

Optimize synthesis planning

Reaxys Predictive Retrosynthesis, powered by *Iktos*, combines AI with high-quality reaction data to deliver more efficient synthesis routes quickly.

Monte Carlo tree search and forward synthesis prediction combine to generate diverse and robust retrosynthetic routes, considering chemo-, regio- and stereo-selectivity.

Tailor searches to project needs

- Dynamic price control on starting materials
- Shipping time filter
- Include and/or exclude intermediates
- Break or protect bonds



16.3M

chemical reactions



453K

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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