Subject: retrosyntheis tools
Posted by scottwabc01 on Wed, 22 Sep 2021 09:48:48 GMT
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hi all,
Please any one can point me to retrosynyesis tools we can use from data warrior?
your help is much appreciated

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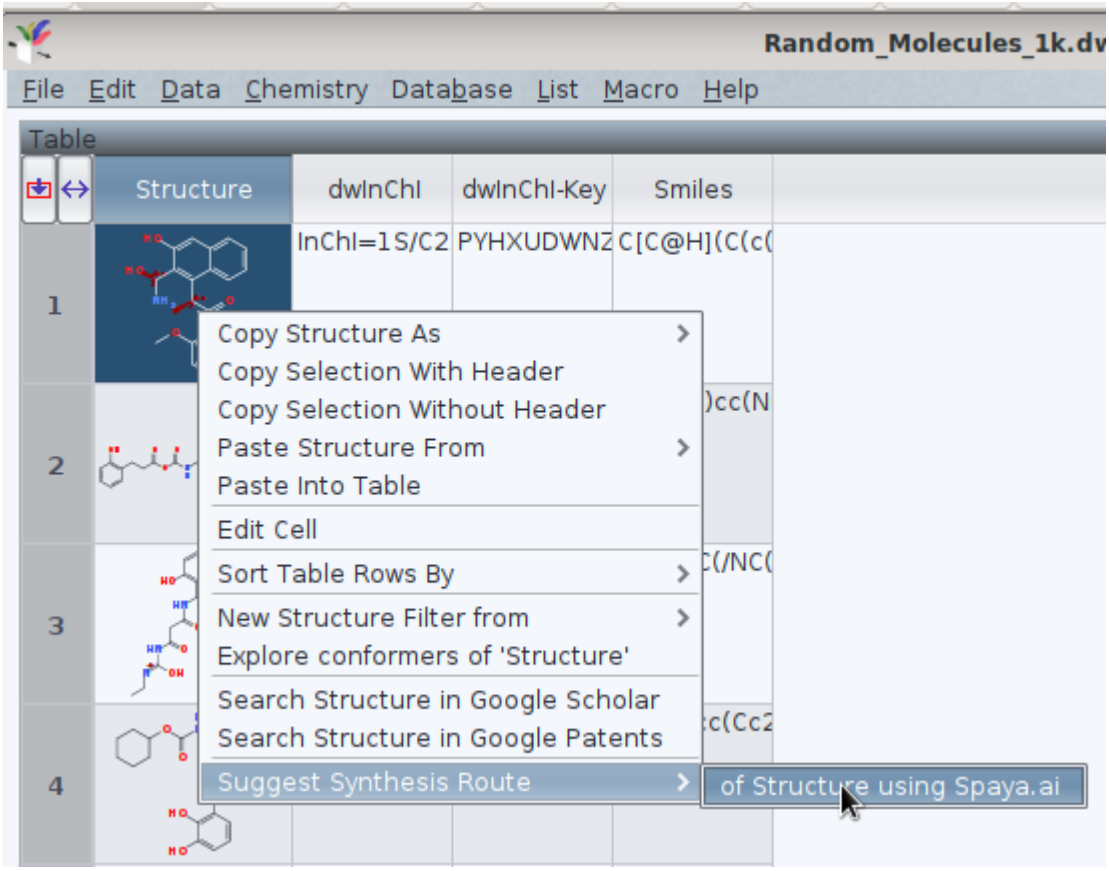
If your organization supports an account on spaya.ai, then a right-click on the structure of interest offers access to suggestions. You have 30 days to venture out and get familiar enough with this service to come to a decision to purchase their service, or not.

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.

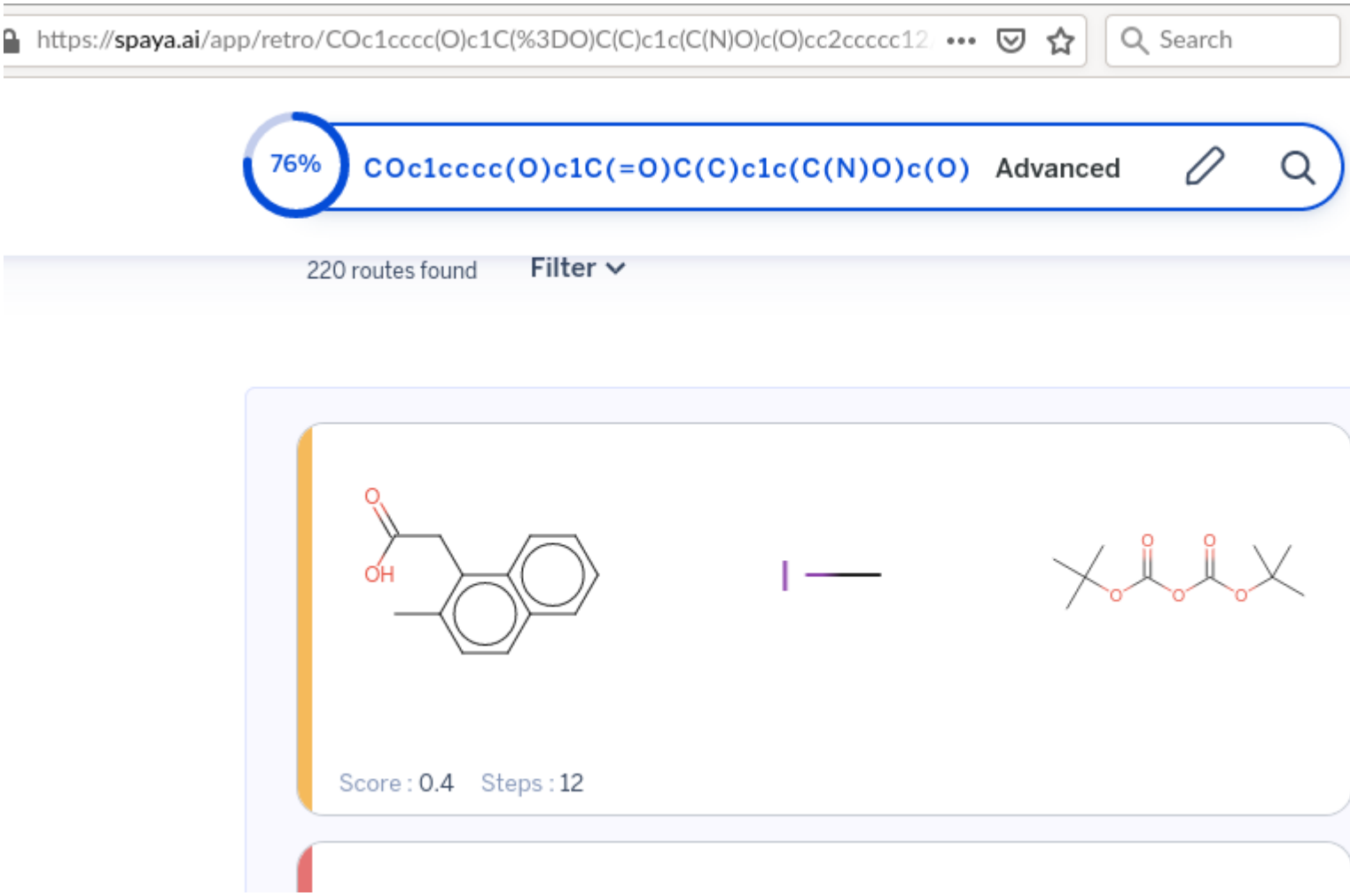
[1a] Genheden, S., Thakkar, A., Chadimová, V. et al. AiZynthFinder: a fast, robust and flexible open-source software for retrosynthetic planning. J Cheminform 12, 70 (2020) (https://doi.org/10.1186/s13321-020-00472-1)
[1b] Retrosynthetic accessibility score (RAscore) – rapid machine learned synthesizability 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 1177 times



2) suggestion_spaya.png, downloaded 1171 times



Subject: Re: retrosyntheis tools
Posted by scottwabc01 on Fri, 24 Sep 2021 14:15:56 GMT
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Thank you, very helpful

Subject: Re: retrosyntheis tools
Posted by Paul Smith on Fri, 24 Sep 2021 14:44:05 GMT
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To add on what has been said on Spaya retrosynthesis tool, they organize some webinars that can be very useful to attend: there is one on September 28th. Video recordings are also available on Youtube.

In a nutshell, I can recommend Spaya which is a reliable, easy to use, and comprehensive tool and where you can select building blocks providers of interest for a given compound price.

Subject: Re: retrosyntheis tools
Posted by scottwabc01 on Fri, 24 Sep 2021 16:02:30 GMT
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Thank you for the heads up, I will try yo register to their webinar on 28th.

Subject: Re: retrosyntheis tools
Posted by scottwabc01 on Wed, 26 Jan 2022 10:57:45 GMT
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Hi All,
Any one can point me to relevant retrosyntheis articles?
Thanks in advance

Subject: Re: retrosyntheis tools
Posted by Drobert on Wed, 26 Jan 2022 11:03:35 GMT
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Hi,
here is the link to the latest ChemRxiv about Spaya.
I have found it very interesting to be honest.
Have a good reading!

Subject: Re: retrosyntheis tools
Posted by nbehrnd on Thu, 27 Jan 2022 06:54:38 GMT
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Your question does not clarify if your interest is about the classical rules, or about contemporary implementation of retrosynthethic algorithms into computer programs. For the former (humanoid recognition of pattern, disconnection into known precursors) E. J. Corey was one prominent author who formalized the approaches.[1, 2] But there are plenty publications about the later as well[3,4,5] and a listing here is opinionated and incomplete. You may use the references below to expand the bibliographic search further.

Norwid

[1] Corey, Nobel lecture in Angewandte 1991, 30, 455-465;
https://doi.org/10.1002/anie.199104553.
[2] E. J. Corey, X-M. Cheng (1995). The Logic of Chemical Synthesis. New York: Wiley. ISBN 978-0-471-11594-6.

Angewandte 2016, 55, 5904-5937; https://doi.org/10.1002/anie.201506101
[4] Badowski, T. et al. Synergy Between Expert and Machine-Learning Approaches Allows for Improved Retrosynthetic Planning. Angewandte 2019, 55, 725-730;

https://doi.org/10.1002/anie.201912083
[5] Thakkar, A. et al. Retrosynthetic accessibility score (RAscore) – rapid machine learned synthesizability classification from AI driven retrosynthetic planning. Chem. Sci. 2021, 12, 3339-3349; https://doi.org/10.1039/D0SC05401A.

Subject: Re: retrosyntheis tools
Posted by Drobert on Mon, 31 Jan 2022 16:19:46 GMT
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To add to this topic, I have recently read the ChemRxiv paper on Spaya:
Integrating Synthetic Accessibility with AI-based Generative Drug Design - https://chemrxiv.org/engage/chemrxiv/article-details/61c19ee 67f367e034f5adb11

In a general way, I have found Spaya software very fast, robust and informative for my research. You can also access a free trial version of it by registering on their website - https://spaya.ai/.

Subject: Re: retrosyntheis tools
Posted by scottwabc01 on Tue, 01 Feb 2022 15:15:08 GMT
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Drobrt,
Thank you, will read the article and get back.
Sound very intersting
Scott

Subject: Re: retrosyntheis tools
Posted by scottwabc01 on Tue, 01 Feb 2022 15:33:23 GMT
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Thank you Norwid, very helpful

Subject: Re: retrosyntheis tools
Posted by scottwabc01 on Wed, 23 Feb 2022 10:48:24 GMT
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Hi, I recently tried chiral pool functionality in Spaya. It seems like a good function. Any one else has tried it?

Subject: Re: retrosyntheis tools
Posted by Drobert on Wed, 23 Feb 2022 10:50:27 GMT
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Hi Scott, I have tried it and it definitely works well.

Subject: Re: retrosyntheis tools
Posted by scottwabc01 on Wed, 23 Feb 2022 10:51:32 GMT
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Good to hear your thoughts Drobert

Subject: Re: retrosyntheis tools
Posted by scottwabc01 on Wed, 23 Mar 2022 10:39:22 GMT
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Hi All,
I wonder if there are any up coming training/webinar sessions for retrosyntheis.

Subject: Re: retrosyntheis tools
Posted by Drobert on Wed, 23 Mar 2022 11:13:28 GMT
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Hi,

There are these upcoming webinars that you might be interested in attending:

Spaya: AI-driven accurate synthetic accessibility - from ‘precise analysis to massive scoring’ on March 29th, 2022 at 10am CEST and 5pm CEST.

Registration link for 10am CEST session:
https://us06web.zoom.us/webinar/register/9716470199061/WN_OP 3Ax_6zQ-GDddfeQfgxxA

Registration link for 5pm CEST session:
https://us06web.zoom.us/webinar/register/1516470198529/WN_ao isMzAzR5OnOjVSmXnsIA

Best,
Robert

Subject: Re: retrosyntheis tools
Posted by scottwabc01 on Wed, 23 Mar 2022 11:49:20 GMT

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Hi All,
I wonder if there are any up coming training/webinar sessions for retrosyntheis.

Subject: Re: retrosyntheis tools
Posted by scottwabc01 on Wed, 23 Mar 2022 11:50:20 GMT
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Thank you Robert

Subject: Re: retrosyntheis tools
Posted by nbehrnd on Thu, 24 Mar 2022 07:57:08 GMT
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For the interested reading this thread a bit later, by today, a brief (i.e., non-exhaustive) search on youtube yields three webinars potentially relevant to and about Spaya in particular. In chronological order of the recording:

+ AI for Retrosynthesis Spaya webinar; by June 10th, 2020 [1]
+ Retrosynthesis in the AI era: opportunities and pitfalls; by September 23, 2020 [2]
+ AI Enhanced Retrosynthesis webinar: Spaya for Chemists; by March 30th, 2021 [3]

Norwid

[1] https://www.youtube.com/watch?v=M7vH9xMdLgw
[2] https://www.youtube.com/watch?v=I2cdBHaWDxE
[3] https://www.youtube.com/watch?v=mPaGnc_kfww