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Subject: Became enamine database a sub-set of chemspace?

Posted by [nbehrnd](#) on Sun, 06 Mar 2022 11:14:01 GMT

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After updating DW 5.5.0 for Linux with the development release by 2022-02-19, I noticed the GUI's entry «Database» does not/does not anymore include an entry to search specifically for enamines.[1] Is the assumption correct that this database became a sub-set of Database -> Search ChemSpace Chemicals?[2]

The search function DW offers with this entry is really helpful which includes to identify sources of isotopically labeled compounds (D/2H, 13C, etc.).

Norwid

[1] In the documentation/help, cf. chapter External Databases -> The Enamine Building Block Database

[2] <https://chem-space.com/>

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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 guarantees 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

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