

# Services for Systems Biology: Software packages CellNetAnalyzer (CNA) and CNAPy

de.NBI-SysBio

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## Short description of the project

Methods and integrated software tools supporting the construction, simulation, and analysis of **mathematical models of biological systems** are an important field of bioinformatics. As part of the **de.NBI-SysBio** service center, this project provides user services for the comprehensive software packages CellNetAnalyzer (CNA) and CellNetAnalyzer for Python (CNAPy), which both enable a GUI-based analysis of metabolic and other cellular networks.

## de.NBI services

CellNetAnalyzer (CNA; runs with MATLAB) and CNAPy (runs with Python) are two comprehensive packages with a **GUI** and an extensive **library of (partially unique) algorithms** for the systems biology analysis of cellular networks. Various methods are provided for exploration, analysis and computational design of **metabolic networks** based on **constraint-based modeling techniques**. In CNA, **regulatory and signal transduction networks** can also be modeled and analyzed using formalisms such as **interaction graphs, logical (Boolean) networks and logic-based differential equations**. The GUIs in CNA and CNAPy rely both on the concept of **interactive network maps** while CNAPy provides many more advanced features for an interactive exploration of metabolic network models. CNA and CNAPy offer also an **API** for a command line mode and are widely used in teaching and research.

## Progress report

- Several **new versions** of our software packages CNA and CNAPy have been released in the last two years providing various new and extended features. This includes:
  - The integration of the **StrainDesign** package [3] in CNAPy could be finished. Another functional extension of CNA and CNAPy concerns balancing of biomass reaction stoichiometry and measured fluxes in FBA published in [4].
  - Escher metabolic network maps** can be used and edited in CNAPy.
  - The installation procedure for CNAPy has been significantly simplified. It is now also available on PyPI.
  - Extended functionalities in connection with scenarios in CNAPy.
- Apart from workshops and training courses (see below), we provided extended user support such as answering specific questions or inquiries via emails, phone calls, or communications in the user forum.
- We are members of the ELIXIR Community “Microbial Biotechnology”.
- A presentation on CNAPy was also given at the Metabolic Pathway Analysis conference 2023 in Seoul.

## de.NBI training and education

We offered several training courses and workshops (partially jointly with other members of de.NBI-SysBio):

- 13-14 June 2023 (in Riga, Latvia): Workshop on CNA and CNAPy at the “Biomodeling Spring school”
- 28-30 Nov 2023 (in Magdeburg): “Tools for Systems biology modeling and data exchange: CellNetAnalyzer, COPASI, SABIO-RK, FAIRDOMHub/SEEK”
- 7 Feb 2024 (in Lisbon; workshop as part of the OLISSIPO winter school): “Constraint-based modeling and design of metabolic networks with CellNetAnalyzer and CNAPy”
- 5-6 Nov 2024 (online): “Constraint-based modeling and design of metabolic networks with CellNetAnalyzer and CNAPy”

## Publications

[1] von Kamp A, Thiele S, Hädicke O, Klamt S (2017) Use of CellNetAnalyzer in metabolic engineering and biotechnology. *Journal of Biotechnology* 261:221-228.

[2] Thiele S, von Kamp A, Bekiaris PS, Schneider P, Klamt S (2022) CNAPy: a CellNetAnalyzer GUI in Python for analyzing and designing metabolic networks. *Bioinformatics* 38:1467-1469.

[3] Schneider P, Bekiaris PS, von Kamp A, Klamt S (2022) StrainDesign: a comprehensive Python ackage for computational design of metabolic networks. *Bioinformatics* 38:4981-4983.

[4] von Kamp A, Klamt S (2023) Balancing biomass reaction stoichiometry and measured fluxes in flux balance analysis. *Bioinformatics* 39:btad600.

## General information on the project

- 0.5 FTE paid by de.NBI (+ 0.5 FTE „Eigenbeitrag“ from MPI)
- 1 FTE from MPI

