



# Insilico Discovery™ – Test Your Hypotheses and Predict Cellular Responses

Insilico's mission is to shorten and simplify the product development processes of its customers by facilitating the quantitative analysis and prediction of cellular responses *in silico*. For this purpose, Insilico continuously develops high-end software tools, of which Insilico Discovery<sup>™</sup> is the tool of choice for modelling and simulation experts.

For both biotechnological process development as well as safety and efficacy testing of new drugs, it is of utmost importance to understand the mechanisms in the cell which lead to the observed phenotype. With Insilico Discovery<sup>™</sup>, it is possible to build compartmentalised network models reflecting these intracellular mechanisms. »Omics« data such as gene sequence, transcript, metabolite and protein data can be integrated into one Insilico Cell<sup>™</sup> model and analysed from a systems point of view.

Established steady-state as well as dynamic simulation methods allow to quantify uptake and excretion rates as well as intracellular fluxes and metabolite concentrations. In addition to that, Insilico Discovery<sup>™</sup> provides the option to test millions of different cellular scenarios automatically and predict how the cell will likely respond. This is helpful especially in applications which otherwise would mean vast amounts of lab work, e.g. systematic testing of gene targets and their combinations in metabolic engineering. Depending on the complexity and number of tests, computing resources can be flexibly utilised from desktop use to external high-performance computing at one of Europe's fastest computer clusters.



#### **Key Features**

Reconstruction and Visualisation of Compartmented Genome-Based Metabolic Networks

Link to Gene Regulation and Signalling Networks

Over 8,000 Biochemical Reactions Covered

Integration of All Kinds of »Omics« data

Detailed Quantification, Analysis and Visualisation of Intracellular Fluxes

Prediction of Cellular Response to Changes in External or Internal Conditions

Access via Secure Web Services

High-Performance Computing with up to 100,000 Processors

Training Workshops Available

#### Key Benefits

Gain Deepened Understanding of Cellular Mechanisms

Save Lab Work by Testing Different Scenarios at the Computer

Identify the Most Promising Actions to Be Taken in Bioprocess Optimisation

Enhance Drug Safety and Efficacy

**Claim Novel Intellectual Property** 

**Reduce Development Risk** 

Shorten Time to Market

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### Insilico Discovery™

Our software product Insilico Discovery<sup>™</sup> is a core component of Insilico's technology platform and can be licensed for in-house use.

Insilico Discovery<sup>™</sup> comprises three different modules allowing for (i) model reconstruction, (ii) integration and visualisation of experimental data and (iii) simulation of network models. Simulation methods include transient <sup>13</sup>C flux analysis, Metabolic Flux analysis (MFA), Flux Balance Analysis (FBA), Minimisation of Metabolic Adjustment (MOMA) and simulation of kinetic differentialalgebraic systems.

Our customers benefit from Insilico Discovery<sup>TM</sup> by achieving their goals with less time and effort, while at the same time improving their insights into cellular mechanisms.

#### Selected features of Insilico Discovery™

Insilico Discovery<sup>™</sup> is the software tool of choice for customers interested in:

- the reconstruction and visualisation of compartmented genome-based metabolic networks via an easy-to-use graphical user interface
- the detailed quantification and analysis of intracellular flux distributions
- predicting concentrations of intra- and extracellular metabolites
- identifying bottlenecks in cellular reaction pathways
- predicting the effect of single and multiple gene perturbations
- access to high performance computer clusters with up to 100,000 processors, facilitating different complex computations in parallel
- browsing the results of Insilico's network solutions.

With Insilico Discovery<sup>™</sup>, users can run hypothesis tests in silico. This example shows simulated effects of three overexpression and downregulation scenarios of selected metabolic genes (green, black, red) in comparison to initial process characteristics (blue dots). Scenarios with low by-product and high product yield (red) will be recommended for implementation, thus sparing our customers tedious consecutive wet-lab experiments.



**Insilico Biotechnology** is a market-leading company providing solutions and software for the simulation of living cells. An interdisciplinary team of experts offers customised solutions for the efficient manufacturing of biotechnological products and for the testing of pharmaceuticals by using high-performance computing and Insilico's proprietary software platform. For world-leading companies from the chemical and pharmaceutical industries, Insilico's technology lowers time, risk and costs of development processes. Founded in 2001, Insilico is a privately held company based in Stuttgart, Germany.