

ChemOffice Professional



The Scientifically Intelligent Productivity Suite for Chemists and Biologists

The ChemOffice Professional® offers a suite of industry leading scientifically intelligent productivity tools that help researchers transform their workflows. With new additions like the ChemDraw Cloud and PerkinElmer Signals™ Notebook, ChemOffice Professional empowers chemists and biologists alike to visualize and capture their research, efficiently keep track of their work, and gain a deeper understanding of their results and make decisions with greater confidence.

Create Publication-Ready Drawings Effortlessly

- Quickly and accurately draw and edit peptide and nucleotide sequences and chemical structures in ChemDraw desktop, ChemDraw Cloud or in Signals Notebook
- Produce structures in seconds with advanced Name-Structure features supporting expanding library including popular pharmaceutical products and ChemACX acronyms
- Copy/Paste peptide and nucleotide sequences from the web or text files and have the sequence laid out with control over block size and length
- Manage multiple structures with dynamic auto-number feature
- Draw Gel Electrophoresis plates and TLC plates quickly and precisely
- Quickly generate systematic IUPAC names from structures
- Use advanced clean-up tools for molecules, reactions and biopolymers to create attractive and accurate diagrams
- Manage multiple structures at once with automatic numbering
- Ensure that papers are publication-ready with pre-stored publication format guidelines for the major chemical and scientific journals

Calculate Efficiently and Accurately – Every Time

- Automatically calculate, track and update stoichiometry data for chemical reactions
- Calculate values for physical properties, view and edit structures in a variety of modes, automatically create databases and forms for importing, exporting and printing data
- Explore important bioavailability properties such as acid dissociation, distribution and aqueous solubility for putative compounds using specialized calculators for pKa, LogD and LogS
- Add chemical intelligence to Microsoft® Excel® spreadsheets. Build and manipulate chemical structures, compute chemical properties and use structure and substructure searches to locate and group compounds
- Use CLogP to calculate the n-octanol/water partition coefficients for estimating the distribution of drugs within the body
- Perform enhanced retrosynthesis analyses on molecules to identify the reactions that are required to create a bond or set of bonds emanating from a single atom.

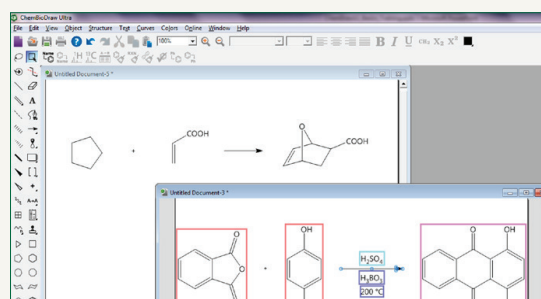


Figure 1: Color-coded parsing of a reaction using Reaction Interpreter.

Structure	Name	BP	MP	ClogP	KOW	Molwt	Newtsp
1	1-Fluoro-4-isobutylbenzene	446.6903	226.49	3.533	1.65	45.0662	12.7579
2	1-bromo-4-butylbenzene	514.552	300.7	4.537	1.67	52.525	11.57703
3	1-chloro-4-(tert-pentyl)benzene	495.5277	284.51	4.816	2.37	54.1297	11.23556

Figure 2: Calculation of chemical properties in ChemDraw for Excel.

Analyze and Visualize for Deeper Insight into Results

- Explore the 3D shape and properties of compounds with the Chem3D® molecular modeling and protein visualization tool
- Build small molecules and simultaneously view the 3D structure
- Perform RGroup Analysis, read graphic files from the database, Python programming and improved tautomeric searching
- Predict ¹H (proton) and ¹³C NMR spectra. Spectra and peaks are linked to the structure for clear interpretation
- Predict a range of properties including BP, MP and more
- Visualize and correlate structures and numeric data with the ChemBioFinder scientific personal database system
- Calculate and display structure activity relationships, clustering relationships, and statistical data, including histograms, scatter, logarithmic plots, and dendrograms
- Create compound profiles and visually compare and rank structures based on values of selected properties and the cost profile associated with each property
- Assess the feasibility of chemical synthesis using an enhanced retrosynthesis tool. This tool searches a cloud-based database of reactions as part of the assessment measure.

Access ChemDraw from your web browser with ChemDraw Cloud

Available for ChemDraw Professional and ChemOffice® Professional.

ChemDraw Cloud provides easy access to your ChemDraw files from any web browser and allows users to access ChemDraw documents from any computer with an Internet connection with no need to install any software on your computer.

- Import or export files, enjoy your favorite drawing features and even revision management.
- You can also share your designs with colleagues in a single click!
- All editing/viewing/managing of ChemDraw documents is done in a web browser (including tablet and mobile devices)
- All documents are stored, encrypted, and backed-up securely on ChemDraw Cloud servers
- Documents can be exported or printed with publication-quality output
- Documents stored in ChemDraw Cloud can be directly accessed/used from ChemDraw desktop or Signals Notebook
- Documents stored in ChemDraw Cloud can be shared with other platform users without distributing/emailing copies

Communicate and Collaborate with your Colleagues and the World

- Enjoy seamless workflows between ChemDraw desktop and Signals Notebook. Browse and open any ChemDraw file you have in your Signals Notebook directly from ChemDraw and when you're done - save your updated drawing back. What's more, you can even enjoy all of the ChemDraw Direct features directly in the ChemDraw module built right into Signals Notebook.
- Use ChemDraw Cloud to save, share and import structures, reactions and drawings with colleagues around the world
- Quickly and accurately search for chemical structures in Microsoft® Office® applications, the ChemDraw suite, ISIS files and more
- Works with the Microsoft® ActiveX® plugin for querying online chemical databases and viewing and publishing online structures
- Search with structural, numeric, and text data via user-customizable forms, including structural, sub-structural, and similarity queries, as well as linking to related data in sub-forms
- Search PerkinElmer Informatics databases for chemical structures in real time as you draw
- Export and import structure files in all the common interchange formats, including molfile, SDfile, SMILES, InChI and more