ChemOffice Professional

The Scientifically Intelligent Productivity Suite for Chemists and Biologists

ChemOffice Professional® software offers a broad suite of industry-leading, scientifically intelligent productivity tools that help researchers transform their workflows. Built on the industry-leading ChemDraw® application, ChemOffice Professional software delivers the tools researchers need to conduct their science. With 3D structures, predicted and experimental spectral results, cloud-based sketching capabilities, and access to a modern cloud-based documentation and scientific collaboration, ChemOffice Professional software 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 – for better, more confident decisions.

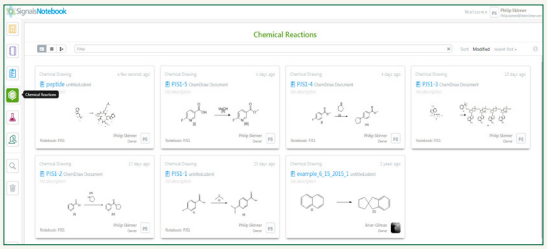

Figure 1: Reaction Interpretation in PerkinElmer Signals™ Notebook Individual Edition.

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.
- Search for molecules and reactions in Elsevier® Reaxys® from the comfort of the ChemDraw application.
- Look up commercial vendors and pricing information from our ChemACX® database of over 10 million substances.
- Look up a CAS registry number through ChemACX.com and return the corresponding chemical structure.
- Manage, curate, and share libraries of HELM monomers within your organization: the latest version of the Pistoia Alliance HELM Format is now supported.
- 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 the ChemDraw application by developing your own JavaScript add-ins. A folder or URL can be specified to dynamically access a remote repository of add-ins to deliver custom capabilities.

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.
- Convert names into structures, and structures into names, including accessing extensive libraries of popular pharmaceutical compounds and commercially available compounds from the ChemACX database. CAS registry numbers from ChemACX database records can be converted into structures.
- Quickly import, create, edit, and share complex biomolecules using the HELM toolbar, including import/export using the HELM notation format.
- 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 software.
- Use advanced cleanup tools for molecules, reactions, and biopolymers to easily produce attractive and accurate diagrams.
- Ensure that papers are publication-ready with prestored 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/paste allows for simpler pasting of SMILES, Mol, or InChI into chemical structures.
- Easily toggle or force a Kekule or delocalized representation of aromatic rings.

PerkinElmer®
For the Better

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, Signals™ Notebook Individual Edition.
- Draw reaction schemes using web-enabled ChemDraw Sketcher software – 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 anytime, wherever it resides.
- A cloud-based solution means no installation, frequent updates, seamless upgrades, no migrations – and no overhead.

Analyze and Explore Your Reactions

- Identify similar reactions from the public literature with integration with CAS SciFinder and Elsevier Reaxys (additional SciFinder and Reaxys licenses required).
- Easily manage the numbering of your molecules with dynamic reaction autonumbering.
- Automatically calculate, track, and update stoichiometry data for chemical reactions.

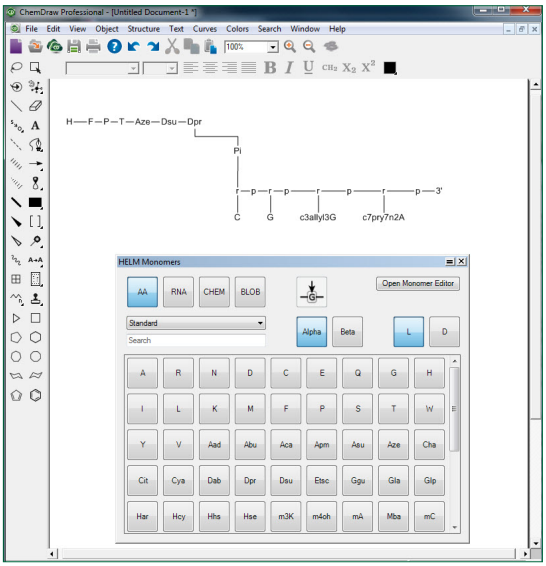

Figure 3: Create novel, complex biopolymers with the new HELM editor.

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 predictivity.
- Explore the 3D shape and properties of compounds with the Chem3D® molecular-modeling and protein-visualization tool. Chem3D Ultra is now compatible with GAMESS 18, Gaussian 16W, and MOPAC 2016.
- 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 the ChemDraw application by developing your own JavaScript add-ins.

ChemDraw Everywhere

- Store, retrieve, and edit your ChemDraw documents on the go, using the ChemDraw Cloud platform.
- All documents are stored, encrypted, and backed up securely on ChemDraw Cloud servers.
- Embed the ChemDraw application into your custom web applications with ChemDraw JavaScript (with ChemOffice Professional site license).

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