspelled or ambiguous names.

![Chemical Structures]

- Dichloropyridine
  - This name appears to be ambiguous

Name > Struct only in Ultra (not pro); Ambiguous names added in ver. 12
Standards Compliance

• **We work with IUPAC**
  - Participation in new standards development
  - Advocate for customers during standards development

• **Areas of Leadership**
  - Structure diagram representation
  - Stereochemical representation
  - Interpretation of chemical nomenclature

• **Publication References:**

  Graphical representation of stereochemical configuration (IUPAC Recommendations 2006)

  Graphical representation standards for chemical structure diagrams (IUPAC Recommendations 2008)

Jonathan Brecher
CambridgeSoft Corporation, 100 CambridgePark Drive, Cambridge, MA 02140, USA
Structure-To-Name Enhancements

Bridged and Fused Ring Systems and Ring Assemblies
ChemDraw NMR Prediction
- Helps Confirm Chemical Structures -

- $^1$H NMR includes splitting Patterns
- Calculate predicted $^{13}$C NMR spectrum

Protocol of the H-1 NMR Prediction:

<table>
<thead>
<tr>
<th>Node</th>
<th>Shift</th>
<th>Best + Inc.</th>
<th>Comment (ppm rel. to TMS)</th>
</tr>
</thead>
<tbody>
<tr>
<td>OH</td>
<td>3.58</td>
<td>2.00</td>
<td>alcohol</td>
</tr>
<tr>
<td>CH</td>
<td>1.47</td>
<td>1.51</td>
<td>general corrections</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-0.02</td>
<td>cyclopentane</td>
</tr>
<tr>
<td></td>
<td>1.51</td>
<td>-0.02</td>
<td>$\delta$ beta -C from methine</td>
</tr>
<tr>
<td></td>
<td>1.51</td>
<td>-0.02</td>
<td>$\delta$ beta -C from methine</td>
</tr>
<tr>
<td>CH2</td>
<td>1.60;</td>
<td>1.345000</td>
<td>cyclopentane</td>
</tr>
<tr>
<td></td>
<td>1.51</td>
<td>-0.04</td>
<td>$\delta$ beta -C from methylene</td>
</tr>
<tr>
<td>CH2</td>
<td>1.60;</td>
<td>1.345000</td>
<td>cyclopentane</td>
</tr>
<tr>
<td></td>
<td>1.51</td>
<td>-0.04</td>
<td>$\delta$ beta -C from methylene</td>
</tr>
<tr>
<td>CH</td>
<td>3.25</td>
<td>1.50</td>
<td>methine</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.73</td>
<td>$\delta$ alpha -O</td>
</tr>
</tbody>
</table>
### MNova Lite Import File Formats

<table>
<thead>
<tr>
<th>Data Format</th>
<th>Vendor</th>
<th>Dimensions</th>
</tr>
</thead>
<tbody>
<tr>
<td>VXR/Unity/Inova</td>
<td>Varian</td>
<td>1D **</td>
</tr>
<tr>
<td>Gemini/VXR</td>
<td>Varian</td>
<td>1D</td>
</tr>
<tr>
<td>XWIN-NMR/UXNNMR</td>
<td>Bruker</td>
<td>1D **</td>
</tr>
<tr>
<td>Aspect 2000/3000</td>
<td>Bruker</td>
<td>1D</td>
</tr>
<tr>
<td>Win-NMR</td>
<td>Bruker</td>
<td>1D</td>
</tr>
<tr>
<td>JEOL GX/EX</td>
<td>JEOL</td>
<td>1D</td>
</tr>
<tr>
<td>CDFF Nuts</td>
<td>AcomNMR</td>
<td>1D **</td>
</tr>
<tr>
<td>JCAMP-DX 5.0</td>
<td>IUPAC</td>
<td>1D</td>
</tr>
<tr>
<td>NTNMr</td>
<td>Tecmag</td>
<td>1D</td>
</tr>
<tr>
<td>SwaN-MR</td>
<td>Menarini</td>
<td>1D</td>
</tr>
<tr>
<td>SIEMENS NMR</td>
<td>Siemens</td>
<td>1D</td>
</tr>
<tr>
<td>SIEMENS NMR</td>
<td>Nicolet/GE</td>
<td>1D</td>
</tr>
</tbody>
</table>

- Basic NMR processing and analysis - ideal for multiple chemists running large numbers of routine experiments
- Complements ChemDraw’s NMR prediction capabilities

Ultra feature (not in ChemDraw Pro)
ChemBioDraw
- New Chemistry Features-

- Disulfide bonds in peptide sequences
- Nucleic and amino acid sequence wrapping and shaping
- Peptide termini display
- Adding bonds to sequence residues
- Rotation About Arbitrary Centers
- Export to SVG *(Windows only)*
- Macintosh PDF Export and Printing
- Improvements in Struct → Name and Name → Struct
Why Move to .NET?

- **.NET Development Directly Benefits You**
  - .NET improves productivity
    - Less time spent on infrastructure
    - More time spent adding value
    - Developers are more productive in .NET

- .NET improves quality
  - Managed code means fewer mistakes
  - Framework usage means higher performance

- .NET is an enabling technology
  - New features in framework yield new features in products
  - .NET is the future of Windows – WPF, Silverlight, etc.
Microsoft Platform Support

- Windows 2000
- Windows XP
- Windows Vista
- Windows 7
- Office XP
- Office 2003
- Office 2007
- Office 2010
ChemDraw for Excel
- Store & Organize Chemicals in Excel -

Ultra feature (not in ChemDraw Pro, and not in ActiveX)

Chemically active structure

Substructure search available utilizing ChemDraw toolbar
Additional Features - ChemDraw for Excel -

- Compatible with Microsoft Office 2007
- New Interface
- New Property Window
- Floating Dialog Box
- .NET Add-in
- New Context Menu

Excel-2007 interface: new in version 12
TLC Plate and Table Tools
- Draw Tables and TLC Plates -

Ultra feature
(not in ChemDraw Pro, and not in ActiveX)
- Highest Presentation Quality Graphics
  - Adjustable Shapes

- Structure perspective on all chemical objects
- Rotatable and adjustable geometric shapes – rectangles and ovals
- Color-faded geometric shapes – rectangles and ovals
- Advanced BioDraw templates and toolbar
- Electronic Lab Notebook integration with CambridgeSoft’s BioDraw program
- High-color documents
- Sample Templates
ChemDraw allows the illustration of...
- Biological pathways
- Cell macro-structures
- Plasmid maps

Combine Biology illustrations with...
- Chemical structures and reactions
- Models from Chem3D
Quality Visualization on the Desktop
- Structural insights, Team collaboration -

- Medicinal and cheminformatics groups can access high quality, easy to use visualization and computation tools at a low cost
- Visualize results from Computational Chemistry Group - assist in designing the next round of synthetic targets
- Protein and Nucleic Acid Ribbon Diagrams provide insight into tertiary and quaternary structure of proteins and protein complexes
A Connolly Surface which excludes the ligand
Live Models in PPT
- Collaboration and Communication -

- Embed Chem3D models in PowerPoint file
- Rotate and zoom Chem3D models while giving a presentation!
ChemBio3D does its best to build a correct 3D conformation as you build the molecule in the 2D panel.

MMFF94 calculations make an even more energy minimized structure.

Ultra feature (not in ChemDraw Pro, and not in ActiveX)
ChemBio3D’s ongoing commitment is to interface with well-respected and widely used 3rd party modeling programs.

- Common interface
- Unified display model
- Common Look and Feel
  - GAMESS
  - MOPAC
  - GAUSSIAN
  - JAGUAR
- ChemBio3D plays nice
  - Thin interface to 3rd party packages
  - Exposes options from other packages
CHEMBIOFINDER

- What’s new in ChemFinder versions 11 & 12
- Interface to online databases
- Statistical Analysis

Ultra feature (not in ChemDraw Pro, and not in ActiveX)
ChemBioFinder - Chemical Database Management System

- View and Build Your Own Chemical Databases
- Create your own forms
- Store chemical structures, physical properties, notes and tables of data
- Integrated with ChemDraw
- Search data by
  - Chemical structure (including sub-structure)
  - Wild card text searches
  - Numeric range searches

Ultra feature (not in ChemDraw Pro, and not in ActiveX)
Data visualization and analysis right in ChemBioFinder

No need to switch back and forth to other apps

Analyses are saved with the form
Visually compare and rank structures based on values of selected properties and the cost profile associated with each property.
Clustering

- Discover similarities between structures based on structure and/or properties
- Single or multi-dimensional
- Interactive display; dendrogram and clustering

New in version 12
Ultra feature
(not in ChemDraw Pro, and not in ActiveX)
ChemBioViz - Statistica Integration -

- Export directly from ChemBioFinder with the click of a button
- Utilize all of Statistica’s many statistical analysis tools

New in version 12 Ultra feature (not in ChemDraw Pro, and not in ActiveX)
OTHER APPLICATIONS in the SUITE

- ChemBioOffice Overview
  - 5 Minutes
- ChemBioDraw
  - 10 Minutes
- ChemBio3D
  - 10 Minutes
- ChemBioFinder
  - 5 Minutes
- Other Applications
  - 2 Minutes
- Ultra feature
  - (not in ChemDraw Pro, and not in ActiveX)
ChemScript
- Chemical Scripting Language -

Powerful scripting language for the Searching, Manipulation and calculation of Chemical Structures

- Based on over 20 years of development from the people who brought you ChemDraw
- Allows manipulation of 2D & 3D chemical structures
- Access to a wide range of property calculations
- Wide range of chemical structures available (Substructure, Similarity, Maximum Common Substructure)
- Clean and Align structures
- Apply business rules (nitro group transformation, tautomeric forms)
- Accessible through popular, robust development environments (Python, .Net etc)
- Salt stripping functionality with customisable salt table
- Supports wide variety of file formats (CDXML, SD, Mol, SMILES, InChI)

Ultra feature (not in ChemDraw Pro, and not in ActiveX)
ChemScript - Improvements -

- ChemScript Integration
- Launch custom python scripts from ChemDraw
- Apply custom drawing rules using ChemScript
- Launch external applications from ChemBioDraw
- Automate workflow from ChemBioDraw

New in version 12; Ultra feature (not in ChemDraw Pro, and not in ActiveX)

# ChemScript code

```python
scaffoldStruct.readData(fileData)

...

if scaffoldStruct.atomByAtomSearch(regMol) != None:
    scaffoldStruct.overlay(regMol)

...
```
ChemBioFinder/Office
- Find molecules of interest on your computer

- Little known but extremely useful utility
- Search drives, desktop, or network for structures, reactions
- All search types: sub, full-structure, similarity, formula, molecular weight
- Search databases, structure files, MS Office documents
- Double-click calls up original source
- Refine and export hit list to any destination