intellegens

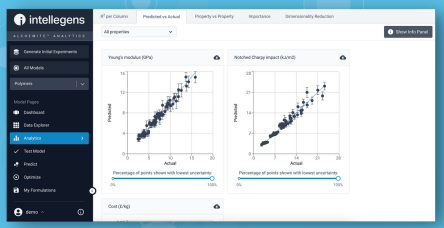
Applied machine learning

Accelerate innovation for chemicals and formulations

Optimize chemicals, formulations, and chemical processes, exploiting all available data

Design more effective and efficient experimental programs, saving months of work

Find novel solutions to market, regulatory, and environmental challenges

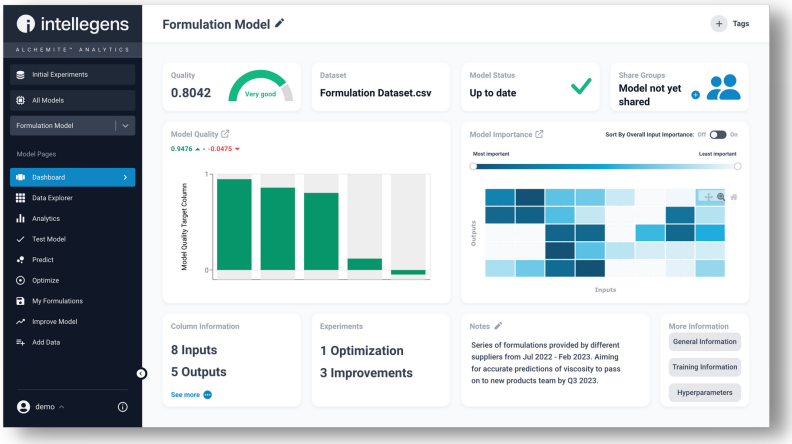


Analyzing predicted property data for polymers in the Alchemite™ Analytics user interface.

Are you developing new chemical compounds, designing formulations, or aiming to improve chemical processes? What if you could reduce the amount of costly experiment, find new solutions, and speed up process improvement decisions – all by making more effective use of your data?

Leaders in chemical and process innovation want to apply novel machine learning technologies to extract more value from their experimental, simulation, or production data. But most machine learning approaches fail when applied to real-world data from these sources, because such data is often messy and incomplete. The answer is the Alchemite™ software from Intellegens, built on a method originally developed at the University of Cambridge.

Alchemite™ applies advanced deep learning that can build models from this sparse, noisy data. It is easy to apply to practical problems in the chemical process industries. Identify vital relationships in your data. Design new chemistries, formulations, and materials. Propose optimal process parameters. And guide planning of experimental projects to dramatically reduce cost and time.



Assessing a formulation design experimental campaign in the Alchemite™ Analytics platform, which provides researchers with quick, easy access to advanced machine learning methods and analysis in a web browser user interface.

Case studies

Formulation development – **Domino Printing Sciences** accelerated a key project on ink formulations, decreasing time-to-market by cutting months out of experimental timescales. Similar applications have included development of plastics, coatings, paints, foodstuffs, and pharmaceuticals.

Design of catalysts – **Johnson Matthey** accurately modeled 16 key performance targets for automotive catalysts, proposing new solutions that have now been experimentally validated.

Flavours and fragrances – **IFF** successfully predicted the sensory properties of chemical compounds based on sparse physicochemical and sensory data, saving costly experimental time and resource.

Drug discovery – **AstraZeneca** and **Optibrium** successfully combined descriptors, in silico, and in vitro data to predict PK parameters and curves.

Alchemite for chemicals and process development

With the **Alchemite™ Analytics** software, scientists can apply powerful machine learning methods through an easy-to-use browser interface. **Alchemite™ Engine** gives data scientists flexible API access to the full power of the Alchemite™ algorithm, enabling them to integrate it with in-house systems and workflows.

- Gap-fill and validate sparse, noisy data from suppliers, experiment, simulation, and production
- Auto-generate models that identify key relationships within your data
- Quantify uncertainty to support a rational business case for key decisions
- Suggest what experiment(s) to do next, increasing the efficiency of experimental programs
- Identify the optimal chemistry or formulation for your product
- Propose optimized process parameters to improve quality and performance.

Next steps

Contact us to book a demo tailored for your application.Visit our website to download white papers and subscribe to our newsletter. Or follow us on social media.

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