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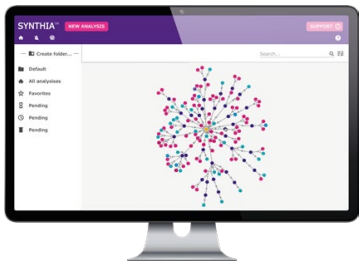
RetroSynthetIQ

SYNTHIA™
Retrosynthesis Software

Newsletter



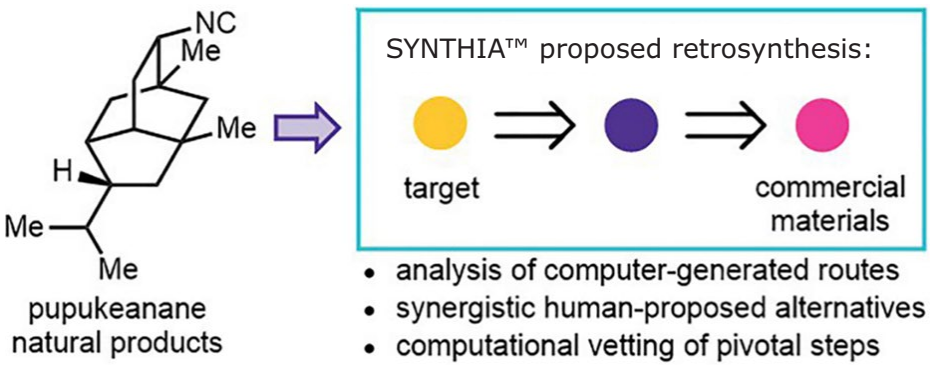
Welcome to **RetroSynthetIQ,** our inaugural Quarterly Newsletter! Below you will find valuable information that includes Cheminformatics research as well as tips & tricks to get the most out of your SYNTHIA™ subscription. We hope that you will find this Newsletter engaging and useful to enhance your workflow & productivity.

Feel free to schedule a meeting with the SYNTHIA™ team for further information.

The Distillate

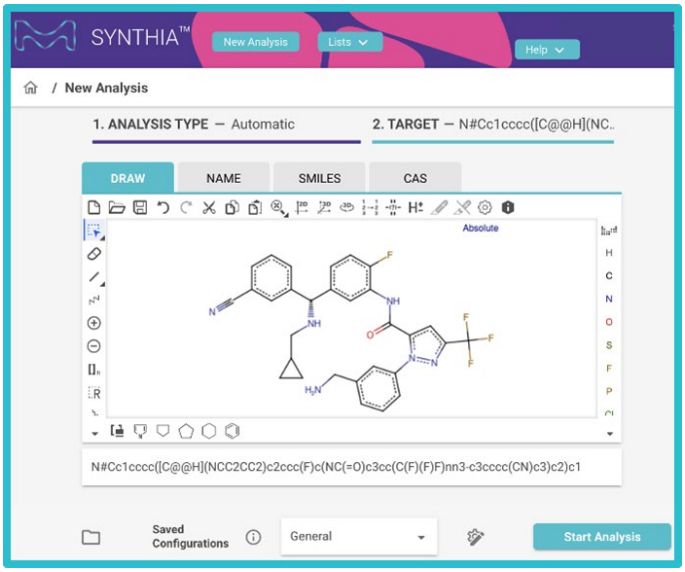
Computer-Aided Synthesis Planning (CASP) is gaining popularity and being used in labs around the world to help speed & enhance route selection and drive innovation in compound design. This month's featured publication was recently published in the journal Tetrahedron and focuses on strategies and tactics used towards the synthesis of pupukeanane natural products. Research groups at UC Berkely and the University of Notre Dame used Synthia™ Retrosynthesis Software to develop novel routes to several pupukeanane natural products.

Read it here



Molecule of the Month

Synthia™ Retrosynthesis Software is a decision support platform that helps synthetic chemists and process chemists alike tackle structurally diverse chemical targets, both previously reported in the literature or completely unknown (like e.g., novel drug candidates or recently isolated natural products).



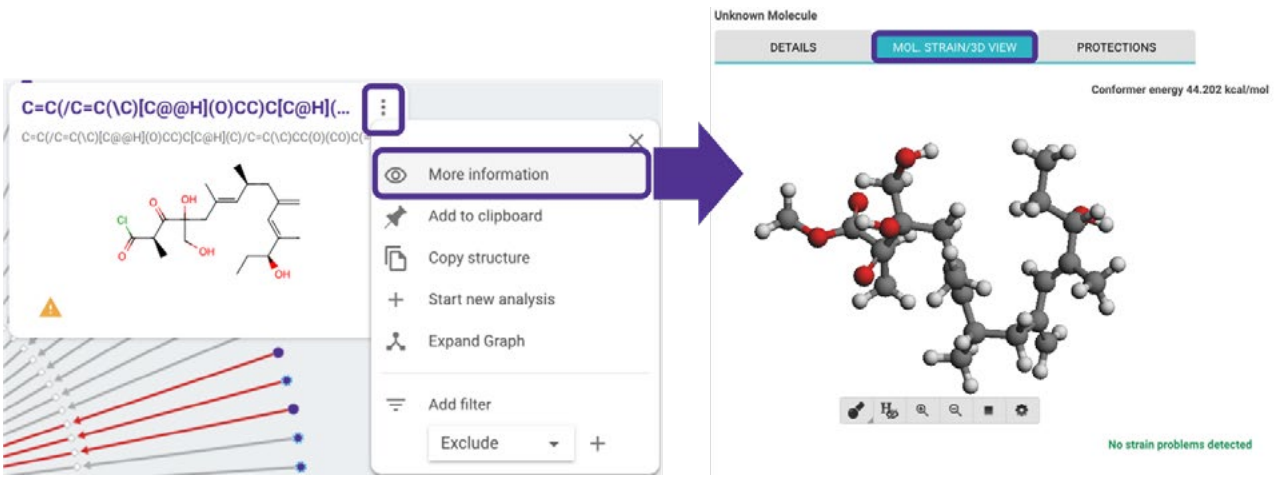
In one of the recent editions of “Small Molecules of the Month” Drughunter presented an oral plasma kallikrein inhibitor, berotralstat, which was recently approved as the first non-steroidal treatment of hereditary angioedema (HAE).

In a recent post on Linkedin, Dr. Ewa Gajewska presented a pathway that was planned by Synthia™ Retrosynthesis Software. Using one of our default search configurations, SYNTHIA™ designed an efficient, convergent, chiral synthesis starting with moderately priced commercial compounds.

Synthia™ Retrosynthesis Software can spark creativity in your synthetic planning by quickly designing routes for target molecules based on your requirements. Follow our Linkedin series to see how SYNTHIA™ lets you go from imagining what’s possible to testing what’s probable.

DID YOU KNOW?...

You can use SYNTHIA™ 3D View to see the molecular conformation of any structure. Open the MOL STRAIN/3D VIEW tab under the molecule details to see the calculated lowest energy and a 3D structural representation. You can switch between ball and stick, line, or space-filling representations and turn the structure in the viewer to see the bonds of interest. This is especially useful for evaluating ring-closing or other intra-molecular reactions for likelihood of success. To find this view, click on any molecule node and open the 3-dot menu--> More Information--> MOL STRAIN/3D VIEW tab.

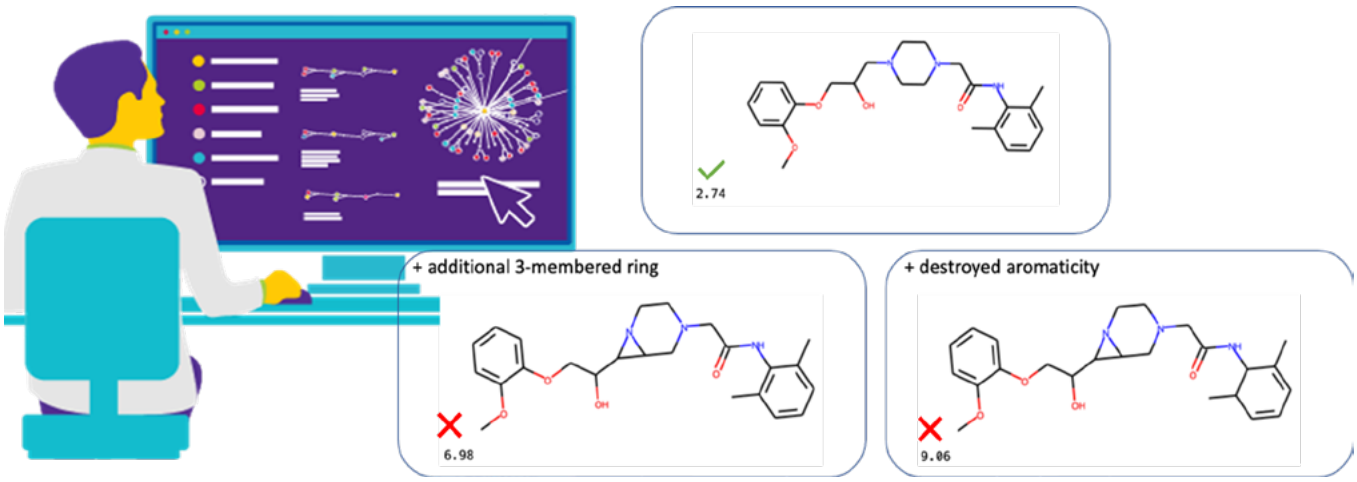


Developer Updates: Synthetic Accessibility Score (SAS)

Synthia™ Retrosynthesis Software is constantly being improved according to your specifications and needs. Our software updates provide new features that align with your workflows and applications.

The SYNTHIA™ Synthetic Accessibility Score (SAS) API is a brand new addition from our development team.

SYNTHIA™ SAS predictions are extremely useful in the drug design process (e.g., high-throughput virtual screening) to quickly limit large sets of drug candidate molecules to the ones that could be obtained in the shortest time. Hundreds of thousands of molecules can be synthesized per hour by utilizing the database of more than 100k expert coded rules.



Connect With Us!

Come Visit us at MilliporeSigma's SYNTHIA™ Booth.

We hope to see you in October at the 18th DDIP in Boston, MA.

Learn More

Book a time slot for a 30-minute live demo session on 'SYNTHIA™ advanced techniques' using the link below.

Schedule A Demo

SYNTHIA™ .EDU

Our team is here for you! We have helped dozens of researchers demonstrate greater value to their organization with direct support. From Monthly Trainings to Webinars and even one-on-one “office hours,” we have an experienced and highly technical team ready to support your biggest challenges. Click to register for one of our support offerings.

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SYNTHIA™ Training 2

SYNTHIA™ Office Hour

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