WHITE PAPER

Tips for Improving Polymer Science with ChemDraw

Changing Times Demand Better Technology Solutions

Introduction

"The pandemic and resulting economic crisis gave plastics a major image makeover amongst consumers; there is now a widely held view that plastic products are safer and cleaner than the recycled and reusable solutions being touted earlier and are at the forefront of the fight to contain the spread of contagion. Gone are the days when plastics will be spoken of only in terms of environmental leakage and a ban."1

"Plastics will also benefit from increased spending on household cleaning, hygiene, and personal protection products, as well as higher domestic food consumption from a more homebased life."1

While progress in polymer science has been revolutionary, abundant opportunities remain for creating new polymeric materials and modifying existing polymers for new applications.

> *"A strategic inflection point is a time in the life of business when its fundamentals are about to change. That change can mean an opportunity to rise to new heights, but it may just as likely signal the beginning of the end."*
>
> -- Andrew Grove, former CEO of Intel

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.

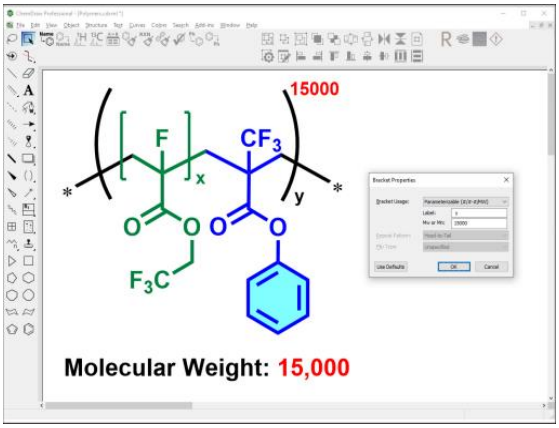

Figure 1. The new Parametrizable brackets in ChemDraw 19.1).

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 12 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. Note for SR: Recycle the paragraph we already wrote about ACX Explorer in other white papers.

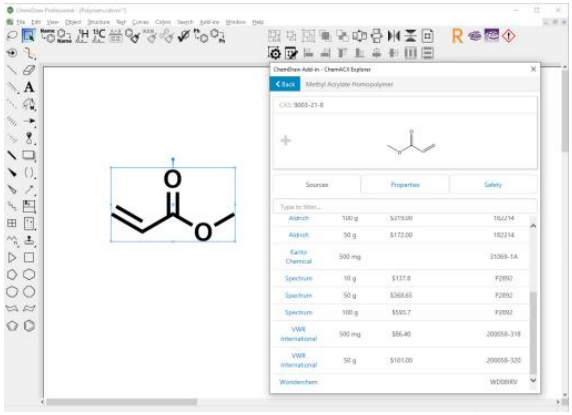

Figure 2. ChemACX Explorer helps you find suppliers and pricing information.

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.

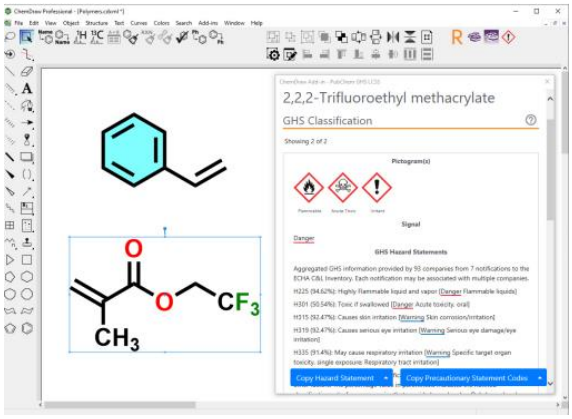

Figure 3. Get access to H and P phrases with the PubChem Laboratory Chemical Safety Sheet add-in.

4. Identify the Best Synthetic Routes: ChemDraw works hand in hand with all the major chemical literature databases through direct integrations with both CAS SciFinder, 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 SciFinder, SciFindern or Reaxys subscription.

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 versions to meet your specific needs.

Reference

1.IHS Market https://ihsmarkit.com/research-analysis/how-is- polymer-demand-impacted-by-the-covid19-pandemic.html

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