GECKO Documentation

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SysBioChalmers

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CHAPTER 1

About GECKO

The **GECKO** toolbox is a Matlab/Python package for enhancing a **G**enome-scale model to account for **E**nzyme **C**onstraints, using **K**inetics and **O**mics. It is the companion software to this publication, and it has two main parts:

- `geckomat`: Matlab+Python scripts to fetch online data and build/simulate enzyme-constrained models.
- `geckopy`: a Python package which can be used with cobrapy to obtain a ecYeastGEM model object, optionally adjusted for provided proteomics data.

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CHAPTER 2

geckomat: Building enzyme-constrained models

2.1 Required software - Python module

- Python 2.7
- setuptools for python 2.7
- SOAPpy:

```
easy_install-2.7 SOAPpy
```

2.2 Required software - Matlab module

- MATLAB (7.5 or higher) + Optimization Toolbox.
- The COBRA toolbox for MATLAB.
- The RAVEN toolbox for MATLAB.
- The libSBML MATLAB API (version 5.17.0 is recommended).

2.3 Usage

- **For creating an enzyme constrained model:**
  - Update the following data files in `/databases` with your organism infomation:
    * `databases/prot_abundance.txt`: Protein abundance Data from Pax-DB. If data is not available for your organism, then a relative proteomics dataset (in molar fractions) can be used instead. The required format is a tab-separated file, named as `databases/relative_proteomics.txt` , with a single header line and 2 columns; the first with gene IDs and the second with the relative abundances for each protein.

    * databases/uniprot.tab: Gene-proteins data from uniprot.
    * databases/chemostatData.tsv: Chemostat data for estimating GAM (optional, called by fitGAM.m).
    * databases/manual_data.txt: Kcat data from eventual manual curations (optional, called by manualModifications.m).
  - Adapt the following functions in /geckomat to your organism:
    * geckomat/enhanceGEM.m
    * geckomat/change_model/manualModifications.m
    * geckomat/limit_proteins/sumProtein.m
    * geckomat/limit_proteins/scaleBioMass.m
    * geckomat/kcat_sensitivity_analysis/changeMedia_batch.m
    * geckomat/change_model/removeIncorrectPathways.m (optional, called by manualModifications.m)
    * geckomat/limit_proteins/sumBioMass.m (optional, called by sumProtein.m & scaleBiomass.m)
    * geckomat/limit_proteins/fitGAM.m (optional, called by scaleBiomass.m)
  - Run geckomat/get_enzyme_data/updateDatabases.m to update ProtDatabase.mat.
  - Run geckomat/enhanceGEM.m with your metabolic model as input.

- **For performing simulations with an enzyme-constrained model:** Enzyme-constrained models can be used as any other metabolic model, with toolboxes such as COBRA or RAVEN. For more information on rxn/met naming convention, see the supporting information of Sanchez et al. (2017)

CHAPTER 3

geckopy: Integrating proteomic data to ecYeastGEM

If all you need is the ecYeastGEM model to use together with cobrapy you can use the `geckopy` Python package.

3.1 Required software

- Python 2.7, 3.4, 3.5 or 3.6
- cobrapy

3.2 Installation

```
pip install geckopy
```

3.3 Usage

```
from geckopy import GeckoModel
import pandas
some_measurements = pandas.Series({'P00549': 0.1, 'P31373': 0.1, 'P31382': 0.1})
model = GeckoModel('multi-pool')
model.limit_proteins(some_measurements)
model.optimize()
```

CHAPTER 4

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