Reaxys®

Release notes for September 2021

Retrosynthesis release notes

Improved Synthesis Planning in Reaxys

Feedback from Reaxys users and the broader research community is important to our development plans. Synthesis planning is a major area of interest to our users, especially those interested in synthetic organic chemistry.

Therefore, throughout 2021, we are exponentially improving the synthesis planning capability in Reaxys. Earlier in the year we announced the release our Predictive Retrosynthesis module and now we are happy to announce that we have made significant steps forward in better supporting retrosynthesis from published literature for all our customers.

This release includes a complete redesign of our synthesis planning environment. The new Retrosynthesis feature allows chemists to start their retrosynthesis projects by drawing the desired compound, provides in one view all the information needed to decide which route to take to the lab and enables project management and options for easier collaboration.

Users can now:

- Easily search for relevant synthesis route for a known substance (published retrosynthesis)
- Users can organize their retrosynthesis projects in the central projects space and easily access:
    - Literature references for each reaction step
    - Reaction condition and experimental procedure
    - Commercial availability of starting materials
    - Export retrosynthesis route data in multiple formats

What is included in the current release:

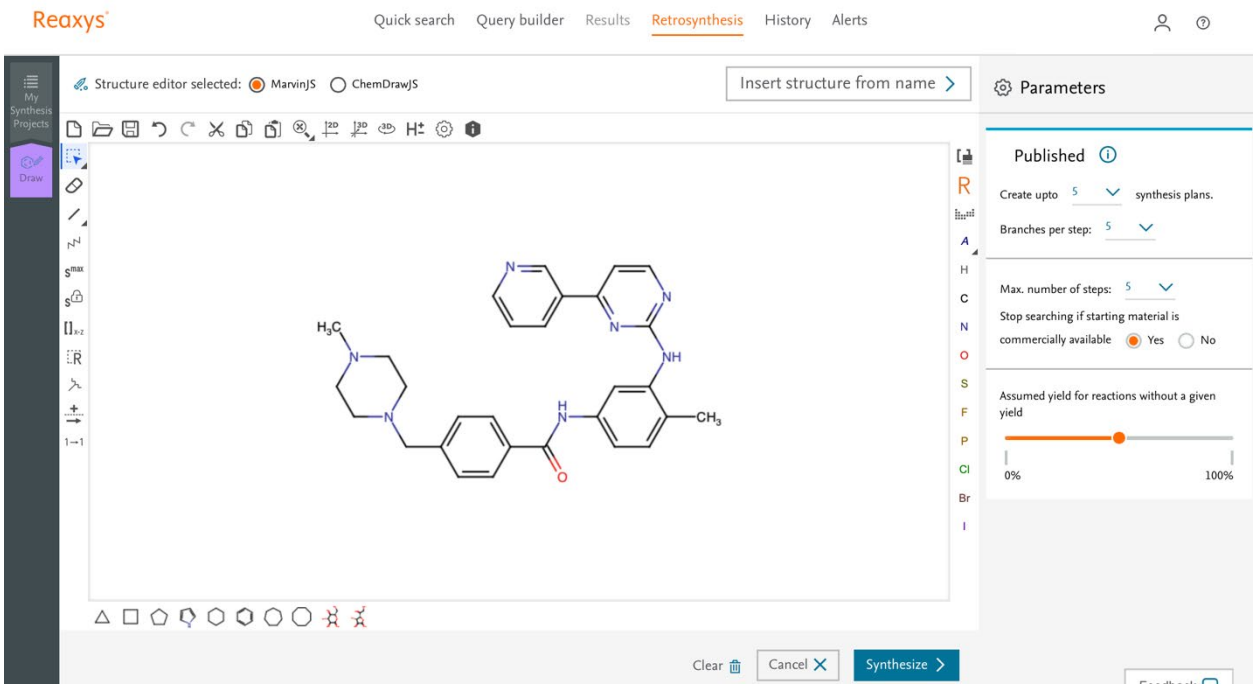
- Redesign of Synthesis Planner to Retrosynthesis enabling users to launch a retrosynthesis search from ChemDraw JS or Marvin JS drawing tool
- Intuitive visualisation options with relevant literature references easily accessible to enable informed decision making
- Option to seamlessly integrate Reaxys predictive retrosynthesis module (additional subscription required).

What's next

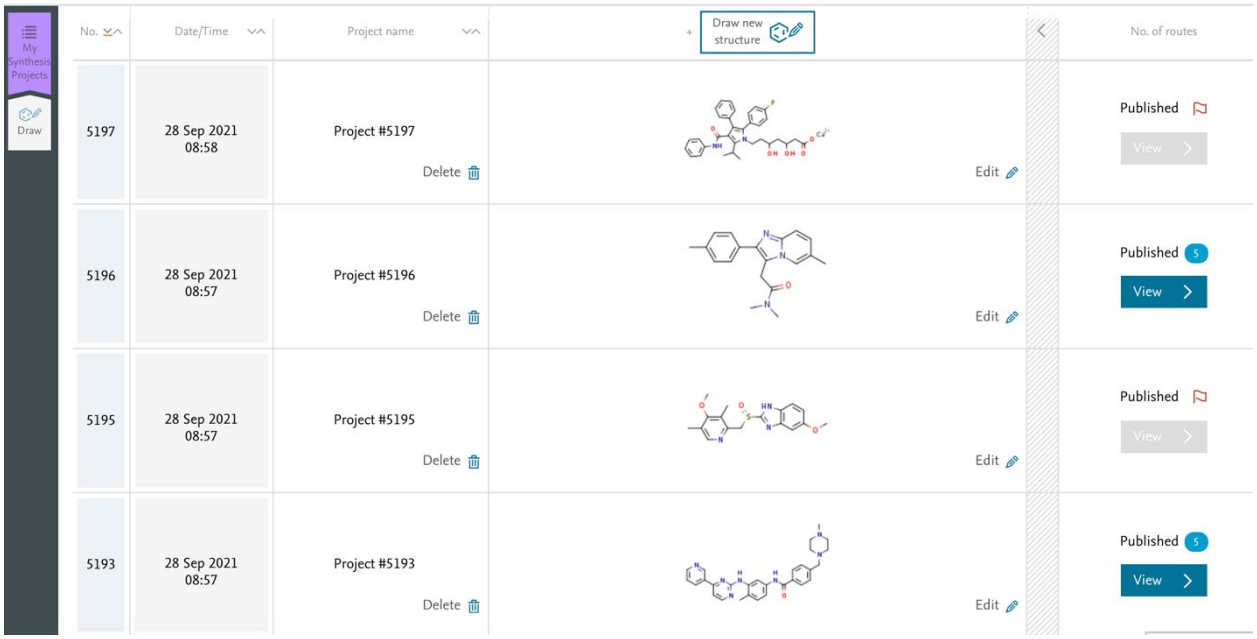
- Further development to enable users to extend / edit the synthesis route giving them the ability to add new steps at any stage of the synthesis tree and to also remove single steps or complete branches

- Further development to enable users to define ‘bonds to be broken’ and ‘bonds to be protected’ in the target molecule when starting the retrosynthesis search
- Predictive retrosynthesis model update with the latest Reaxys reactions dataset

Users can now draw the desired compound by selecting the Retrosynthesis feature on the top bar and define the parameters for the project from the options on the left side menu:



Review, edit or delete Retrosynthesis projects:



Analyse results by reviewing experimental conditions, procedures, and literature reference for each reaction step: