

Success story

A better way to screen molecules – and save resources – with help from the Umetrics® Suite of Data Analytics Solutions

Trial and error. That's one way to discover which molecules to use to create a new plasticizer with specific qualities. But it has its limits. It doesn't do the best job of putting accumulated knowledge to good use as there are usually only a few people with the right knowledge and experience to contribute to development. A leading producer of specialty chemicals used the Umetrics Suite as part of a new tool and a new way of working with the aim of streamlining their work through better use of information – saving time and resources.

Can we use data-driven methods? Market demand gives rise to opportunities for tailoring products and chemicals – with specific properties. *“The traditional way to do it is to list a candidate set of molecules based on domain knowledge and experience,”* says a specialist in chemometrics at the company. *“We wanted to find a better method – to complement domain knowledge with data-driven methods based on multivariate data analysis to enhance our understanding and increase awareness. That way we could make sure that the whole project team could contribute in a more efficient way – with the hope of saving time and resources in the long run.”*

“Virtual Lab” With SIMCA® at Its Core

The company was already using parts of the Umetrics Suite elsewhere in their work, so the decision to use SIMCA® as the core of the new multivariate data analytics-based method, called the Virtual Lab, was easy to make. The resulting tool combines a computational solution for calculation with the multivariate engine in SIMCA®, which visualizes the different molecules in relation to each other. That visualization aids in interpretation, and makes it easier to screen molecules with good properties. And thus to complement domain knowledge and experience with data-driven methods.

A Collaborative – Cost-Effective – Method

SIMCA® structured and visualized the computed properties of each molecule in a way that allowed project teams to compare performance with respect to the specifications for the plasticizers. As a result, the entire team of specialists, chemists and engineers was able to participate in a discussion on how to proceed. It was the combination of data-driven methods and specific domain knowledge and experience that really made the difference.

“We could test new ideas in Virtual Lab, for example, and then the specialists could challenge the results before a product was synthesized. This was an effective screening tool for new candidate molecules,” says the specialist in chemometrics. *“The true value lies in the way the visualization opens up a forum for communication.”*

What Works for Plasticizers, Works for Lubricants Too

“What we were able to achieve with SIMCA® and Virtual Lab in our plasticizer project was quite convincing,” he continues. *“We were able to make use of data we would otherwise simply have archived, and to work more collaboratively. We made the workflow more efficient by creating a script to automate it, and I was satisfied enough to test the principles*

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Specialist in chemometrics



on a similar project around lubricators. In my opinion, there are many areas where SIMCA and Virtual Lab would be a valuable tool. For example, it could be used to recommend products based on customer preferences."



The customer:

A world leader in several sectors of the specialty chemicals market for a wide variety of industries and applications.

The challenge:

Find a way to enhance understanding of plasticizers through more effective work principles based on data-driven methods, with saving resources as a goal.

The solution:

A new work method based on SIMCA[®], which visualizes the performance of molecules relative to each other.

The result:

Enhanced understanding, a tool that facilitates screening and communication, and the potential for saving resources.

SIMCA[®] from Sartorius Data Analytics

SIMCA[®] is a multivariate data analysis solution with an intuitive graphical interface. It gives you the flexibility to handle complex data in many forms.

SIMCA[®] is part of the Umetrics[®] Suite of Data Analytics Solutions, a family of proven data analytics solutions that work seamlessly together.

Sartorius Data Analytics

Phone: +46 40 664 25 80
E-mail: umetrics@sartorius.com

