Subject: Re: retrosyntheis tools
Posted by nbehrnd on Thu, 23 Sep 2021 19:10:19 GMT
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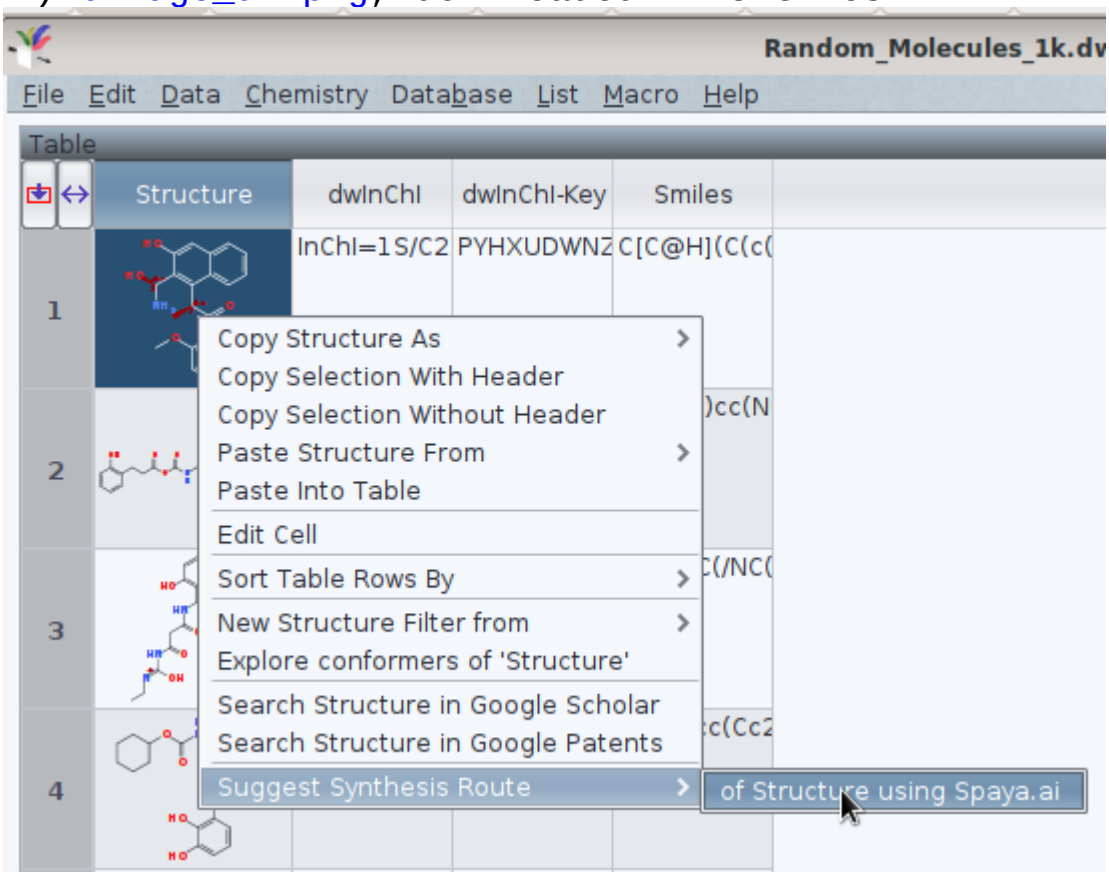
If your organization supports an account on spaya.ai, then a right-click on the structure of interest offers access to suggestions. You have 30 days to venture out and get familiar enough with this service to come to a decision to purchase their service, or not.

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 1175 times

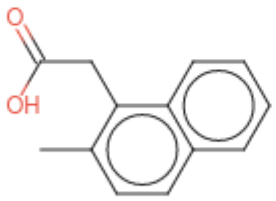


2) suggestion_spaya.png, downloaded 1169 times

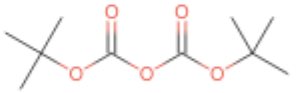
https://spaya.ai/app/retro/COc1cccc(O)c1C(%3DO)C(C)c1c(C(N)O)c(O)cc2ccccc12 ••• Search

76% COc1cccc(O)c1C(=O)C(C)c1c(C(N)O)c(O) Advanced

220 routes found Filter







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