

## PDxPop 5

The Companion Graphical Interface for NONMEM®

### Enhanced NONMEM population modelling & analysis

PDxPop software seamlessly integrates with existing tools and its own automated methods to expedite the iterative process of population pharmacokinetic modelling and analysis. Working in concert with NONMEM®, the “gold standard” in Population Pharmacokinetic and Pharmacokinetic-Pharmacodynamic modelling, R and/or S-Plus® for graphics and statistics and MS Word® and Excel®, PDxPop, available in Windows, Linux & Mac OS, delivers optimal flexibility with increased efficiency and functionality.

### PDxPop 5.2 is fully compatible and synergistic with NONMEM 7.3 and higher

#### New or Improved in PDxPop 5.2:

- Advanced NONMEM 7.3 run arguments as checkboxes and with a command line text box
- Enhanced run options for multiple estimation method runs gently stop single or batches of control stream runs, skip to next estimation method, choice to display numerical iterations or not during the run
- NONMEM 7.3 short-hand syntax (such as \$OMEGA VALUES (0.2,0.001) and \$THETA (0,2,100)x5) can be interpreted by PDxPop
- Standardised visual predictive check and Prediction corrected predictive check added
- Bootstrap evaluation employs NONMEM 7.3’s bootstrap method with stratification, and parses the job across multiple CPU’s

PDxPop 5.2 has been developed in accordance with a robust software development life cycle (SDLC) process with supporting documentation according to industry level quality standards. The software has been fully tested, is functioning as expected, is scientifically sound and fit for use for a graphical user interface for statistical analysis, and acceptable for release to customers.

- Diagnostic summary statistics and plots for the Bayesian analysis contain multiple quantile values and positions (2.5, 5, 10, 25, 50, 75, 90, 95, 97.5%)
- Control stream file wizards allow easy employment of new estimation options for PK and User Models
- Easily implement MPI or FPI parallelisation of NONMEM runs introduced in NONMEM 7.2
- Up to 100 CPUs can be utilised for multi-CPU problems
- Fully controllable Look-and-Feel for PDxPop GUI, allowing color palette and font size changes
- Easy access to Configuration Editor with keyboard shortcuts
- Easy access to switch between R and S-Plus using keyboard shortcut or mouse-clicks
- Creates both R and S-Plus plots simultaneously for all evaluation methods
- Able to install and register past (NONMEM 7.1.2) to present (NONMEM 7.3.0) to future NONMEM (NONMEM 7.9.0) releases

## Data Management Interface

- Quickly view, edit or plot data sets in MS Excel or R/S-Plus for initial exploration of data
- Easily perform a single split of a data set to create an index and validation data set for modelling and model validation steps or multiple splits for model evaluation methods

## Modelling Interface

- Implements NONMEM 7.3 additional command line arguments via the PDxPop GUI
  - Improved in PDxPop 5.2 are all NONMEM 7.3 additional command line arguments
- Wizard for NONMEM “parafiles” to control MPI & FPI parallel computing
- Run batches in parallel on multi-core systems to save time
- Create, sort, view, edit or copy control stream
- Automate the creation and error proofing of control stream files with control stream wizards or use a standard template
- Point-and-click to easily select, prioritise and compile the control streams to be run: individually or in batches
- View progress before analysis is complete through View Intermediate Results feature or real-time plotting of the objective function value or any model parameter as a function of the iteration number

## Output Interface

- Post-process NONMEM output not run from PDxPop for easy access to PDxPop graphical and statistical methods
- More efficiently utilise outputs, perform analyses, applying
- R/S-Plus and MS Excel functions
- Output is produced in formats designed to streamline the analysis and reporting process:
  - Standard NONMEM results with additional information on the control stream used
  - Enhanced Output Summary Results: including final estimates for theta, omega and sigma and their associated standard deviation, %CV, %RSE, intervals, AIC and SBC

- Fully automated diagnostic plots using R/S-Plus or MS Excel
- Automated R/S-Plus plots of estimated parameters (qqplots, histograms) and etas (pairs plots, histograms)
- Automated R/S-Plus plot comparisons between two runs
- Automated Bayesian parameter history plots
- Access Custom User-written R/S-Plus scripts from PDx-Pop

## Model Evaluation Interface

- WALD approximation methodology implemented to aid in covariate model building
  - Improved in PDxPop 5.2 to run in multi-CPU mode
- Automated bootstrap analysis to determine intervals of parameters – Improved in PDxPop 5.2 to run in multi-CPU mode
  - Improved in PDxPop 5.2 to access NONMEM’s \$SIM bootstrap capability along with its full range of arguments, e.g. STRAT and STRATF etc
- Automated objective function and to determine asymmetric confidence intervals
- Automated leverage analysis to determine model stability and influence of atypical individuals
  - Improved in PDxPop 5.2 to run in multi-CPU mode
- Automated random initial parameter estimate variation
  - Improved in PDxPop 5.2 to run in multi-CPU mode
- Automated Visual Predictive Check implementation
- Automated Multiple MCMC Chains
  - Improved in PDxPop 5.2 to run in multi-CPU mode
- More automated model evaluation features are being implemented with each new release

## Tracking & Audit Trail

- The Run Log tracks all steps in the analysis. View, print or save this important information as a file
- Maintain an electronic journal associated with the analysis to record important information: comments on runs, models used, decisions made on outputs, etc

## Tools and Utilities

- Initiate MPI registration via PDxPop toolbar
- Graphical NONMEM installation tool and Fortran compiler tester for all compilers supported by PDx-Pop
- PDF format PDxPop User Manual, support document, and “tool tips” accessible through the interface
- HTML and PDF version of NONMEM help accessible through the interface
- System diagnostics test to trouble-shoot potential configuration issues
- Library of NONMEM control streams and data for all standard NONMEM models

## System Requirements

### Platform

- Intel or AMD Pentium processor with minimum 1 GB of RAM (2 GB for Windows Vista or 7)
- Windows XP, Vista or 7, Linux (Ubuntu tested), or Mac OS X (Snow Leopard tested)
- Graphics card and monitor capable of minimum resolution of 1280x800
- CD-ROM disk drive
- Microsoft Mouse or other compatible pointing device.
- 100 MB free disk space for all required software (Interface space = 25 MB)
- ~100 MB of swap space/virtual memory.
- Linux and Mac OS versions have only R as visualisation tool

## Required Software

- NONMEM 7 Level 1.0 or higher
- Intel Visual Fortran\* (versions 8.0 or higher), GNU g95 (version 0.92! or higher), gfortran (version 4.5.0 or higher)
- MS Excel 97 or higher and Word 97 or higher
- Internet Explorer 7.0 or higher or any other browser

## Recommended Software

- R version 3.1.3 (or higher) or S-Plus for Windows 8.2 (or higher) required for model evaluation features)
- Xpose 4.0 for R or 3.104 for S-Plus (available at <http://xpose.sourceforge.net/>) \*Intel Visual Fortran requires Microsoft Visual Studio



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