
Subject: retrosynthesis 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 retrosynthesis tools we can use from data warrior?
your help is much appreciated

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>)

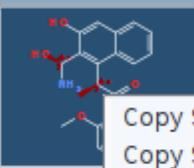
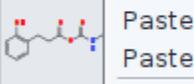
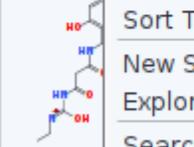
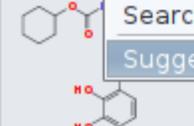
File Attachments

1) [bridge_dw.png](#), downloaded 797 times

Random_Molecules_1k.dv

File Edit Data Chemistry Database List Macro Help

Table

	Structure	dwlInChI	dwlInChI-Key	Smiles
1		InChI=1S/C2	PYHXUDWNZ	C[C@H](C(c
2	)cc(N
3				C(/NC(
4				cc(Cc2

Context menu for row 1:

- 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
- Suggest Synthesis Route > of Structure using Spaya.ai

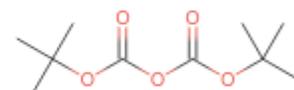
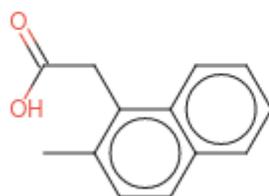
2) [suggestion_spaya.png](#), downloaded 802 times

76%

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



220 routes found Filter



Score : 0.4 Steps : 12

Subject: Re: retrosynthesis tools

Posted by [scottwabc01](#) on Fri, 24 Sep 2021 14:15:56 GMT

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Thank you, very helpful

Subject: Re: retrosynthesis 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: retrosynthesis 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: retrosynthesis 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 retrosynthesis articles?
Thanks in advance

Subject: Re: retrosynthesis 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: retrosynthesis 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 retrosynthetic 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: retrosynthesis 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/61c19ee67f367e034f5adb11>

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: retrosynthesis 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 interesting
Scott

Subject: Re: retrosynthesis tools

Posted by [scottwabc01](#) on Tue, 01 Feb 2022 15:33:23 GMT

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Thank you Norwid, very helpful

Subject: Re: retrosynthesis 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: retrosynthesis 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: retrosynthesis 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: retrosynthesis 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 retrosynthesis.

Subject: Re: retrosynthesis 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_OP3Ax_6zQ-GDddfeQfgxxA

Registration link for 5pm CEST session:

https://us06web.zoom.us/webinar/register/1516470198529/WN_aoisMzAzR5OnOjVSmXnslA

Best,
Robert

Subject: Re: retrosynthesis 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 retrosynthesis.

Subject: Re: retrosynthesis tools

Posted by [scottwabc01](#) on Wed, 23 Mar 2022 11:50:20 GMT

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Thank you Robert

Subject: Re: retrosynthesis 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=l2cdBHaWDxE>

[3] https://www.youtube.com/watch?v=mPaGnc_kfww
