# Infinity Pharmaceuticals Standardizes on MATLAB® for Drug Discovery Data Analysis



Calculating IC50 curves with MATLAB.

In the race to deliver drugs to market more quickly, biopharmaceutical companies need to classify and interpret data at unprecedented rates with tools that eliminate redundant analysis tasks and promote collaboration among scientists.

Infinity Pharmaceuticals, an early stage biopharmaceutical company focused on the discovery of new cancer medicines, has standardized on MATLAB® for drug discovery data analysis. Infinity uses MATLAB to calculate all IC50 curves, the concentration of a drug that is required to inhibit 50% of enzyme activity.

"The open architecture of MATLAB was critical to building applications that enable collaborative scientific processes," says Andy Palmer, senior vice president of operations and organization at Infinity Pharmaceuticals.
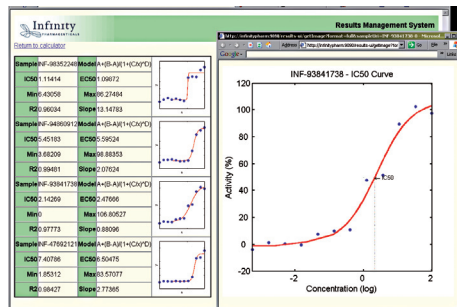
## THE CHALLENGE

Infinity sought to standardize on a data analysis tool that would integrate with their in-house applications and provide efficient analysis of large data sets.

To avoid manually entering results into a central database, they decided to automate the process of capturing, analyzing, and visualizing data.

Infinity would require software that enabled them to standardize on various calculations and ensure the integrity of their screening results across projects.

"We needed a tool that enabled our researchers to solve the same problems in a consistent and proven environment," explains Nick Encina, senior informatics

analyst at Infinity Pharmaceuticals. "Our researchers need to be confident in their results and the comparison of results from different experiments."

## THE SOLUTION

Infinity chose MATLAB to integrate with their existing applications and calculate their IC50 curves.

"With its powerful engine and analysis capabilities, MATLAB was the clear choice for us," explains Encina. "No other product on the market came close to matching all of its capabilities."

Encina and his colleagues developed an automated process by which the data generated by a scientist's instrument is read directly into a database. Using MathWorks tools, project teams review, analyze, and annotate data by removing outliers and dynamically refitting the curves.

"Automating our data analysis process with MATLAB ensures that no data is lost," says Encina.

To calculate the IC50 curves, Infinity developed a Web-based interface that uses Java to communicate with MATLAB. The

## THE CHALLENGE

To standardize on a data analysis tool that handles large data sets and integrates with existing systems

## THE SOLUTION

Use MATLAB to automate the process of capturing, analyzing, visualizing, and importing data

## THE RESULTS

- Development costs reduced by $100,000
- Future cost savings expected
- Quality results delivered consistently

## The MathWorks

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interface prompts scientists to perform their calculations. Parameters from the interface use M-file templates to execute scripts in MATLAB.

Scientists used MATLAB and the Statistics Toolbox to perform batch calculations of hundreds of thousands of data points. They plotted the curves for visualization using the Curve Fitting Toolbox. Visualizations along with IC50 values and coefficients in response elements are displayed to scientists in a browser. The IC50s persist in a database to ensure that data is retained.

Once the scientists approve the modifications, they update the values stored in the database with a single click and publish it to the project leaders and scientific leadership teams for immediate notification.

Engineers are also using MATLAB and related toolboxes across a wide variety of internally developed applications, including KI calculations for finding the enzyme inhibition constant. Using MathWorks tools, Infinity ensures that values are calculated consistently across all experimental results.

"Using MATLAB to create the KI toolset only took days, compared with months with previous tools," notes Encina.

Infinity is also using MATLAB for cluster analysis and analytical chemistry result derivation.

## THE RESULTS

- **Development costs reduced by $100,000.** "With MATLAB, we reduced our development time significantly," explains Dennis Underwood, vice president of discovery informatics and computational science at Infinity Pharmaceuticals. "That has resulted in an annual savings of $100,000."
- **Future cost savings expected.** With the integration of their in-house tools with MATLAB completed, scientists can focus on developing algorithms even more quickly. "We estimate that we can develop future algorithms in MATLAB in just a few days compared to perhaps months," says Underwood. "This could save us hundreds of thousands of dollars more."
- **Quality results delivered consistently.** By standardizing on MATLAB, researchers can confidently use each other's data and results for analysis and eliminate redundant experiments.

*To learn more about Infinity Pharmaceuticals, visit* **www.ipi.com**

## APPLICATION AREAS
- Computational biology
- Data analysis
- R&D

## PRODUCTS USED
- MATLAB
- Statistics Toolbox
- Curve Fitting Toolbox

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