CNApy Users Guide

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Abstract

Introduction

This is the user manual of CNApy. CNApy is a graphical interface for the modelling and analysis of metabolic networks on the basis of constraint-based (stoichiometric) modeling approaches. It allows

- the import/export of SBML models
- creating COBRApy/CNA models
- linking a graphical representation to the model data
- convenient exploration and editing of the model
- model analysis with standard and advanced constraint-based methods
- and saving everything as a CNApy *.cna project

The methods provided for model analysis (some of them are part of CNApy but most are functions from CNA and COBRApy) include:

- Flux balance analysis
- Parsimonious flux balance analysis
- Flux variability analysis
- Minimal cut sets
- Elementary modes
- Phase plane analysis
- Yield optimization

CNApy is available at https://github.com/cnapy-org/CNApy under the [Apache-2.0 License](#).

We appreciate any comments or suggestions for improvements and we are greatly interested in your feedback which you can give at our [User Forum](#).

For feature requests and bug reports please use our [Issue tracker](#)

Thank you for using CNApy!

Installation

The easiest way to install CNApy is using conda. First install conda and then:

- Create a conda environment with all dependencies

```
conda create -n cnapy-1.0.0 -c conda-forge -c cnapy cnapy=1.0.0
```

- Activate the cnapy conda environment

```
conda activate cnapy-1.0.0
```

- Run CNApy

```
cnapy
```

On windows you may also use the [graphical installer](#).

The rest of this document is a full list of formatting elements/features supported by Manubot. Compare the input (`.md` files in the `/content` directory) to the output you see below.

Basic formatting

Bold text

Semi-bold text

<div align="center">Centered text</div>

<div align="right">Right-aligned text</div>

Italic text

Combined *italics and **bold***

~~Strikethrough~~

1. Ordered list item
2. Ordered list item
   a. Sub-item
   b. Sub-item
      i. Sub-sub-item
3. Ordered list item
   a. Sub-item

- List item
- List item
- List item

subscript: H_2O is a liquid

superscript: 2^{10} is 1024.

[unicode superscripts](#)⁰¹²³⁴⁵⁶⁷⁸⁹

[unicode subscripts](#)₀₁₂₃₄₅₆₇₈₉

A long paragraph of text. Lorem ipsum dolor sit amet, consectetur adipiscing elit, sed do eiusmod tempor incididunt ut labore et dolore magna aliqua. Ut enim ad minim veniam, quis nostrud exercitation ullamco laboris nisi ut aliquip ex ea commodo consequat. Duis aute irure dolor in reprehenderit in voluptate velit esse cillum dolore eu fugiat nulla pariatur. Excepteur sint occaecat cupidatat non proident, sunt in culpa qui officia deserunt mollit anim id est laborum.

Putting each sentence on its own line has numerous benefits with regard to [editing](#) and [version control](#).

Line break without starting a new paragraph by putting
two spaces at end of line.

Document organization

Document section headings:

Heading 1

Heading 2

Heading 3

Heading 4

Heading 5

Heading 6

A heading centered on its own printed page

Horizontal rule:

`Heading 1`'s are recommended to be reserved for the title of the manuscript.

`Heading 2`'s are recommended for broad sections such as *Abstract*, *Methods*, *Conclusion*, etc.

`Heading 3`'s and `Heading 4`'s are recommended for sub-sections.

Links

Bare URL link: https://manubot.org

[Long link with lots of words and stuff and junk and bleep and blah and stuff and other stuff and more stuff yeah](#)

[Link with text](#)

[Link with hover text](#)

[Link by reference](#)

Citations

Citation by DOI [1].

Citation by PubMed Central ID [2].

Citation by PubMed ID [3].

Citation by Wikidata ID [4].

Citation by ISBN [5].

Citation by URL [6].

Citation by alias [7].

Multiple citations can be put inside the same set of brackets [1,5,7]. Manubot plugins provide easier, more convenient visualization of and navigation between citations [2,3,7,8].

Citation tags (i.e. aliases) can be defined in their own paragraphs using Markdown's reference link syntax:

Referencing figures, tables, equations

Figure 1

Figure 2

Quotes and code

> Quoted text

> Quoted block of text
>
> Two roads diverged in a wood, and I—
> I took the one less traveled by,
> And that has made all the difference.

Code `in the middle` of normal text, aka `inline code`.

Code block with Python syntax highlighting:

```python
from manubot.cite.doi import expand_short_doi

def test_expand_short_doi():
    doi = expand_short_doi("10/c3bp")
    # a string too long to fit within page:
    assert doi == "10.25313/2524-2695-2018-3-vliyanie-enhansera-copia-i-
        insulyatora-gypsy-na-sintez-ernk-modifikatsii-hromatina-i-
        svyazyvanie-insulyatornyh-belkov-vtransfetsirovannyh-geneticheskih-
        konstruktsiyah"
```

Code block with no syntax highlighting:

```
Exporting HTML manuscript
Exporting DOCX manuscript
Exporting PDF manuscript
```

Figures

Figure 1: A square image at actual size and with a bottom caption. Loaded from the latest version of image on GitHub.

Figure 2: An image too wide to fit within page at full size. Loaded from a specific (hashed) version of the image on GitHub.

Figure 3: A tall image with a specified height. Loaded from a specific (hashed) version of the image on GitHub.

Figure 4: A vector `.svg` image loaded from GitHub. The parameter `sanitize=true` is necessary to properly load SVGs hosted via GitHub URLs. White background specified to serve as a backdrop for transparent sections of the image.

Tables

Table 1: A table with a top caption and specified relative column widths.

Bowling Scores	Jane	John	Alice	Bob
Game 1	150	187	210	105
Game 2	98	202	197	102
Game 3	123	180	238	134

Table 2: A table too wide to fit within page.

	Digits 1-33	Digits 34-66	Digits 67-99	Ref.
pi	3.14159265358979323 846264338327950	28841971693993751 0582097494459230	78164062862089986 2803482534211706	`piday.org`
e	2.71828182845904523 536028747135266	24977572470936999 5957496696762772	40766303535475945 7138217852516642	`nasa.gov`

Table 3: A table with merged cells using the `attributes` plugin.

	Colors	
Size	**Text Color**	**Background Color**
big	blue	orange
small	black	white

Equations

A LaTeX equation:

$$\int_0^\infty e^{-x^2} dx = \frac{\sqrt{\pi}}{2} \tag{1}$$

An equation too long to fit within page:

$$\begin{aligned} x = a + b + c + d + e + f + g + h + i + j + k + l + m + n + o + p + q + r + s + t \\ + u + v + w + x + y + z + 1 + 2 + 3 + 4 + 5 + 6 + 7 + 8 + 9 \end{aligned} \tag{2}$$

Special

⚠ **WARNING** *The following features are only supported and intended for* `.html` *and* `.pdf` *exports. Journals are not likely to support them, and they may not display correctly when converted to other formats such as* `.docx` *.*

<div style="border:1px solid;padding:1em;">LINK STYLED AS A BUTTON</div>

Adding arbitrary HTML attributes to an element using Pandoc's attribute syntax:

> Manubot Manubot Manubot Manubot Manubot. Manubot Manubot Manubot Manubot. Manubot Manubot Manubot. Manubot Manubot. Manubot.

Adding arbitrary HTML attributes to an element with the Manubot `attributes` plugin (more flexible than Pandoc's method in terms of which elements you can add attributes to):

> Manubot Manubot Manubot Manubot Manubot. Manubot Manubot Manubot Manubot. Manubot Manubot Manubot. Manubot Manubot. Manubot.

Available background colors for text, images, code, banners, etc:

white `lightgrey` grey darkgrey black lightred lightyellow lightgreen lightblue lightpurple red orange yellow green blue purple

Using the Font Awesome icon set:

✔ ? ★ 🔔 ✖ •••

🏛 Light Grey Banner
useful for *general information* - manubot.org

❶ Blue Banner
useful for *important information* - manubot.org

🚫 Light Red Banner
useful for *warnings* - manubot.org

References

1. **Sci-Hub provides access to nearly all scholarly literature**
   Daniel S Himmelstein, Ariel Rodriguez Romero, Jacob G Levernier, Thomas Anthony Munro,
   Stephen Reid McLaughlin, Bastian Greshake Tzovaras, Casey S Greene
   eLife (2018-03-01) https://doi.org/ckcj
   DOI: 10.7554/elife.32822 · PMID: 29424689 · PMCID: PMC5832410

2. **Reproducibility of computational workflows is automated using continuous analysis**
   Brett K Beaulieu-Jones, Casey S Greene
   Nature biotechnology (2017-04) https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6103790/
   DOI: 10.1038/nbt.3780 · PMID: 28288103 · PMCID: PMC6103790

3. **Bitcoin for the biological literature.**
   Douglas Heaven
   Nature (2019-02) https://www.ncbi.nlm.nih.gov/pubmed/30718888
   DOI: 10.1038/d41586-019-00447-9 · PMID: 30718888

4. **Plan S: Accelerating the transition to full and immediate Open Access to scientific publications**
   cOAlition S
   (2018-09-04) https://www.wikidata.org/wiki/Q56458321

5. **Open access**
   Peter Suber
   MIT Press (2012)
   ISBN: 9780262517638

6. **Open collaborative writing with Manubot**
   Daniel S Himmelstein, Vincent Rubinetti, David R Slochower, Dongbo Hu, Venkat S Malladi,
   Casey S Greene, Anthony Gitter
   Manubot (2020-05-25) https://greenelab.github.io/meta-review/

7. **Opportunities and obstacles for deep learning in biology and medicine**
   Travers Ching, Daniel S Himmelstein, Brett K Beaulieu-Jones, Alexandr A Kalinin, Brian T Do,
   Gregory P Way, Enrico Ferrero, Paul-Michael Agapow, Michael Zietz, Michael M Hoffman, …
   Casey S Greene
   Journal of The Royal Society Interface (2018-04-04) https://doi.org/gddkhn
   DOI: 10.1098/rsif.2017.0387 · PMID: 29618526 · PMCID: PMC5938574

8. **Open collaborative writing with Manubot**
   Daniel S Himmelstein, Vincent Rubinetti, David R Slochower, Dongbo Hu, Venkat S Malladi,
   Casey S Greene, Anthony Gitter
   PLOS Computational Biology (2019-06-24) https://doi.org/c7np
   DOI: 10.1371/journal.pcbi.1007128 · PMID: 31233491 · PMCID: PMC6611653