CambridgeSoft Solutions

Learn

5 Minutes
• ChemBioOffice
5 Minutes
• ChemBioDraw and Chem3D
60 Minutes
• ChemBioFinder

Over

5 Minutes
• Electronic Lab Notebook
10 Minutes
• BioAssay and Inventory

Lunch

10 Minutes
• CambridgeSoft Solutions Overview

CambridgeSoft
Life Science Enterprise Solutions
Naturwissenschaftliche Unternehmenslösungen
Solutions globales pour les sciences de la vie
ライフサイエンス・エンタープライズ・ソリューション
ChemBioOffice
- The Desktop Productivity Toolkit for Scientists -

For your office

For your web designer

For your scientists
ChemBioOffice Ultra

Core Applications

ChemBioDraw Ultra
ChemBio3D Ultra
ChemBioFinder/
ChemBioViz Ultra

Additional Components

ChemDraw and
CombiChem for Excel
Struct = Name
Chem NMR
ChemScript Pro

Core Applications

E-Notebook
Ultra
Inventory Ultra
BioAssay Ultra

Additional Components

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

Additional Components

Mnova Lite
STATISTICA
Base
GAMESS

Workgroup and Enterprise
Level software to share and
Partner Software

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Life Science Enterprise Solutions
ChemBioOffice Site Subscriptions

- Unlimited usage within institution
- Desktop or Workgroup (for individual or shared environments)
- All departments have access to required software
- Software updates and administrator support included
- Software can be used on any machine (lab, laptop, home)
- Individual online software downloads = less administration
- Site licenses reduce support load
- Multi-year site licenses reduce long-term cost

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CHEMBIODRAW

- 5 Minutes
  - ChemBioOffice Overview

- 5 Minutes
  - ChemBioDraw and ChemBio3D

- 60 Minutes
  - ChemBioFinder

- 10 Minutes
  - Electronic Lab Notebook

- 10 Minutes
  - BioAssay, Inventory, Sharing of data
## 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 Using 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 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
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
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**
- 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
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 Area, tPSA was added to the Chemical Properties in version 9.0*
**Structures from Names**  
- And Vice Versa -

- **Isotopes**
  - $^{18}$O
  - $^{18}$O acid-d

- **Lambda convention**
  - $N$-(1H-1λ4,2,3-Thiadiazol-1-ylidene)carbamic acid

- **Porphyrrins**
  - Ring systems
  - Most salts
  - Structures with a net charge
  - Simple mixtures and multi-component systems
  - Heterocycles
  - Bicyclics
  - Simple Inorganics

- **Inner salts**
  - 2-Methyl-1-(3-sulfopropyl)naphtho(1,2-d)thiazolium inner salt

- 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:
**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

[Chemical Structures Image]
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>Base + 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>1.56</td>
<td>general corrections</td>
</tr>
<tr>
<td>CH</td>
<td>1.47</td>
<td>1.51</td>
<td>cyclopentane</td>
</tr>
<tr>
<td>CH</td>
<td>1.30</td>
<td>-0.02</td>
<td>2 beta -C from methine</td>
</tr>
<tr>
<td>CH</td>
<td>1.30</td>
<td>-0.04</td>
<td>cyclopentane</td>
</tr>
<tr>
<td>CH</td>
<td>1.52</td>
<td>-0.04</td>
<td>1 beta -C from methylene</td>
</tr>
<tr>
<td>CH</td>
<td>1.56</td>
<td>-0.02</td>
<td>cyclopentane</td>
</tr>
<tr>
<td>CH</td>
<td>1.56</td>
<td>-0.04</td>
<td>3 beta -C from methylene</td>
</tr>
<tr>
<td>CH</td>
<td>3.25</td>
<td>1.50</td>
<td>methine</td>
</tr>
<tr>
<td>CH</td>
<td>3.25</td>
<td>1.50</td>
<td>1 alone -O</td>
</tr>
</tbody>
</table>
New Sequence tool
- Easily Create Amino Acid, DNA, RNA Sequences -

- Draw peptide and nucleotide sequences
- Several modes:
  - Single-letter amino acid tool
  - Three-letter amino acid tool
  - DNA tool
  - RNA tool
- Termini are labeled depending on the type of sequence drawn
- Expand and contract single or multiple labels and sequences
Expand Generic Structures

ChemDraw interprets and explicitly expands generic structures…

- Nicknames stay as nicknames (although you can “expand labels”)
- 2-bromophenol deduplicated versus 6-bromophenol
- R-groups within R-groups ok; “mix-and-match” all ok!
PolymerDraw
- Repeat Pattern -

A: Repeat pattern head-to-tail

\[
\begin{align*}
\text{[O-O]}^* & = \text{[O-O-O-O-O-O]}^* \\
\end{align*}
\]

B: Repeat pattern head-to-head

\[
\begin{align*}
\text{[O-O]}^{hh}^* & = \text{[O-O-O-O-O-O]}^* \\
\end{align*}
\]

C: Repeat pattern either/unknown

\[
\begin{align*}
\text{[O-O]}^{eu}^* & = \begin{bmatrix}
\text{[O-O-O-O-O-O]}^* \\
\text{[O-O-O-O-O-O]}^*
\end{bmatrix}_{\text{mix}}
\end{align*}
\]
ChemDraw for Excel
- Store, Search, Organize Chemicals in Excel -

Chemically active structure

Substructure search available utilizing ChemDraw toolbar
TLC Plate, Table Tools, Arrows, Pen Tool
- Facilitates Easy Drawing -
ChemBioDraw
- New Biology Features-

- Advanced BioDraw templates and toolbar
- Electronic Lab Notebook integration with CambridgeSoft’s BioDraw program
- High-color documents
- Sample Templates
ChemBioDraw
- Document Settings -

Available Style Sheets

Document Settings

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

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

Units: Inches

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

Bond Indicators:
- Show Query Indicators
- Show Reaction Indicators
- Show Sequence Bonds
I/Draw mode allows the user to work as though he or she is working within ISIS/draw.
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
Model Explorer Tree Control

- Efficiently explore the structure of large molecules -
Surface Display Options
- Visualization of binding sites -

A Connolly Surface which excludes the ligand
Display of Hydrogen Bonds
- Selective Display highlights interactions of interest -
Fast Automatic Overlay
- Rigid molecule overlays made simple -
• Embed Chem3D models in PowerPoint file
• Rotate and zoom Chem3D models while giving a presentation!
Live Models
- For those without Chem3D installed -

- Create animated GIF files for websites or presentations that work regardless of whether Chem3D is installed on the computer.
MMFF94 Force Field Minimization
- Before and after peptide minimization -

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.
ChemBio3D 3rd Party Pairings
- Gaussian, Jaguar, MOPAC, GAMESS -

Gaussian
• Predict NMR, IR and Raman spectra
• Support multi-step jobs and partial optimizations
• New DFT tab
• Monitor Gaussian Link processes

Jaguar
• Surfaces: Total Charge Density surface, Total Spin Density surface, Molecular Electrostatic Potential surface and Molecular Orbital surface

GAMES
• General Atomic and Molecular Electronic Structure System

MOPAC
• Molecular Orbital PACage
• Semi empirical quantum chemistry program based on Dewar and Thiel's NDDO approximation
Chem3D
- New Features-

- MMFF94 Force Field Calculation Improvements
- ChemDraw Panel and Structure Browser
- Running Molecular Dynamics using the MMFF94 force field
- Conformation Sampling, the Stochastic Method
Chem3D
- New Feature Benefits -

**MMFF94 Force Field Calculation Improvements**
- Faster processing times on force field calculations

**ChemDraw Panel and Structure Browser Improvements**
- Run MMFF94 from within Structure Browser
- Live link between 2D and 3D and vice versa
- Type in chemical names or SMILES strings to draw structures

**Running Molecular Dynamics using the MMFF94 force field**
- Faster and better force field calculations during molecular dynamics analysis

**Conformation Sampling, the Stochastic Method**
- Ability to find local energy minimizations of molecules
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
Data visualization and analysis right in ChemFinder
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.
ChemBioFinder/ChemBioViz
- Clustering -

**Clustering**

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

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

Statistica Integration
ELECTRONIC LAB NOTEBOOK

- 10 Minutes
  - Electronic Lab Notebook

- 5 Minutes
  - ChemBioFinder

- 60 Minutes
  - ChemBioDraw and ChemBio3D

- 5 Minutes
  - ChemBioOffice Overview

- 10 Minutes
  - BioAssay, Inventory, Sharing of Data

- 10 Minutes
  - Overview
E-notebook Ultra Desktop
- Chemistry Notebook; Eliminate hours writing & searching lab results -

- Work Offline Functionality
- Reaction Section
- Stoichiometry Grid
- Reaction Conditions
- Audit Trail
- AutoText
Biology Notebook Configuration
- Free-form interface with enhanced searchability -

NEW!

Ability to add as many sections as needed

Free-form drawing section

Seamless integration with Microsoft Office 2007
E-notebook Office 2007 Compatibility
- Work seamlessly with Office 2007 -
- Better searching -

- When typing a word to search, the contents and the names of collections and documents are searched and the results displayed.
- Search all MS Office text.

Here is an example of a simple text query where we search for the word “offline.”

Here are the results from that search.

Here we have clicked on one of the results of the search and find the word “offline” in a word document.
Audit Trail and Security
- Maintain 21CFR Part 11 Compliance -

Location of audit trail
E-signatures

• Electronically sign with co-authors and witnesses. Storage in a separate database to protect IP.

Rendering of experiment into one, nicely formatted document.
BIOASSAY AND INVENTORY

- 10 Minutes
  - BioAssay,
  - Inventory,
  - Sharing of Data

- 10 Minutes
  - Electronic Lab Notebook

- 5 Minutes
  - ChemBioFinder

- 60 Minutes
  - ChemBioDraw
  - ChemBio3D

- 5 Minutes
  - ChemBioOffice Overview

- 5 Minutes
  - ChemBioDraw
  - ChemBio3D

- 60 Minutes
  - ChemBioDraw
  - ChemBio3D

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What is BioAssay?

- Import and storage of assay data
- Automated handling of assay workflows
- Graphical outputs and heat maps
- Mathematical manipulation and analysis of assay information
Making BioAssay Work - Data sources

**Plate Setup Data**
- Defines what type of plate you are working with. (Ex: 96-well, 384-well)

**Well Setup Data**
- Defines what substance is in each well of the plate. (Ex: Empty, compound, negative control, positive control)

**Protocol Setup Data**
- Defines what actions and calculations you want to take place upon import of data

**Raw Data**
- Can be virtually anything and can be in plate block format, columnar data or a custom format that you can define
BioAssay
- New Features -

- Excel Analysis
  - Export data from BioAssay into Excel
  - Automatically launch a specified excel macro or add-in to be run to process the data
  - Import the manipulated data back into BioAssay using a pre-defined file import template
Inventory Ultra
- Desktop Chemical Inventory Management -

- SQL Server Role-based Security
- Cascading Location Model
- Audit Trail - logs all changes relating to Locations, Containers, and Substances
- Utility to import Excel data
- Structure intelligence using MolServer – can be deployed on the DB server
- Integration with ChemACX.com
- Reconcile location contents
Inventory Ultra
- Intuitive Layout -

Inventory location hierarchy

Contents of one location

Tabs contain data for each substance

Option to rectify contents of location

Contents of one location for each substance

Inventory Manager - Logged on as Invadmin

List of substances with details such as name, CAS, substance, barcode, container status, and expiration date.

Inventory Manager - Logged on as Invadmin

Inventory location hierarchy with options to add new location, edit location, move location, delete location, and more.

Option to rectify contents of location
Interface with ChemACX

- Access to thousands of commercially available chemicals -

Search the ChemACX database or your Inventory database

Results can be added to your shopping cart for manager approval + ordering
New Request Management Functionality
- Request chemicals for management approval -

- Requests and Request management
- Shopping Carts
- Toolbars
Labeling
- Create and print barcodes from your printer -
Sharing Data
- Applicable for ELN, BioAssay, Inventory -

ELN, BioAssay, Inventory

Desktop
- Individual use
  - Individual Database
    - Forms unique to user
      - No costly duplication or irretrievable work

Workgroup
- Data shared among users
  - Read or read/write access to notebooks for each user

Enterprise
- Data shared among users
  - Read or read/write access to notebooks for each user

Cloud
- Data shared among users
  - Read or read/write access to notebooks for each user

Forms unique to user

Customizations to meet requirements

Drastically reduced IT and maintenance costs
Sharing Data
- Benefits -

- Search (structure, text, scientist, etc.)
- Avoid duplication
- Standardized formatting
- IP protection
- Audit Trail
- Backups
- Reports
Cloud Computing
- Benefits -

• Infrastructure investment
  • Acquisition cost
  • Installation cost
  • Adoption cost
  • Support cost

• Coherent and resilient environment – not a brittle “software stack”

• Scalability in response to changing need
  • Integratability/Interoperability with legacy assets and other services
  • Configurability/Programmability from data, through logic, up into the user interface without compromising robust multi-tenancy
Cloud Computing
- Technical Details -

Single tenancy gives each customer a dedicated software stack – and each layer in each stack still requires configuration, monitoring, upgrades, security updates, patches, tuning and disaster recovery.

On a multi-tenant platform, all applications run in a single logical environment: automatically upgraded and maintained. Ongoing improvements appear to all customers at once.
Cloud Computing - ROI -

Faster Results; Lower Risks; Predictable Costs

On-Premise Operations:
53% of software projects cost
189% of original estimate\(^1\)

Cloud Computing:
Average 49% ROI within 10 Months\(^2\)

Value

Fixed Costs and Excess Operating Expenses

Upgrade Expense & Opportunity Costs

Buying Function, not Infrastructure

Value

Time

\(^1\) Standish Group, Chaos Report 2006
\(^2\) Third-Party CustomerSat Research on 4,165 Salesforce.com customers, February 2008

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# Cloud Computing Security

<table>
<thead>
<tr>
<th>Facility Security</th>
<th>Network Security</th>
<th>Platform Security</th>
</tr>
</thead>
<tbody>
<tr>
<td>• 24x365 on site security</td>
<td>• Fault tolerant and redundant external firewall</td>
<td>• SaaS “Type II” facility</td>
</tr>
<tr>
<td>• Biometric readers, Security guards</td>
<td>• Intrusion detection systems</td>
<td>• Optional strict password policies</td>
</tr>
<tr>
<td>• Anonymous exterior</td>
<td>• Best practices secure systems management</td>
<td>• SAS 70 Audited</td>
</tr>
<tr>
<td>• Silent alarm</td>
<td>• 3rd party vulnerability assessments</td>
<td></td>
</tr>
<tr>
<td>• CCTV</td>
<td></td>
<td></td>
</tr>
<tr>
<td>• Motion detection</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>