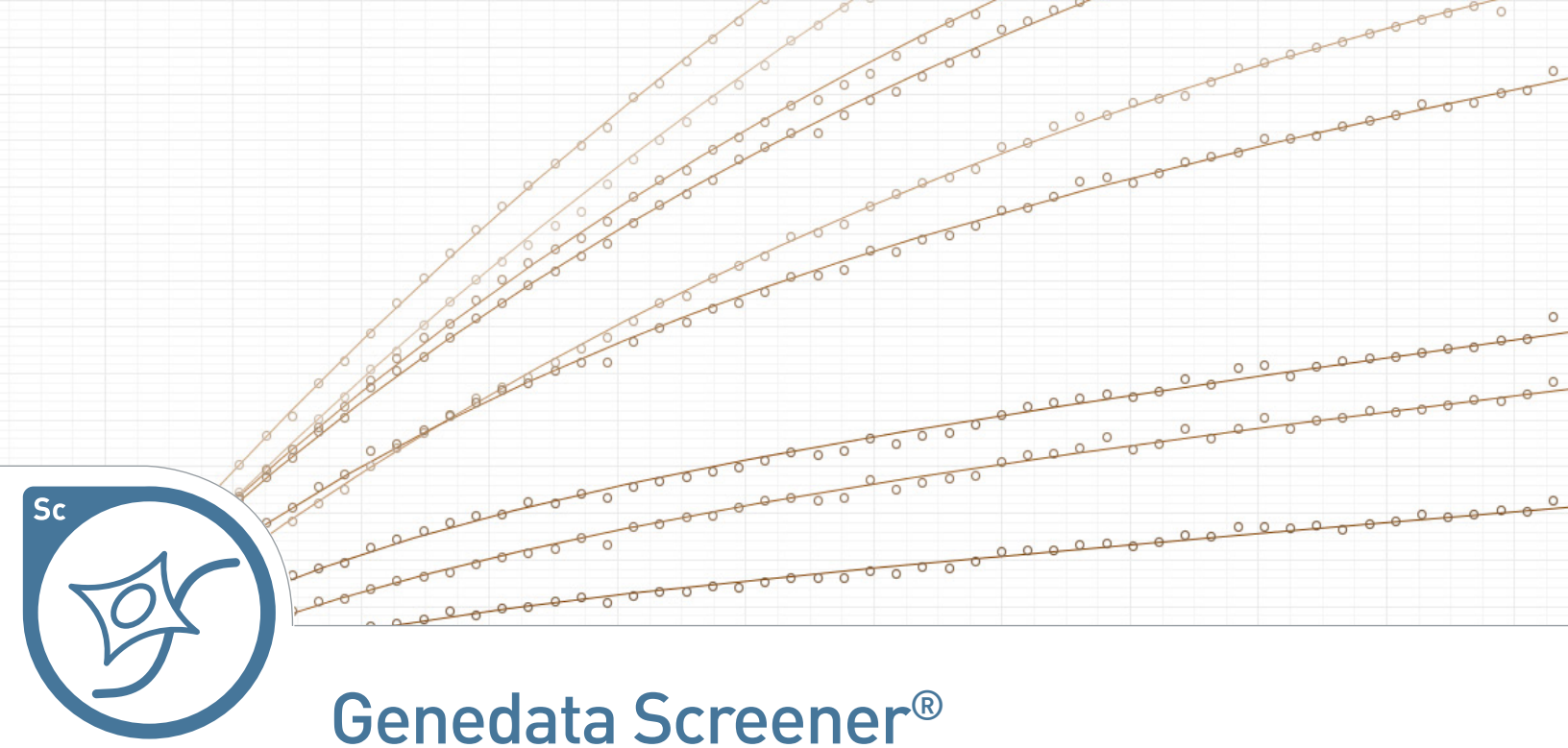
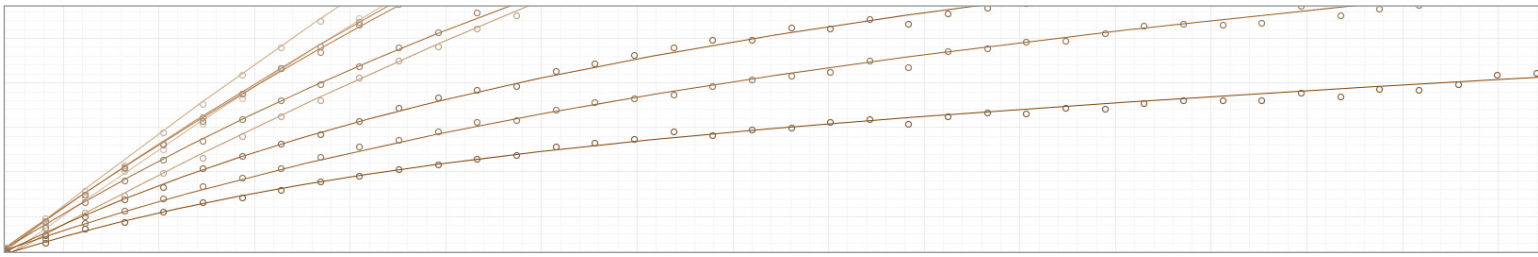


Genedata Screener®

for Mechanistic Analysis

Early inclusion of mechanistic information is becoming key for modern drug discovery programs. Kinetic information in particular increases the yield of high quality lead candidates by better selection and speeds up their propagation by instilling higher confidence in their potential. To supply this information, Genedata Screener allows processing of biophysical and mechanistic assays in scalable high throughput. The software reliably provides consistent results and makes all detailed mechanistic parameters available to project scientists across the organization.

Genedata
solutions in silico



Better Decisions

Screener for Mechanistic Analysis is designed to import the raw data from instruments providing kinetic information, analyzing binding curves from all your instruments in the same workflow. The software provides technology-specific methods and allows easy comparison between experiments. You can store original data and results centrally, automatically propagate them to your corporate data warehouse, and browse through all results from all experiments at sufficient detail from any corporate location.

Screener for Mechanistic Analysis brings full integration of your mechanistic data into your research process, helping decision makers everywhere make better decisions.

Consistent Results

With Screener, data reliability increases.

The automatic transfer of all mechanistic data eliminates manual cut and paste errors that easily occur when using spreadsheets. Following the automated data import, the analysis workflow is also set up to be consistent, so that all results are comparable between experiments, regardless of who has performed the analysis.

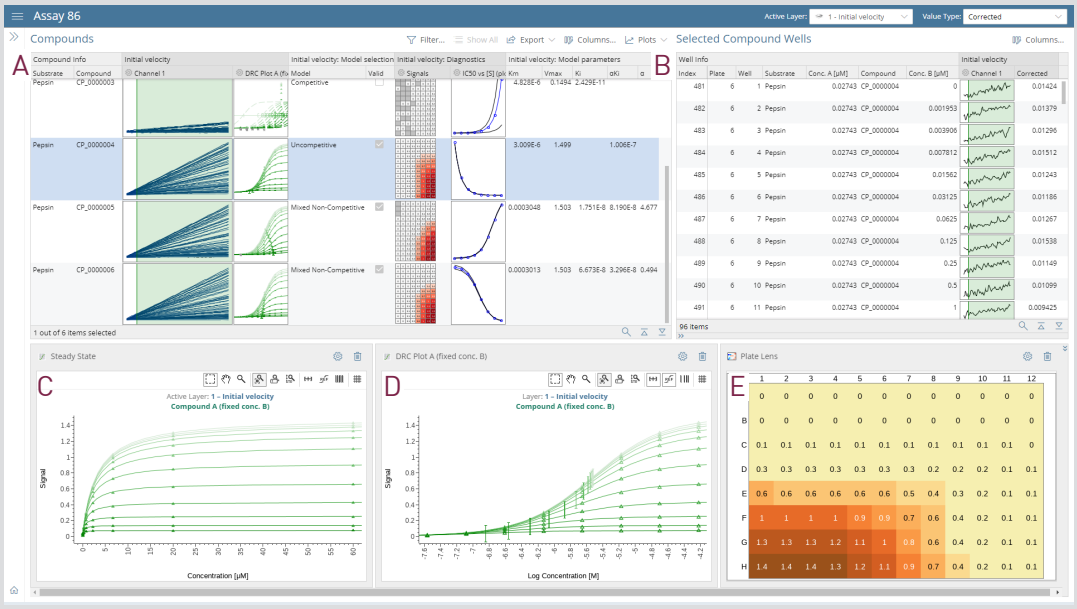
In addition, best-practice calculations and methods specifically designed for mechanistic analysis are available directly from the interface, ensuring that the same best-practice methods are used for all applicable analyses across the company.

Flexible Analysis

The correct balance between automation and flexibility is sometimes difficult to achieve. Genedata Screener solves this challenge by offering full automation combined with in-depth diagnostics, review, and re-processing options. Binding curves can be viewed next to final results and processing steps found sub-optimal can be adjusted interactively. New calculation methods can be added or edited by the user based on findings during the analysis.

This balance between automation and interactivity allows you to efficiently achieve high quality results that you can immediately share (including raw data) with your colleagues and collaborators.

Slow Inhibitor Binding Experiment



(FIG. 1) A modality of inhibition experiment in Genedata Screener.
A) The Compound Table displays the analysis results, which are based on fitted modality of inhibition. The model is automatically selected by Genedata Screener based on the data, but can also be manually overwritten by the user. Fit results include model validity, Km, Vmax, Ki and αKi.
B) The table shows the calculated slope of the progress curves for the selected compound wells.
C, D) The plot shows the fitted dose response curves. The points correspond to the calculated slopes and each curve stands for a fixed inhibitor concentration. The concentration axis is displayed in linear and logarithmic units respectively.
E) The plate lens shows the calculated slope for each well. It gives a graphical representation of the response over the dilution series.

Fast and Scalable

Desktop applications can work well when analyzing data at lower volumes, but as soon as experiments increase in number or size, these analysis methods do not scale.

With Screener for Mechanistic Analysis, the analysis of 50 compounds is as quick as the analysis of 5. Data loads and processes in seconds and views reload instantly. Method or data corrections are immediately implemented across the entire data set and high-level overviews allow you to easily review complete experiments.

All this enables time savings of up to 80% when going from spreadsheets and manual analysis to Genedata Screener.

Built-in Business Logic

Screener for Mechanistic Analysis builds on the proven screening analysis and workflow logic of Genedata Screener. Along with direct integrations with instruments used for mechanistic analysis, methods are included for applications such as kinetic probe competition assays (kPCA), kinetic analysis with one or two-step binding or reversibility, and competitive/non-competitive/uncompetitive modalities of inhibitor binding.

The open infrastructure of Genedata Screener also allows you to implement company-specific processing methods and business rules, so that you can always choose the optimal way to analyze your data.

Solution of Choice

The world's top pharma and contract research organizations rely on Screener for a streamlined analysis. Screener manages massive as well as complex data sets, and uncovers relevant information with powerful analysis methods.

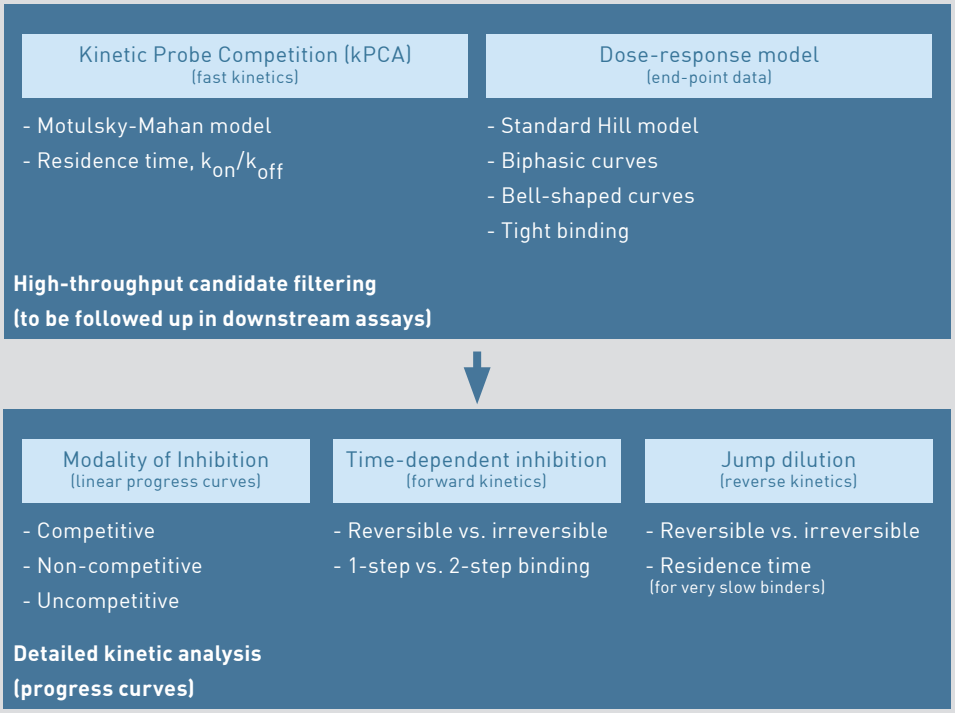
Screener for Mechanistic Analysis complements existing R&D data analysis pipelines, addresses challenges specific to this domain and feeds results back into the main discovery data stream. Furthermore, Screener makes the results accessible beyond the screening laboratory.

Supporting all in vitro screening, Genedata Screener improves screening productivity, eliminates redundancies, and drives innovative research.

Covering the Mechanistic Analysis Workflows

(FIG. 2) A schematic representation of the mechanistic analysis workflows with the respective types of experiments and analyses.

- *kPCA: Determines k_{on}/k_{off} and residence time early in the drug discovery process.*
- *Dose-response model: A portfolio of models allows an initial qualification of the type of binding observed.*
- *Modality of Inhibition: Classifies the modality of inhibition and calculates the affinity of compounds.*
- *Time-dependent inhibition: Determines kinetic parameters (using global or local fit models) of reversible and irreversible binders acting via a one- or a two-step process.*
- *Jump dilution: Complements the time-dependent inhibition analysis with confirmation or rejection of reversibility status and the determination of k_{off} for very slow binders.*



Genedata Screener

Genedata Screener analyzes, visualizes, and manages screening data from in-vitro screening assay technologies across the enterprise, including very complex as well as ultra-high throughput experiments. Its screening-oriented business logic enables rapid processing and comprehensive analysis of complete campaigns.

Services and Support

Genedata offers a range of services and support, from installation and customization of Screener to global roll-out support, training, data analysis, application consulting and IT consulting services, all tailored to the specific needs of your organization. Our services team consists of highly skilled professionals with extensive domain knowledge in screening and software technology, bringing specialized know-how and experience to your organization.

Experienced Partner

With nearly two decades of experience in industrial screening data analysis and global enterprise deployments of Genedata Screener, Genedata is an ideal collaboration partner for companies wanting to advance their screening operations. In addition to the steadily evolving Screener software, Genedata offers extensive opportunities for custom or co-development of specific new functionalities, procedures, or methodologies to support your current and future needs.

Next Steps

To find out more about Genedata Screener, please visit www.genedata.com/screener.

For a conversation about your screening analysis needs or to schedule a live demonstration, please contact us at screener@genedata.com.

Genedata Screener® is part of the Genedata portfolio of advanced software solutions that serve the evolving needs of drug discovery, industrial biotechnology, and other life sciences.

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