ChemOffice Professional® offers a broad suite of industry-leading, scientifically intelligent productivity tools that help researchers transform their workflows. Built off of the industry leading chemical drawing application ChemDraw, ChemOffice brings the tools a researcher needs to conduct their science. From 3D structures to predicted and experimental spectral results, cloud based sketching capabilities and access to a modern cloud based documentation and scientific collaboration platform, 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.

Highlights

• Create Publication-Ready Drawings Effortlessly with the industry leading ChemDraw application

• Document, store, retrieve and share your experimental records with access to PerkinElmer Signals™ Notebook Individual Edition, a modern, cloud-based Scientific collaboration platform

• Load and process 1D NMR and LC/GC/MS data directly on your desktop with Mnova ChemDraw Edition

• Build custom chemically-intelligent web applications with ChemDraw® JavaScript (ChemDraw JS, available with a ChemOffice Site License only)

• Expand the capabilities of ChemDraw by developing your own JavaScript-based add-ins.

Create Publication-Ready Drawings Effortlessly

• Create structures and reactions effortlessly, consistent with IUPAC, FDA and publication standards. Atoms on molecules can now be numbered following their IUPAC nomenclature name.

• Convert names into structures, and vice versa including accessing extensive libraries of popular pharmaceutical compounds and commercially available compounds from ChemACX. CAS Registry Numbers from ChemACX records can now be converted into structures

• Quickly import, create, edit and share complex biomolecules using the HELM toolbar, including import/export using the HELM notation format developed by the Pistoia Alliance

• No Mouse Needed! Create your structures and reactions as fast as you can type with Enhanced hotkeys

• Draw biological pathways, including GPCRs, ligand receptors, DNA, lipid bilayers and antibodies using BioDraw

• Use advanced clean-up tools for molecules, reactions and biopolymers to easily produce attractive and accurate diagrams

• Ensure that papers are publication-ready with pre-stored publication format guidelines for the major chemical and scientific journals

• Import/Export using common standards such as SMILES, Mol, SDFile, InChI, HELM, FASTA and CDXML. Improved copy/pasting allows for simpler pasting of SMILES, Mol or InChI into chemical structures.

Figure 1: Reaction Interpretation in PerkinElmer Signals™ Notebook Individual Edition.

Figure 2: Prediction of spectral and structural properties via ChemNMR and Chem3D.
Document, Store, Retrieve and Share your Science

- Create, manage and share experiments and notebooks with your colleagues, with access to the new scientific collaboration platform, PerkinElmer Signals™ Notebook Individual Edition
- Draw reaction schemes using a web enabled ChemDraw sketcher, the stoichiometry is calculated for you
- Add data from any source, of any type, from any browser
- Free text and chemical search and query help you find your data, whenever, wherever
- A cloud based solution means no installation, frequent updates, seamless upgrades, no migrations – no overhead

Analyze and Explore Your Reactions

- Identify similar reactions from the public literature with integration with SciFinder (Additional SciFinder license required)
- 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
- Easily manage the numbering of your molecules with dynamic Reaction Auto-numbering
- Automatically calculate, track and update stoichiometry data for chemical reactions

Predict and Calculate Efficiently and Accurately – Every Time

- Predict and calculate values for physiochemical properties important for bioavailability and stability, such as mp, bp, cLogP, pKa, LogD, and LogS
- Predict 1H and 13C 1D NMR spectra, including varying solvent and frequency, update with your own experimental data to improve the predictivity
- Explore the 3D shape and properties of compounds with the Chem3D® molecular modeling and protein visualization tool
- 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
- Extend the capabilities of ChemDraw by developing your own JavaScript-based add-ins.

ChemDraw Everywhere

- Store, retrieve and edit your ChemDraw documents on the go, using ChemDraw Cloud
- Web based ChemDraw sketcher allows access from any device
- All documents are stored, encrypted, and backed-up securely on ChemDraw Cloud servers
- Embed ChemDraw into your custom web applications with ChemDraw JavaScript (with ChemOffice Professional Site License)

Figure 3: Create novel, complex biopolymers with the new HELM editor.