



# Transforming drug research through AI/ML integration

## Clinical Pharmacology Modeling Solution

**The LabVantage@Analytics Clinical Pharmacology Modeling Solution** has been designed to provide a complete solution for laboratory personnel using a model-informed, drug development (MIDD) process. Seamlessly integrated with LabVantage LIMS, the solution provides a set of high throughput, template-driven utilities, enabling laboratory scientists to:

- Accelerate their analysis turnaround times
- Ensure analysis consistencies
- Increase computational efficiency
- Reduce overall time and cost required to bring drugs to market

A primary challenge faced by scientists and researchers working in laboratories is to be able to process bioanalytical data into meaningful parameters in their drug research and development processes.

The necessary computation and analyses require heavy usage of statistical computational techniques on the sample data residing in the laboratory information management systems (LIMS). In most of the cases, there is little or no integration between the LIMS software and the analytical tools used for such computations. This makes retrieval of the relevant data from the LIMS and the subsequent postback of the computed analyses to the LIMS a cumbersome and an inefficient process. Furthermore, the computational tools available in most of the cases are fairly rudimentary and do not offer the range of statistical capabilities as required in various stages of research and development.

This results in increased turnaround times, reduction of process efficiency, and an overall delay in the whole drug development lifecycle.

# Overview of Solutions

## Pharmacokinetic Modeler

The PK Modeler solution is designed to help researchers study the correlations between drug concentration and their pharmacologic responses. The module is bundled with modeling design templates based on dosing (Single/Multiple), method of elimination (Linear/ Michaelis Menten), or route of administration (IV Bolus, IV Infusion, Extravascular). Some of the key features are:

- Support for compartmental/non-compartmental analysis on individual/pooled data
- Bioavailability calculations
- Calculation of best-fit parameter for individual subjects
- Derivation of clearance rate, half-life, etc.
- Modeling for population pharmacokinetics.
- Use non-linear, mixed-effects models that can estimate the parameter distribution for the population, as well as assess the contribution of inter-individual variations physiologically and pathologically (covariates) to individual parameter values

## Pharmacodynamics Modeler

The goal of our PD modeling solution is to link the effect either to drug concentration or to drug doses when the drug-induced response is generated by a simple or a multiple receptor activation. The solution is pre-packaged with time-independent models for describing the balanced relationship between concentration and effects. Model library includes:

- Linear
- Log-linear
- Ordinary Emax Model
- Ordinary Inhibition Emax Model
- Sigmoid Emax Model (Hill)
- Sigmoid Inhibition Emax Model (Hill)

## Bioanalytical Calibration Curve Library

The Bioanalytical Calibration Curve Library provides a set of pre-packaged statistical algorithms for generating the best-fit standards curve. Known concentrations of the analyte being assayed are used in order to predict the unknown concentrations of analytes of interest.

Features include:

- Assortment of curve-fitting models (linear/non-linear) – examples include: 4PL Marquardt, 5PL Marquardt, Linear, Quadratic, Log-Log, exponential, etc.
- Ability to specify weights for regression models (1, 1/x, 1/x<sup>2</sup>, 1/y, 1/y<sup>2</sup>, 1/f, 1/f<sup>2</sup>)
- Ability to: select/omit standards, preconfigure or calculate limits of quantification and limits of detection, and set up and configure run acceptance templates
- Incorporation of aliquot factor and/or dilution factor
- Scenario analysis options

## Immunogenicity Cut Point Analyzer

The goal of the Immunogenicity Cut Point Analyzer is to: (i) determine the cut point of a substance, or the level at which a substance is considered reactive for anti-drug antibodies, and (ii) facilitate cut point calculations by using parametric/non-parametric approaches and application of the calculated cut points across screening, confirmatory, and titer cases with workflows. The module provides:

- Computation of various cut points and associated metrics such as:
  - Screening cut point
  - Confirmatory cut point
  - Specificity cut point
  - Assay sensitivity
- Configuration for various types of controls such as:
  - Screen negative and positive controls
  - Immuno-depletion Controls (Titer ELISA)
  - RIP Negative Controls (Titer RIP)
  - Positive Titer Control

## Business Benefits

- **Drastic reduction in computational errors due to template-driven utilities**
- **Major improvement in turnaround time due to faster processing**
- **Increase in computation accuracy and precision stemming from access to a huge number of computational algorithms**
- **Increased lab efficiency and throughputs**
- **Reduced cost associated with poor quality**

- Computation options include the following:
  - Parametric computations – Tests for normality using the Shapiro-Wilk test and features for variable transformation to address non-normalities
  - Non-parametric computations – A percentile-based approach with adjustments for outliers
  - Computation and use of additive or multiplicative correction factors
  - Incorporation of floating cut points
  - Interpretations using a library of tests and functions such as ANOVA, Levene's test, etc.

- Application of cut points with workflow configurations
- General configuration options such as: expected slope, specificity assay, CV configuration, report defaults, sharing immunodepletion, as well as samples in immunodepletion of unknowns, etc.
- Dynamic criteria setting for determining positive/negative status using absolute or percentage difference

### Reports and Dashboards

The Clinical Pharmacology Modeling solution is complete with a self-sufficient reporting and dashboard solution. It contains pre-built reports and dashboards for each of the core modules within the solution. Furthermore, the solution also offers laboratory business users the flexibility to design custom reports and dashboards of their laboratory data by using the powerful out-of-the-box business intelligence (BI) utility.

### Powered by **tcg mcube**

LabVantage@Analytics is powered by **tcg mcube**. **tcg mcube** is an advanced analytics and AI Platform, which allows users to create compelling business solutions for tackling complex industry problems. With its modular architecture, **tcg mcube** handles multiple data types, and it provides an efficient "cut-and-fit" into legacy environments if needed. Its mantra: Velocity to Value.



Ingest structured and unstructured data from diverse sources



Store ingested data within big data stores and data lakes



Provide a library of algorithms for machine learning



Create stunning visualizations using a powerful BI library

## Technical Features

Seamless, bidirectional integration with LabVantage LIMS allows for easy lookup and writeback of laboratory data	Inbuilt connectors for ingesting data from external sources for additional computation
Integrated solution with each function available as an independent, plug-and-play module	Detailed audit trail management and logging features for every user action performed
Self-service business intelligence capabilities allowing the generation of custom dashboards and reports	Access to hundreds of statistical algorithms for performing additional computations
Export features for computed data in all standard formats for downstream consumption	Configurable workflow-based approval process for each analysis task
Centralized access management and single sign-on through LIMS	Configurable alerts and notifications for individual roles and users



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### ABOUT LABVANTAGE SOLUTIONS

A recognized leader in enterprise laboratory software solutions, LabVantage Solutions dedicates itself to improving customer outcomes by transforming data into knowledge. The LabVantage informatics platform is highly configurable, integrated across a common architecture, and 100% browser-based to support hundreds of concurrent users. Deployed on-premise, via the cloud, or SaaS, it seamlessly interfaces with instruments and other enterprise systems – enabling true digital transformation. The platform consists of the most modern laboratory information management system (LIMS) available, integrated electronic laboratory notebook (ELN), laboratory execution system (LES), scientific data management system (SDMS), and our advanced analytics solution (LabVantage Analytics); and for healthcare settings, a laboratory information system (LIS). We support more than 1500 global customer sites in the life sciences, pharmaceutical, medical device, biobank, food & beverage, consumer packaged goods, oil & gas, genetics/diagnostics, and healthcare industries. Headquartered in Somerset, NJ, with global offices, LabVantage has, for four decades, offered its comprehensive portfolio of products and services to enable customers to innovate faster in the R&D cycle, improve manufactured product quality, achieve accurate record-keeping, and comply with regulatory requirements. For more information, visit [labvantage.com](http://labvantage.com).

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