

Optimize synthesis planning

Reaxys Predictive Retrosynthesis, *powered by Pending.AI*, combines AI with high-quality reaction data to efficiently deliver innovative synthesis routes.

This synthesis tool combines three neural networks with Monte Carlo tree search to quickly generate robust routes.

Tailor searches to project needs

- Price control on starting materials
- Shipping time filter
- Setting route diversity
- Break or protect bonds



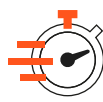
18.3M

chemical reactions



425M

retrosynthetic rules



<10

minutes
to get results



150M

commercially
available materials



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Explore the intuitive interface of Reaxys Predictive Retrosynthesis

The screenshot displays the Reaxys Predictive Retrosynthesis interface. On the left, a retrosynthetic route is shown with three steps. Red circles with numbers 1 through 6 highlight key features: 1. A link to literature (Reaction ID: 4271399), 2. End in purchasable starting materials, 3. Access experimental procedures to execute plans, 4. Published, predicted and custom routes in one view, 5. Tailor results by editing synthesis routes, and 6. Export easily to collaborate on route design. The right panel shows the details for the selected reaction, including the reaction scheme, conditions, and experimental procedure. The experimental procedure describes the synthesis of 4-bromo-5-fluoro-2,3-dimethyl-1H-indole-7-carboxylic acid from 4-bromo-5-fluoro-2-hydrazinylbenzoic acid hydrochloride and 2-butanone.

Scientifically robust predictions

- 1 Link to literature that informed the routes
- 2 End in purchasable starting materials
- 3 Access experimental procedures to execute plans

Intuitive experience

- 4 Published, predicted and custom routes in one view
- 5 Tailor results by editing synthesis routes
- 6 Export easily to collaborate on route design

Customizable

- Integrate reaction data
- Select preferred vendors
- Integrate starting materials

More routes, faster with API

Reaxys Predictive Retrosynthesis offers an API to process more molecules, faster.

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