

Instructions for COBRA Toolbox modeling

As a start, the COBRA Toolbox is initiated in Matlab to build the Xcc model from the SBML file by:

(The Matlab command is displayed in *italics*)

```
initCobraToolbox
```

```
model = readCbModel
```

Browse and select “suppl_data2_XccB100_COBRA_model.xml”

Change the objective of the model, for instance, to set the biomass as objective function:

```
model = changeObjective (model, 'biomass1')
```

To simulate growth on glucose and nitrate, for instance, declare the other carbon import reactions to zero:

```
model = changeRxnBounds (model, 'Sulfate_exchange', -1, 'l')  
model = changeRxnBounds (model, 'Frc_exchange', 0, 'l')  
model = changeRxnBounds (model, 'Suc_exchange', 0, 'l')  
model = changeRxnBounds (model, 'Man_exchange', 0, 'l')  
model = changeRxnBounds (model, 'Malate_exchange', 0, 'l')  
model = changeRxnBounds (model, 'NH3_exchange', 0, 'l')  
model = changeRxnBounds (model, 'Nitrate_exchange', -2, 'l')  
model = changeRxnBounds (model, 'Glc_exchange', -2, 'l')  
model = changeRxnBounds (model, 'Gal_exchange', 0, 'l')  
model = changeRxnBounds (model, 'GlcNAc_exchange', 0, 'l')
```

```
solution = optimizeCbModel (model)
```

- The calculated growth rate is f: 0.0503.

To analyze the impact of a single gene deletion, set the specific reaction rate to zero:

```
model = changeRxnBounds (model, 'tkr', 0, 'b')  
solution = optimizeCbModel (model)
```

- The calculated growth rate is 0 (f).

To perform single gene deletions of all genes with MOMA:

```
grRatioMOMA = singleGeneDeletion (model, '1MOMA')
```

To plot the results:

```
plot (1:length(grRatioMOMA), [sort (grRatioMOMA)], 'x')
```

We recommend the following literature references related to the COBRA Toolbox for further readings (Becker et al., 2007; Schellenberger et al., 2011).