

Bio334 metabolic modelling cheatsheet

For more python tricks & tips, have a gander at <https://www.pythoncheatsheet.org>

Dataframes using pandas

```
import pandas as pd
# Making a dataframe
dataframe = pd.DataFrame([[1,2], [3,4]], columns=["colm1", "colm2"])
# Accessing values in a dataframe
index = 0 # Getting a value from the first row
val = dataframe.loc[index, "column_name"]
# Getting all values from a column: This returns a pandas series
vals = dataframe["column_name"]
# Accessing multiple values: This returns a pandas series
index = [0,10,14]
vals = dataframe.loc[index, "column_name"]
# Accessing multiple values: This returns a numpy array
vals = dataframe.loc[index, "column_name"].values
# Getting maximum and minimum values
valmax = dataframe.loc["column_name"].max()
valmin = dataframe.loc["column_name"].min()
# Getting unique values
vals = dataframe["column_name"].unique()
```

Doing a for-loop over values in a dataframe:

```
for row in range(dataframe.shape[0]):
    print(dataframe.loc[row, "column_name"])
```

Plotting using matplotlib

```
import matplotlib.pyplot as plt
import numpy as np
# Making up some data
x = np.linspace(0,20,21)
y = x**2
# Making a plot
plt.plot(x,y,marker='o',linestyle='none')
plt.xlabel('here is x')
plt.ylabel('here is y')
plt.title('A simple plot')
plt.show()
```

Quick cobrapy functions

```
import cobra
# Read in an sbml model
model = cobra.io.read_sbml_model('model_name.xml')
# Performing fba
solution = model.optimize()
# Quick overview of results
model.summary()
# To see reaction fluxes
solution.fluxes
# Deleting reactions
from cobra.flux_analysis import single_reaction_deletion
deletion_results = single_reaction_deletion(model, model.reactions[:])
# Flux variability analysis
from cobra.flux_analysis import flux_variability_analysis
fva_result = flux_variability_analysis(model, model.reactions[:])
```