

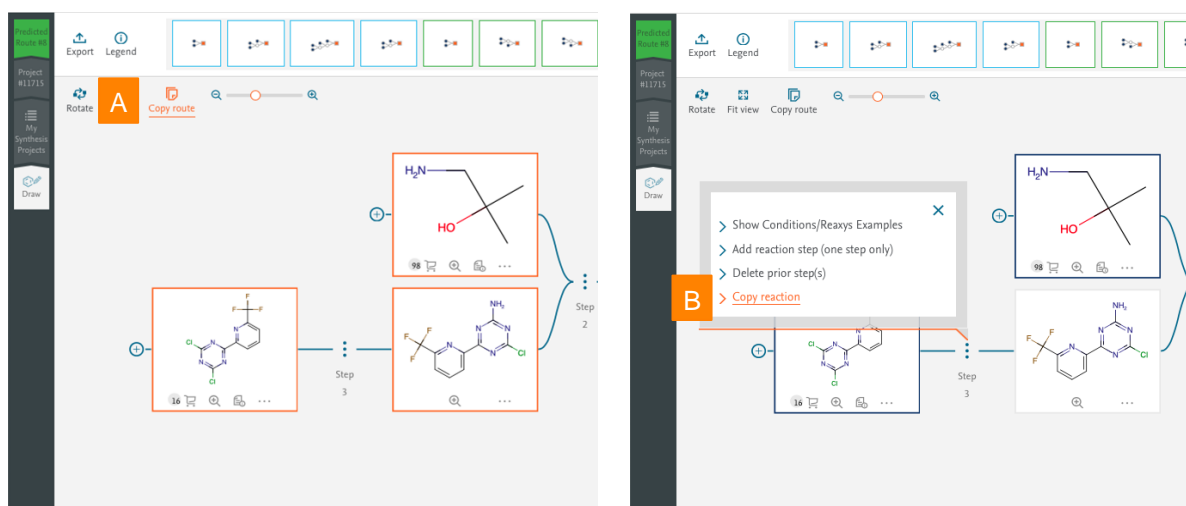
## Release notes for March 2022

Guided by customer feedback, Reaxys is continuously improving the Predictive Retrosynthesis module and our Retrosynthesis feature, so users can have better options for project management and collaboration.

What is included as part of this release?

### I. Improvements to export and collaboration options

- i. **Copy synthesis tree to preferred drawing tool:** Users can now copy the entire synthesis tree to the clipboard (A) and paste it into other external tools, like Marvin or ChemDraw, to more easily publish or share with colleagues.
- ii. **Copy reaction step:** Users can now copy an individual reaction step from the synthesis tree to the clipboard (B), so that they can paste it into MarvinJS or ChemDrawJS for querying in Reaxys, or into other external tools for publishing or sharing with colleagues.
- iii. **Export retrosynthesis plans as RD file:** In addition to exporting synthesis plans, users can now export synthesis trees in Reaction Data File format (.rdf), so that they can reimport them into many chemoinformatic tools for analysis and modelling (e.g. using RDKit, CDKit, etc.).



## II. More options to start and set up your retrosynthesis search

- Transfer from Reaxys reactions results page to retrosynthesis:** Users can better control the start point of a retrosynthesis search (C).
- “Last step only” option for published retrosynthesis:** Users can now run “last step only” search for published retrosynthesis (D). This option was previously only available for predicted retrosynthesis.

The screenshot shows the Reaxys interface. On the left is a 'Filters' sidebar with various search criteria like 'By Structure', 'Yield', 'Reagent/Catalyst', etc. The main area displays a reaction (Reaction ID: 29206092) with a 'Transfer to retrosynthesis' button. Below the reaction, a table lists conditions and references.

Conditions	Yield	Reference
With copper(I) iodide; potassium carbonate; N,N-dimethylethylenediamine in 1,4-dioxane at 85°C; for 18h; Reflux; Inert atmosphere; Experimental Procedure	85.4%	Current Patent Assignee: TEMAPHARM SP. Z O.O. - WO2010/14022, 2010, A1 Location in patent: Page/Page column 6-7 <a href="#">Full Text</a> <a href="#">Details</a> <a href="#">Abstract</a>
With copper(I) iodide; potassium carbonate; N,N'-dimethylethylenediamine in water; toluene for 24h; Solvent; Reflux; Green chemistry;	84.1%	Wang, Culling; Bai, Xiao; Wang, Rui; Zheng, Xudong; Ma, Xiumei; Chen, Huan; Ai, Yun; Bai, Yajun; Liu, Yifeng [Organic Process Research and Development, 2019, vol. 23, # 9, p. 1918 - 1925] <a href="#">Full Text</a> <a href="#">Details</a> <a href="#">Abstract</a>

2 out of 2

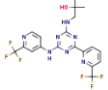

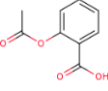

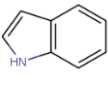

The screenshot shows the Reaxys interface with the 'Structure editor selected' set to 'MarvinJS'. The main area displays a chemical structure. On the right, the 'Parameters' panel is visible, showing options for 'Published' and 'Length & depth of synthesis plans'. The 'D' (Last step only) option is selected.

Parameters

- 10 min processing time
- STD SIAL LN EM U2 U5 T1 building blocks
- [Edit](#)
- ☒ Published
- Length & depth of synthesis plans
- Full routes: 5
- ☒ Last step only
- Branches per step: 5
- Max. number of steps: 5
- Stop searching if building block is commercially available: ☒ Yes ☐ No
- Assumed yield for reactions without a given yield: 0% to 100%

### III. Better visibility of commercial substances' availability

- i. **Projects page:** The shopping cart for commercially available substances and the View Details icon will be shown on the projects page (E).
- ii. **Edit synthesis plan pop-up:** Users can make a more informed choice when selecting which published and/or predicted reaction step to add to the synthesis plan by having the shopping cart and View Details icon displayed.

0 selected Delete					Draw new structure		No. of routes	
No.	Date/Time	Project name						
<input type="checkbox"/>	11715	27 Feb 2022 06:47	Project #11715 Delete		 42	Edit	Predicted 3 Published 4 View	
<input type="checkbox"/>	11698	27 Feb 2022 02:10	Project #11698 Delete		 95	Edit	Predicted 0 View	
<input type="checkbox"/>	11688	28 Feb 2022 09:53	Project #11688 Delete		 83	Edit	Customized 5 Published 5 View Feedback	

#### What's next:

- Break and Protect Bonds: New Retrosynthesis features will give chemists more ability to obtain relevant results by defining which bonds to break or protect.
- An updated Predictive Retrosynthesis model with the latest reaction data, increasing the coverage of reactions and providing better predictions.