

FLYER



# Using the Power of ChemDraw in a JavaScript Sketcher

Deployed as You Want



# ChemDraw® JS is a pure JavaScript sketcher with the chemical intelligence and esthetics of ChemDraw on the desktop available as a zero download component for use in web browsers and other apps.

Already used as the sketcher in McGraw-Hill Education's Connect Chemistry online courses and in the Revvity Signals™ Notebook collaborative science platform, ChemDraw Cloud, Lead Discovery (Powered by Tibco™ Spotfire®), and Revvity Signals™ Lead Discovery, ChemDraw JS is now available for customer deployment to enable chemical intelligence into web browsers and other applications.

## ChemDraw Chemistry

ChemDraw JS has the same underlying chemical smarts as ChemDraw on the Desktop. It comes equipped with all the familiar tools you need to draw structures, reactions, mechanisms and text:

- Ring, chain and bond tools
- Arrows
- Text tool for chemical labels and captions
- Charges
- Query features: generic atoms, atom lists, bond type and topology
- Valence checker
- Marquee and Lasso selection tools
- Eraser
- Templates: Amino acids, Bicyclics, Cycloalkanes
- Acyclic Chain tool
- Expand/Contract Labels
- Round-Trip editing into MS Office documents (requires browser clipboard extension)

## ChemDraw JS Productivity

In addition to the basic drawing tools, ChemDraw JS provides several ways to speed up the creation of publication quality diagrams:

- Hotkeys to quickly add atoms and change the nature of bonds in molecules
- New reaction shortcut
- Copy/paste to duplicate structures
- Structure and reaction clean-up

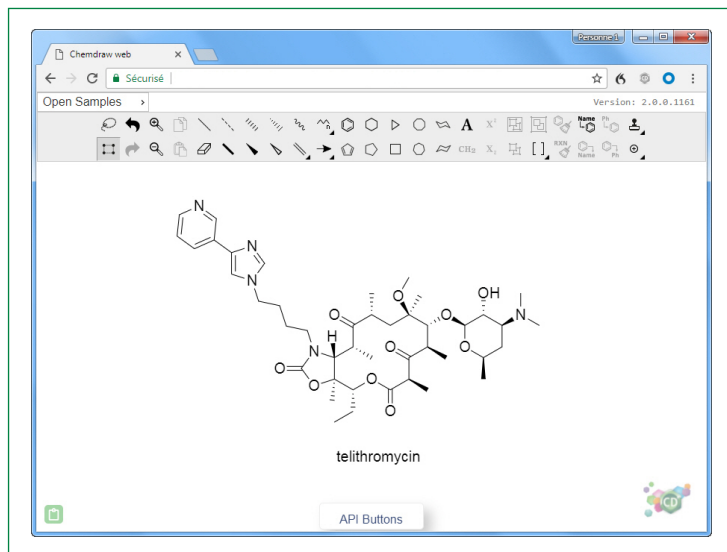


Figure 1. ChemDraw JS Drawing Pane.

## ChemDraw JS Sharing

ChemDraw JS generates and reads the same file formats used by ChemDraw Desktop so that files can be easily shared. Additional formats are also available for sharing with other applications:

- CDXML
- molfile and rxnfile
- SMILES
- InChI and InChIKey
- Chemical drawings copied from ChemDraw Desktop, or from other third-party editors, can be directly pasted into ChemDraw JS for immediate exchange of structures and reactions between desktop and web browsers.
- Chemical drawings embedded in MS Office applications (Windows) can be copied/pasted into ChemDraw JS without loss of information (requires browser extension).

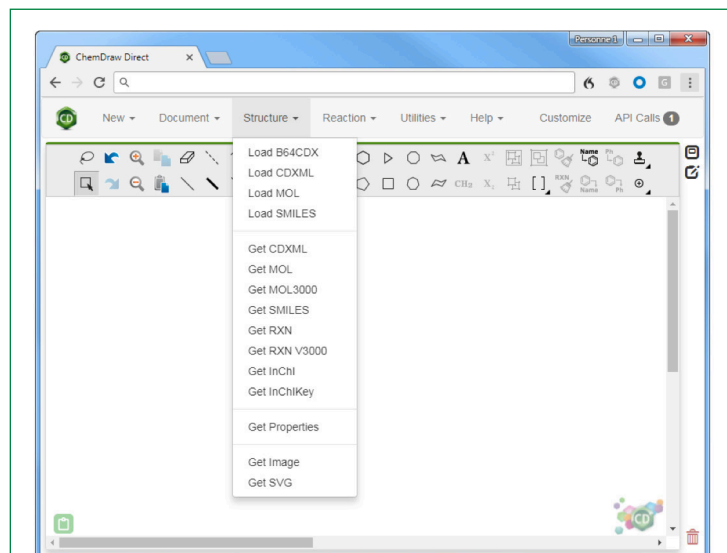
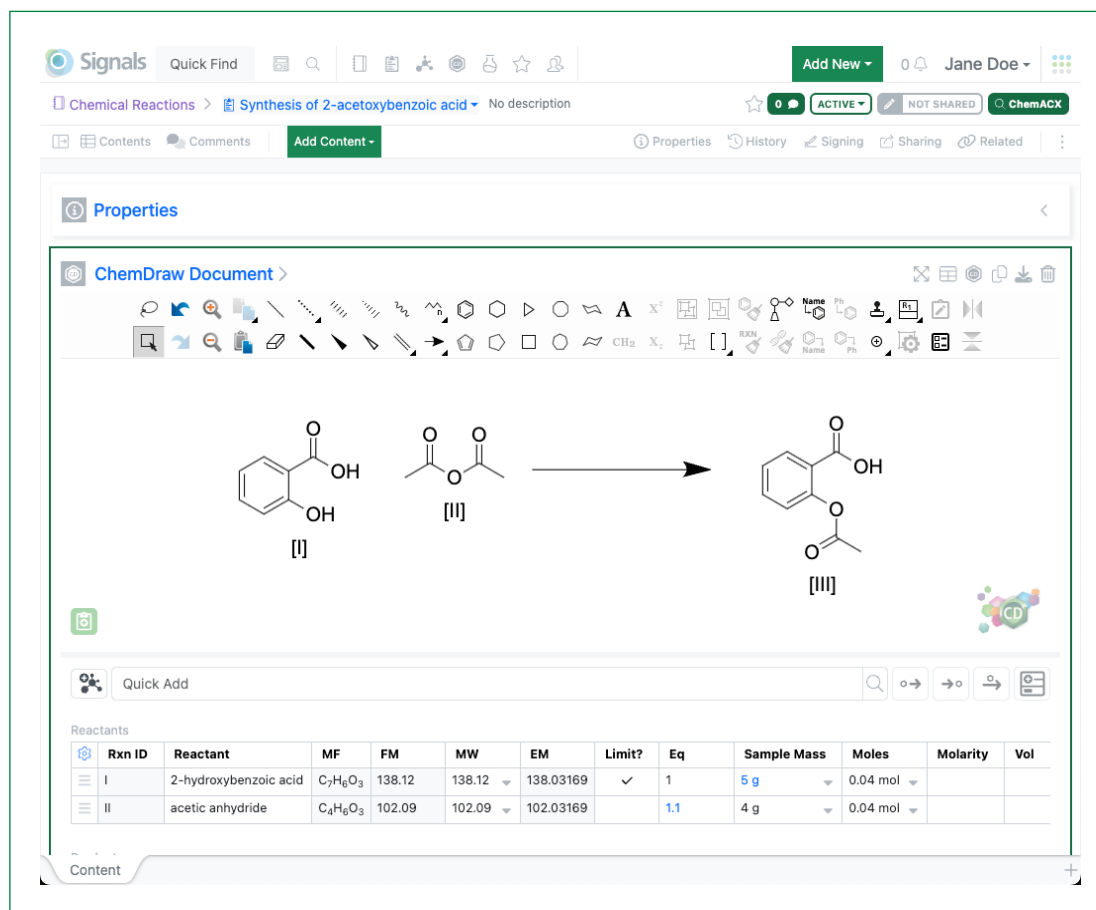


Figure 2. Available API calls for ChemDraw JS.

# ChemDraw® JS Deployment

ChemDraw JS is supplied with a fully documented User's Guide, Installation Guide and Developers' Guide. The latter includes instructions on how to load and to embed ChemDraw JS into an application, and details of how to make API calls to generate the various file formats that are available.



The screenshot displays the Revvity Signals™ Notebook interface. At the top, there is a navigation bar with 'Signals', a search bar, and user information 'Jane Doe'. Below this is a breadcrumb trail: 'Chemical Reactions > Synthesis of 2-acetoxybenzoic acid'. The main workspace is titled 'ChemDraw Document' and contains a chemical reaction sketcher. The reaction shows 2-hydroxybenzoic acid (labeled [I]) reacting with acetic anhydride (labeled [II]) to produce 2-acetoxybenzoic acid (labeled [III]). Below the reaction is a 'Reactants' table:

Rxn ID	Reactant	MF	FM	MW	EM	Limit?	Eq	Sample Mass	Moles	Molarity	Vol
I	2-hydroxybenzoic acid	C <sub>7</sub> H <sub>6</sub> O <sub>3</sub>	138.12	138.12	138.03169	✓	1	5 g	0.04 mol		
II	acetic anhydride	C <sub>4</sub> H <sub>6</sub> O <sub>3</sub>	102.09	102.09	102.03169		1.1	4 g	0.04 mol		

Figure 3. ChemDraw JS Sketcher in Revvity Signals™ Notebook.