AI enhanced retrosynthesis solution for chemists

Reaxys®

Any AI tool can provide suggestions, Reaxys offers solutions

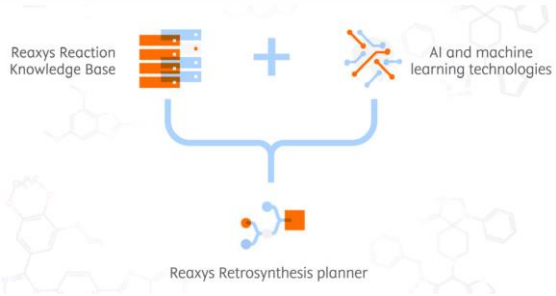
ghp International Life Sciences Awards

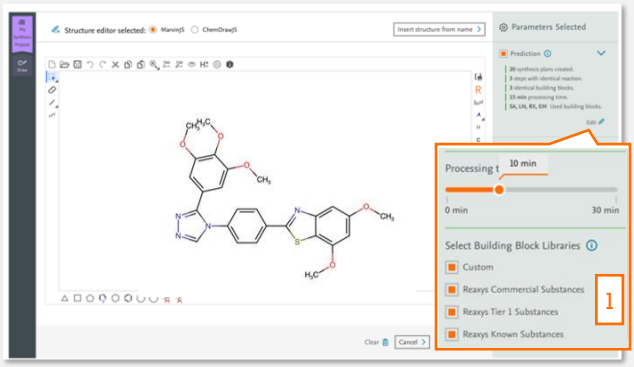
Elsevier Information Systems GmbH

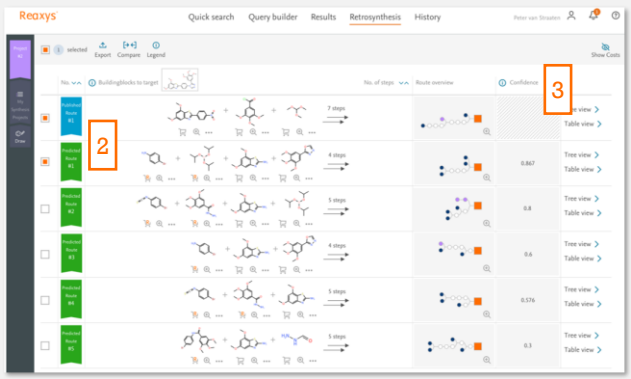
Best Chemistry Predictive Analytics Specialists

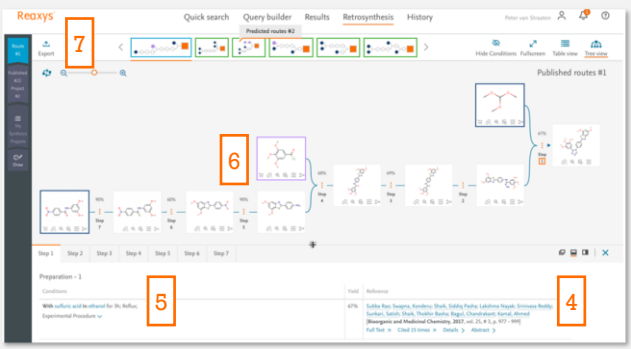
Reaxys Predictive Retrosynthesis, developed in collaboration with Dr. Mark Waller of Pending.AI, leverages cutting-edge deep learning technology and **high-quality reaction data** from the **largest database of chemical reactions to generate scientifically robust predictions.**

- ✓ Neural networks coupled with Monte-Carlo tree search
- ✓ >15m single step chemical reactions with >400,000 auto-extracted rules
- ✓ Customizable to your needs – Integrate reaction data, starting materials or preferred vendors for more relevant results.









1. **Tailored results -** Edit retrosynthesis parameters for diversity, speed and choose libraries of building blocks to meet your needs
2. **User Friendly -**Published and predicted routes for a target molecule in one view.
3. **Build Confidence -** The route confidence scoring system ranks routes.
4. **Literature Precedence -** Link to literature references for published routes, and to the literature that informed predicted routes.
5. **Execute Your Plan** - Easily access experimental procedures for similar reactions that informed the predicted route.
6. **Purchasable Starting Materials** - Unique to Reaxys is that routes always provide purchasable starting materials, or in-house integrated stockroom compounds or proprietary molecules.
7. **Easily Export -**Routes can be exported in multiple formats for sharing and adding to electronic lab notebooks

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Contact us today to discuss how the Reaxys Retrosynthesis engine can support your research and development