ACD/LABS [ADVANCED CHEMISTRY DEVELOPMENT, INC.]

Transforming Solvent Selection with AI-Powered Predictions at Covestro

Covestro, a world-leading manufacturer of high-quality polymer materials, faced a familiar challenge in chemical research—choosing the right solvent. Solvent selection is central to reaction success, efficiency, and cost, yet chemists often rely on a narrow set of solvents. Covestro wanted to broaden solvent exploration, reduce trial-and-error, and make predictive insight accessible across research teams.

Challenges in Solvent Selection

Solvent choice can strongly influence experimental outcomes, but limited familiarity and the cost of broad screening often restrict options to, typically, 5–10 common solvents. Routine requests for solubility guidance often fall to property data specialists and computational chemists, creating bottlenecks and diverting their effort from higher-value science.

These challenges are common across research organizations, where teams must balance speed, cost, and scientific rigor. A scalable, accessible method for pre-screening solvents can reduce friction and improve outcomes across multiple projects, setting the stage for a more data-driven approach.

After finding no commercial or open-access tool that addressed these challenges, the team at Covestro developed a deep learning AI-powered solvent selection tool – Solvent Recommender.

AI-Powered Solution: Solvent Recommender

Solvent Recommender is trained on experimental data from diverse small organic molecules across 78 common solvents, and ranks solvents for each new molecule from best to worst based on predicted activity coefficient. Using an ensemble of message-passing neural networks, the model provides fast, practical solvent guidance for chemists.

Rather than predicting absolute solubility, it provides a comparative measure of which solvents are more likely to perform effectively relative to others. This focus on relative performance has proven highly actionable in the research environment, where speed and direction matter most.

The tool was deployed across research teams at Covestro and integrated into existing digital infrastructure, making it easily accessible. Chemists can input a new molecule and receive an ordered list of solvent recommendations within moments, dramatically reducing the time between idea and experiment.

How Scientists at Covestro Use Solvent Recommender

Researchers and engineers across Covestro use the tool in diverse contexts, from synthesis exploration and optimization involving protecting group chemistry, to process research and kilogram-scale synthesis of heterocyclic building blocks. It has also supported solvent selection for specialized NMR experiments on uncommon side components, identification of separation solvents for chemical recycling, and estimation of solvent–antisolvent pairs for complex organic molecules. The model is used daily and independently by R&D staff across the organization.

"Solvent Recommender has seen widespread adoption throughout our chemical development pipeline. It helps our scientist identify the best solvent choices across many types of projects and supports a wide range of synthesis, analytical, and process applications," Jens Langanke, Head of R&D Simulations & Data Science, Covestro.

Benefits of AI-Powered Solvent Recommendation at Covestro

The deployment of Solvent Recommender reshaped workflows across Covestro R&D and has delivered many benefits:

Resource Optimization

Routine predictions that previously fell to computational chemists and property data specialists are now automated and accessible to all. Experts can focus on complex scientific challenges, reallocating intellectual capital to higher-value scientific work.

Broader Exploration of Solvents

Chemists now evaluate over 70 solvents instead of the usual 5 to 10. Ranked recommendations encourage exploration of less familiar solvent options, expanding scientific creativity and increasing the chances of identifying optimal solvents earlier in the research process.

Streamlined Workflows

Solvent selection is now a digital-first process. Researchers now start with Solvent Recommender to narrow down solvent candidates, making lab experiments more targeted and efficient, conserving valuable laboratory time, equipment, and materials.

Improved Collaboration

The tool has established a clearer workflow across disciplines. Chemists use Solvent Recommender independently, consulting experts only for complex cases. This reduces bottlenecks, improves efficiency, and supports autonomous, coordinated teamwork.

Enhanced Decision-Making

Embedding Solvent Recommender into the organization's digital ecosystem gives chemists access to complementary predicted property data. This enables evaluation of solvents and molecules in context with other physicochemical properties, supporting more informed experimental decisions.

Empowering R&D with Digital Tools

The development and deployment of Solvent Recommender fundamentally changed how Covestro approaches both experimental and digital solvent selection. What was once a narrow, resource-intensive manual experimental process has become a broad, data-driven, and highly efficient workflow.

Thoughtfully designed AI tools delivered both scientific and organizational benefits to Covestro. By democratizing access to predictive insights, the company fostered a culture of independence and exploration while simultaneously increasing efficiency and productivity.

With Solvent Recommender in place, Covestro optimized workflows and laid the foundation for continued digital transformation in chemical R&D and early product development. The deployment highlights the impact of digital solutions in driving innovation and efficiency, and shows how AI can accelerate discovery in the chemical sciences.

Learn More

Just as Covestro transformed its solvent selection process, your teams could benefit from broader solvent exploration, more efficient workflows, and reduced reliance on routine expert input. Solvent Recommender is available as an add-on to PhysChem Suite, helping your scientists make smarter, faster decisions. Contact us to discover how it can support your research and drive similar gains in efficiency and innovation.