

## What's new in version 2.11.0

- Chemical database integration with DigitalGlassware's RecipeBuilder

We have now introduced the capability of linking your chemical database with RecipeBuilder, facilitating the population of the chemical scheme and chemical tables within a Recipe from your chemical database. This chemical information is captured within our Practical Chemistry Markup Language (PCML) that underpins our DigitalGlassware Recipes.

For version 2.11.0 we have linked our Molecular Information/ Identity System (MIS) which is derived from the [open source PubChem database](#), and provides access to chemical names, structures and specific chemical information. This new feature can be accessed in several ways

### 1. Automatically draw structures based on the chemical name or SMILES

Within the Recipe Overview screen in the Create a Recipe screen, our chemical sketching tool ICEdit has received an update! A new icon has been introduced that allows you to add structures to ICEdit by searching the MIS either using chemical names or SMILES. This icon is currently linked to MIS as standard, and can also be linked to your database if required. A new Extract button can then extract the chemical structures to the Recipe's chemical table.

### 2. Automatically extract chemical information in the chemical table

If your database is integrated with DigitalGlassware then chemicals can be added directly to the chemicals table using the new database integration feature as well. This is achieved by clicking the "Add a Row" icon as normal, but now selecting your database from the dropdown menu as the data source. From here you can add your chemical name or chemical identifier to add that chemical to the chemical table.

The screenshot displays the 'Version 2.11 of DigitalGlassware: Chemical Database Integration' interface. The main workspace is titled 'Recipe Scheme' and contains a toolbar with various icons for editing and a prominent 'EXTRACT' button. Below the toolbar is a large empty area for drawing chemical structures. To the right, a 'Meta' panel lists several fields: 'author' (Deepmatter), 'owner' (Deepmatter), 'publication' (Enter recipe Publication...), 'version' (1.0), 'version-author' (Deepmatter), 'version-owner' (Deepmatter), 'custom-tag' (Enter recipe Custom tag...), and 'creation-date' (25 May 2022). At the bottom left, there is a 'Synopsis' section with the text 'Enter Recipe Synopsis here...'.