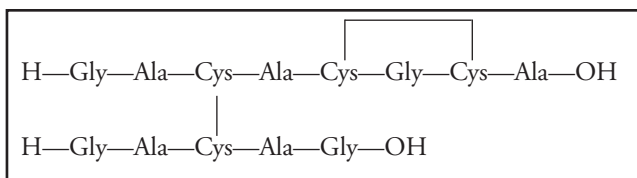


ChemBioDraw Ultra 12.0

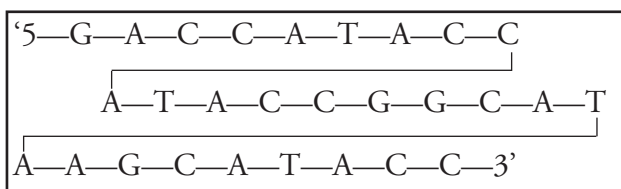
CHEMBIODRAW IS THE INDUSTRY standard software used by scientists worldwide to draw accurate, chemically-aware structures for use in database queries, and preparation of publication-quality graphics, and create publication-quality biological pathways graphics and plasmid maps. This document highlights new features which have been added to the ChemBioDraw Ultra application in version 12.

Sequence Tool Enhancements

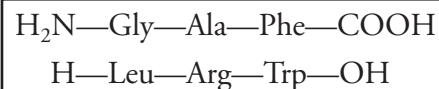
Disulfide Bonds can now be created between residues. Using the standard bond tool, it is now possible to join the -SH groups in order to form a disulfide bond:



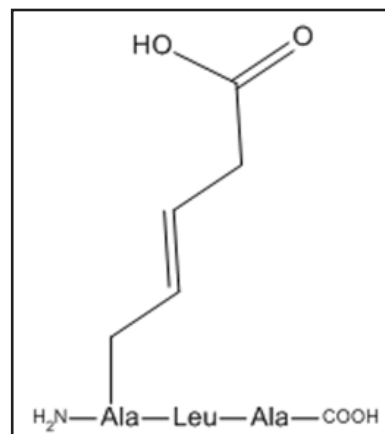
Sequence Wrapping and Shaping is now possible for multi-line sequences. While using the sequence tool, the sequence can be continued on a new line by pressing the Enter key. Users can also arbitrarily reshape a sequence after it has been typed by selecting groups of residues and dragging them to different places on the screen using the marquee tool:



Peptide Termini Display options are now also available, so users can choose to display peptide termini using either H/OH or H₂N/COOH:



Sequence residues (DNA, RNA, or peptide) can be modified using the bond tools. Modifications are local to the individual labels. The user selects the atom to which the bond will be attached on expansion and the modified structures can be expanded and contracted as usual.



Struct>Name and Name>Struct version 12 Improvements

Name>Struct recognizes ambiguous chemical names. The software now reports if a name was ambiguous, and indicates and that generated structure might not have been the one intended by the author.

Struct>Name now handles naming of new structural motifs:

- Ring Assemblies
- Fused Ring Systems
- Bridged Fused Ring Systems
- Bridged Ring Systems (polyalicyclic hydrocarbons, von Baeyer hydrocarbons)

All specifications subject to change without notice.

US 1 800 315-7300 INT'L 1 617 588-9300 FAX 1 617 588-9390 EMAIL info@cambridgesoft.com

EU 00 800 875 20000 UK +44 1223 464900 JP 0120 73 800 WWW www.cambridgesoft.com

MAIL CambridgeSoft Corporation 100 CambridgePark Drive Cambridge, Massachusetts 02140 USA

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ChemBioDraw Ultra 12.0

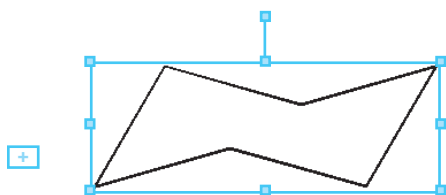
ChemNMR — User Correctable Databases for Proton Prediction

User Correctable Databases for Proton Prediction are now available in version 12, allowing users to add their own shift correction data for proton prediction which can supplement the existing data used by the ChemNMR algorithm. Users of MestreNova and ACD Labs can produce and output the correction data as an SDF file which can then be merged into the existing database used by the ChemNMR algorithm.

Rotation about Arbitrary Centers

This is now possible with modification of the Lasso and Marquee tools to include an additional adjustment handle on selection. The '+' handle indicates the center of rotation, which by default is the center

of the selection rectangle. When moving the cursor over this handle, the icon will change to a double-arrow icon, indicating that this point can be dragged. If the '+' handle is close to an atom, its position will be adjusted such that it lies directly over that atom, allowing rotation about a particular atom of interest. Rotation will now be centered on the selected origin.



ChemScript Integration

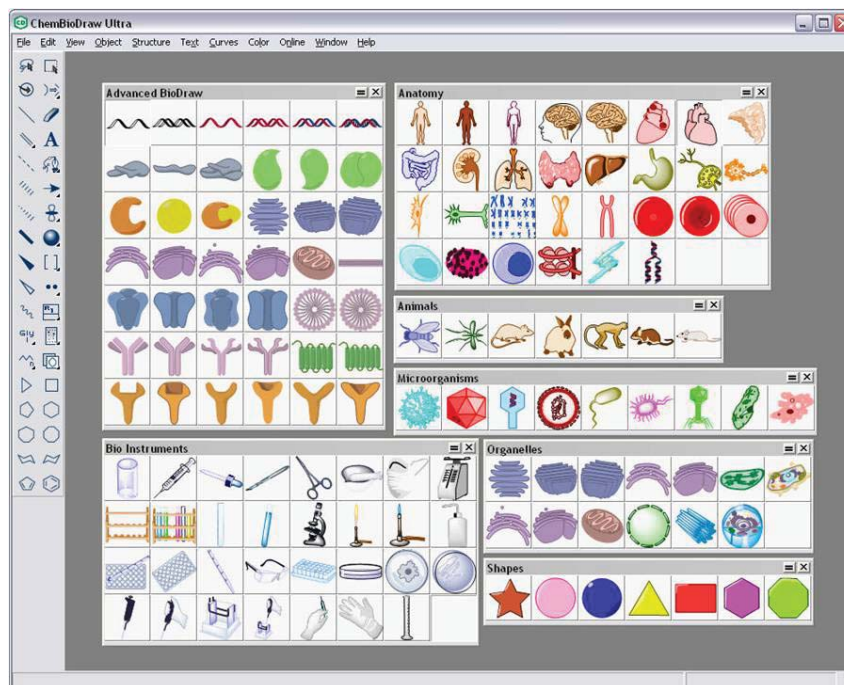
ChemScript algorithms applying chemistry business rules to molecules can now be accessed directly from the ChemBioDraw menu bar. ChemScript is the CambridgeSoft chemical scripting environment, where chemical business rules can be applied to chemical objects by using customizable scripts.

Export to SVG

ChemBioDraw can now export drawings to the Scalable Vector Graphics (SVG) format, an XML-based format for describing two-dimensional vector graphics.

High-color Documents

ChemDraw 12.0 removes the previous restriction of 24 colors per document, allowing documents which can contain over 16 million colors.



BioDraw Enhancements – Pathways Templates and New Elements

A set of *high-color advanced BioDraw Pathways Templates* are now included with the software showing publication-quality renderings of biological systems.

Additional Advanced BioDraw Elements are now available on the BioDraw toolbar including new elements for channels, enzymes, kinases, nuclear pores, receptors and more.



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US 1 800 315-7300 INT'L 1 617 588-9300 FAX 1 617 588-9390 EMAIL info@cambridgesoft.com

EU 00 800 875 20000 UK +44 1223 464900 JP 01 20 73 800 WWW www.cambridgesoft.com

MAIL CambridgeSoft Corporation 100 CambridgePark Drive Cambridge, Massachusetts 02140 USA

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www.cambridgesoft.com