GERMAN NETWORK FOR BIOINFORMATICS INFRASTRUCTURE

de.NBI/ELIXIR-DE projects at Heidelberg University

Frank T. Bergmann, Leonid Kostrykin, Ursula Kummer, Karl Rohr, on behalf of all PIs at
Heidelberg University, Heidelberg, Germany

Contract Nr. W-de.NBI-016

Summary: The project encompasses the following ELIXIR-Resources: COPASI, KNIME, Galaxy Image Analysis, Precog and Mechnetor, as well as the maintenance of and service via the de.NBI-Cloud at Heidelberg University. In addition, OmniPath, a resource for knowledge of intra- and intercellular signaling has been supported and an ELIXIR-Officer was financed. Finally, training in the context of each of these resources has been conducted.

COPASI (PI Kummer, Bergmann)

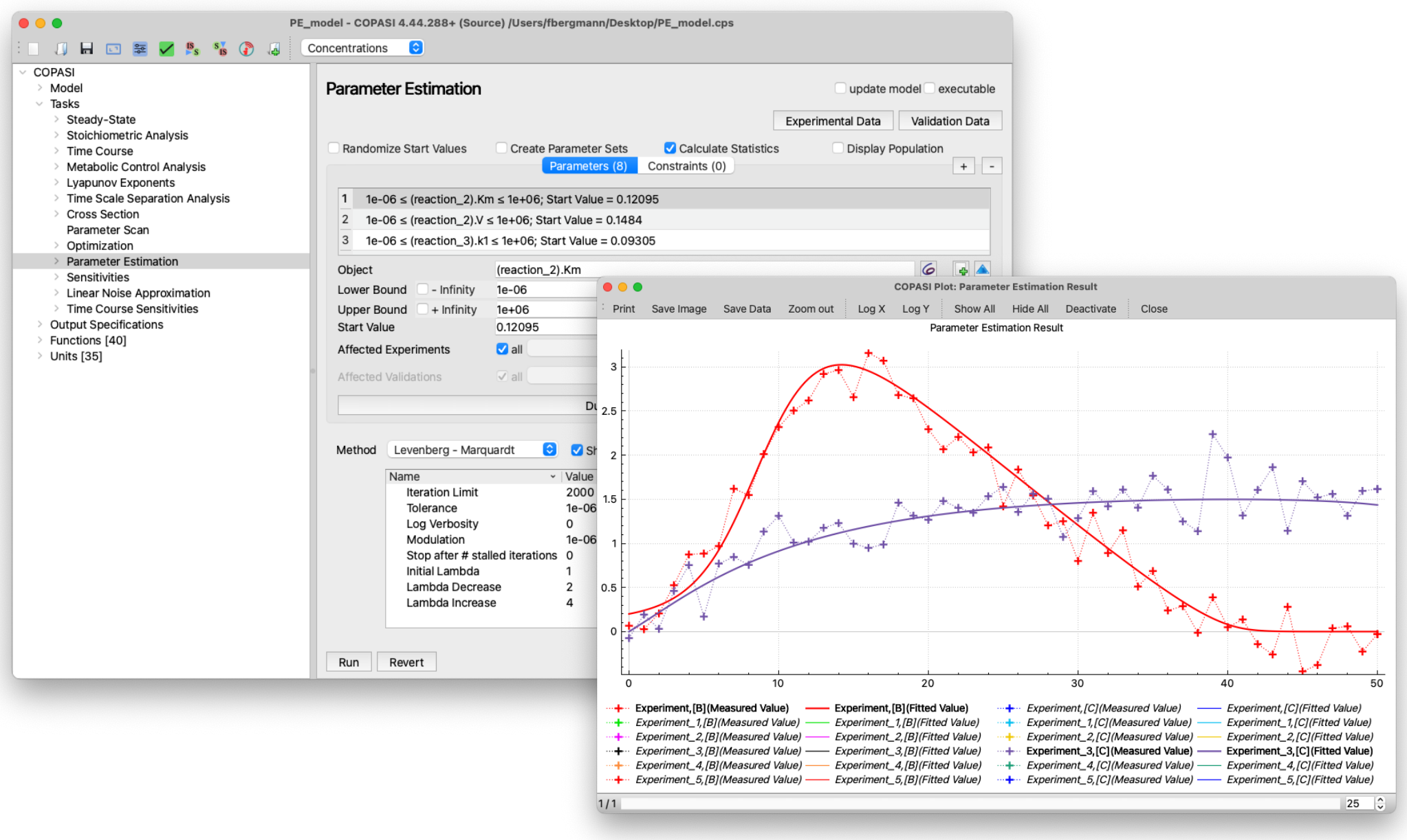
COPASI (Hoops et al., 2006, Mendes et al., 2009), developed in the group of Ursula Kummer at Heidelberg University, together with the group of Pedro Mendes (Connecticut, USA), is a systems biology software that integrates standard and novel algorithms for the modeling, simulation and analysis of process-based non-spatial models, mostly at the cellular level. COPASI supports both ODE-based as well as stochastic (discrete particle based) formalisms. In addition, COPASI features include steady state calculation, sensitivity analyses, optimization, parameter fitting, parameter scanning and computing nonlinear dynamical systems properties such as Lyapunov exponents, among others

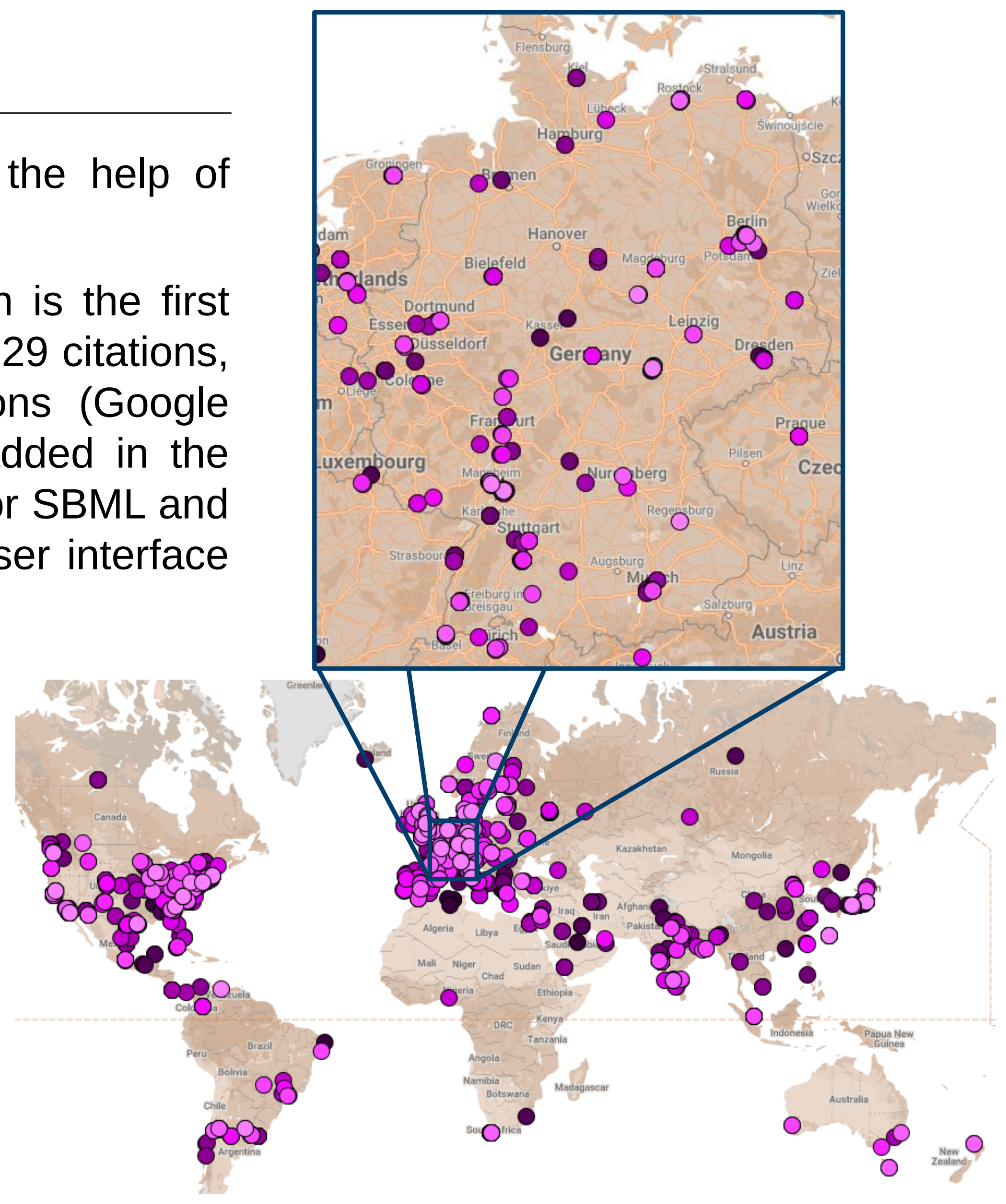
In the reporting period we released six new versions of COPASI and track their download numbers through GitHub. These releases had a total download of 556.962 times. We offered 4 training courses / workshops on COPASI. Our user forum has currently 458 registered members. In the reporting period we had 243 posts on the forum.

Recent Publication:
Bergmann FT, (2023). BASICO: A simplified Python interface to COPASI. Journal of Open Source Software, 8(90), 5553.

We continue to monitor publications produced with the help of COPASI on our website at http://copasi.org/Research.

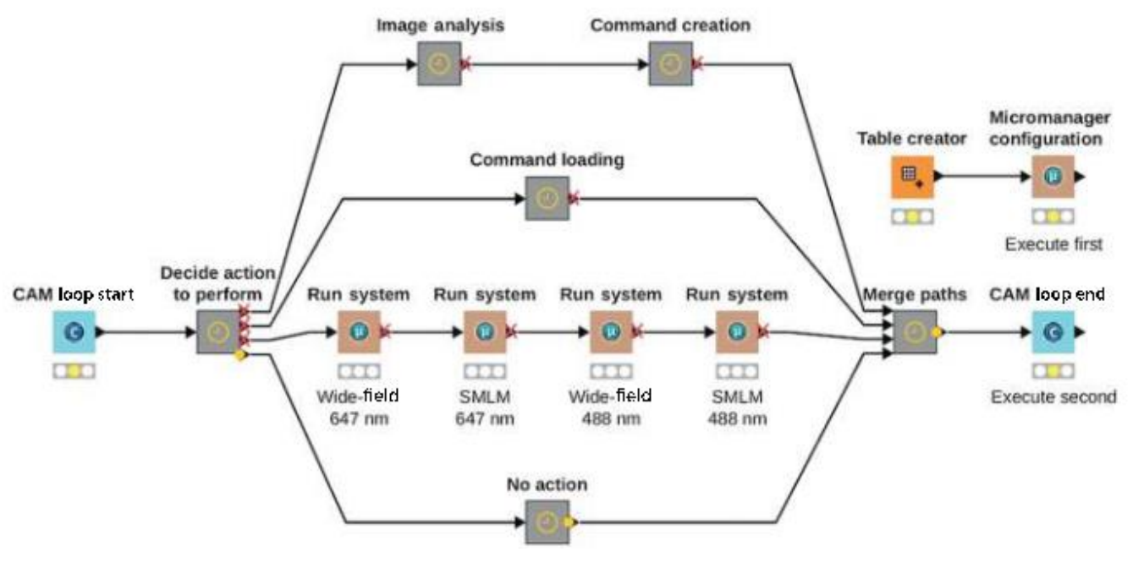
Citations of Hoops et al., Bioinformatics (2006) which is the first publication on COPASI: 2023 – 167 citations, 2024 – 129 citations, total citations of the origin publication: 3057 citations (Google Scholar) or 1768 (Web of Science). New features added in the reporting period, include enhanced standard support for SBML and SED-ML, improved plotting capabilities and general user interface improvements.





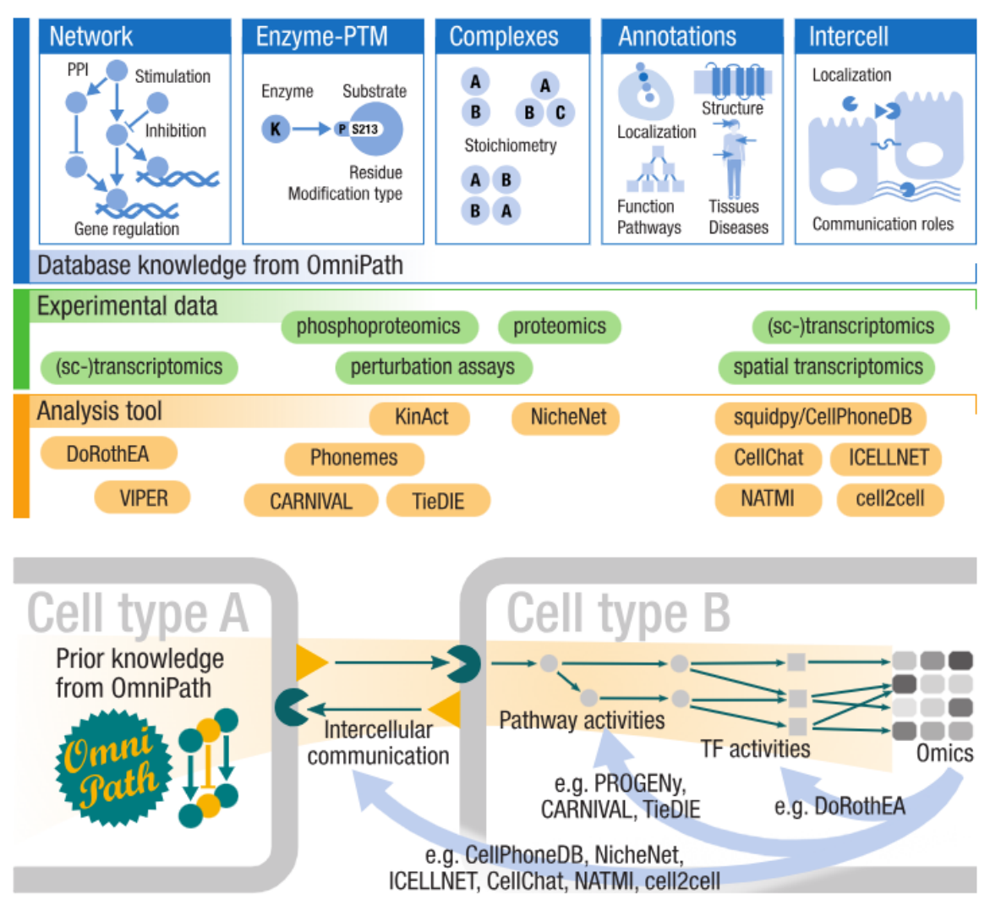
KNIME (PI Erfle):

During the project, automated image analysis workflows were developed and extended in the analysis platform KNIME with special focus on systemic phenotyping of cells. The developed workflows allow users to perform high-throughput analysis of microscopy data, without the need of extensive programming or image analysis know-how.



OmniPath (PI Saez-Rodriguez):

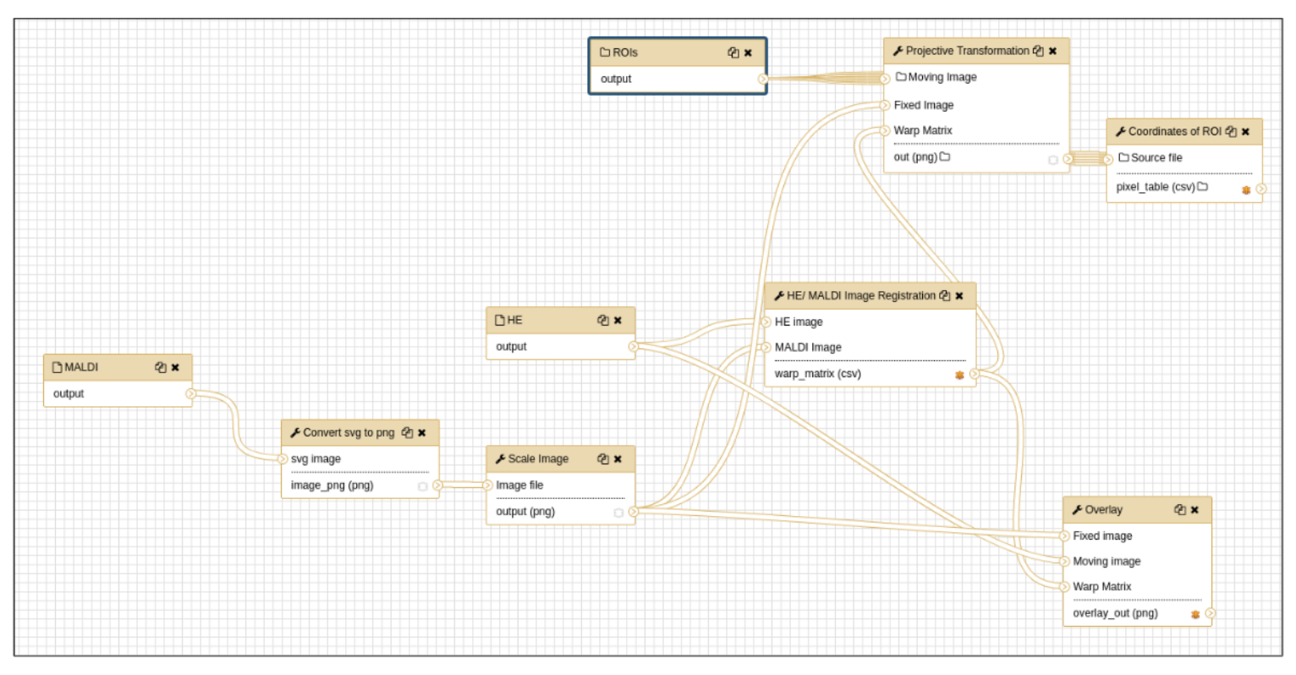
OmniPath is a comprehensive database of molecular biology knowledge. It integrates data from over 100 resources, covering protein-protein and gene regulatory interactions, enzyme-PTM relationships, protein complexes, protein annotations, and intercellular communication. This database is particularly useful for building and analyzing signaling networks, which can help in understanding and treating diseases like cancer and fibrosis.



Galaxy Image Analysis (PI Rohr, Kostrykin):

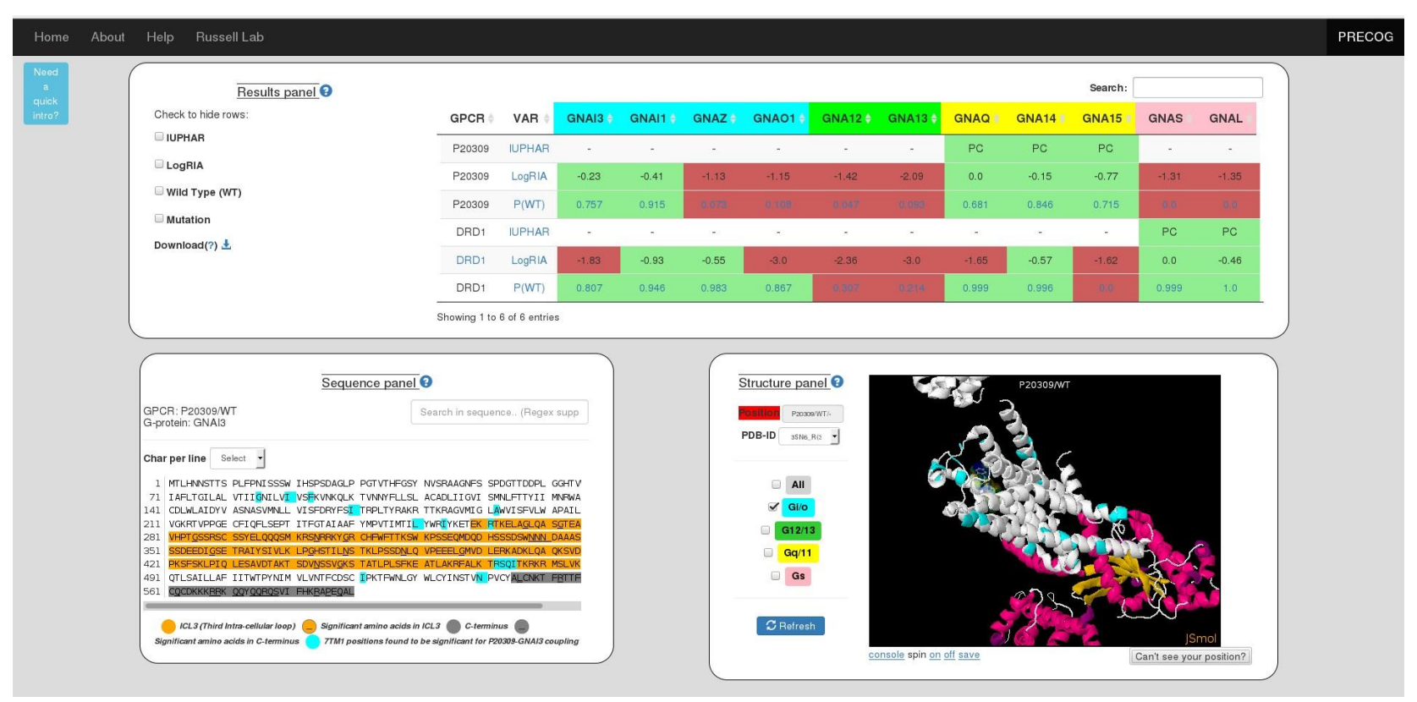
Dr. Leonid Kostrykin (ELIXIR Germany Officer of HD-HuB) contributed tools and software packages for Galaxy Image Analysis (GIA) and Conda. GIA is an ELIXIR Service for web-based analysis of microscopy images and is available on the European Galaxy Server. From January 2023 to October 2024, four Conda packages were added or updated, reaching more than 16.000 downloads. In total, all our contributed Conda packages had more than 2.500.000 downloads in this period. GIA was extended by more than 10 tools and more than 30 tools were updated. The developed tools are deployed via the de.NBI-Cloud.

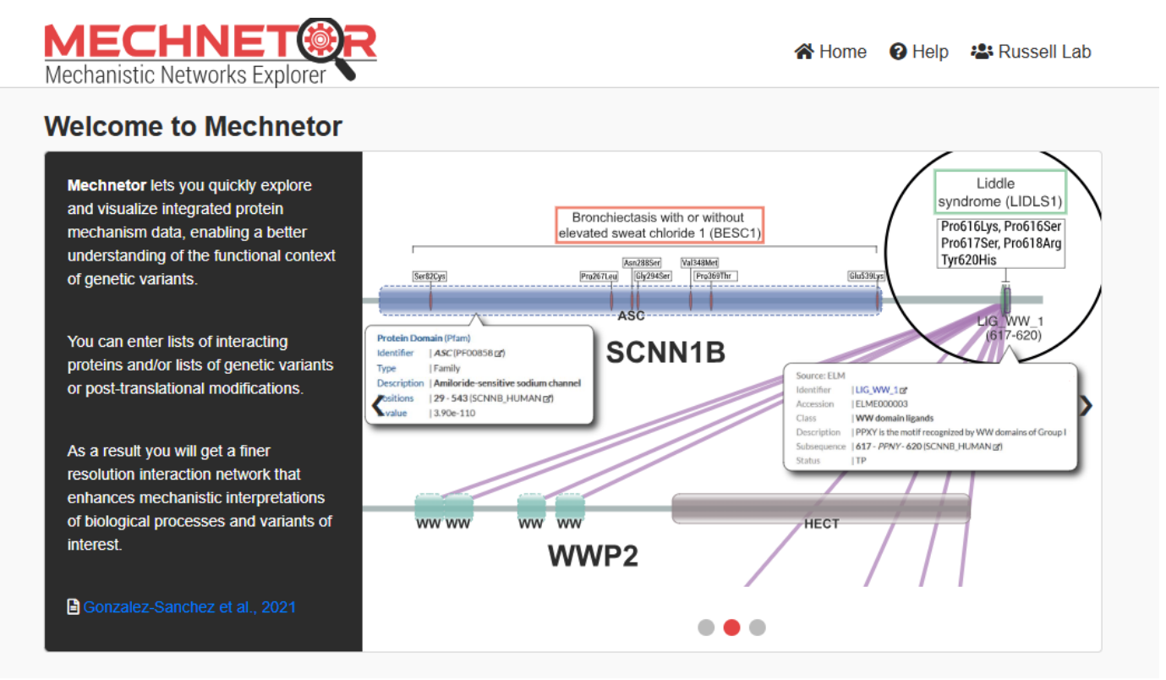
Tutorials on the Galaxy Training Network were updated and extended, and a de.NBI training course on microscopy image analysis was given. Dr. Leonid Kostrykin is active in several entities (ELIXIR Galaxy Community, ELIXIR Tools Platform, EuroBioimaging FAIR Image Data Workflows Expert Group) and contributed to several events (European Galaxy Days 2023, ELIXIR BioHackathon Europe 2023, NFDI4BIOIMAGE Hackathon Next Generation Bioimage Analysis Workflows 2023, Galaxy Community Conference 2024, ELIXIR BioHackathon Europe 2024). His contributions to the Galaxy platform were recognized in the recent overview paper authored by the Galaxy Community (Nucleic Acids Research 2024).



Precog and Mechnetor (PI Russell):

PRECOG (Predicting coupling probabilities of G-protein coupled receptors) lets you predict coupling probabilities of Class A GPCRs to 11 G-proteins based on input sequence information (either WT or mutated)





Mechnetor is designed to explore and visualize integrated protein mechanism data, helping to understand the functional context of genetic variants.

Finances:

LIBIS which is financed by the MWK in Baden-Württemberg and comprises the own contribution to de.NBI finances the tools, whereas money from the FZJ is used for the de.NBI-Cloud, teaching activities and ELIXIR-activities.
The position of **Dr. Leonid Kostrykin** as the ELIXIR Germany Officer of HD-HuB is provided via FZJ.

GEFÖRDERT VOM
Bundesministerium für Bildung und Forschung