



## CHALLENGE

Compiling and analyzing huge quantities of data in a drug discovery environment.

## SOLUTION

JMP® enables the computational chemists at AstraZeneca to manipulate and analyze large data sets to help pinpoint molecules active for a specific target.

## RESULTS

Scientists at AstraZeneca make the most of JMP's visualization capabilities and robust analytics to conduct research more quickly and effectively, which helps the company bring quality drugs to the market faster.

## MORE INFORMATION

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# Computational Chemistry at AstraZeneca

The global pharmaceutical company's quest to more quickly bring new medicines to market

Manipulating data sets that sometimes contain up to a million rows is a daunting task—and one that is made much easier for the computational chemists at AstraZeneca with JMP on the job.

“We have large quantities of different types of data that need bringing together and analyzing in a robust manner,” explains Dr. Paula Kitts, a computational chemist with AstraZeneca in Alderley Park, England.

Kitts is involved in using small molecule and protein modeling to aid molecular design. Essentially it's drug discovery. “The computational chemistry part of it is actually trying to look at things we can either calculate computationally or trying to build statistical models to predict things that will help chemists decide what to make next. We try to help them design molecules that will potentially be active against a particular target,” she explains.

Because this entails gathering huge amounts of data, the computational chemists are especially keen on the data analysis tools and techniques found in JMP. The software enables them to quickly gather large, complicated sets of data, and presents the information in a visually appealing,

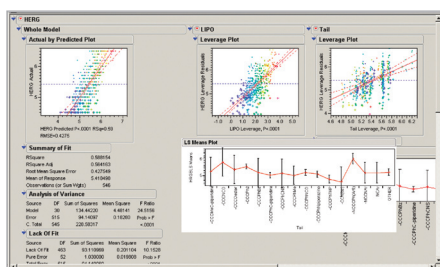
easy-to-read manner so they can quickly see patterns or problems. “It's really, really quick. In other software you can do the work, but everything is not in one place,” says Kitts. “With JMP, you can use just one piece of software to do everything, where previously we'd be using three or four different pieces of software.”

The research of the computational chemists plays a crucial role in their work on multidisciplinary project teams that includes medicinal chemists, bioscientists, and physical chemists.

Being able to do research more effectively is key to helping this leading global pharmaceutical company in its quest to more quickly bring to market new medicines designed to fight disease in areas such as gastrointestinal, cardiovascular, neuroscience, respiratory, inflammation, cancer, and infection.

## Increased Capabilities Improve Efficiency

Much of what underlies the work that the scientists at AstraZeneca undertake is data manipulation. That's why JMP's compatibility with many data sources allows direct interrogation of discovery data. “I can open any table of data without having to do any processing



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“In some cases, I don’t know how I would do the job if I didn’t have JMP.”

Dr. Paula Kitts  
computational chemist at AstraZeneca  
Alderley Park, England

of that data. I can bring it all in using JMP, and then I can manipulate it and transform it very quickly myself,” Kitts explains. “That wasn’t always the case with other software we used.”

Access to the database especially helps, for example, when AstraZeneca uses JMP in high throughput screening. “We test the corporate compound collection against particular targets and might end up with up to a million rows of data against a particular target that we’re interested in. Obviously, it’s useful that we can just open that straight into JMP,” Kitts says.

The ability to open the data straight from the database using JMP also saves time—it means opening one table instead of innumerable ones. Kitts cites an example where she had six compounds in 15 different tests. “You can imagine if I had to open that many large tables, it’d be horrendous,” she says. Instead she can retrieve one view of all the data through JMP. With one quick look, she can see if something has gone wrong in a particular test.

Because using JMP is so quick, it also helps the scientists perform “what-if” scenarios. “You can try lots of different

things. You can do some investigation to see what the data looks like. If you’ve done it wrong, it’s so quick you can just do it again.”

JMP is definitely a timesaver. A prime example is the scripting function of JMP used to do repetitive processes, for instance, if you wanted to do a particular analysis once a week. “Once you actually decide what that analysis is, you want to save it and do it again—and not have to think about it every time,” Kitts explains. It might take her an hour to do an analysis. But the next time, because she has already saved the script, it will take her a minute or less—saving an hour every time she needs to repeat the analysis with new data.

### Moving Forward

AstraZeneca is a longtime SAS customer and continues to use SAS in many diverse areas including discovery statistics, biostatistics, and clinical programming. Over time, the company has also grown the use of JMP in computational chemistry and continues to expand its use by medicinal and physical chemists in this department. This expansion is mainly due to Kitts and the other 120 JMP users at

Alderley Park discovering that the software is fast and intuitive. According to Kitts, AstraZeneca computational chemists, in particular, enjoy the fact that they do not need to write programs when using JMP, which saves time and effort.

Kitts has been using JMP since she started at AstraZeneca in 1997. During that time the software has gone through several upgrades. “We have upgraded and updated JMP. It looks similar, but it’s always obvious where the improvements are. And it is always improving.”

JMP has been so successful in helping AstraZeneca’s computational chemists at Alderley Park that the company is promoting the use of the software within other groups. The company now provides its own JMP training, and the software’s user-friendly attributes are particularly helpful as AstraZeneca trains new users.

“JMP is easy to use even if you have never seen it before,” Kitts says. “New people don’t generally need to go on the training, even though we have training courses in-house. We find that we just sit down with the new starters for half an hour, they get the hang of it quite quickly.”

And the scientists at AstraZeneca have quite quickly learned that JMP enables them to do their research more effectively and more rapidly, making the software a necessary part of their workplace. “In some cases,” Kitts says, “I don’t know how I would do the job if I didn’t have JMP.”

