



Anatune

Challenge

Deliver sophisticated chemical analysis services, including advanced data processing, that push the limits of chemistry.

Chemical attraction: JMP® and DOE team up for better chemistry

Anatune is a leading provider of robotic solutions for chemical analysis. JMP® helps the company perform the sophisticated analytics that set it apart from the competition.

For many industries, chemical analysis is mission critical. Makers of fragrances, for example, need to identify the compounds that give natural aroma sources their signature scents. And the stakes are high: the success of new product lines, the cost-savings of an innovative packaging material, the reputation of a trusted brand. That's why enterprises across industries turn to Anatune, a leading provider of automated robotic solutions for chemical analysis. The company offers end-to-end services and support, from automated sample prep to analysis, from data processing to consulting. But chemical analysis can be costly and time consuming. To remain competitive, Anatune must optimize the processing and analysis of chemical data. And for that, it relies on JMP.

Taking the measure of business progress

Founded in Cambridge, England, in 1996, Anatune serves customers in the United Kingdom and Ireland, and has partnerships with market-leading makers of instrumentation for chemical analysis. The company provides solutions focused on chromatography and mass spectrometry, analytical technologies used to separate, identifying and measure substances in samples of all kinds. These techniques are considered a gold standard in forensic substance identification, because they're used to perform a 100 percent statistically specific test that positively identifies the presence of even tiny amounts of a particular substance.

"In chemistry, you only make progress if you measure things properly," says Ray Perkins, CEO of Anatune. "And much of what our customers need to measure is 'only just possible.' We provide not only the instrumentation but also the support that enables our customers to push the limits of analytical chemistry."

A key differentiator for Anatune is its focus on the use of automation and robotics in chemical analysis. By using robotics, the company can

automate repetitive tasks that analysts would otherwise have to perform. That saves time and money. It also makes for more accurate testing. And it frees up scientists for activities where they can add more value.

"Our solutions are modular, so they can be comprehensive, with different robots handling different tasks," says Camilla Liscio, PhD, an applications chemist with Anatune. "One advantage of robots is that they perform a given task the same way every time. That's especially important, for example, if you want to control different experimental parameters, because you can eliminate biases due to human error. Another advantage is that the analysts can then focus on the data analysis."

Anatune can provide companies with a complete solution, from the development of the best analytical approach to the installation of the equipment. Customers are then trained to fully understand their solution and make the most out of it. "That's one way JMP enters the picture," Liscio says. "JMP is a very useful tool for our method-development stage because it gives us the best answers to what we're looking for."

A match made in heaven

Another way Anatune uses JMP is as part of its design of experiments (DOE) approach to chemical analysis. "In the lab, the most common approach to method optimization is to change one experimental variable at a time, while keeping the other variables fixed," Liscio explains. "But that often leads analysts into exploring only part of the



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Camilla Liscio, Applications Chemist



relevant experimental space, especially when multi-parameter processes are involved."

In contrast, a multivariate approach provides information about a larger region of the experimental space, which can allow analysts to fully explore the problem and uncover the best solution. It also provides a shorter path for getting to that solution. "My own experience using DOE has been very positive," Liscio says. "It has shortened my method-development times by 50 percent or more. And I love the certainty of knowing I've found the best possible combination of parameters."

Anatune uses DOE for a variety of processes. The most complex is analytical sample prep, which involves several stages, each of which can include multiple parameters such as time, temperature and mixing speed. "It's very hard to find the optimal combination working one variable at a time, especially because you're looking at the interactions among parameters," Liscio explains. "So that's an area for DOE to shine. DOE helps you identify the significant factors and the best conditions for those factors."

The company also finds DOE a perfect fit for its differentiating focus on automation. "Automation and DOE are a match made in heaven," Liscio says. "Automation is an analytical tool that can give you the best method, while DOE is a statistical tool that can give you the best answer." The challenge of DOE, though, is its potential complexity from a statistical perspective. "I'm a chemist, not a statistician or an IT person," Liscio says. "So while I saw the potential of DOE and was eager to use it, I was put off by the data processing. That's why JMP is so valuable."

From enormously complex to 'super easy'

In fact, DOE provided Liscio's - and Anatune's - introduction to JMP. "DOE is the most efficient way to develop analytical methods, but it has required a grasp of statistics that puts it beyond the reach of most

people," Liscio contends. "But with JMP, anyone can use DOE, because the software does the difficult work. JMP provides a structural and very elegant way to tackle very complicated analytical challenges."

And complicated analytical challenges are what Anatune faces every day. The data it processes can be enormously complex, depending on the number of samples, the method of testing and the application. "But once you put it in JMP, it's straightforward," Liscio says. "You just copy and paste on the response column, and from there, it's super easy."

A good example of Anatune's use of JMP is in chemical analysis for the fragrance industry. One of the company's customers needed to identify the compounds in the aroma of flowers so that it could create an aroma profile for each flower and categorize each species botanically. But aromas can involve many compounds in various concentrations, and identifying those compounds can be exceedingly difficult. "We have a technique that exhaustively extracts volatile compounds from a sample and preconcentrates them onto an adsorbent trap," Liscio explains. "The analytes are then released from the trap with temperature and analyzed by GC-MS. The advantage of this technique is that it's efficient at sampling and concentrating volatile compounds such as fragrance compounds. However, the optimization of several parameters is required to obtain a good method. And JMP is very effective for this application."

Liscio reports that method development like this would take a week or longer if performed one variable at the time. With JMP and DOE, that time is reduced to two days or less. "And it probably takes only 10 minutes to put it together in JMP," she says. Results like these have made Liscio a strong JMP proponent. "I want every customer to have this base analytical toolkit - JMP to do the method of optimization, automation to perform the experiments, and JMP for data processing to help with the data analysis. "The more I use JMP, the more opportunities I see for other areas where JMP can be used."

Solution

Employ a design of experiments (DOE) methodology to optimize multivariate chemical analysis delivered via robotic lab systems; integrate JMP to provide a reproducible and robust solution for customers regardless of data complexity.

Results

By using JMP to run multivariate experiments, Anatune has shortened development time by 50 percent. These efficiencies enable Anatune to better serve its customers with market-leading automated chemical-analysis solutions.

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