

Subject: Re: retrosynthesis tools

Posted by [nbehrnd](#) on Thu, 23 Sep 2021 19:10:19 GMT

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If your organization supports an account on spaya.ai, then a right-click on the structure of interest offers access to suggestions. You have 30 days to venture out and get familiar enough with this service to come to a decision to purchase their service, or not.

They are not the only ones in the field to predict reactions/to offer retrosynthesis (e.g, <https://rxn.res.ibm.com/>, or <https://askcos.mit.edu/retro/>); you may enter the targeted structure by the SMILES string DataWarrior can assign to the molecule structures. If you have access to and some familiarity with Python, AiZynthFinder by the Reymond group may be an interesting example (open source code, permissive MIT licence), too.

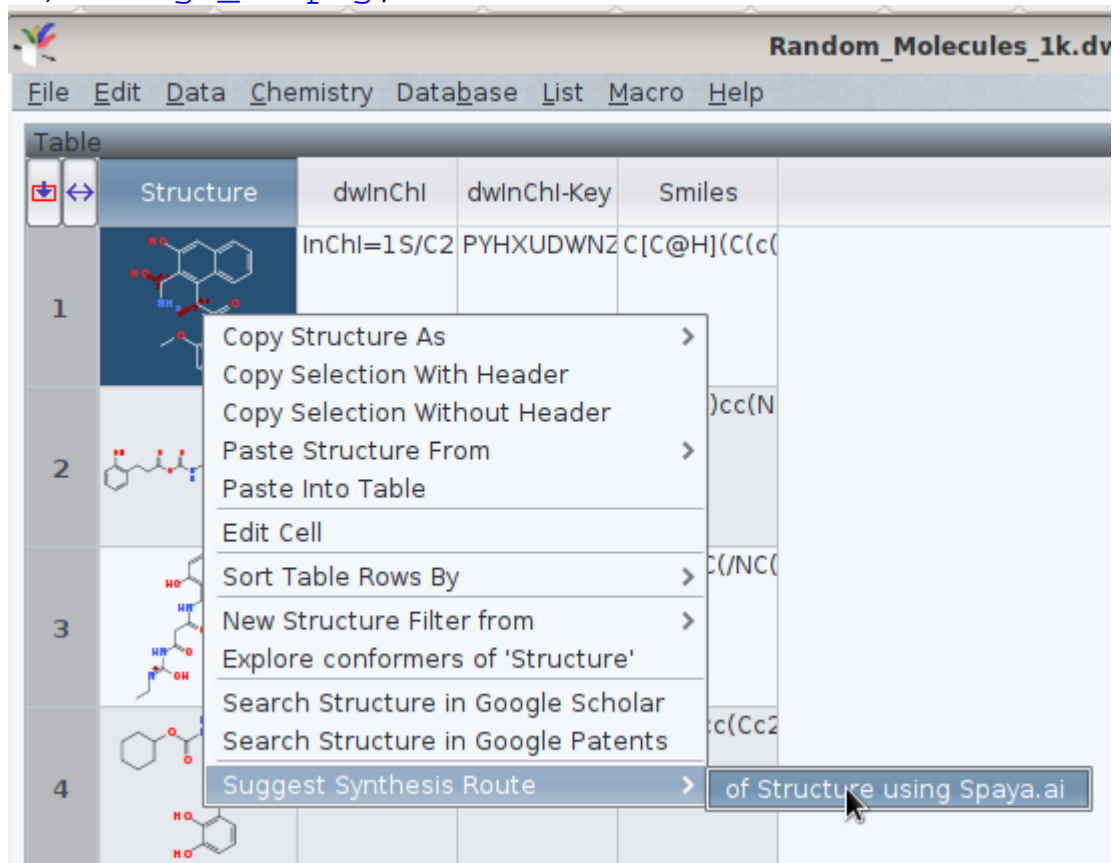
[1a] Genheden, S., Thakkar, A., Chadimová, V. et al. AiZynthFinder: a fast, robust and flexible open-source software for retrosynthetic planning. J Cheminform 12, 70 (2020)

(<https://doi.org/10.1186/s13321-020-00472-1>)

[1b] Retrosynthetic accessibility score (RAscore) – rapid machine learned synthesizability classification from AI driven retrosynthetic planning, Thakkar et al. Chem. Sci., 2021,12, 3339-3349 (<https://doi.org/10.1039/D0SC05401A>)

File Attachments

1) [bridge_dw.png](#), downloaded 855 times



The screenshot shows the DataWarrior application window titled "Random_Molecules_1k.dv". The menu bar includes File, Edit, Data, Chemistry, Database, List, Macro, and Help. Below the menu is a table with columns for Structure, dwinChI, dwinChI-Key, and Smiles. The table contains four rows of chemical structures. A context menu is open over the first row, listing options such as "Copy Structure As", "Copy Selection With Header", "Copy Selection Without Header", "Paste Structure From", "Paste Into Table", "Edit Cell", "Sort Table Rows By", "New Structure Filter from", "Explore conformers of 'Structure'", "Search Structure in Google Scholar", "Search Structure in Google Patents", and "Suggest Synthesis Route". The "Suggest Synthesis Route" option is highlighted, and a tooltip next to it says "of Structure using Spaya.ai".

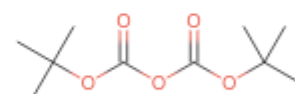
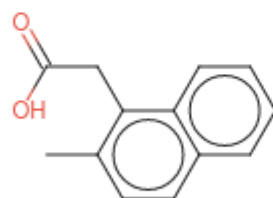
2) [suggestion_spaya.png](#), downloaded 863 times

76%

COc1cccc(O)c1C(=O)C(C)c1c(C(N)O)c(O) Advanced



220 routes found Filter



Score : 0.4 Steps : 12