

# Pfizer Guides Lab Experiments Using Computational Analysis with MathWorks Tools

Drug discovery and development traditionally have been labor intensive and computationally complex. Wet-bench experiments can consume weeks of a researcher’s time as parameters and conditions are tested. Analyzing the results of these experiments has been slowed by limited computational and analyst resources to process the results.

Using MathWorks tools, Pfizer, Inc. is trying to improve the efficiency of wet-bench experiments by performing computational analysis to help guide experiments and analyze results. With these types of approaches, biologists can narrow the range of parameters to be explored and quickly identify the most significant outcomes, saving potentially weeks or months of wet-bench work.

“With the tools that we developed using MATLAB®, our biologists can better understand the space they are working in and limit the experiments that they need to run,” explains Bart Hendriks, senior scientist at Pfizer. “The tools help them choose the experiments that the models suggest will have the biggest impact, helping to reduce the reliance on intuition.”

## THE CHALLENGE

Pharmaceutical researchers typically begin the drug discovery process by identifying a target, an illness, or physiological condition to treat with a new drug. Wet-bench biologists then develop assays to screen enormous libraries of compounds to detect whether and how drugs under development would affect the target. They must then test the promising compounds and their impact on the target.



GUI developed with MATLAB to analyze a compound transport model.

With the high number of parameters involved in these assays, biologists need modeling and simulation tools to target experiments that produce valuable results in less time. Pfizer analysts seek to develop user-friendly tools for bench biologists to perform some of their own analysis without requiring a staff of dedicated analysts to develop programs for each set of experiments.

## THE SOLUTION

Hendriks led a grass-roots initiative at Pfizer’s Research Technology Center that used MATLAB and the MATLAB Compiler to develop and deploy predictive models of biology with the aim of streamlining the production and analysis of lab results. The intended users are biologists in Pfizer’s target biology and ADME/toxicology groups, who would use the tools to predict the best assay conditions for experiments and to examine aspects of drug transport.

Hendriks first used the MATLAB tools by developing a computational model. To construct these models, he used MATLAB for everything from solving relatively simple algebraic equations to more complex systems of ordinary differential equations.

## THE CHALLENGE

To streamline drug discovery by enabling biologists to guide experimentation with computational analysis

## THE SOLUTION

Use MathWorks tools to develop and deploy easy-to-use applications for analyzing and predicting lab results

## THE RESULTS

- Focus on research maintained
- Biologist efficiency improved
- Grass-roots effort initiated

“ Using tools that we developed with MATLAB, our biologists perform computations beyond what they could have done or even considered doing in Excel. ”

Bart Hendriks, Pfizer

For analyzing drug transport, Hendriks used MATLAB to nondimensionalize ordinary differential equations to identify the system's principle controlling parameters.

Hendriks then worked with biologists, who would ultimately use the tool, to design a user interface. Using the MATLAB development environment, he created graphical user interfaces (GUIs) that enable researchers with no programming knowledge to immediately use the tools.

The GUIs enable biologists to vary a range of parameters, including mechanisms of inhibition for compounds, protein expression levels, and rate constants describing some of the physics of the system, such as permeability of compounds. Leveraging the plotting capabilities of MATLAB, Hendriks incorporates sophisticated graphs into the GUIs to help biologists interpret complex results.

“The interactive GUIs that we develop with MathWorks tools allow me to communicate convincing and clear analysis results to biologists,” says Hendriks. “This is much more effective than our previous approach using PowerPoint slides.”

Based on feedback from biologists, Hendriks fine-tunes each interface and then uses the MATLAB Compiler to build a stand-alone version of the tool. The compiled tool is then deployed to biologists for use on their own desktops.

Currently, a small group of biologists within Pfizer are applying MATLAB based tools as part of a proof-of-concept initiative. “As we demonstrate the benefits of computational analysis and define a new workflow with MathWorks tools, we may look forward to expanding this approach to other areas within Pfizer,” notes Hendriks.

## THE RESULTS

### ■ Focus on research maintained.

“MathWorks tools let me concentrate on the biology and scientific questions instead of getting into the details of software application development,” says Hendriks. “Developing these tools in any other way would have meant dedicating additional resources—resources that are not available given the number and priority of other ongoing projects.”

■ **Biologist efficiency improved.** By incorporating analytical expertise into easy-to-use tools, Hendriks enables Pfizer biologists to guide laboratory activities by performing sophisticated analysis themselves. “The tools provide a framework for research. For example, they can recommend proper assay conditions and also help researchers understand what the tradeoffs are if they stray from those recommendations,” says Hendriks.

### ■ Grass-roots effort initiated.

“MathWorks tools enabled me to start this program with limited resources, time, and effort,” says Hendriks. “Without these tools, it is unlikely we would do this work, because it would simply be beyond the scope of my programming expertise.”

To learn more about the Pfizer Research Technology Center, visit

[www.pfizerrtc.com](http://www.pfizerrtc.com)

[www.mathworks.com](http://www.mathworks.com)

## APPLICATION AREAS

- Algorithm development
- Biotechnology, pharmaceutical, and medical
- Data analysis
- Modeling and simulation

## PRODUCTS USED

- MATLAB
- MATLAB Compiler