



## Review on CambridgeSoft ChemBioDraw Ultra 13.0v

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**ABSTRACT:** ChemBioDraw Ultra 13.0v is a software package for drawing and creating chemical formulas used mainly for chemists and biologists around the world to create a real imaging based on computational chemistry, molecular studies for publication, scientific intelligent 2D/3D drawings for use in ELN's for publications and databases, and query databases for chemicals. Scientists can now quickly, effectively and accurately communicate their research results and may expose their ideas easily using an extensive set of templates biological / chemical and preconceived drawing objects to create compelling illustrations of cells and metabolic pathways, including live chemical objects as needed. A unique design solution addressed both chemists and biologists as who they can trust this software package can take care of accuracy and representation of organic substances, organometallic, polymeric and bio-polymeric (including amino acids, peptides, and DNA and RNA sequences), and to deal with advanced stereochemistry as well. Scientists can thus save valuable time and increased data accuracy by using ChemBioDraw Ultra 13.0v package to predict the physicochemical properties, generate spectra, generate IUPAC nomenclature and to calculate correctly the stoichiometry of the reaction. Finding compounds or structures of interest much faster and higher accuracy regardless of chemistry or type of structure analyzed. Better results from searches in databases and reduced time spent in searching for a specific compound creates more time for creative science.

**Key words:** Perkin-Elmer, CambridgeSoft, chemical compound draw, computational chemistry

### I. INTRODUCTION

ChemBioDraw Ultra version 13.0 is currently one of the software packages to the latest scientific design, believed on previous versions as standard by most experts in the field. Growing number of users who benefit from ease of use, high quality production, the chemical robustness of embedded intelligence, the rich set of biological tools available and their integration into ChemOffice suite and the joining together of several other top third party partners together with the continuous improvement and diversification incorporated elements make this product a true industry leader.

ChemBioDraw base includes optional versions of well-known program STATISTICA for more detailed numerical analysis, another industry leader and quickly process Lite MNova NMR spectra on the desktop, regardless of the instrument which was obtained thanks to advanced conversion system and data analysis incorporated. It includes also software that operates scripting language called ChemScript incorporated in the software package to automate processes related to structure and analyze batch type and connection to other freeware or proprietary software code.

ChemBioDraw bestows upon chemists and biologists with a rich set of easy to use tools for quickly creating articles and publishing significant scientific drawings of molecules, reactions and biological entities, pathways and related properties generation, systematic name and spectra.

### ChemBioDraw Ultra 13.0

This innovative application for chemists and biologists design offers all the features that ultimately recommends it as pack leader of industrial design, publishing and analytical features in ChemDraw combined with the biology and biochemistry characteristics in BioDraw Ultra package, providing a complete solution for drawing chemical structures and also can design combined with an analysis of biological pathways, becoming a valuable tool in both pure research and in educating future professionals in the field.

ChemBioDraw Ultra includes a rich and varied assortment of chemical structure analysis tools such as prediction of  $^{13}\text{C}$  and  $^1\text{H}$ -NMR spectra prediction for spectra with peak splitting and highlighting, and the choice of solvent, Struct=Name, ChemDraw/Excel, stoichiometric analysis, number property, including pKA, and logS related logD live structure-linked database gateway live, fragmentation tools, TLC plate and gel electrophoresis, drawing tools, and 3D structures live about 2D structure. ChemBioDraw Ultra offer also customization options for nicknames, templates and hotkeys, and adds a new feature that allows the user to save data in Dropbox (this option requires a permanent internet connection). A new toolbar allows the creation of biopolymers peptides, DNA and RNA sequences, including beta acids and D-amino acid disulfide and lactam bridges and linkers and protection groups.

Trace elements to the design of biological pathways include membranes, DNA, enzymes, receptors, and reaction arrows. tRNA, ribosomes, helix proteins, Golgi bodies, G-proteins, immunoglobulins, mitochondrion, new pen tool, free-hand annotation and mapping tool type plasmid are also included, thus the easiest way of drawing them currently existing in the market.

#### **ChemDraw ActiveX/Plugin Pro 13.0**

This premier ActiveX control type/Plug-in allows querying chemical databases and online data viewing and publishes online structures. Installation program automatically installs this plugin required application and ActiveX controls on browser type/existing web browsers.

#### **Chem3D Pro 13.0**

This application is first class desktop molecular modeling and protein visualization provides support open GL graphics at state-of-the-art, and stereo hardware. If it is required to build small molecules using the ChemDraw interface this can be seen as 3D structure that appears simultaneously, the software can perform basic molecular modeling calculations such as the dihedral driver, MM2 experiments, experiments of mechanics and molecular dynamics. It can also perform calculations "ab initio" through a GUI interface for GAMESS (free application when used in academia but require user registration [1]). This option is available only for Windows versions.

#### **ChemBioFinder Ultra 13.0**

ChemBioFinder Ultra is the ultimate system management databases for chemical structure and information databases appeal through the program after registration as a user. Browse, create, search, and update local databases with structural data, numeric and text through custom user forms, including structural queries, sub-structural-based similarity and link to related data existing sub-forms. Calculate values for physical properties view and edit structures in a variety of very complex ways to create new databases automatically and including forms for imported data, export and print. The user can easily manage saved searches, preferential access to certain databases and database structural view through Windows Explorer dock able application software. Other features include the ability to program can make RGroup analysis, graphic files to read from the database, to program in Python language and seek tautomeric forms a clearly improved compared to previous versions. This option is available only for Windows versions.

#### **ChemBioViz Pro 13.0**

ChemBioViz Pro is a program package type very rich set of tools used in visualizing numerical data from ChemBioFinder. This set of tools enables calculation and display structure activity relationship type,

relationship type clustering and calculating and displaying statistical data, including the real-time display of histograms, scatter type applications, graphics and even logarithmic dendrograms. Descriptive statistics include minimum, maximum, average, median deviation, standard, and more. The user can create composite profiles and comparative view can also classify structures based on values of selected properties and even a profile of costs associated with each property. It is also possible to create plots under the ChemBioFinder for different sub-forms. ChemBioViz is a visualization application type structure that works with Ultra ChemBioFinder application also allows users to correlate biological activity with chemical structures related. ChemBioViz turns ChemBioFinder data provided by a comprehensible graphical format, it allows scientists to easily discern correlations between structure and activity. ChemBioViz application generates the late running interactive window that contains a variety of data types and also allows researchers to analyze these data using a variety of statistical analytical tools at hand. Users can then filter their data on any field in the database, in order to examine subsets of data to locate trends and correlations. This option is available only for Windows versions.

#### **ChemDraw/Excel Pro 13.0**

ChemDraw/Excel allows specialists can create interactive interfaces chemical calculation in real time as the familiar Microsoft Excel environment permits. Construction and manipulation of chemical structures using Microsoft Excel application, chemical properties and structure calculation, and use substructure search in order to locate any group of compounds. This option is available only for Windows versions.

#### **ChemBioFinder for Office 13.0**

ChemBioFinder for Office is the main conversion program which allows locating the file, search for structure in the documents on computer or other units on the network. The program can read many types of structural extension files such as CDX, MOL, SDF, rxn and SKC, and search results can be displayed or converted to SDfiles. This option is available only for Windows versions.

#### **BioDraw Ultra 13.0**

BioDraw Ultra application allows drawing and annotating biological pathways quick and straightforward, adding a level unmatched in terms of uniformity and high degree of detail. Design elements type tool boxes include membranes, DNA, enzymes, receptors, and reaction arrows, tRNA, ribosomes, helix proteins, Golgi bodies, G-proteins, immunoglobulins, mitochondrion and a Plasmid Map Tool type.

The latest version of BioDraw Ultra includes a new feature consisting in the presence of a new tool bar for drawing and editing bio-polymers peptide and nucleotide sequences using single and three letter codes, including beta and D-amino acids. The sequences can be expanded and contracted sulfur and lactam bridges can be easily added.

### ChemNMR Pro 13.0

ChemNMR software application can be used to accurately estimate  $^{13}\text{C}$  and  $^1\text{H}$  NMR spectra and chemical shifts. Chosen molecule and its spectrum appear in a new window. Chemical shifts are displayed directly on the molecule and the spectrum is directly linked to the structure so that clicking on a peak in the spectrum obtained fragment program stresses related to the molecule. Through the application ChemNMR 13.0, the solvent can be specified which can be either DMSO or  $\text{CDCl}_3$ .

### Struct=Name Pro 13.0

The application Struct=Name contains some leading comprehensive methods for converting chemical structures into chemical names and International Union of Pure and Applied Chemistry (IUPAC) names for structures. During the development of these versions this application suffered the most noticeable improvements. The application can be used for most types of compounds, including some charged compounds and even salts, bridge systems and molten tone, symmetrical structures extremely isotopically labeled compounds and many other types of inorganic and organometallics.

### MestRe Nova Std/Lite

MestRe Nova (MNova) Std/Lite is an application-dimensional (1D) used only data processing, visualization and analysis of NMR spectral type. The lite/standard offers a variety still limited conversion facilities for most formats NMR spectrometry type and includes a conventional processing, the display and plotting, normal capabilities offered by program type NMR spectra visualization and some techniques a more advanced processing. MNova Std/Lite is a 1D version restricted MNova program that provides the user basic processing and some analysis capabilities. MNova full version is available either through the online store, or directly on the company website SciStore research section Mestrelab.

### What's new?

New Features in version 13.0 [2, 3]

- Biopolymer toolbar with disulfide and lactam bridges, beta and D-amino acids, DNA, RNA, protecting groups and linkers.

- Paste peptide, DNA and RNA sequences and have them interpreted chemically with sequence wrapping and shaping.
- New Gel Electrophoresis Plate Tool provides arbitrary rotation for lane labels, drag and position band labels, paste data from Excel or other sources, and copy and paste between lanes.
- Calculators for pKa, LogD and LogS enable scientists to explore important bioavailability properties such as acid dissociation, distribution and aqueous solubility for putative compounds.
- Collaboration is easier than ever as scientists can now use Dropbox™ to save, share and import ChemBioDraw structures, reactions and drawings using a secure, sharable Cloud location.

### Installation

The purchased version is a Windows only version so below are the software requirements (Table 2).

### ChemBioDraw Ultra 13.0v Windows only [4-6].

To install the software the user must first **sign in to the CambridgeSoft Website**

1. If ChemBioDraw has been downloaded in the past, log in to the following site using previous existing account [5, 6].
2. After logging in, locate the **Services** section on the right side of the page and click the **My Site Subscription** link.
3. Locate the **Accessing Registered User Software** section and click on the **Download Site Subscription Software** link.
4. Read the sections on the next page carefully - the **First** section contains a link to **Windows** software.
5. Click the **Click Here to Download Software 1** link in the appropriate section.
6. After the software begins downloading click the **BACK** button in browser.
7. Locate the **Services** section on the right side of the page and click on **My Downloads**. Keep this page open once it loads.

### Install ChemBioDraw Ultra 13 [7]

1. Before installation be sure that the computer meets the system requirements listed above.
2. When the download is finished, locate the **<name>.exe** (Windows) file and double-click to launch the installer.
3. In the **CambridgeSoft Software Activation** window, enter the required information and click **Activate over Internet**.
4. This information can be found in the **My Downloads** page which was opened earlier.

5. In the CambridgeSoft ChemBioDraw Ultra 13.0 Wizard window, click **Next** >.
6. In the License Agreement window, select **I accept the terms in this license agreement**, and click **Next** >.
7. In the **Select Type** window, choose the Default setup and click **Next** >.
8. In the **Select Features** window, click **Next** >.
9. In the **Select Features** window, select **MNova NMR Lite/Std** and click **Next** >(this is optional).
10. In the **Ready to Install** window, click **Install**.
11. In the **Installation Complete** window, click **Finish** [7].

The process is very smooth and fast, so an average user can do it without any problems.

#### Getting Started

To run ChemBioDraw application on a Windows PC you must follow the following procedure: open **Start Menu** and navigate to **Start>All Programs >ChemBioDraw 20xx>ChemBioDraw Ultra xx**.

A tutorial about how to use ChemDraw can be also achieved from internet resource [8].

#### Program Interface

As previous versions the interface is almost the same, but with some modifications on Calculations Menu, according to the new introduced features. See editions comparison (Table 1).

#### Speed and Accuracy of computations

Compared with the previously released version of ChemDraw 10.0v and ChemDraw Ultra 12.0v on which the first and second authors used at University of KwaZulu-Natal, South Africa and Center for Organic Chemistry, Romania, respectively. Presently the new version of ChemBioDraw Ultra 13.0v introduce higher speed computation, more accurate compound IUPAC nomenclature, a much friendlier interface when it's coming to presenting the results.

Following example is used to express this improvement:

**Table 1: Comparison of ChemDraw 10.0v, ChemBioDraw 12.0v, and 13.0v editions.**

ChemDraw 10.0[9]	ChemBioDraw 12 [10, 11]	ChemBioDraw 13.0[12]
ChemDraw Ultra	ChemBioDraw Ultra 12.0	ChemBioDraw Ultra 13.0
	MestRe-C Standard	MestRe Nova Std/Lite
Chem3D Std	Chem3D 12.0 Pro	Chem3D Pro 13.0
	ChemFinder 12.0 Standard	ChemBioFinder Ultra 13.0
ChemFinder Pro	ChemFinder/Office 12.0	ChemBioFinder for Office 13.0
ChemDraw Plugin Pro Chem3D Plugin Std	ChemDraw and Chem3D ActiveX Pro Controls & Plugins	ChemDraw ActiveX/Plugin Pro 13.0
N/A	ChemInfo (Index, RXN, NCI & AIDS) Databases	N/A
N/A	E-Notebook 12.0 Pro	N/A
N/A	N/A	ChemBioViz Pro 13.0
N/A	N/A	ChemDraw/Excel Pro 13.0
N/A	N/A	BioDraw Ultra 13.0
N/A	N/A	ChemNMR Pro 13.0
N/A	N/A	Struct=Name Pro 13.0

Note: N/A means not available.

**Table 2: Requirements comparison between ChemDraw 10.0v ChemBioDraw 12.0v, and 13.0v.**

<b>ChemDraw 10.0</b> [9]	<b>ChemBioDraw 12</b> [13]	<b>ChemBioDraw Ultra 13.0v</b> [14]
<b>OS:</b> Windows 95, 98, 2000, Me, XP, Windows NT 4.0 RAM 64 Mb.	<b>OS:</b> Windows 2000 SP4, XP Professional SP3 (32 bit only), Vista 32-bit only (Vista Home/Home Premium are not supported), or Windows 7 32 bit (Professional and Ultimate), Windows 7 Professional, Ultimate & Enterprise 64 bit (BioAssay NOT supported).	<b>OS:</b> Windows XP Professional SP3 (32 bit), Windows Vista Business and Ultimate (32 bit), Windows 7 Professional and Ultimate (32 bit) (STATISTICA is not included), Windows 7 Professional and Ultimate (64 bit) (STATISTICA is not included).
<b>Plugin:</b> Internet Explorer 4.0-6.x or Netscape 4.0-6.x Other IE 3.x or greater required for Help and Online Menu.	<b>Plugin/Control:</b> ChemDraw plugin/ActiveX control supports Netscape® 7.x, Firefox 8.x, Chrome 7.0, and Microsoft IE 6.x. and 7.0 (32 bit) 8.0 (32 bit) only. The Chem3D ActiveX control supports IE 6.x and 7.0 (32 bit) 8.0 (32 bit) only.	<b>Plugin/Control:</b> ChemDraw plugin/ActiveX control supports: Microsoft Internet Explorer 7.x (32 bit only) Microsoft Internet Explorer 8.x (32 bit only) Microsoft Internet Explorer 9.0 (32 bit only), Firefox 12.0 and Chrome 19.x.
N/A	<b>RAM:</b> RAM 512 MB (minimum) 1GB (preferred).	<b>RAM:</b> 512 MB (minimum) 1GB (preferred).
Disk Space: Ultra-70 Mb, Pro-40 Mb, Std-30 Mb Processor: Intel or AMD faster than a 486.	N/A	N/A
<b>Microsoft Office:</b> MS Office 97 or greater required for Excel and Word Add-Ins.	<b>Microsoft Office:</b> Microsoft Office 2000 (Not supported by ChemDraw for Excel and Combi for Excel add-ins or E-Notebook), XP, 2003 and 2007, limited 2010 (32-bit) support.	<b>Microsoft Office:</b> Microsoft Office 2003 Microsoft Office 2007 Microsoft Office 2010 32-bit (There are some known problems with Office 2010, please see compatibility page for more information [15]).
N/A	<b>Client:</b> RAM 512 MB (minimum) 1GB (preferred).	N/A
N/A	<b>Server:</b> RAM 2 GB (minimum) - for E-Notebook Client Server configuration if the database files and the SQL Server 2005 (Express edition) are present on the Server.	N/A
N/A	<b>Server Software:</b> Windows XP Professional SP2 (32 bit only) or Vista 32-bit only (Vista Home/Home Premium are not supported) or Windows 2003 R2 SP2 or Windows 2008.	N/A
N/A	<b>Other:</b> SQL Server 2005 Express edition with SP2.	N/A
N/A	<b>Screen:</b> Resolution: 800x600 or higher.	<b>Screen:</b> Resolution: 1024x768 or higher.
N/A	NOTE: ChemBioDraw Ultra 12.0v does not support case sensitive SQL. The SQL Server needs to be in the same domain as the clients. The SQL Server port should be added to the firewall for the clients to be able to see it.	N/A

Note: N/A means not available.

In order to evaluate the correctness of IUPAC names of the heterocyclic compounds two of the dihydropyrimidines that are mono and di-substituted analogues (**1** and **2**) known for anti-TB properties [16] have been considered for on three version of the Perkin-Elmer Cambridge ChemDraw software.

Table 3: IUPAC comparison of dihydropyrimidine analogues on three versions of the Cambridge ChemDraw version.

SI No	Chemical Structure	ChemDraw 10.0v[16]	ChemBioDraw Ultra 12.0v	ChemBioDraw Ultra 13.0v
1		2-(3-Bromophenylamino)-6-(4-chlorophenyl)-5-(methoxycarbonyl)-4-methyl-3,6-dihydropyrimidin-1-ium chloride	2-((3-Bromophenyl)amino)-6-(4-chlorophenyl)-5-(methoxycarbonyl)-4-methyl-3,6-dihydropyrimidin-1-ium chloride	2-((3-Bromophenyl)amino)-6-(4-chlorophenyl)-5-(methoxycarbonyl)-4-methyl-3,6-dihydropyrimidin-1-ium chloride
2		6-(4-Chlorophenyl)-2-(2-hydroxy-4-nitrophenylamino)-5-(methoxycarbonyl)-4-methyl-3,6-dihydropyrimidin-1-ium chloride	6-(4-Chlorophenyl)-2-((2-hydroxy-4-nitrophenyl)amino)-5-(methoxycarbonyl)-4-methyl-3,6-dihydropyrimidin-1-ium chloride	6-(4-Chlorophenyl)-2-((2-hydroxy-4-nitrophenyl)amino)-5-(methoxycarbonyl)-4-methyl-3,6-dihydropyrimidin-1-ium chloride

## CONCLUSION

The software is continuously improved; the optimizations are more than visible, so is definitely to be considered as a major release and not as an improved and patched release. We are very pleased by the featured options that this release offered to us and we warmly recommend to anyone to go for this new and improved major release.

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### Competing interests

The authors declare that they have no competing interests.

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