# Integrating Lead Discovery

BY ALISSA POH

Like most other industries, pharma has its trends and recurring themes. Of late, a good many companies have been partnering with vendors to customize software for data consolidation. One such partnership, between Amgen and in-silico solutions specialist Genedata, yielded Amgen Lead Discovery Informatics (ALDI).

**Best Practices Winner:** Amgen
**Project:** Amgen Lead Discovery Informatics
**Category:** Drug Discovery and Development
**Nominated by:** Genedata

There's always need for a more consistent view of research data—small wonder, given that many companies are really patchwork quilts of M&As. "Scientists tend to store their data in ways they like and can easily manipulate and view," says Randal Chen, Amgen's director of information systems. These seemingly small nuances in storage formats, he adds, actually add up to a large difference.

The Tripos-Wyeth-Accenture initiative—Next-Gen Discovery IT (see "Triple Play," *Bio•IT World*, Nov 2008)—is another example, albeit a more generic solution tying together Wyeth's disparately-located databases. On the other hand, Chen notes that ALDI focuses on managing voluminous information from Amgen's high-throughput screens.

"We'd acquired several other bio/pharma companies over the years, which gave us complementary core capabilities for finding new lead compounds," says Bill Goode, a senior systems analyst within Amgen's research informatics department, and project manager for ALDI. "But we also had to deal with the drawback of numerous legacy tools, different practices and workflows." As such, Amgen's research and information systems groups spearheaded ALDI as an effort to select a commercially available platform that would align the company's multiple research sites, as well as support standardized methods for data analysis and progressing compounds.

Amgen and Genedata collaborated on the ALDI project, with the goal of developing a product capable of not only handling large volumes of information but also integrating with other Amgen systems. The choice of Genedata's Screener came after extensive review of products on the market, as well as a joint Amgen-Genedata workshop to establish a framework for additional customization. "We had to see how Amgen's requirements and our existing [Screener] product would fit together," says Stephan Heyse, head of lead discovery informatics at Genedata.

Bill Goode, Amgen Inc.; Kurt Zingler, Genedata (USA)

## Agile Development

The collaborators agreed to use an agile approach that broke development into "sprints." Two-thirds of each three-week cycle were spent writing new software on Genedata's part, followed by a week of testing by Amgen's end users. Goode says this allowed for quick feedback and course correction as bugs and feature gaps were found. Heyse adds that it "took a lot of risk out of the whole project, as there was always control from both sides as to where this was heading."

Heyse was enormously impressed that, right from the start, Amgen had "done all the work in aligning the overall project goals. They had a clear vision and a practical way of approaching it. We saw even then how much Screener could deliver and what was missing."

Goode agrees that defining ALDI's goals from the outset was vital in ensuring its successful implementation. The team sought an overall performance increase; better quality control in distinguishing compounds of interest from artifacts; a shorter period of data analysis for new assays without needing to increase support staff; and improved consolidation of workflows.

"The results were fairly impressive," he says. "Our productivity increased by 50 percent on average—sometimes as high as 80 percent. Screener offered a bunch of intrinsic tools that allowed us to... rescue compounds we hadn't previously identified as true actives. We removed the support staff bottleneck—it takes one week at most now to analyze new assay data. We also worked with our lead discovery scientists to define best practices, and [integrated these with Genedata's] modules for curve-fitting, kinetics analysis, and hit selection that have had enormous impact on the quality of our data."

Given these results, end user accolades, and the fact that ALDI was implemented in under a year, the collaborators felt that their system was ready to withstand scrutiny as a Best Practices entry—and they weren't disappointed. "[The award] establishes that this type of software development, in this space, is valuable, and that the overall strategy we laid out for handling scientific data also worked,"

says Goode. "It's a great validation by our industry peers."

Amgen is looking to reap ALDI's benefits beyond lead discovery into therapeutics and eventually large-molecule studies. One unexpected benefit from this collaboration, says Goode, is that "our system's foundation won't need retooling or major redesign; we can build on other areas without rewriting the software from the ground up."

Amgen viewed the ALDI project as a partnership. "Genedata brought their best expertise out from the very beginning," says Goode. "It was much more a technical and scientific collaboration as opposed to them trying to sell us a piece of software."

On Genedata's part, Heyse was impressed by Amgen's general lack of micromanagement. "They didn't feel a need to specify every single detail in advance—we were simply told to go ahead and do our work, which was great," he says. "You could say we 'sprinted' at this together." •