WHITE PAPER

Tips for Improving Polymer Science with ChemDraw

Changing Times Demand Better Technology Solutions

Introduction

Plastic materials have become integral to modern life, offering versatility and functionality across numerous applications. Since the invention of the first synthetic plastic, Bakelite, in the early 20th century, plastics have evolved into a cornerstone of industrial production and consumer goods. They are lightweight, durable, and moldable, making them ideal for packaging, construction, automotive, and medical devices. However, the environmental impact of conventional plastics, primarily derived from petroleum, has raised significant concerns regarding pollution and sustainability.

As a response to these challenges, researchers are exploring greener alternatives, including bioplastics made from renewable resources. This shift is essential not only for reducing our carbon footprint but also for promoting a circular economy that prioritizes recycling and biodegradability, ensuring that plastic materials can be used responsibly in the future.

Always present to support innovation, ChemDraw® offers features that enable the accurate description and reporting of discoveries in plastic and polymer material sciences. Let's explore them!

A Better Path to Discovery and Communication

ChemDraw, a leading chemical drawing and publishing solution, makes the path to polymers discovery and communication faster, easier, and more compelling. Here are some tips and tricks for improving your path to polymers discovery and communication.

1. Smart Polymer Brackets: Whether their molecular weights are known, analytically determined, or unknown, ChemDraw can handle any polymers through a new, unified type of brackets. Those new brackets allow calculation OR definition of the synthesized polymer average molecular weight. Simply measure it through an analytical method like GPC and use the calculated MW for the polymer you draw. Alternatively, you can enter the supplier-provided Mw when using a commercial substance to enable easy stoichiometry calculations with built- in ChemDraw tools.

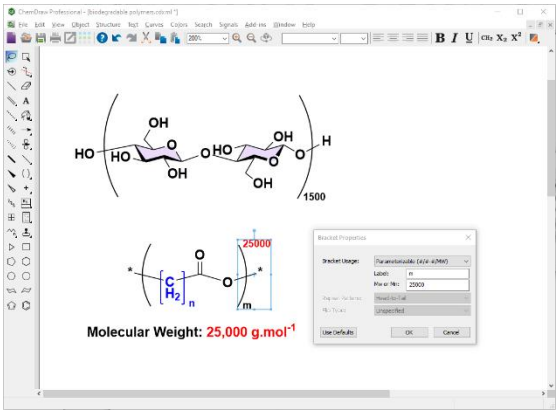

Figure 1. The new Parametrizable brackets in ChemDraw

2. Easily Source Reagents: ChemACX Explorer, a modern add-in informs you of the availability of commercial reagents, including vendor and pricing information, updated on a regular basis in ChemACX, Revvity's database of over 27 million commercially available chemical compounds. Simply search by name, CAS Registry Number or even substructure or similarity search and add the reagent to your canvas.

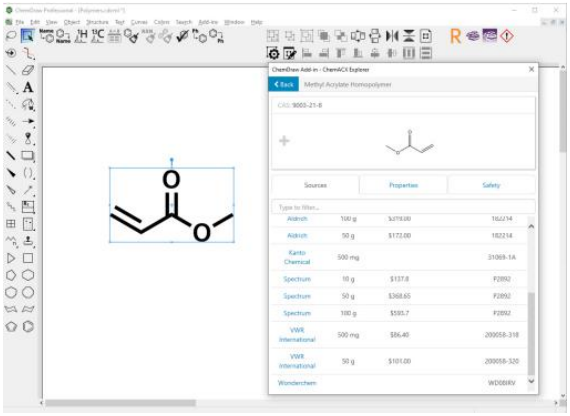

Figure 2. ChemACX Explorer helps you find suppliers and pricing information.

3. Safety First! We know how important access to safety data is for any chemist, as the first step before commencing bench work. We also know how time-consuming it can be to dig that information up, from a book or from a website. To this end, we recently introduced a powerful feature in ChemDraw under the form of the PubChem safety add-in. One of the largest public chemical databases available, PubChem holds the safety information (GHS Symbols, Hazard and Precautionary Phrases) for more than 120,000 chemical reagents and molecules. The PubChem Library Chemical Safety Sheet (LCSS) add-in ChemDraw gives you instant access to critical safety assessments, and lets you copy H and P phrases from specific safety agencies to your clipboard for you to paste into your experimental procedure in an electronic format, for example in Signals Notebook or in MS Word.

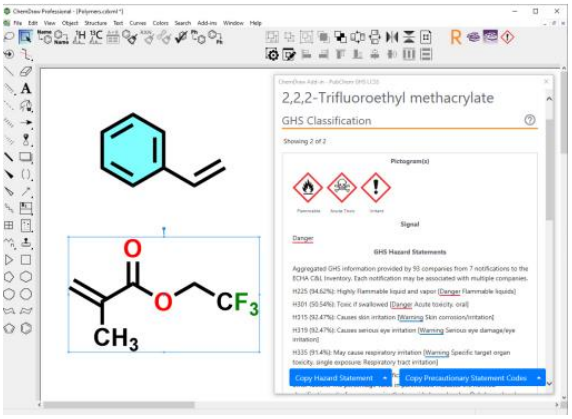

Figure 3. Get access to H and P phrases with the PubChem Laboratory Chemical Safety Sheet add-in.

4. Identify the Best Synthetic Routes: ChemDraw works hand in hand with all the major chemical literature databases through direct integrations with CAS SciFinder-n™ and Elsevier Reaxys®. Simply draw and select a molecule or a reaction to look into the literature from the comfort of ChemDraw and retrieve experimental procedures, yields and extensive literature references from your favorite databases. Note that those features require an active subscription to SciFinder-n or Reaxys.

5. Focus on Your Research Not on Drawing: Depicting and sharing your chemistry has never been easier nor faster. ChemDraw's revolutionary hotkeys systems changed the chemical drawing paradigm on computers by allowing you to draw molecules and reactions literally as fast as you can type them on a keyboard. Hotkeys are intuitive, quick and easy: simply press "f" over an atom to change it to a fluorine, press "Shift+f" to make it a "CF3". "s" is sulfur, while "Shift+s" is for silicon. In addition, ChemDraw's smart copy/paste function lets you Ctrl/Cmd + C SMILES text strings (found on chemical vendors websites or Wikipedia entries) and

Ctrl/Cmd + V them into ChemDraw directly as a structure. And if chemistry classes were not your forte, the user-favorited Name-to-Structure function will take the guessing and drawing completely out of the equation.

Summary

With its origins as a chemical drawing tool, ChemDraw has evolved steadily to become the leading chemically-intelligent solution for multiple disciplines from specialty chemistry to pharmaceutical drug discovery.

Some chemists love to draw and some don't. But all of you have to share, report on, and publish your work in various formats, up to and including filing with the United States Patent and Trademarks Office. No matter which kind of chemist you are, or what your drawing and publishing requirements might be, ChemDraw has the powerful features and integrations with critical external chemistry databases to help you publish beautiful drawings in seconds not minutes or hours. It is the gold standard for chemical drawing software. Plus, it is available in three offerings to meet your specific needs.

Features described in this white paper are available with a ChemDraw Professional or a Signals ChemDraw license. To learn more about our offerings, check our product page at https://revvitysignals.com/products/research/chemdraw

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