Reaxys®

AI-enhanced predictive retrosynthesis

Fast. Robust. Easy to use.

Superior technology

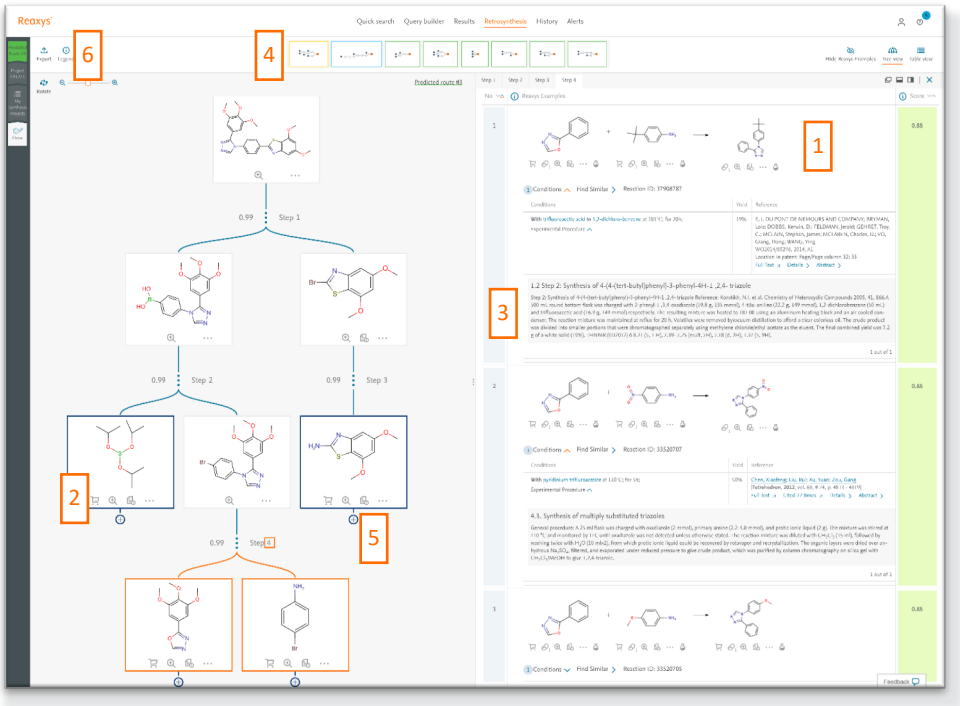
- 3 neural networks
- Monte Carlo tree search
- Results in 10 minutes

Unmatched data set

- >15M single step reactions
- >100M virtual negative reactions
- >400k auto-extracted rules

Customizable

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



Scientifically robust predictions

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

Intuitive experience

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

Reaxys Predictive Retrosynthesis

elsevier.com/solutions/reaxys/predictive-retrosynthesis