



## Takeda Streamline Analytical Handling with ACD/Spectrus Processor

Push-back to learning more software to process analytical data leads to a new unified approach to analytical data handling.



Matthew Jones  
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Analytical Research

When Matthew Jones decided to buy new UPLC equipment for the Open Access LC/MS lab from a different vendor than the existing instrumentation, his decision was motivated by the need for a fit-to-purpose instrument. The new instrument would provide increased flexibility and throughput. The medicinal chemistry group, however, were hesitant to use the new instrument because they had to learn yet another piece of specialized software to analyze their UPLC/MS traces.

The drive to investigate a new solution was simplification of analytical data processing and interpretation into a single software environment and to reduce IT support. The chemistry group had numerous vendor software tools on their computers and managing the different versions of the different pieces of software was becoming an issue. "Spectrus Processor seemed to meet all our needs," says Jones.



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A successful trial of ACD/Spectrus Processor by eight scientists representing process and medicinal chemistry groups and the analytical research team, led to a Discovery-wide purchase for the Boston site (approx. 80 users).

“Learning from past mistakes I decided we needed to identify a few champions from the Process and Medicinal Chemistry groups to be involved in the software evaluation from the very beginning. They would in turn be the ones to introduce this new software to their colleagues. They were very enthusiastic and there was little push-back. The team was given 2 months to learn Spectrus Processor before the old software was removed from their computers. It's fairly intuitive and the users have been happy with it.”

Spectrus Processor is now handling analytical data from ~15 different instruments including 400 and 500 MHz NMR machines, numerous UPLC instruments, XRPD, TGA, DSC, and IR instruments; all from different instrument vendors. “Some purification work is still being done using instrument vendor software when it's more ideally suited to that work,” adds Jones, “but all our routine analyses are being processed and reported using Spectrus Processor.”

How does Spectrus Processor compare with the software it replaced? “It's very comparable to the third party software we were using for NMR and LC/MS,” Jones explains. Initial concerns about its ability to handle 2D NMR proved to be unfounded and it is used daily for LC/MS analysis. They had a pleasant surprise when it came to interpretation of infrequently used IR spectroscopy. He admits, “In the short time I played with the IR tools in Spectrus Processor I was able to get more out of the data than with the original instrument vendor software.”

Being able to build on the Spectrus Processor software, Jones hopes to realize his long term vision—a single platform for handling and sharing live analytical information.

### **About Takeda Pharmaceutical Company Limited**

Located in Osaka, Japan, Takeda is a research-based global company with its main focus on pharmaceuticals. As the largest pharmaceutical company in Japan and one of the global leaders of the industry, Takeda is committed to strive towards better health for people worldwide through leading innovation in medicine. Additional information about Takeda is available through its corporate website, [www.takeda.com](http://www.takeda.com).



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