

# Syngenta and Elsevier *accelerate* AI-enabled synthesis with route-level planning and machine-ready reaction data





The combination of trusted literature data and proprietary chemistry enables end-to-end synthesis workflows — from planning to execution to learning. Discover how Syngenta and Elsevier worked together for faster, more sustainable small molecule discovery in crop protection.

## Background

AI has transformed many areas of drug and materials discovery. **Synthetic route design and execution**, however, has historically benefited less from digital innovation beyond electronic lab notebooks (ELNs). In Crop Protection R&D, where speed, robustness and sustainability matter, Syngenta set out to change this. (1, 2, 3, 4). The goal was to modernize how chemists plan, run and learn from reactions. Data is structured from the outset around its intended use in predictive models and synthesis planning tools.

To do this, Syngenta's **Computer-Aided Synthesis Team** drives the implementation of a software platform that integrates **computer-aided synthesis planning (CASP)**, predictive reactivity models and structured reaction data capture, supported by systematic access to **Reaxys reaction data**.

*“Integrating Reaxys data into our workflow for systematic access was a breakthrough moment for our strategy.”*

**Marco Stenta**

Computational Chemist, Syngenta

## The challenge: modern models need modern reaction data

Syngenta's R&D teams operate in a **proprietary reactivity space**, where many experiments are not published and where internal know-how is a competitive advantage. As Syngenta began retraining state-of-the-art reactivity models to reflect this, the team encountered a common barrier: **legacy ELN records were optimized for human reading and basic searches, not for machine learning**.

To unlock reliable model training and validation, Syngenta launched a change program to help bench scientists execute reaction protocols with **structured, machine-ready reaction data capture**, including consistent identifiers, controlled vocabularies and ontology-driven classification. Consequently, reaction outcomes can be reused at scale for modeling and decision-making.

1. Lopantsyna, N., et al. (2025). “NOCTIS: open-source toolkit that turns reaction data into actionable graph networks.” *Journal of cheminformatics* 18(1): 6.  
2. Pasquini, M. and M. Stenta (2023). “LinChemin: SynGraph—a data model and a toolkit to analyze and compare synthetic routes.” *Journal of cheminformatics* 15(1): 41.  
3. Pasquini, M. and M. Stenta (2024). “LinChemin: Route Arithmetic Operations on Digital Synthetic Routes.” *Journal of chemical information and modeling*.  
4. Toniato, A., et al. (2023). “Fast Customization of Chemical Language Models to Out-of-Distribution Data Sets.” *Chemistry of Materials*.

## Why Reaxys: expanding beyond proprietary data while preserving differentiation

As reactivity modeling matured, Syngenta's Reaction Data Scientists recognized that internal data alone, however valuable, was not sufficient to fully exploit modern modeling strategies. Access to **Reaxys reactivity data** enabled a two-step approach:

1. **Pre-train "general chemistry" models** on the broad, curated Reaxys corpus to capture widely observed reactivity patterns and reaction precedents.
2. **Fine-tune** those models on Syngenta's proprietary reaction data to tailor predictions to Syngenta's unique chemistry space and experimental practices.

In parallel, Reaxys supports day-to-day scientific work through **integrated search**: chemists can quickly identify reaction precedents, evaluate starting material availability, and drill down into underlying literature context via the Reaxys web interface, directly from Syngenta's internal workflows.

*"High-quality, curated reaction data was our starting point for building reliable synthesis planning models. Think of it as the general discovery chemistry foundation — Reaxys gave us that foundation at scale. We then layered in our proprietary agrochemical knowledge, so the models speak the language of our chemistry, not just chemistry in general."*

**Guillaume Berthon**

Head of Digital Chemical Synthesis Crop Protection Research, Syngenta

## From point solutions to a single synthesis platform

Syngenta initially validated individual capabilities (federated chemical search across internal and external sources, reactivity prediction and structured reaction data capture) before integrating them into a unified platform that provides a **start-to-end experience**:

- **Plan**: compare whole synthetic routes provided by CASP tools and manual entry, using multiple criteria (e.g., precedents, feasibility, starting materials, sustainability considerations).
- **Execute**: run experiments with structured protocols designed to generate machine-ready reaction data.
- **Analyze and learn**: feed harmonized internal and Reaxys-derived insights into models for retrosynthesis, product prediction and condition optimization while keeping expert chemist judgment central to critical steps such as reaction interpretation.

This integration expands the scope of scientific investigation beyond proprietary datasets while preserving Syngenta's ability to differentiate through its internal chemistry and expert-led decision-making.





## Impact

Since implementing this platform, Syngenta has reported **reductions in route design time**, improved operational efficiency through integrated search and stronger confidence in model-supported decisions. Adoption has expanded to the **majority of chemists across Syngenta Crop Protection Research sites**. The platform also supports multi-parameter route assessment, including sustainability-focused criteria such as solvent and waste considerations.

*“Integrating Reaxys data into our workflow for systematic access was a breakthrough moment for our strategy. It allowed us to combine trusted literature precedents with our proprietary chemistry, and to build workflows where data is captured for learning — not just recorded for compliance.”*

**Marco Stenta**  
Computational Chemist, Syngenta

## About Syngenta

Syngenta is a leading science-based agriculture company that helps farmers grow resilient, healthy crops while promoting sustainable farming practices that protect and preserve the planet.

## About Elsevier

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