Kinetica 5
Version Release
Description

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SCIENTIFIC

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VERSION RELEASE DESCRIPTION

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Version Release Description

Document History			
Version	**Description**	**Written/Revised by**	**Date**
r1	Kinetica v 5.0 VRD	Mari Kuwata	09-Dec-2008

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1. INTRODUCTION

1.1 Purpose

This Version Release Description is meant to describe in detail the contents of this release. This document will be identified as Thermo Fisher Scientific Document Number 0847 r1. It identifies and describes the release notes for Kinetica. The intended audience includes all users of the software.

1.2 Scope

This Version Release Description is limited to Kinetica™ Stand Alone v5.0

1.3 Inventory of Materials Released

1) Application CD ROM (version 5.0)
2) Version Release Description for Kinetica™ v5.0, Document Number 0847 r1
3) Kinetica™ v5.0 User Manual
4) Kinetica™ v5.0 Installation Guide
5) Kinetica™ v5.0 Basic Reference Guide

1.4 Reference Documents

1) Kinetica™ v5.0 System Design Specification Document Number: 0842 r1
2) Kinetica ™ v5.0 Functional Requirements Specification Document Number: 0840 r1
3) Test Plan for Kinetica ™ v5.0 Document Number: 0846 r1
4) Test Summary Report for Kinetica ™. V5.0 Document Number: 0848 r1

2. Release Notes

2.1 Version Description

Kinetica™ is comprised of the following modules:

Module	Description
General	Overall
Kinetica	Data Analysis
Import Assistant	Data Import
Table Assistant	Exporting tables
NCA Assistant	Non Compartmental Properties
Designer	Create A Compartmental Moment through visual 'Symbolic modeling'
Population Designer	Create A Population Moment through visual 'Symbolic modeling'
Chart Wizard	Create Graphs and Plots of Data

2.2 New/Modified Functionality for This Release

Description of New Functionality
• New non-compartmental analysis method for sparse sampling design takes into account repeat animal use to compute the standard error of the AUC. Method is based on the Bailer-Satterwaithe (also known as the Jia-Needleman-Bailer) method. • Non-compartmental analysis for steady state profiles has extended capability to perform regression of the terminal phase concentration-time points. The method has a more extensive data handling for starting concentrations, including user-defined time-point such that the system will use the corresponding concentration as the initial concentration. • Superposition method for variable dosing intervals is a model-independent method to estimate steady-state profiles based on single-dose profile. • Computation of the last AUC triangle whereby the last concentration is flagged as a BLQ adheres to BLQ handling specifications. • Observed Clast is output from the AUC* method as a parameter of the method. • BLQ handling in the non-compartmental analysis methods (AUC*, AUC steady-state, AUC steady-state with Lz, Sparse AUC) allows user to map a separate LLOQ column and use LLOQ, LLOQ/2, LLOQ/3 and LLOQ/4 in the pharmacokinetic computations. • Textual comments can be incorporated to the worksheet level in Kinetica, the comments from Watson for a particular concentration can also be imported into the worksheet level. • Table structure for sparse sampling design provides listing of individual sparse concentration data • Table structure for sparse sampling design provides summary statistics for the composite data • Descriptive statistics in Table Assistant takes into account BLQ specifications (default, BLQ as 0, BLQ as missing, user-defined BLQ based on a separate LLOQ column) from user in the computation of summary statistics for the concentration-time profiles. • Additional menu item called graphs to separate statistical and graphical functionalities. • Addition of a “Intelligent Spreadsheet” icon in the Study pane for quick import of data in the “wide” and “long” format into the Kinetica structure. • Rename of “All variable” icon to “Dataset variable” and “Study variable” icon to “Global variable”. In the Insert menu, “Study” fields renamed to “Global” fields to be consistent with the naming convention. • New method called “Run Macro” to run appended macro. • Interface to Sigma Plot version 9.0 is achieved through specific Table Assistant structures. The interface will bring data from the Kinetica structure to the Sigma Plot spreadsheet in a format that is ready to create graphs within Sigma Plot.

Description of New Functionality
• Mean Curve method is an additional method that allows user to specify line patterns, thickness, color, symbol, etc. Mean curve graphical control and settings are part of the method global option. • In the mean curve in the Global pane, user can set the gallery name as option to where the graph should be sent.

3. MATERIALS UTILIZED for TESTING

The following materials were used during test execution.

3.1 Hardware

10 GB hard drive
512 MB RAM
866 Mhz processor

3.2 Software

Windows XP Professional (SP2)
MS Office 2003
Kinetica™ 5.0

4. Issues and Workarounds

4.1 Issues Addressed since Previous Release (v4.4)

Issue Number	Description	Closure Notes
03-003833-raer (3786)	Attached is a kinetica file that has a problem when using the NCA Assistant. Basically, if the units for dose (mg) is different units than concentration (nM) the CL and Vss are miscalculated when using the wizard (Kinetica dose not convert the dose correctly even though the molecular weight is entered). If you go back to the method and go to the units page and just click molecular weight and recalculate, the error is rectified. Please give me a call if you need any further information or clarification of the problem.	This issue has been corrected and verified in this release of Kinetica.
03-003988-heer (3944)	We have problems with the AUCinter method. In a multiple dose study we would like to calculate AUC0-24 and AUC648-672. Concentration values below LLOQ should be set to zero. An example data set is attached. The calculation of AUC0-24 is correct. However, the second integrated AUCinter method calculates only up to Tlast and not up to the defined TEnd. Did we do something incorrect or is this an program error? Is there an easy way to overcome this problem? I would appreciate it if you could check this issue as soon as possible. Thanks for your help.	This issue has been corrected and verified in this release of Kinetica.

Issue Number	Description	Closure Notes
04-005402-boon (5112)	Test Step 12 : In NCA Assistant, Step 4 of 5, user should be able to right click on a point in the graph and change the properties (symbol, line, etc.). This can be done and the changes are seen when [Apply] is hit. However, when [OK] is hit, the settings are not saved and the graph resets to the original settings .**Kinetica**	This issue has been corrected and verified in this release of Kinetica.
05-007867-jene (6939)	When there is a syntax error in the kinetica basic code the program does not indicate at witch line the error is. Please see the attached file (Showstopper issue)	This issue has been corrected and verified in this release of Kinetica.
05-007898-jebo (6962)	When using Break Points it is not possible to execute macros Create a new empty kdb file Paste the following code in the macro editor dim test as string test = "Hello" msgbox test test = "Bye" msgbox test Execute the code Set a break point in the last line Execute the code	This issue has been corrected and verified in this release of Kinetica.

5. Re-Validation Suggestions

As Kinetica™ v5.0 is considered a major release by Thermo Fisher Scientific, we recommend the following suite of test scripts be executed.

Test Scripts	Test Scripts
KMS001- Compare Kinetica Population PK/PD Analysis results and testing data	KS001- Validity of the PK/PD Models
KMS002- Kinetica Population Analysis Function using Available Template	KS002- Changes to Data Analysis
KMS003-Non-CompartmentalCalculation Extravascular	KS003- Modify Kinetica PK/PD Analytical Study
KMS004-Non-Compartmental Calculation IV Bolus	KS004- Data Entry, Exporting Reports in Kinetica
KMS005- Non-Compartmental Calculation IVInfusion	KS004- Data Entry, Exporting Reports in Kinetica
KMS006- Non-Compartmental Calculation Steady State	KS006- Exporting Tables and Reports
KMS007- Single Dose PK Fitting	KS007- Define, Modify and Save Analysis Models

Test Scripts	Test Scripts
KMS008-Multiple Dose PK Fitting	KS008- Trapezoidal Study Analysis
KMS009- Simulation of Kinetica ™	KS009- Stopping Calculation Process
KMS010- PD Fitting	KS010- Kinetica's Table Assistant Defining Significant Figures
KMS011- PK/PD Fitting	KS011- Documentation of Input Commands and All Data Analysis
KMS012 - Kinetica ™ Statistical Methods Calculation (SAS or Excel Compare)	KS012- Residual Plots
KMS013 - Parameter Plotting	KS013-Ability to Automatically Adjust Units of Mass or Volume
KMS014- Categorical Plotting	KS014- Ability to Correct PK Parameter Values
KMS015 - Unit conversion in method AUC*	KS015- Data Points Used in the T-Half Life Calculation
KMS016 - Column Operation / Calculation	KS016- Ability to Define and/or Remove Data Points
KMS017- Urinary Template Calculations	KS017- Adding New Data or Replacing Existing Study Data
KMS018 - Absorption Template Calculations	KS018- Options on Treating Concentrations
KMS019- Binding Template Calculations	KS019- Viewing Graphs in Batch Mode
KMS020 -Enzyme Template Calculations	KS020- Ability to View Concentration vs. Time Data
KMS021- Convolution/Deconvolution Template Calculations	KS021- PK/PD Analysis and AUC Method
KMS024 - NCA Assistant Method in Non-Compartmental Calculation	KS022- Electronic Help System
KMS025- User Designed Model Fitting	KS023- Concentration-Time Modeling
KMS026- Fitting Multiple Profiles Simultaneously	KS025- Concentration-Time Modeling
KMS027 - Compare Kinetica Population PK/PD Analysis	KS026- Kinetica Dataset Column Filter Import
KMS028- Compare Kinetica Population PK/PD Analysis Multi Dose	KS029- Kinetica Macro Privileges

Test Scripts	Test Scripts
KMS029 - Compare Kinetica Population PK/PD Analysis results and testing data	KS030- Privilege-Based Ability to Perform Kinetica Clipboard Operations
KMS030-Population PK Validation Model (Standalone only)	KS031- Watson™ Import
KMS031 - Sparse AUC method to handle sparse sampling	KS032- Kinetica – Method/Insertion-Deletion
KMS032 - Rename Partial AUC checkbox	KS033- Kinetica™ – AUC
KMS033 - Compute last AUC triangle	KS034- Kinetica™ – Filter
KMS034 -Superposition method with variable dosing intervals	KS036- Kinetica™ – Graphing
KMS035- Output observed Clast from the AUC* method	KS038- Superposition and Modified Wagner
KMS036- Enable Text in the worksheet columns	KS039- PK/PD Analytical Study
KMS037 - AUC steady state with Lz	KS040- Kinetica Multiple X and Y imports
KMS038- Include a hard-coded method	KS041- Kinetica™ – Filter (Standalone Specific)
KMS039- SigmaPlot Interface	KS042- Kinetica License Expiration
KMS040- Mean Curve by Group graphical settings	KS043- Table structure for toxic kinetic study to list individual sparse data
	KS044- Descriptive statistics
	KS045- SAS transport file
	KS046- Allow user to insert their license
	KS047- Regroup and rearrangement of menu items
	KS048-Parsing of Spreadsheet data to the Kinetica Structure
	KS049- Changed variable name in study pane