Subject: Re: Became enamine database a sub-set of chemspace? Posted by thomas on Sun, 06 Mar 2022 16:57:10 GMT

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Enamine building block retrieval was replaced by a commercial building block retrieval with the option to select among multiple providers of which one is Enamine. The change was done in two places, the 'Database' menu and in the combinatorial library dialog when suggestion commercially available reactants. The idea behind is to gradually allow more providers to add their chemicals to the database.

The Chemspace search function was not changed. Technically, the ChemSpace search uses the API and server at chem-space.com, which garanties that the database is always up-to-date, but it does not support atom and bond query features and no exclude groups. The 'Commercial Building Block' search on the other hand are typically weeks or sometimes even months old, depending on when the last update for a specific provider was done. However, the search is faster, it supports price and package size and atom/bond query features, and exclude groups.

Thomas