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# **GECKO Documentation**

*Release 1.3.1*

**SysBioChalmers**

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# CHAPTER 1

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## About GECKO

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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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## geckomat: Building enzyme-constrained models

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### 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 information:
    - \* databases/chemostatData.tsv: Chemostat data for estimating GAM (optional).
    - \* databases/manual\_data.txt: Kcat data from eventual manual curations (optional).
    - \* databases/prot\_abundance.txt: Protein abundance Data from Pax-DB.
    - \* databases/uniprot.tab: Gene-proteins data from uniprot.

- Adapt the following functions in /geckomat to your organism:
  - \* geckomat/get\_enzyme\_data/preprocessModel.m
  - \* geckomat/change\_model/manualModifications.m (optional)
  - \* geckomat/change\_model/removeIncorrectPathways.m
  - \* geckomat/limit\_proteins/sumBioMass.m (If chemostat data is provided)
  - \* geckomat/limit\_proteins/scaleBioMass.m (If chemostat data is provided)
  - \* geckomat/kcat\_sensitivity\_analysis/changeMedia\_batch.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. \(2017\)](#)

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## geckopy: Integrating proteomic data to ecYeastGEM

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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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### Contributors

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