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Practical Work: Free and Open Source Software

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PART 1 –Theoretical Study of the Tool: CellDesigner

1. General presentation of the tool

CellDesigner is a free and open-source software used for the graphical modeling and visualization of biochemical networks and cellular processes. It provides a graphical user interface that allows users to represent molecular interactions in a clear and structured manner. CellDesigner is mainly used in the field of systems biology to describe and analyze complex biological mechanisms inside the cell.

(Source: CellDesigner Official Website; Funahashi et al., 2008)

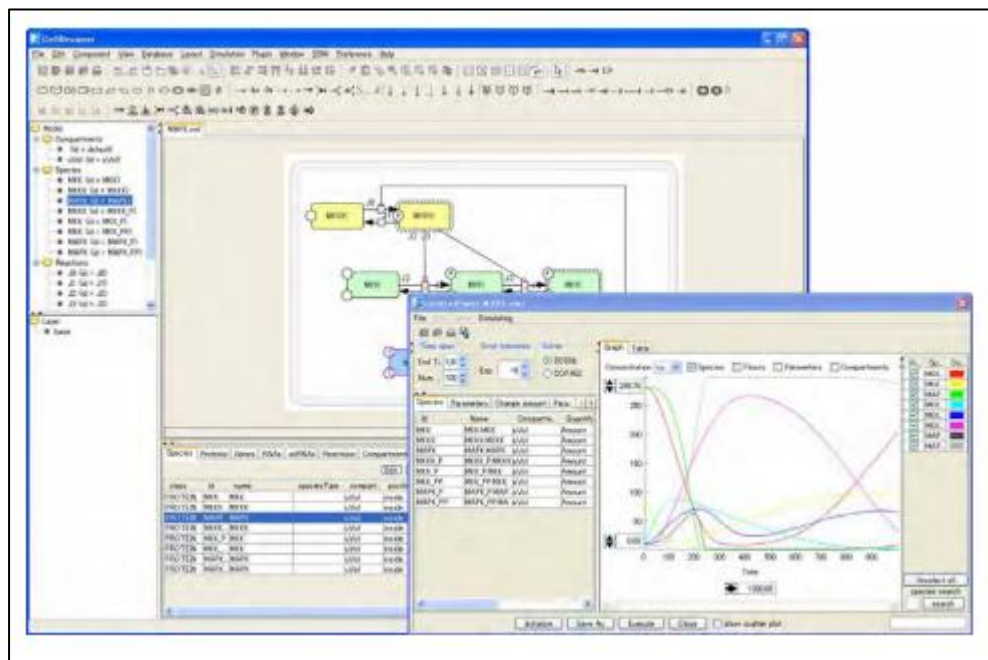


Figure 1. Graphical user interface of CellDesigner showing elements used for modeling biochemical networks. (Source: CellDesigner Official Startup Guide)

2. Main functionalities

CellDesigner offers several functionalities for modeling biological systems. It allows users to draw biochemical reaction networks, including metabolic pathways and signaling pathways. The software supports the representation of molecules, reactions, and their interactions using standardized graphical symbols. In addition, CellDesigner enables the creation, import, and export of models in the Systems

Biology Markup Language (SBML) format, which facilitates model sharing and interoperability with other systems biology tools.

(Source: CellDesigner Documentation; Funahashi et al., 2008)

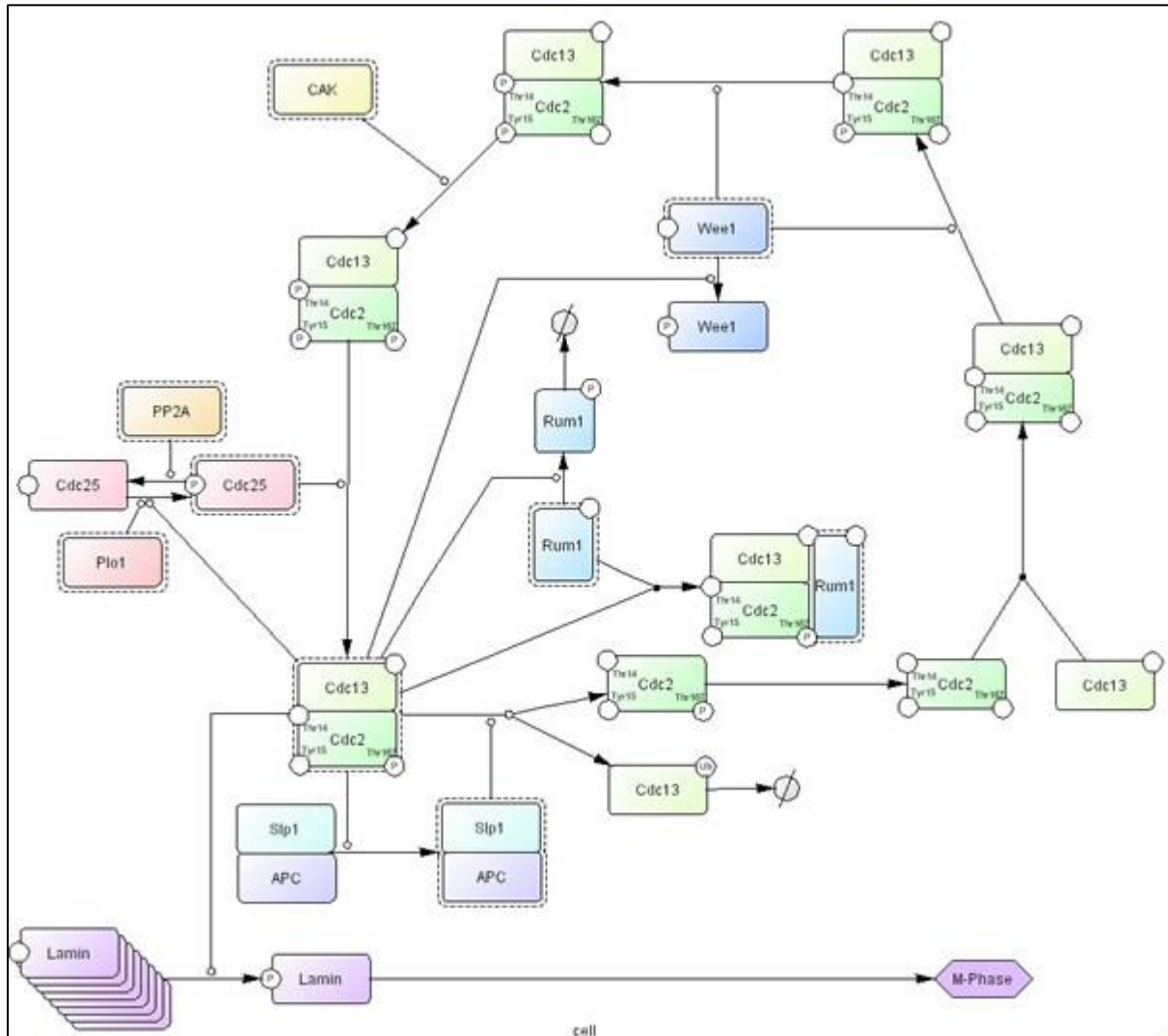


Figure 2. An example of a process diagram representation in CellDesigner illustrating biochemical reactions and molecular state transitions.

(Source: CellDesigner Process Diagram Documentation)

3. Technical aspects

CellDesigner is a free software developed using the Java programming language. It is a multiplatform tool that can be used on Windows, Linux, and macOS operating systems. The software supports the Systems Biology Markup Language (SBML), which allows biological models to be exchanged with other systems biology tools.

CellDesigner is also compatible with the Systems Biology Workbench (SBW) environment.

(Source: CellDesigner Official Website; CellDesigner Documentation)

4. Strengths

CellDesigner has several strengths that make it a useful tool in systems biology. One of its main advantages is its graphical user interface, which allows users to model biological networks without the need for programming skills. The use of standardized symbols improves the clarity and readability of the models. In addition, CellDesigner is widely used in academic research and education, which contributes to its reliability and availability of documentation.

(Source: CellDesigner Official Website; Funahashi et al., 2008)

5. Limitations and weaknesses

Despite its strengths, CellDesigner has some limitations. The software primarily focuses on the graphical representation of biochemical networks and does not provide advanced computational simulation capabilities directly within the tool. As a result, users often need to export models to other specialized software to perform detailed simulations and quantitative analyses. In addition, managing and visualizing very large and complex networks can become challenging.

(Source: Funahashi et al., 2008; CellDesigner Documentation)

6. Conclusion

In conclusion, CellDesigner is a powerful and accessible tool for the graphical modeling of biochemical networks and cellular processes. Its strengths lie in its user-friendly interface, standardized symbols, and wide adoption in academic research and education. However, its limitations include restricted computational simulation capabilities and challenges with very large networks. Overall, CellDesigner remains a valuable resource for researchers and students in the field of systems biology, particularly for visualizing and understanding complex biological interactions.

(Source: Funahashi et al., 2008; CellDesigner Official Website)

PART 2 – Practical Study

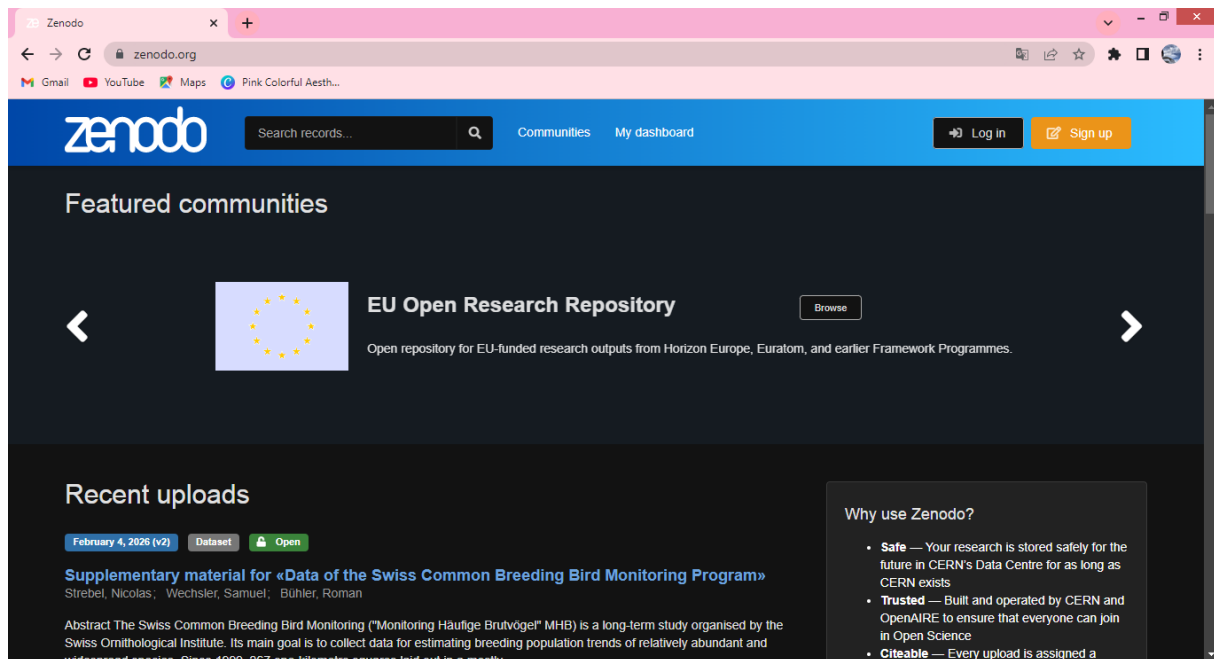
1. Presentation of Zenodo

Zenodo is an open-access research data repository developed by CERN and supported by the European Open Science Cloud. Its main objective is to allow researchers to share, preserve, and make accessible scientific outputs such as datasets, publications, software, and presentations. Zenodo supports open science by providing free access to research results and assigning a Digital Object Identifier (DOI) to each uploaded record.

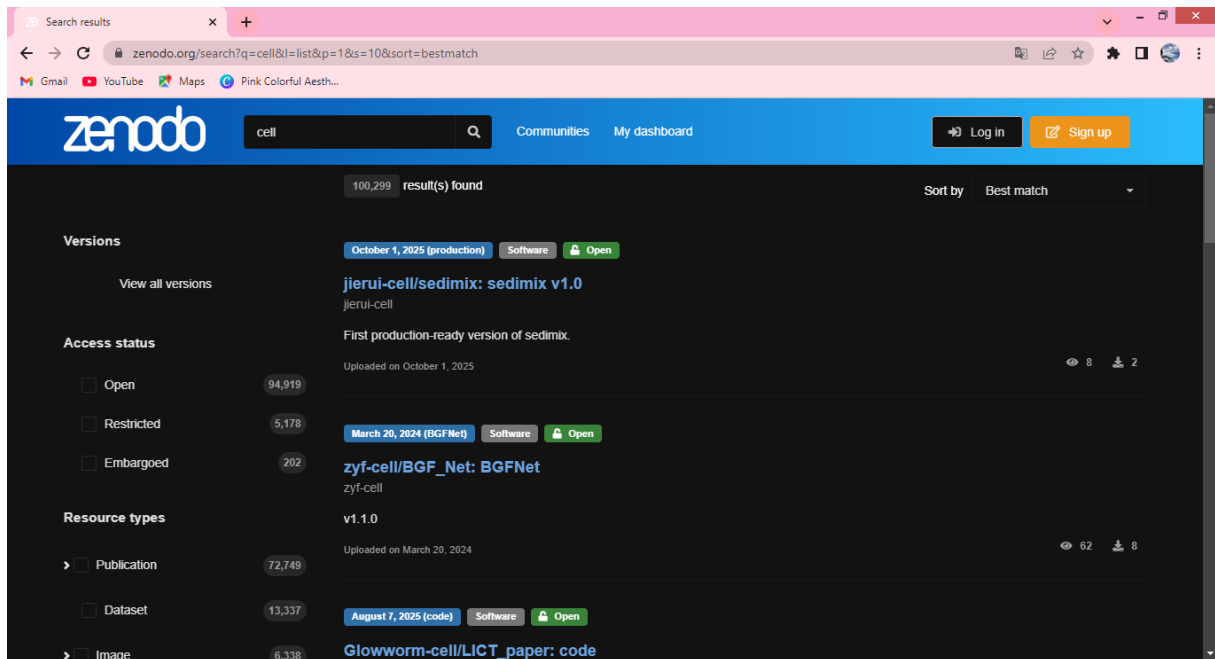
Zenodo hosts different types of content, including datasets, research articles, software code, images, and posters. It is widely used in natural and life sciences, as it enables researchers to share biological and biomedical data in a structured and transparent way. By promoting data sharing and long-term preservation, Zenodo plays an important role in open science and scientific collaboration.

2. Description of the steps carried out

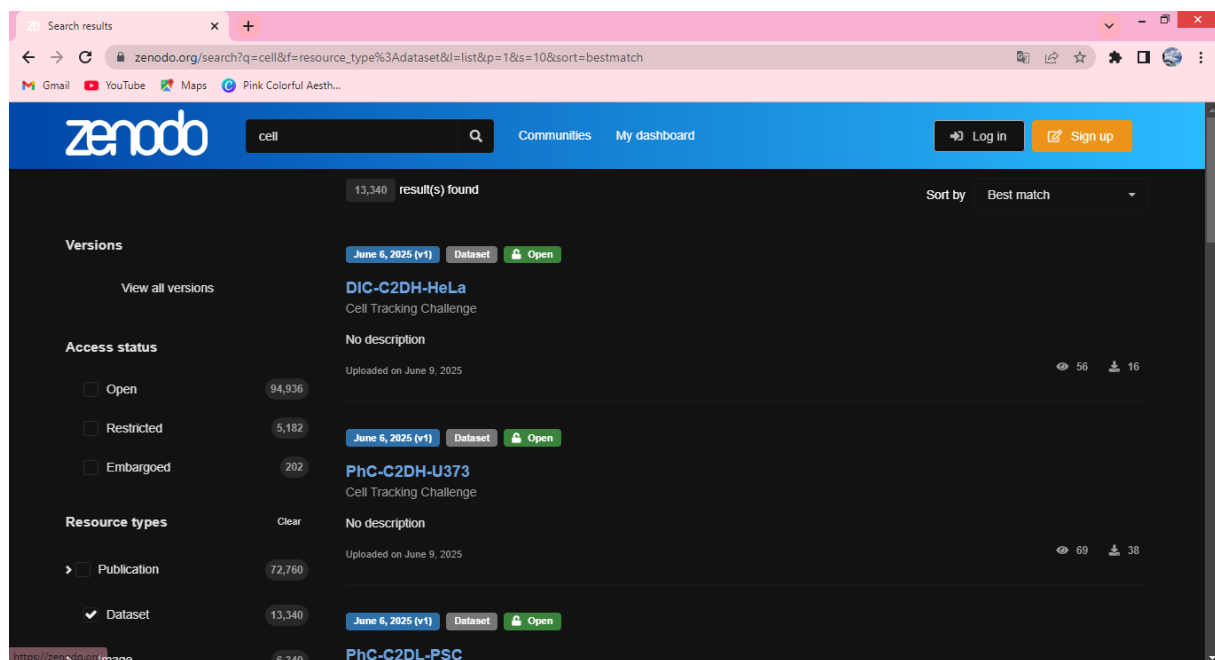
- The Zenodo platform was accessed through its official website (<https://zenodo.org/>). The homepage provides access to search tools, recent uploads, and different categories of scientific content.



- A search was performed on the Zenodo platform using the keyword "cell" in order to find datasets related to cellular biology.



- To focus only on datasets, a filter was applied by selecting the Resource type "Dataset".



- A relevant dataset related to cellular biology was selected based on the clarity of its description and the availability of complete metadata.

The screenshot shows the Zenodo record page for a dataset. The header includes the Zenodo logo, a search bar, and navigation links for 'Communities' and 'My dashboard'. The dataset is published by Dryad on February 1, 2013, and is version v1. The title is 'Data from: RNAi screening reveals a large signaling network controlling the Golgi apparatus in human cells'. The authors listed are Chia, Joanne; Goh, Germaine; Racine, Victor; Ng, Susanne; Kumar, Pankaj; and Bard, Frederic. The dataset has 160 views and 934 downloads. The description states: 'The Golgi apparatus has many important physiological functions, including sorting of secretory cargo and biosynthesis of complex glycans. These functions depend on the intricate and compartmentalized organization of the Golgi apparatus. To investigate the mechanisms that regulate Golgi architecture, we developed a quantitative morphological assay using three different Golgi compartment markers and quantitative image analysis, and performed a kinome- and phosphatome-wide RNAi screen in HeLa cells. Depletion of 159 signaling genes, nearly 20% of genes assayed, induced strong and varied perturbations in Golgi morphology. Using bioinformatics data, a large regulatory network could be constructed. Specific subnetworks are involved in phosphoinositides regulation, acto-myosin dynamics and mitogen activated protein kinase signaling. Most gene depletion also affected Golgi functions, in particular glycan biosynthesis, suggesting that signaling cascades can control glycosylation directly at the Golgi level. Our results provide a genetic overview of the signaling pathways that control the Golgi apparatus in human cells.'

- The selected dataset was downloaded directly from the Zenodo platform using the download option provided on the dataset page.

The screenshot shows the 'Files' section of the Zenodo record page. It displays a table of files with columns: Replicate, Well, GeneSymbol, Site, index, selected, seg.nbPixels, seg.center.x, and seg.center.y. The table lists 9 files, all with 'Rep1' as the replicate and '003' as the well. The 'GeneSymbol' column lists 'Monensin' for all entries. The 'index' column ranges from 3 to 9. The 'selected' column shows values like 1.000000e+000, 0.000000e+000, and 0.000000e+000. The 'seg.nbPixels' column ranges from 8.355000e+003 to 8.070000e+003. The 'seg.center.x' column ranges from 1.902437e+003 to 6.421317e+002. The 'seg.center.y' column ranges from 1.64861e+003 to 1.35681e+003. Below the table, there is a 'Download all' button. To the right of the table, there is a 'Keywords and subjects' section with the following keywords: Glycosylation, Golgi, RNAi screening, and Imaging. Below this, there is a 'Details' section with the DOI '10.5061/dryad.1m2p3', the resource type 'Dataset', and the publisher 'Zenodo'. At the bottom, there is a 'Rights' section with the license 'Creative Commons Zero v1.0 Universal'.

3. Dataset metadata

Table 1. Metadata of the selected dataset according to the Dublin Core standard.

Metadata Element	Information
Title	Data from: RNAi screening reveals a large signaling network controlling the Golgi apparatus in human cells
Creators	Joanne Chia, Germaine Goh, Victor Racine, Susanne Ng, Pankaj Kumar, Frederic Bard
Date Published	February 1, 2013
Description	Dataset detailing RNAi screening results and large regulatory networks controlling the Golgi apparatus in human cells
Type	Dataset
Files	GolgiRef_Cell_features.txt, Kinome_Cell_features.txt
Size	19.7 GB
Identifier	DOI: 10.5061/dryad.1m2p3
Publisher	Zenodo

References

- CellDesigner Official Website. Available at: <https://www.celldesigner.org>
- CellDesigner Documentation. Available at:
<https://www.celldesigner.org/documentation>
- CellDesigner Official Startup Guide. Available at:
<https://www.celldesigner.org/documents.html>
- Funahashi, A., Morohashi, M., Kitano, H., & Tanimura, N. (2008). CellDesigner: a process diagram editor for gene-regulatory and biochemical networks. *Biosilico*, 1(5), 159–162.