Reaxys
Predictive Retrosynthesis

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

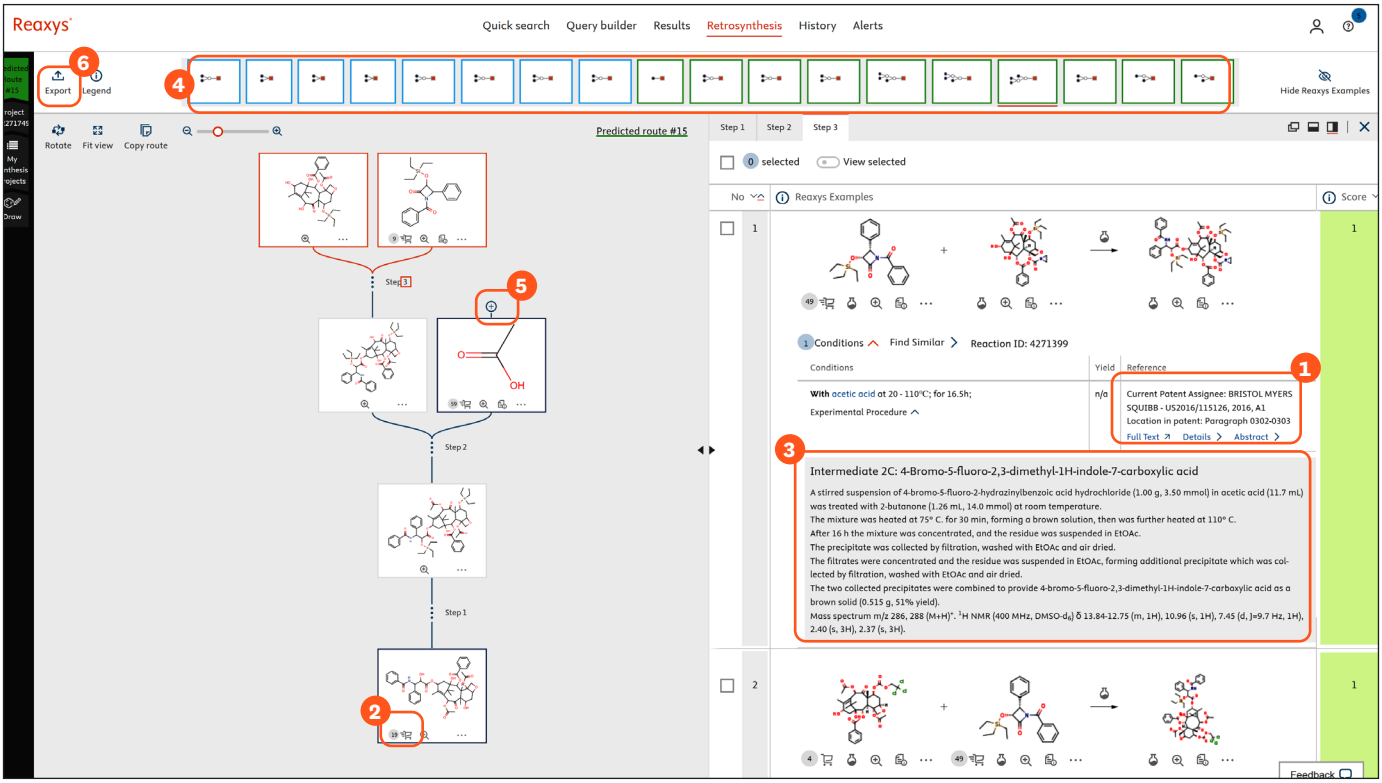
<10
minutes
to get results

150M
commercially
available materials

ELSEVIER

Advancing human progress together

Explore the intuitive interface of Reaxys Predictive Retrosynthesis



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.

Advance your research with Elsevier's Reaxys Predictive Retrosynthesis and a portfolio of solutions for pharmaceutical R&D and chemicals and materials development. Discover, innovate and develop with confidence, supported by trusted quality information, innovative technology and scientific expertise. Let's shape progress together.

Learn more about Reaxys Predictive Retrosynthesis: elsevier.com/products/reaxys/predictive-retrosynthesis