

ChemDraw Ultra 6.0. CD-ROM. CambridgeSoft Corp. 1999. US\$ 599 (educational). www.camsoft.com.

Current software offers a variety of ways for scientists to communicate chemical structures and reactions, in addition to the more traditional methods. Therefore, a software package that offers the flexibility of being able to prepare drawings of a high quality and then work towards making them presentable via all available media is to be welcomed. ChemDraw Ultra 6.0 embraces this role well.

Like its predecessors, ChemDraw Ultra 6.0 presents the user with an interface that is logically laid out and instinctive to use. By selecting the required ring or bond tools from the palette provided, molecules can easily be constructed and manipulated to result in well-presented formulae. Text within a drawing can quickly be altered via a tool bar. Of particular advantage with this latest version is the possibility to draw dashed arcs and circles using the tools palette. These tasks now seem effortless. A quick reference card is provided for both Windows and Macintosh platforms with concise descriptions of all menus, screen and tool elements, and tips for working with drawings. Structures can be cleaned up if desired and, for those creating drawings for publication, style sheets are available for most chemistry journals; alternatively, it is easy to create your own.

The level of chemical intelligence available with ChemDraw Ultra 6.0 is impressive. Whilst drawing you can choose to be supported by the program's 'Show Chemical Warnings' function; this highlights any parts of the structure showing any chemical irregularities with a distinctive red box. The 'Check Structure' function will then elaborate on the warnings if needed. Labour-saving features such as HotKeys, which can be used to label atoms and automatically inserts any additional hydrogens, or Nicknames, which allows abbreviations to be created for functional groups without losing their chemical significance, are still available. Structures can then be analysed for molecular weight and other chemical properties. A list describing these is quickly generated via the add-on ChemProp.

In addition, the program can assign *R/S*, *r/s*, or *E/Z* stereochemistry to a compound according to Cahn-Ingold-Prelog rules. The stereocentres automatically appear in the drawing and alter instantaneously when the corresponding changes are made to the compound. Structures can also be selected and their IUPAC names generated using a link with AutoNom 2.1; this appears beneath the structure with any of the above stereochemistry retained in the name. By placing the name within the same window as the structure it avoids the awkwardness of having to toggle

between several naming and drawing windows. The names can sometimes contain superfluous hyphens, but these are easily edited. Structures can also be created from names and most organic nomenclature is accurately recognised.

ChemDraw Ultra 6.0 can be used to predict ^{13}C and ^1H NMR shifts for a compound with ChemNMR. The estimations are fast and easy to obtain and the selected molecule appears in a new window labelled with the estimated shifts, the corresponding line spectrum, and a text description of the prediction. The accuracy of the values given by the molecule are coloured according to confidence and the correlation between the spectrum and the structure is highlighted by moving the mouse arrow over either.

Query structures can be drawn specifying the properties of atoms, bonds, and other query attributes, such as listing alternative R groups on a parent structure, before exporting to a chemical database for searching. Similarly, reactions can be atom-to-atom mapped, either automatically or manually, and the reaction centres defined for creating records or for querying in a reaction database.

It is possible to create posters or multipage documents within one file which saves time for those drawing structures for presentation or publication. Files can be transferred across Macintosh and Windows platforms, and to and from additional applications. This program also comes packaged with ChemFinder for creating chemical databases or querying existing ones, and Chem3D for molecular modelling. Plugins are also provided for publishing structures or searching chemical databases on the web. A chapter of the ChemDraw Ultra 6.0 manual is dedicated to its extensive capabilities for sharing information and online technical support is available.

ChemDraw Ultra 6.0 is a powerful package, beneficial for scientists in both industry and academia, or scientific publishers. The features it contains make it an ideal teaching tool, or a supportive program for preparing accurate structures or reactions for communicating to a wide number of destinations. The luxury of accessing structure names, NMR predictions, etc., via the one interface saves the time and expense associated with having additional programs to perform these tasks. I would highly recommend this program as a valuable addition to your software.

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