

Release notes for August 2022

The Reaxys Team continue to strive to make improvements to your experience within the product. This release focuses on improving some Retrosynthesis functionalities:

Enriched information about commercially available substances

- (1) **New Icon:** A new rapid delivery shopping cart icon (A) will be displayed for substances which can be shipped in up to 5 days



- (2) **More Information:** Upon hovering over the shopping cart icon, the tooltip will provide users with information about Shipping Time, Best Price (USD/g) and Largest Available Package Size. Information will be displayed as per below category

Shipping time	<ul style="list-style-type: none"> • Up to 5 days • Up to 10 days • Up to 4 weeks • Up to 12 weeks – custom synthesis
Largest available package size	<ul style="list-style-type: none"> • Up to 1 mg • Up to 1 g • Up to 1 kg • Up to 10 kg • Greater than 10 kg • Greater than 1 tonne

In cases where this information is not provided by the supplier, users will see “Please contact supplier”

This information will further help researchers in making make or buy decision for substances and selecting synthesis route(s) for a given molecule.

Enhancement to edit synthesis plans pop-up, for customization of published and/or predicted retrosynthesis

- (1) **Increased number of published and predicted reaction step options:** When editing synthesis routes, users will be able to review all the single step published and/or predicted reactions (B), to find the best suited step to add to their route.
- (2) **Yield based sorting of published reaction step:** To review example reactions effectively, published reaction step(s) will be sorted by decreasing yields (C), so users will be able to select reaction step(s) with highest yield first.

1 selected Add >

Published (27)

Predicted (65)

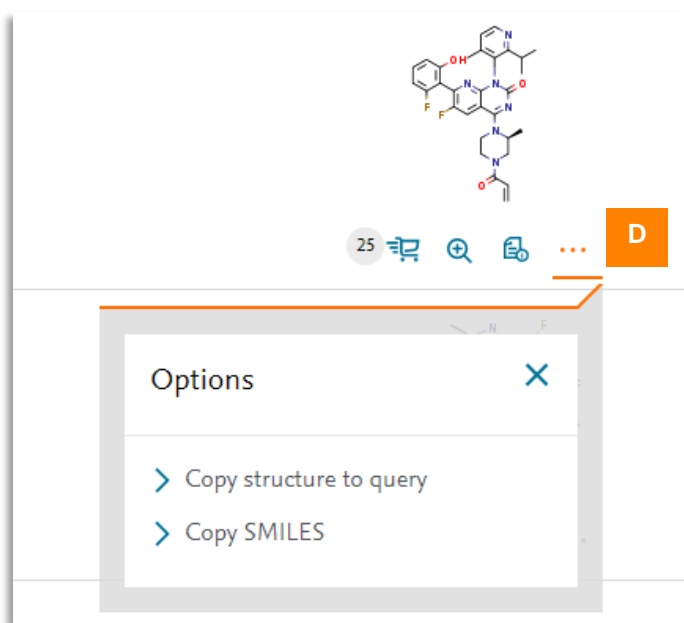
Optional single step to be added	Conditions	Yield	Reference
<div><div><div><div><div><div></div></div></div><div><div><div></div></div></div></div><div><div><div></div></div></div></div></div>	<div>With lithium aluminium tetrahydride In tetrahydrofuran at -10 - 20°C; for 2 h</div> <div>Experimental Procedure ✓</div>	91% C	<div>Current Patent Assignee: HANGZHOU BIO SINCERITY PHARMA TECH COP - CN110156754, 2019, A</div> <div>Location in patent: Paragraph 0020-0021;</div> <div>Full Text Details Abstract</div>
<div><div><div><div><div><div></div></div></div><div><div><div></div></div></div></div><div><div><div></div></div></div></div></div>	<div>With lithium aluminium tetrahydride In tetrahydrofuran at 0°C; for 3h; Inert atmosphere;</div> <div>Experimental Procedure ✓</div>	87.2%	<div>Current Patent Assignee: SINO BIOPHARMACEUTICAL LIMITED - CN106316935, 2017, A</div> <div>Location in patent: Paragraph 0085; 0086; 0087; 0088; 0089</div> <div>Full Text Details Abstract</div>
<div><div><div><div><div><div></div></div></div><div><div><div></div></div></div></div><div><div><div></div></div></div></div></div>	<div>With sodium tris(acetoxy)borohydride In 1,2-dichloro-ethane at 20°C; for 10h;</div> <div>Experimental Procedure ✓</div>	91%	<div>Current Patent Assignee: TIANJIN TASLY GROUP COMPANY., LTD.; CHINA PHARMACEUTICAL UNIVERSITY - CN112390793, 2021, A</div> <div>Location in patent: Paragraph 0052</div> <div>Full Text Details Abstract</div>
<div><div><div><div><div><div></div></div></div><div><div><div></div></div></div></div><div><div><div></div></div></div></div></div>	<div>Stage #1: 4-ethylpiperazine; 6-amino-3-pyridinecarbaldehyde In 1,2-dichloro-ethane at 20°C; for 2h;</div> <div>Stage #2: With sodium tris(acetoxy)borohydride In 1,2-dichloro-ethane at 20°C; for 8h;</div> <div>Experimental Procedure ✓</div>	91%	<div>Current Patent Assignee: CHINA PHARMACEUTICAL UNIVERSITY - CN113105434, 2021, A</div> <div>Location in patent: Paragraph 0054-0057</div> <div>Full Text Details Abstract</div>
<div><div><div><div><div><div></div></div></div><div><div><div></div></div></div></div><div><div><div></div></div></div></div></div>	<div>Stage #1: 4-ethylpiperazine; 6-amino-3-pyridinecarbaldehyde In 1,2-dichloro-ethane at 20°C; for 2h;</div> <div>Stage #2: With sodium tris(acetoxy)borohydride In 1,2-dichloro-ethane at 20°C; for 8h;</div> <div>Experimental Procedure ✓</div>	91%	<div>Current Patent Assignee: CHINA PHARMACEUTICAL UNIVERSITY - CN113149978, 2021, A</div> <div>Location in patent: Paragraph 0062-0065</div> <div>Full Text Details Abstract</div>

B

1 2 3 >

Easier transfer and copy of structure from retrosynthesis page

Upon clicking the '3 dots' icon next to the structure (D) users will see options to copy the structure for quick search in Reaxys or copy the structure as SMILES



Improved accessibility of retrosynthesis pages

Retrosynthesis pages on Reaxys have been enhanced to conform with Web Content Accessibility Guidelines and can now be accessed via tabbing