

## SBML Model Report

# Model name: “Messiha2013 - combined glycolysis and pentose phosphate pathway model”



May 5, 2016

## 1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Vijayalakshmi Chelliah<sup>1</sup> and Kieran Smallbone<sup>2</sup> at November ninth 2008 at no o’ clock in the morning. and last time modified at April eighth 2016 at 5:38 p. m. Table 1 gives an overview of the quantities of all components of this model.

Table 1: Number of components in this model, which are described in the following sections.

| Element           | Quantity | Element              | Quantity |
|-------------------|----------|----------------------|----------|
| compartment types | 0        | compartments         | 2        |
| species types     | 0        | species              | 76       |
| events            | 0        | constraints          | 0        |
| reactions         | 34       | function definitions | 0        |
| global parameters | 10       | unit definitions     | 5        |
| rules             | 4        | initial assignments  | 0        |

## Model Notes

Messiha2013 - combined glycolysis and pentose phosphate pathway model

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[BIOMD0000000502](#) and [MODEL1303260018](#) are combined to examine the response to oxidative stress.

This model is described in the article: [Enzyme characterisation and kinetic modelling of pentose phosphate pathway in yeast](#). Hanan L. Messiha, Edward Kent, Naglis Malys, Kathleen M. Carroll, Pedro Mendes, Kieran Smallbone *PeerJ PrePrints* 1:e146v2

Abstract:

We present the quantification and kinetic characterisation of the enzymes of the pentose phosphate pathway in *Saccharomyces cerevisiae*. The data are combined into a mathematical model that describes the dynamics of this system and allows for the predicting changes in metabolite concentrations and fluxes in response to perturbations. We use the model to study the response of yeast to a glucose pulse. We then combine the model with an existing glycolysis one to study the effect of oxidative stress on carbohydrate metabolism. The combination of these two models was made possible by the standardized enzyme kinetic experiments carried out in both studies. This work demonstrates the feasibility of constructing larger network models by merging smaller pathway models.

This model is hosted on [BioModels Database](#) and identified by: [BIOMD0000000503](#).

To cite BioModels Database, please use: [BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models](#).

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## 2 Unit Definitions

This is an overview of nine unit definitions of which four are predefined by SBML and not mentioned in the model.

### 2.1 Unit `substance`

**Name** mmol

**Definition** mmol

### 2.2 Unit `mM`

**Name** mM

**Definition**  $\text{mmol} \cdot \text{l}^{-1}$

### 2.3 Unit `mM_per_s`

**Name** mM per s

**Definition**  $\text{mmol} \cdot \text{l}^{-1} \cdot \text{s}^{-1}$

## 2.4 Unit per\_s

**Name** per\_s

**Definition**  $s^{-1}$

## 2.5 Unit per\_mM\_per\_s

**Name** per\_mM\_per\_s

**Definition**  $\text{mmol}^{-1} \cdot \text{l} \cdot s^{-1}$

## 2.6 Unit volume

**Notes** Litre is the predefined SBML unit for volume.

**Definition** l

## 2.7 Unit area

**Notes** Square metre is the predefined SBML unit for area since SBML Level 2 Version 1.

**Definition**  $\text{m}^2$

## 2.8 Unit length

**Notes** Metre is the predefined SBML unit for length since SBML Level 2 Version 1.

**Definition** m

## 2.9 Unit time

**Notes** Second is the predefined SBML unit for time.

**Definition** s

# 3 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

| Id            | Name          | SBO | Spatial<br>Dimensions | Size | Unit  | Constant                            | Outside |
|---------------|---------------|-----|-----------------------|------|-------|-------------------------------------|---------|
| cell          | cell          |     | 3                     | 1    | litre | <input checked="" type="checkbox"/> |         |
| extracellular | extracellular |     | 3                     | 1    | litre | <input checked="" type="checkbox"/> |         |

### 3.1 Compartment `cell`

This is a three dimensional compartment with a constant size of one litre.

**Name** `cell`

### 3.2 Compartment `extracellular`

This is a three dimensional compartment with a constant size of one litre.

**Name** `extracellular`

## 4 Species

This model contains 76 species. The boundary condition of 48 of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 8 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

| Id    | Name  | Compartment | Derived Unit                      | Constant                 | Boundary Condition                  |
|-------|-------|-------------|-----------------------------------|--------------------------|-------------------------------------|
| ADP   | ADP   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input type="checkbox"/>            |
| ATP   | ATP   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input type="checkbox"/>            |
| AcAld | AcAld | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input type="checkbox"/>            |
| BPG   | BPG   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input type="checkbox"/>            |
| DHAP  | DHAP  | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input type="checkbox"/>            |
| F16bP | F16bP | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input type="checkbox"/>            |
| F6P   | F6P   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input type="checkbox"/>            |
| G1P   | G1P   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input type="checkbox"/>            |
| G3P   | G3P   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input type="checkbox"/>            |
| G6P   | G6P   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input type="checkbox"/>            |
| GAP   | GAP   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input type="checkbox"/>            |
| GLC   | GLC   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input type="checkbox"/>            |
| NAD   | NAD   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input type="checkbox"/>            |
| P2G   | P2G   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input type="checkbox"/>            |
| P3G   | P3G   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input type="checkbox"/>            |
| PEP   | PEP   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input type="checkbox"/>            |
| PYR   | PYR   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input type="checkbox"/>            |
| T6P   | T6P   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input type="checkbox"/>            |
| UDP   | UDP   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input type="checkbox"/>            |
| UTP   | UTP   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input type="checkbox"/>            |
| AMP   | AMP   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input checked="" type="checkbox"/> |

| Id    | Name  | Compartment   | Derived Unit                      | Constant                            | Boundary Condition                  |
|-------|-------|---------------|-----------------------------------|-------------------------------------|-------------------------------------|
| NADH  | NADH  | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/>            | <input checked="" type="checkbox"/> |
| UDG   | UDG   | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/>            | <input checked="" type="checkbox"/> |
| ACE   | ACE   | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| EtOH  | EtOH  | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| F26bP | F26bP | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| GLCx  | GLCx  | extracellular | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| GLY   | GLY   | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| SUC   | SUC   | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| TRH   | TRH   | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| ADH1  | ADH1  | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| CDC19 | CDC19 | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| ENO1  | ENO1  | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| ENO2  | ENO2  | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| FBA1  | FBA1  | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| GLK1  | GLK1  | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| GPD1  | GPD1  | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| GPD2  | GPD2  | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| GPM1  | GPM1  | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| HOR2  | HOR2  | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| HXK1  | HXK1  | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| HXK2  | HXK2  | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| PDC1  | PDC1  | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| PDC5  | PDC5  | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| PDC6  | PDC6  | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| PFK1  | PFK1  | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| PFK2  | PFK2  | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| PGI1  | PGI1  | cell          | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |

| Id    | Name  | Compartment | Derived Unit                      | Constant                            | Boundary<br>Condi-<br>tion          |
|-------|-------|-------------|-----------------------------------|-------------------------------------|-------------------------------------|
| PGK1  | PGK1  | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| PGM1  | PGM1  | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| PGM2  | PGM2  | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| RHR2  | RHR2  | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| TDH1  | TDH1  | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| TDH3  | TDH3  | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| TPI1  | TPI1  | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| TPS1  | TPS1  | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| TPS2  | TPS2  | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| UGP1  | UGP1  | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| E4P   | E4P   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/>            | <input type="checkbox"/>            |
| G6L   | G6L   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/>            | <input type="checkbox"/>            |
| NADPH | NADPH | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/>            | <input type="checkbox"/>            |
| P6G   | P6G   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/>            | <input type="checkbox"/>            |
| R5P   | R5P   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/>            | <input type="checkbox"/>            |
| Ru5P  | Ru5P  | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/>            | <input type="checkbox"/>            |
| S7P   | S7P   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/>            | <input type="checkbox"/>            |
| X5P   | X5P   | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/>            | <input type="checkbox"/>            |
| NADP  | NADP  | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input type="checkbox"/>            | <input checked="" type="checkbox"/> |
| GND1  | GND1  | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| GND2  | GND2  | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| NQM1  | NQM1  | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| RKI1  | RKI1  | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| RPE1  | RPE1  | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| SOL3  | SOL3  | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| TAL1  | TAL1  | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| TKL1  | TKL1  | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |

| Id   | Name | Compartment | Derived Unit                      | Constant                            | Boundary<br>Condi-<br>tion          |
|------|------|-------------|-----------------------------------|-------------------------------------|-------------------------------------|
| ZWF1 | ZWF1 | cell        | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |



## 5 Parameters

This model contains ten global parameters.

Table 4: Properties of each parameter.

| Id       | Name | SBO | Value | Unit                              | Constant |
|----------|------|-----|-------|-----------------------------------|----------|
| sum_AxP  |      |     | 6.020 | $\text{mmol} \cdot \text{l}^{-1}$ | ✓        |
| sum_NAD  |      |     | 1.590 | $\text{mmol} \cdot \text{l}^{-1}$ | ✓        |
| sum_UxP  |      |     | 1.398 | $\text{mmol} \cdot \text{l}^{-1}$ | ✓        |
| sum_NADP |      |     | 0.330 | $\text{mmol} \cdot \text{l}^{-1}$ | ✓        |
| Kx5p_TAL |      |     | 0.670 | $\text{mmol} \cdot \text{l}^{-1}$ | ✓        |
| Ke4p_TAL |      |     | 0.946 | $\text{mmol} \cdot \text{l}^{-1}$ | ✓        |
| Kr5p_TAL |      |     | 0.235 | $\text{mmol} \cdot \text{l}^{-1}$ | ✓        |
| Kgap_TAL |      |     | 0.100 | $\text{mmol} \cdot \text{l}^{-1}$ | ✓        |
| Kf6p_TAL |      |     | 1.100 | $\text{mmol} \cdot \text{l}^{-1}$ | ✓        |
| Ks7p_TAL |      |     | 0.150 | $\text{mmol} \cdot \text{l}^{-1}$ | ✓        |

## 6 Rules

This is an overview of four rules.

### 6.1 Rule AMP

Rule AMP is an assignment rule for species AMP:

$$\text{AMP} = \text{sum\_AxP} - [\text{ATP}] - [\text{ADP}] \quad (1)$$

**Derived unit**  $\text{mmol} \cdot \text{l}^{-1}$

### 6.2 Rule NADH

Rule NADH is an assignment rule for species NADH:

$$\text{NADH} = \text{sum\_NAD} - [\text{NAD}] \quad (2)$$

**Derived unit**  $\text{mmol} \cdot \text{l}^{-1}$

### 6.3 Rule UDG

Rule UDG is an assignment rule for species UDG:

$$\text{UDG} = \text{sum\_UxP} - [\text{UTP}] - [\text{UDP}] \quad (3)$$

**Derived unit**  $\text{mmol} \cdot \text{l}^{-1}$

#### 6.4 Rule NADP

Rule NADP is an assignment rule for species NADP:

$$\text{NADP} = \text{sum\_NADP} - [\text{NADPH}] \quad (4)$$

**Derived unit**  $\text{mmol} \cdot \text{l}^{-1}$

7 Reactions

This model contains 34 reactions. All reactions are listed in the following table and are subsequently described in detail. If a reaction is affected by a modifier, the identifier of this species is written above the reaction arrow.

Table 5: Overview of all reactions

| Nº | Id     | Name   | Reaction Equation  | SBO     |
|----|--------|--------|--|---------|
| 1  | ADH    | ADH    | $\text{AcAld} + \text{NADH} \xrightleftharpoons[\text{NAD}]{\text{ADH1, ADH1, AcAld, NADH, EtOH, NAD}} \text{EtOH} + \text{NAD}$             | 0000176 |
| 2  | AK     | AK     | $2 \text{ ADP} \xrightleftharpoons[\text{ATP}]{\text{ADP, AMP, ATP}} \text{ATP} + \text{AMP}$  | 0000176 |
| 3  | ATPase | ATPase | $\text{ATP} \xrightarrow{\text{ATP}} \text{ADP}$   | 0000176 |
| 4  | ENO    | ENO    | $\text{P2G} \xrightleftharpoons[\text{PEP}]{\text{ENO1, ENO2, ENO1, P2G, PEP, ENO2}} \text{PEP}$   | 0000176 |
| 5  | FBA    | FBA    | $\text{F16bP} \xrightleftharpoons[\text{GAP}]{\text{FBA1, FBA1, F16bP, DHAP, GAP}} \text{DHAP} + \text{GAP}$                                 | 0000176 |
| 6  | GPD    | GPD    | $\text{DHAP} + \text{NADH} \xrightleftharpoons[\text{NAD}]{\text{ADP, ATP, F16bP, GPD1, GPD2, DHAP, NADH, G3P, NAD, F16bP}} \text{NAD}$      | 0000176 |
| 7  | GPM    | GPM    | $\text{P3G} \xrightleftharpoons[\text{P2G}]{\text{GPM1, GPM1, P3G, P2G}} \text{P2G}$   | 0000176 |
| 8  | GPP    | GPP    | $\text{G3P} \xrightarrow{\text{HOR2, RHR2, G3P}} \text{GLY}$   | 0000176 |
| 9  | HXK    | HXK    | $\text{GLC} + \text{ATP} \xrightleftharpoons[\text{ADP}]{\text{HXK1, T6P, HXK2, GLK1, HXK1, GLC, ATP, G6P, ADP, T6P, HXK2, ADP}} \text{ADP}$ | 0000176 |
| 10 | PDC    | PDC    | $\text{PYR} \xrightarrow{\text{PDC1, PDC5, PDC6, PDC1, PYR, PDC5, PDC6}} \text{PDC1}$  | 0000176 |
| 11 | PFK    | PFK    | $\text{ATP} + \text{F6P} \xrightarrow[\text{F16bP}]{\text{AMP, F26bP, PFK1, PFK2, PFK2, F6P, ATP, F16bP, ADP, AMP, F26bP}} \text{F16bP}$     | 0000176 |
| 12 | PGI    | PGI    | $\text{G6P} \xrightleftharpoons[\text{F6P}]{\text{PGI1, PGI1, G6P, F6P}} \text{F6P}$   | 0000176 |

| Nº | Id             | Name           | Reaction Equation  | SBO     |
|----|----------------|----------------|--|---------|
| 13 | PGK            | PGK            | $\text{ADP} + \text{BPG} \xrightleftharpoons{\text{PGK1, PGK1, ADP, BPG, P3G, ATP}} \text{ATP} + \text{P3G}$                 | 0000176 |
| 14 | PGM            | PGM            | $\text{G6P} \xrightleftharpoons{\text{PGM1, PGM2, G6P, G1P}} \text{G1P}$   | 0000176 |
| 15 | PYK            | PYK            | $\text{ADP} + \text{PEP} \xrightleftharpoons{\text{CDC19, F16bP, CDC19, PEP, ADP, PYR, ATP, F16bP}} \text{ATP} + \text{PYR}$ | 0000176 |
| 16 | TDH            | TDH            | $\text{GAP} + \text{NAD} \xrightleftharpoons{\text{TDH1, TDH3, TDH1, GAP, NAD, BPG, NADH, TDH3}} \text{BPG} + \text{NADH}$   | 0000176 |
| 17 | TPI            | TPI            | $\text{DHAP} \xrightleftharpoons{\text{TPI1, TPI1, DHAP, GAP}} \text{GAP}$   | 0000176 |
| 18 | TPP            | TPP            | $\text{T6P} \xrightarrow{\text{TPS1, TPS2, T6P}} \text{TRH}$   | 0000176 |
| 19 | TPS            | TPS            | $\text{G6P} + \text{UDG} \xrightarrow{\text{TPS1, TPS2, G6P, UDG}} \text{T6P} + \text{UDP}$                                  | 0000176 |
| 20 | UGP            | UGP            | $\text{G1P} + \text{UTP} \xrightarrow{\text{UGP1, UTP, G1P, UDG}} \text{UDG}$  | 0000176 |
| 21 | acetate_branch | acetate_branch | $\text{AcAld} + \text{NAD} \xrightarrow{\text{AcAld, NAD}} \text{ACE} + \text{NADH}$   | 0000176 |
| 22 | udp_to_utp     | udp_to_utp     | $\text{UDP} + \text{ATP} \xrightarrow{\text{UDP, ATP}} \text{UTP} + \text{ADP}$  | 0000176 |
| 23 | HXT            | HXT            | $\text{GLCx} \xrightleftharpoons{\text{GLCx, GLC}} \text{GLC}$   | 0000185 |
| 24 | GND            | GND            | $\text{P6G} + \text{NADP} \xrightarrow{\text{GND1, GND2, GND1, P6G, NADP, Ru5P, NADPH, GND2}} \text{Ru5P} + \text{NADPH}$    | 0000176 |
| 25 | RKI            | RKI            | $\text{Ru5P} \xrightleftharpoons{\text{RKI1, RKI1, Ru5P, R5P}} \text{R5P}$   | 0000176 |
| 26 | RPE            | RPE            | $\text{Ru5P} \xrightleftharpoons{\text{RPE1, RPE1, Ru5P, X5P}} \text{X5P}$   | 0000176 |
| 27 | SOL            | SOL            | $\text{G6L} \xrightarrow{\text{SOL3, SOL3, G6L, P6G}} \text{P6G}$  | 0000176 |
| 28 | TAL            | TAL            | $\text{GAP} + \text{S7P} \xrightleftharpoons{\text{TAL1, NQM1, TAL1, GAP, S7P, F6P, E4P, NQM1}} \text{F6P} + \text{E4P}$     | 0000176 |

| Nº | Id            | Name          | Reaction Equation  | SBO     |
|----|---------------|---------------|--|---------|
| 29 | TKL_E4P       | TKL (E4P:F6P) | $\text{X5P} + \text{E4P} \xrightleftharpoons[\text{F6P}]{\text{TKL1, R5P, S7P, TKL1, X5P, E4P, GAP, F6P, R5P, S7P}} \text{GAP} + \text{F6P}$ | 0000176 |
| 30 | TKL_R5P       | TKL (R5P:S7P) | $\text{X5P} + \text{R5P} \xrightleftharpoons[\text{S7P}]{\text{TKL1, E4P, F6P, TKL1, X5P, R5P, GAP, S7P, E4P, F6P}} \text{GAP} + \text{S7P}$ | 0000176 |
| 31 | ZWF           | ZWF           | $\text{G6P} + \text{NADP} \xrightarrow[\text{NADPH}]{\text{ZWF1, ZWF1, G6P, NADP, G6L, NADPH}} \text{G6L} + \text{NADPH}$                    | 0000176 |
| 32 | NADPH_oxidase | NADPH oxidase | $\text{NADPH} \xrightarrow{\text{NADPH}} \text{NADP}$  | 0000176 |
| 33 | E4P_sink      | E4P sink      | $\text{E4P} \xrightarrow{\text{E4P}} \emptyset$  | 0000176 |
| 34 | R5P_sink      | R5P sink      | $\text{R5P} \xrightarrow{\text{R5P}} \emptyset$  | 0000176 |

## 7.1 Reaction ADH

This is a reversible reaction of two reactants forming two products influenced by six modifiers.

**Name** ADH

**SBO:0000176** biochemical reaction

### Reaction equation



### Reactants

Table 6: Properties of each reactant.

| Id    | Name  | SBO |
|-------|-------|-----|
| AcAld | AcAld |     |
| NADH  | NADH  |     |

### Modifiers

Table 7: Properties of each modifier.

| Id    | Name  | SBO |
|-------|-------|-----|
| ADH1  | ADH1  |     |
| ADH1  | ADH1  |     |
| AcAld | AcAld |     |
| NADH  | NADH  |     |
| EtOH  | EtOH  |     |
| NAD   | NAD   |     |

### Products

Table 8: Properties of each product.

| Id   | Name | SBO |
|------|------|-----|
| EtOH | EtOH |     |
| NAD  | NAD  |     |

## Kinetic Law

**Derived unit** contains undeclared units

$$v_1 = \text{vol}(\text{cell}) \cdot \frac{[\text{ADH1}] \cdot \text{kcat} \cdot \left( \frac{[\text{AcAld}] \cdot [\text{NADH}]}{\text{Kacald} \cdot \text{Kinadh}} - \frac{[\text{EtOH}] \cdot [\text{NAD}]}{\text{Kacald} \cdot \text{Kinadh} \cdot \text{Keq}} \right)}{1 + \frac{[\text{NADH}]}{\text{Kinadh}} + \frac{[\text{AcAld}] \cdot \text{Knadh}}{\text{Kinadh} \cdot \text{Kacald}} + \frac{[\text{EtOH}] \cdot \text{Knad}}{\text{Kinad} \cdot \text{Ketoh}} + \frac{[\text{NAD}]}{\text{Kinad}} + \frac{[\text{AcAld}] \cdot [\text{NADH}]}{\text{Kinadh} \cdot \text{Kacald}} + \frac{[\text{NADH}] \cdot [\text{EtOH}] \cdot \text{Knad}}{\text{Kinadh} \cdot \text{Kinad} \cdot \text{Ketoh}} + \frac{[\text{AcAld}] \cdot [\text{NAD}] \cdot \text{Knadh}}{\text{Kinadh} \cdot \text{Kinad} \cdot \text{Kacald}} + \frac{[\text{EtOH}]}{\text{Ketoh}}}$$

Table 9: Properties of each parameter.

| Id      | Name | SBO | Value     | Unit                   | Constant |
|---------|------|-----|-----------|------------------------|----------|
| kcat    |      |     | 176.000   | s <sup>-1</sup>        | ✓        |
| Ketoh   |      |     | 17.000    | mmol · l <sup>-1</sup> | ✓        |
| Kinad   |      |     | 0.920     | mmol · l <sup>-1</sup> | ✓        |
| Knad    |      |     | 0.170     | mmol · l <sup>-1</sup> | ✓        |
| Knadh   |      |     | 0.110     | mmol · l <sup>-1</sup> | ✓        |
| Kinadh  |      |     | 0.031     | mmol · l <sup>-1</sup> | ✓        |
| Kacald  |      |     | 0.462     | mmol · l <sup>-1</sup> | ✓        |
| Kiacald |      |     | 1.100     | mmol · l <sup>-1</sup> | ✓        |
| Kietoh  |      |     | 90.000    | mmol · l <sup>-1</sup> | ✓        |
| Keq     |      |     | 14492.754 | dimensionless          | ✓        |

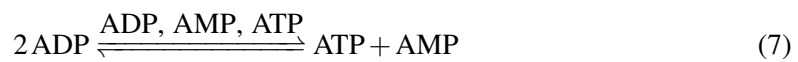
## 7.2 Reaction AK

This is a reversible reaction of one reactant forming two products influenced by three modifiers.

**Name** AK

**SBO:0000176** biochemical reaction

### Reaction equation



### Reactant

Table 10: Properties of each reactant.

| Id  | Name | SBO |
|-----|------|-----|
| ADP | ADP  |     |

## Modifiers

Table 11: Properties of each modifier.

| Id  | Name | SBO |
|-----|------|-----|
| ADP | ADP  |     |
| AMP | AMP  |     |
| ATP | ATP  |     |

## Products

Table 12: Properties of each product.

| Id  | Name | SBO |
|-----|------|-----|
| ATP | ATP  |     |
| AMP | AMP  |     |

## Kinetic Law

**Derived unit**  $0.0010 \text{ mol} \cdot \text{s}^{-1}$

$$v_2 = \text{vol}(\text{cell}) \cdot k \cdot \left( [\text{ADP}] \cdot [\text{ADP}] - \frac{[\text{AMP}] \cdot [\text{ATP}]}{\text{Keq}} \right) \quad (8)$$

Table 13: Properties of each parameter.

| Id  | Name | SBO | Value | Unit  | Constant                            |
|-----|------|-----|-------|---|-------------------------------------|
| k   |      |     | 0.75  | $\text{mmol}^{-1} \cdot \text{l} \cdot \text{s}^{-1}$ | <input checked="" type="checkbox"/> |
| Keq |      |     | 0.45  | dimensionless   | <input checked="" type="checkbox"/> |

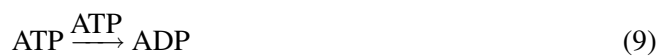
### 7.3 Reaction ATPase

This is an irreversible reaction of one reactant forming one product influenced by one modifier.

**Name** ATPase

**SBO:0000176** biochemical reaction

#### Reaction equation





## Reactant

Table 14: Properties of each reactant.

| Id  | Name | SBO |
|-----|------|-----|
| ATP | ATP  |     |

## Modifier

Table 15: Properties of each modifier.

| Id  | Name | SBO |
|-----|------|-----|
| ATP | ATP  |     |

## Product

Table 16: Properties of each product.

| Id  | Name | SBO |
|-----|------|-----|
| ADP | ADP  |     |

## Kinetic Law

**Derived unit** contains undeclared units

$$v_3 = \text{vol}(\text{cell}) \cdot \frac{\frac{V_{\max} \cdot [\text{ATP}]}{K_{\text{atp}}}}{1 + \frac{[\text{ATP}]}{K_{\text{atp}}}} \quad (10)$$

Table 17: Properties of each parameter.

| Id   | Name | SBO | Value | Unit  | Constant                            |
|------|------|-----|-------|---|-------------------------------------|
| Vmax |      |     | 6.16  | $\text{mmol} \cdot \text{l}^{-1} \cdot \text{s}^{-1}$ | <input checked="" type="checkbox"/> |
| Katp |      |     | 3.00  | $\text{mmol} \cdot \text{l}^{-1}$                     | <input checked="" type="checkbox"/> |

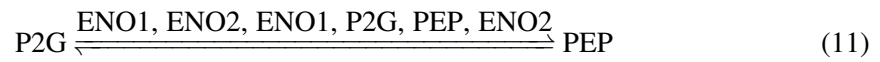
## 7.4 Reaction ENO

This is a reversible reaction of one reactant forming one product influenced by six modifiers.

**Name** ENO

**SBO:0000176** biochemical reaction

### Reaction equation



### Reactant

Table 18: Properties of each reactant.

| Id  | Name | SBO |
|-----|------|-----|
| P2G | P2G  |     |

### Modifiers

Table 19: Properties of each modifier.

| Id   | Name | SBO |
|------|------|-----|
| ENO1 | ENO1 |     |
| ENO2 | ENO2 |     |
| ENO1 | ENO1 |     |
| P2G  | P2G  |     |
| PEP  | PEP  |     |
| ENO2 | ENO2 |     |

### Product

Table 20: Properties of each product.

| Id  | Name | SBO |
|-----|------|-----|
| PEP | PEP  |     |

### Kinetic Law

**Derived unit** contains undeclared units

$$\begin{aligned}
v_4 = \text{vol}(\text{cell}) \cdot \frac{[\text{ENO1}] \cdot \text{kcat\_ENO1} \cdot \left( \frac{[\text{P2G}]}{\text{Kp2g\_ENO1}} - \frac{[\text{PEP}]}{\text{Kp2g\_ENO1} \cdot \text{Keq}} \right)}{1 + \frac{[\text{P2G}]}{\text{Kp2g\_ENO1}} + \frac{[\text{PEP}]}{\text{Kpep\_ENO1}}} \\
+ \text{vol}(\text{cell}) \cdot \frac{[\text{ENO2}] \cdot \text{kcat\_ENO2} \cdot \left( \frac{[\text{P2G}]}{\text{Kp2g\_ENO2}} - \frac{[\text{PEP}]}{\text{Kp2g\_ENO2} \cdot \text{Keq}} \right)}{1 + \frac{[\text{P2G}]}{\text{Kp2g\_ENO2}} + \frac{[\text{PEP}]}{\text{Kpep\_ENO2}}}
\end{aligned} \tag{12}$$

Table 21: Properties of each parameter.

| Id        | Name | SBO | Value  | Unit                   | Constant |
|-----------|------|-----|--------|------------------------|----------|
| kcat_ENO1 |      |     | 7.600  | s <sup>-1</sup>        | ✓        |
| Kp2g_ENO1 |      |     | 0.043  | mmol · l <sup>-1</sup> | ✓        |
| Kpep_ENO1 |      |     | 0.500  | mmol · l <sup>-1</sup> | ✓        |
| kcat_ENO2 |      |     | 19.870 | s <sup>-1</sup>        | ✓        |
| Kp2g_ENO2 |      |     | 0.104  | mmol · l <sup>-1</sup> | ✓        |
| Kpep_ENO2 |      |     | 0.500  | mmol · l <sup>-1</sup> | ✓        |
| Keq       |      |     | 6.700  | dimensionless          | ✓        |

## 7.5 Reaction FBA

This is a reversible reaction of one reactant forming two products influenced by five modifiers.

**Name** FBA

**SBO:0000176** biochemical reaction

### Reaction equation



### Reactant

Table 22: Properties of each reactant.

| Id    | Name  | SBO |
|-------|-------|-----|
| F16bP | F16bP |     |

### Modifiers

Table 23: Properties of each modifier.

| Id    | Name  | SBO |
|-------|-------|-----|
| FBA1  | FBA1  |     |
| FBA1  | FBA1  |     |
| F16bp | F16bp |     |
| DHAP  | DHAP  |     |
| GAP   | GAP   |     |

## Products

Table 24: Properties of each product.

| Id   | Name | SBO |
|------|------|-----|
| DHAP | DHAP |     |
| GAP  | GAP  |     |

## Kinetic Law

**Derived unit** contains undeclared units

$$v_5 = \text{vol}(\text{cell}) \cdot \frac{[\text{FBA1}] \cdot \text{kat} \cdot \left( \frac{[\text{F16bp}]}{\text{Kf16bp}} - \frac{[\text{DHAP}] \cdot [\text{GAP}]}{\text{Kf16bp} \cdot \text{Keq}} \right)}{1 + \frac{[\text{F16bp}]}{\text{Kf16bp}} + \frac{[\text{DHAP}]}{\text{Kdhap}} + \frac{[\text{GAP}]}{\text{Kgap}} + \frac{[\text{F16bp}] \cdot [\text{GAP}]}{\text{Kf16bp} \cdot \text{Kigap}} + \frac{[\text{DHAP}] \cdot [\text{GAP}]}{\text{Kdhap} \cdot \text{Kgap}}} \quad (14)$$

Table 25: Properties of each parameter.

| Id     | Name | SBO | Value  | Unit                   | Constant                            |
|--------|------|-----|--------|------------------------|-------------------------------------|
| kat    |      |     | 4.139  | s <sup>-1</sup>        | <input checked="" type="checkbox"/> |
| Kf16bp |      |     | 0.451  | mmol · l <sup>-1</sup> | <input checked="" type="checkbox"/> |
| Keq    |      |     | 0.069  | mmol · l <sup>-1</sup> | <input checked="" type="checkbox"/> |
| Kdhap  |      |     | 2.000  | mmol · l <sup>-1</sup> | <input checked="" type="checkbox"/> |
| Kgap   |      |     | 2.400  | mmol · l <sup>-1</sup> | <input checked="" type="checkbox"/> |
| Kigap  |      |     | 10.000 | mmol · l <sup>-1</sup> | <input checked="" type="checkbox"/> |

## 7.6 Reaction GPD

This is a reversible reaction of two reactants forming two products influenced by twelve modifiers.

**Name** GPD

**SBO:0000176** biochemical reaction

### Reaction equation



### Reactants

Table 26: Properties of each reactant.

| Id   | Name | SBO |
|------|------|-----|
| DHAP | DHAP |     |
| NADH | NADH |     |

### Modifiers

Table 27: Properties of each modifier.

| Id    | Name  | SBO |
|-------|-------|-----|
| ADP   | ADP   |     |
| ATP   | ATP   |     |
| F16bP | F16bP |     |
| GPD1  | GPD1  |     |
| GPD2  | GPD2  |     |
| DHAP  | DHAP  |     |
| NADH  | NADH  |     |
| G3P   | G3P   |     |
| NAD   | NAD   |     |
| F16bP | F16bP |     |
| ATP   | ATP   |     |
| ADP   | ADP   |     |

### Products

Table 28: Properties of each product.

| Id  | Name | SBO |
|-----|------|-----|
| G3P | G3P  |     |
| NAD | NAD  |     |

## Kinetic Law

**Derived unit** contains undeclared units

$$v_6 = \text{vol}(\text{cell}) \cdot \frac{\frac{V_{\max}}{K_{\text{dhap}} \cdot K_{\text{nadh}}} \cdot \left( [\text{DHAP}] \cdot [\text{NADH}] - \frac{[\text{G3P}] \cdot [\text{NAD}]}{K_{\text{eq}}} \right)}{\left( 1 + \frac{[\text{F16bP}]}{K_{\text{fbp}}} + \frac{[\text{ATP}]}{K_{\text{atp}}} + \frac{[\text{ADP}]}{K_{\text{adp}}} \right) \cdot \left( 1 + \frac{[\text{DHAP}]}{K_{\text{dhap}}} + \frac{[\text{G3P}]}{K_{\text{g3p}}} \right) \cdot \left( 1 + \frac{[\text{NADH}]}{K_{\text{nadh}}} + \frac{[\text{NAD}]}{K_{\text{nad}}} \right)} \quad (16)$$

Table 29: Properties of each parameter.

| Id    | Name | SBO | Value     | Unit  | Constant                            |
|-------|------|-----|-----------|---|-------------------------------------|
| Vmax  |      |     | 0.783     | $\text{mmol} \cdot \text{l}^{-1} \cdot \text{s}^{-1}$ | <input checked="" type="checkbox"/> |
| Knadh |      |     | 0.023     | $\text{mmol} \cdot \text{l}^{-1}$                     | <input checked="" type="checkbox"/> |
| Kdhap |      |     | 0.540     | $\text{mmol} \cdot \text{l}^{-1}$                     | <input checked="" type="checkbox"/> |
| Keq   |      |     | 10000.000 | dimensionless   | <input checked="" type="checkbox"/> |
| Kfbp  |      |     | 4.800     | $\text{mmol} \cdot \text{l}^{-1}$                     | <input checked="" type="checkbox"/> |
| Katp  |      |     | 0.730     | $\text{mmol} \cdot \text{l}^{-1}$                     | <input checked="" type="checkbox"/> |
| Kadp  |      |     | 2.000     | $\text{mmol} \cdot \text{l}^{-1}$                     | <input checked="" type="checkbox"/> |
| Knad  |      |     | 0.930     | $\text{mmol} \cdot \text{l}^{-1}$                     | <input checked="" type="checkbox"/> |
| Kg3p  |      |     | 1.200     | $\text{mmol} \cdot \text{l}^{-1}$                     | <input checked="" type="checkbox"/> |

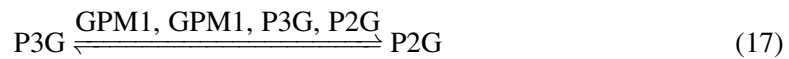
## 7.7 Reaction GPM

This is a reversible reaction of one reactant forming one product influenced by four modifiers.

**Name** GPM

**SBO:0000176** biochemical reaction

### Reaction equation



### Reactant

Table 30: Properties of each reactant.

| Id  | Name | SBO |
|-----|------|-----|
| P3G | P3G  |     |

## Modifiers

Table 31: Properties of each modifier.

| Id   | Name | SBO |
|------|------|-----|
| GPM1 | GPM1 |     |
| GPM1 | GPM1 |     |
| P3G  | P3G  |     |
| P2G  | P2G  |     |

## Product

Table 32: Properties of each product.

| Id  | Name | SBO |
|-----|------|-----|
| P2G | P2G  |     |

## Kinetic Law

**Derived unit** contains undeclared units

$$v_7 = \text{vol}(\text{cell}) \cdot \frac{[\text{GPM1}] \cdot k_{\text{cat}} \cdot \left( \frac{[\text{P3G}]}{K_{\text{p3g}}} - \frac{[\text{P2G}]}{K_{\text{p3g}} \cdot K_{\text{eq}}} \right)}{1 + \frac{[\text{P3G}]}{K_{\text{p3g}}} + \frac{[\text{P2G}]}{K_{\text{p2g}}}} \quad (18)$$

Table 33: Properties of each parameter.

| Id   | Name | SBO | Value  | Unit                   | Constant |
|------|------|-----|--------|------------------------|----------|
| kcat |      |     | 400.00 | s <sup>-1</sup>        | ✓        |
| Kp3g |      |     | 1.20   | mmol · l <sup>-1</sup> | ✓        |
| Keq  |      |     | 0.19   | dimensionless          | ✓        |
| Kp2g |      |     | 1.41   | mmol · l <sup>-1</sup> | ✓        |

## 7.8 Reaction GPP

This is an irreversible reaction of one reactant forming one product influenced by three modifiers.

**Name** GPP

**SBO:0000176** biochemical reaction

## Reaction equation



## Reactant

Table 34: Properties of each reactant.

| Id  | Name | SBO |
|-----|------|-----|
| G3P | G3P  |     |

## Modifiers

Table 35: Properties of each modifier.

| Id   | Name | SBO |
|------|------|-----|
| HOR2 | HOR2 |     |
| RHR2 | RHR2 |     |
| G3P  | G3P  |     |

## Product

Table 36: Properties of each product.

| Id  | Name | SBO |
|-----|------|-----|
| GLY | GLY  |     |

## Kinetic Law

**Derived unit** contains undeclared units

$$v_8 = \text{vol}(\text{cell}) \cdot \frac{\frac{V_{\max} \cdot [\text{G3P}]}{K_{\text{g3p}}}}{1 + \frac{[\text{G3P}]}{K_{\text{g3p}}}} \quad (20)$$

Table 37: Properties of each parameter.

| Id   | Name | SBO | Value | Unit  | Constant                            |
|------|------|-----|-------|---|-------------------------------------|
| Vmax |      |     | 0.883 | $\text{mmol} \cdot \text{l}^{-1} \cdot \text{s}^{-1}$ | <input checked="" type="checkbox"/> |
| Kg3p |      |     | 3.500 | $\text{mmol} \cdot \text{l}^{-1}$                     | <input checked="" type="checkbox"/> |



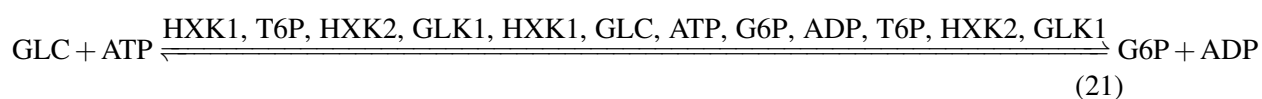
## 7.9 Reaction HXK

This is a reversible reaction of two reactants forming two products influenced by twelve modifiers.

**Name** HXK

**SBO:0000176** biochemical reaction

### Reaction equation



### Reactants

Table 38: Properties of each reactant.

| Id  | Name | SBO |
|-----|------|-----|
| GLC | GLC  |     |
| ATP | ATP  |     |

### Modifiers

Table 39: Properties of each modifier.

| Id   | Name | SBO |
|------|------|-----|
| HXK1 | HXK1 |     |
| T6P  | T6P  |     |
| HXK2 | HXK2 |     |
| GLK1 | GLK1 |     |
| HXK1 | HXK1 |     |
| GLC  | GLC  |     |
| ATP  | ATP  |     |
| G6P  | G6P  |     |
| ADP  | ADP  |     |
| T6P  | T6P  |     |
| HXK2 | HXK2 |     |
| GLK1 | GLK1 |     |

### Products

Table 40: Properties of each product.

| Id  | Name | SBO |
|-----|------|-----|
| G6P | G6P  |     |
| ADP | ADP  |     |

## Kinetic Law

**Derived unit** contains undeclared units

$$\begin{aligned}
 v_9 = \text{vol}(\text{cell}) \cdot & \frac{[\text{HXK1}] \cdot \text{kat\_HXK1} \cdot \left( \frac{[\text{GLC}] \cdot [\text{ATP}]}{\text{Kglc\_HXK1} \cdot \text{Katp\_HXK1}} - \frac{[\text{G6P}] \cdot [\text{ADP}]}{\text{Kglc\_HXK1} \cdot \text{Katp\_HXK1} \cdot \text{Keq}} \right)}{\left( 1 + \frac{[\text{GLC}]}{\text{Kglc\_HXK1}} + \frac{[\text{G6P}]}{\text{Kg6p\_HXK1}} + \frac{[\text{T6P}]}{\text{Kit6p\_HXK1}} \right) \cdot \left( 1 + \frac{[\text{ATP}]}{\text{Katp\_HXK1}} + \frac{[\text{ADP}]}{\text{Kadp\_HXK1}} \right)} \\
 & + \text{vol}(\text{cell}) \cdot \frac{[\text{HXK2}] \cdot \text{kat\_HXK2} \cdot \left( \frac{[\text{GLC}] \cdot [\text{ATP}]}{\text{Kglc\_HXK2} \cdot \text{Katp\_HXK2}} - \frac{[\text{G6P}] \cdot [\text{ADP}]}{\text{Kglc\_HXK2} \cdot \text{Katp\_HXK2} \cdot \text{Keq}} \right)}{\left( 1 + \frac{[\text{GLC}]}{\text{Kglc\_HXK2}} + \frac{[\text{G6P}]}{\text{Kg6p\_HXK2}} + \frac{[\text{T6P}]}{\text{Kit6p\_HXK2}} \right) \cdot \left( 1 + \frac{[\text{ATP}]}{\text{Katp\_HXK2}} + \frac{[\text{ADP}]}{\text{Kadp\_HXK2}} \right)} \\
 & + \text{vol}(\text{cell}) \cdot \frac{[\text{GLK1}] \cdot \text{kat\_GLK1} \cdot \left( \frac{[\text{GLC}] \cdot [\text{ATP}]}{\text{Kglc\_GLK1} \cdot \text{Katp\_GLK1}} - \frac{[\text{G6P}] \cdot [\text{ADP}]}{\text{Kglc\_GLK1} \cdot \text{Katp\_GLK1} \cdot \text{Keq}} \right)}{\left( 1 + \frac{[\text{GLC}]}{\text{Kglc\_GLK1}} + \frac{[\text{G6P}]}{\text{Kg6p\_GLK1}} \right) \cdot \left( 1 + \frac{[\text{ATP}]}{\text{Katp\_GLK1}} + \frac{[\text{ADP}]}{\text{Kadp\_GLK1}} \right)}
 \end{aligned} \tag{22}$$

Table 41: Properties of each parameter.

| Id         | Name | SBO | Value    | Unit                   | Constant |
|------------|------|-----|----------|------------------------|----------|
| kat_HXK1   |      |     | 10.200   | s <sup>-1</sup>        | ✓        |
| Kglc_HXK1  |      |     | 0.150    | mmol · l <sup>-1</sup> | ✓        |
| Katp_HXK1  |      |     | 0.293    | mmol · l <sup>-1</sup> | ✓        |
| Kg6p_HXK1  |      |     | 30.000   | mmol · l <sup>-1</sup> | ✓        |
| Kadp_HXK1  |      |     | 0.230    | mmol · l <sup>-1</sup> | ✓        |
| Kit6p_HXK1 |      |     | 0.200    | mmol · l <sup>-1</sup> | ✓        |
| kat_HXK2   |      |     | 63.100   | s <sup>-1</sup>        | ✓        |
| Kglc_HXK2  |      |     | 0.200    | mmol · l <sup>-1</sup> | ✓        |
| Katp_HXK2  |      |     | 0.195    | mmol · l <sup>-1</sup> | ✓        |
| Kg6p_HXK2  |      |     | 30.000   | mmol · l <sup>-1</sup> | ✓        |
| Kadp_HXK2  |      |     | 0.230    | mmol · l <sup>-1</sup> | ✓        |
| Kit6p_HXK2 |      |     | 0.040    | mmol · l <sup>-1</sup> | ✓        |
| kat_GLK1   |      |     | 0.072    | s <sup>-1</sup>        | ✓        |
| Kglc_GLK1  |      |     | 0.011    | mmol · l <sup>-1</sup> | ✓        |
| Katp_GLK1  |      |     | 0.865    | mmol · l <sup>-1</sup> | ✓        |
| Kg6p_GLK1  |      |     | 30.000   | mmol · l <sup>-1</sup> | ✓        |
| Kadp_GLK1  |      |     | 0.230    | mmol · l <sup>-1</sup> | ✓        |
| Keq        |      |     | 2000.000 | dimensionless          | ✓        |

## 7.10 Reaction PDC

This is an irreversible reaction of one reactant forming one product influenced by seven modifiers.

**Name** PDC

**SBO:0000176** biochemical reaction

### Reaction equation



### Reactant

Table 42: Properties of each reactant.

| Id  | Name | SBO |
|-----|------|-----|
| PYR | PYR  |     |

### Modifiers

Table 43: Properties of each modifier.

| Id   | Name | SBO |
|------|------|-----|
| PDC1 | PDC1 |     |
| PDC5 | PDC5 |     |
| PDC6 | PDC6 |     |
| PDC1 | PDC1 |     |
| PYR  | PYR  |     |
| PDC5 | PDC5 |     |
| PDC6 | PDC6 |     |

### Product

Table 44: Properties of each product.

| Id    | Name  | SBO |
|-------|-------|-----|
| AcAld | AcAld |     |

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{10} = \text{vol}(\text{cell}) \cdot \frac{\frac{[\text{PDC1}] \cdot \text{kcat\_PDC1} \cdot [\text{PYR}]}{K_{\text{pyr\_PDC1}}}}{1 + \frac{[\text{PYR}]}{K_{\text{pyr\_PDC1}}}} + \text{vol}(\text{cell}) \cdot \frac{\frac{[\text{PDC5}] \cdot \text{kcat\_PDC5} \cdot [\text{PYR}]}{K_{\text{pyr\_PDC5}}}}{1 + \frac{[\text{PYR}]}{K_{\text{pyr\_PDC5}}}} + \text{vol}(\text{cell}) \cdot \frac{\frac{[\text{PDC6}] \cdot \text{kcat\_PDC6} \cdot [\text{PYR}]}{K_{\text{pyr\_PDC6}}}}{1 + \frac{[\text{PYR}]}{K_{\text{pyr\_PDC6}}}} \quad (24)$$

Table 45: Properties of each parameter.

| Id        | Name | SBO | Value | Unit                   | Constant |
|-----------|------|-----|-------|------------------------|----------|
| kcat_PDC1 |      |     | 12.14 | s <sup>-1</sup>        | ✓        |
| Kpyr_PDC1 |      |     | 8.50  | mmol · l <sup>-1</sup> | ✓        |
| kcat_PDC5 |      |     | 10.32 | s <sup>-1</sup>        | ✓        |
| Kpyr_PDC5 |      |     | 7.08  | mmol · l <sup>-1</sup> | ✓        |
| kcat_PDC6 |      |     | 9.21  | s <sup>-1</sup>        | ✓        |
| Kpyr_PDC6 |      |     | 2.92  | mmol · l <sup>-1</sup> | ✓        |

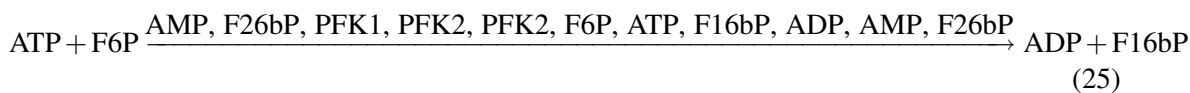
## 7.11 Reaction PFK

This is an irreversible reaction of two reactants forming two products influenced by eleven modifiers.

**Name** PFK

**SBO:0000176** biochemical reaction

### Reaction equation



## Reactants

Table 46: Properties of each reactant.

| Id  | Name | SBO |
|-----|------|-----|
| ATP | ATP  |     |
| F6P | F6P  |     |

## Modifiers

Table 47: Properties of each modifier.

| Id    | Name  | SBO |
|-------|-------|-----|
| AMP   | AMP   |     |
| F26bP | F26bP |     |
| PFK1  | PFK1  |     |
| PFK2  | PFK2  |     |
| PFK2  | PFK2  |     |
| F6P   | F6P   |     |
| ATP   | ATP   |     |
| F16bP | F16bP |     |
| ADP   | ADP   |     |
| AMP   | AMP   |     |
| F26bP | F26bP |     |

## Products

Table 48: Properties of each product.

| Id    | Name  | SBO |
|-------|-------|-----|
| ADP   | ADP   |     |
| F16bP | F16bP |     |

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{11} = \text{vol}(\text{cell}) \cdot [\text{PFK2}] \cdot \text{kcat} \quad (26)$$

$$gR \cdot \frac{[F6P]}{Kf6p} \cdot \frac{[ATP]}{Katp} \cdot \left(1 - \frac{[F16bP] \cdot [ADP]}{[F6P] \cdot [ATP] \cdot Keq}\right) \cdot \left(1 + \frac{[F6P]}{Kf6p} + \frac{[ATP]}{Katp} + \frac{gR \cdot [F6P] \cdot [ATP]}{Kf6p \cdot Katp} + \frac{[F16bP]}{Kf16} + \frac{[ADP]}{Kadp}\right) \cdot \left(1 + \frac{[F6P]}{Kf6p} + \frac{[ATP]}{Katp} + \frac{gR \cdot [F6P] \cdot [ATP]}{Kf6p \cdot Katp} + \frac{[F16bP]}{Kf16} + \frac{[ADP]}{Kadp} + \frac{gR \cdot [F16bP] \cdot [ADP]}{Kf16 \cdot Kadp}\right)^2 + L0 \cdot \left(\frac{1 + \frac{Ciatp \cdot [ATP]}{Katp}}{1 + \frac{[ATP]}{Katp}}\right)^2 \cdot \left(\frac{1 + \frac{Camp \cdot [AMP]}{Kamp}}{1 + \frac{[AMP]}{Kamp}}\right)^2 \cdot \left(\frac{1 + \frac{Cf26bP \cdot [F26bP]}{Kf26bP}}{1 + \frac{[F26bP]}{Kf26bP}}\right)^2$$

Table 49: Properties of each parameter.

| Id   | Name | SBO | Value   | Unit                   | Constant |
|------|------|-----|---------|------------------------|----------|
| kcat |      |     | 209.600 | s <sup>-1</sup>        | ✓        |
| gR   |      |     | 5.120   | dimensionless          | ✓        |
| Kf6p |      |     | 0.100   | mmol · l <sup>-1</sup> | ✓        |

| Id    | Name | SBO | Value                | Unit                              | Constant                            |
|-------|------|-----|----------------------|-----------------------------------|-------------------------------------|
| Katp  |      |     | 0.710                | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> |
| L0    |      |     | 0.660                | dimensionless                     | <input checked="" type="checkbox"/> |
| Ciatp |      |     | 100.000              | dimensionless                     | <input checked="" type="checkbox"/> |
| Kiatp |      |     | 0.650                | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> |
| Camp  |      |     | 0.085                | dimensionless                     | <input checked="" type="checkbox"/> |
| Kamp  |      |     | 0.100                | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> |
| Cf26  |      |     | 0.017                | dimensionless                     | <input checked="" type="checkbox"/> |
| Kf26  |      |     | $6.82 \cdot 10^{-4}$ | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> |
| Cf16  |      |     | 0.397                | dimensionless                     | <input checked="" type="checkbox"/> |
| Kf16  |      |     | 0.111                | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> |
| Catp  |      |     | 3.000                | dimensionless                     | <input checked="" type="checkbox"/> |
| Kadp  |      |     | 1.000                | $\text{mmol} \cdot \text{l}^{-1}$ | <input checked="" type="checkbox"/> |
| Keq   |      |     | 800.000              | dimensionless                     | <input checked="" type="checkbox"/> |

## 7.12 Reaction PGI

This is a reversible reaction of one reactant forming one product influenced by four modifiers.

**Name** PGI

**SBO:0000176** biochemical reaction

### Reaction equation



### Reactant

Table 50: Properties of each reactant.

| Id  | Name | SBO |
|-----|------|-----|
| G6P | G6P  |     |

### Modifiers

Table 51: Properties of each modifier.

| Id   | Name | SBO |
|------|------|-----|
| PGI1 | PGI1 |     |
| PGI1 | PGI1 |     |
| G6P  | G6P  |     |

| Id  | Name | SBO |
|-----|------|-----|
| F6P | F6P  |     |

## Product

Table 52: Properties of each product.

| Id  | Name | SBO |
|-----|------|-----|
| F6P | F6P  |     |

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{12} = \text{vol}(\text{cell}) \cdot \frac{[\text{PGI1}] \cdot \text{kcat} \cdot \left( \frac{[\text{G6P}]}{\text{Kg6p}} - \frac{[\text{F6P}]}{\text{Kg6p} \cdot \text{Keq}} \right)}{1 + \frac{[\text{G6P}]}{\text{Kg6p}} + \frac{[\text{F6P}]}{\text{Kf6p}}} \quad (28)$$

Table 53: Properties of each parameter.

| Id   | Name | SBO | Value   | Unit                   | Constant |
|------|------|-----|---------|------------------------|----------|
| kcat |      |     | 487.360 | s <sup>-1</sup>        | ✓        |
| Kg6p |      |     | 1.026   | mmol · l <sup>-1</sup> | ✓        |
| Keq  |      |     | 0.290   | dimensionless          | ✓        |
| Kf6p |      |     | 0.307   | mmol · l <sup>-1</sup> | ✓        |

## 7.13 Reaction PGK

This is a reversible reaction of two reactants forming two products influenced by six modifiers.

**Name** PGK

**SBO:0000176** biochemical reaction

## Reaction equation



## Reactants

Table 54: Properties of each reactant.

| Id  | Name | SBO |
|-----|------|-----|
| ADP | ADP  |     |
| BPG | BPG  |     |

## Modifiers

Table 55: Properties of each modifier.

| Id   | Name | SBO |
|------|------|-----|
| PGK1 | PGK1 |     |
| PGK1 | PGK1 |     |
| ADP  | ADP  |     |
| BPG  | BPG  |     |
| P3G  | P3G  |     |
| ATP  | ATP  |     |

## Products

Table 56: Properties of each product.

| Id  | Name | SBO |
|-----|------|-----|
| ATP | ATP  |     |
| P3G | P3G  |     |

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{13} = \text{vol}(\text{cell}) \cdot \frac{[\text{PGK1}] \cdot \text{kcat} \cdot \left( \frac{[\text{ADP}]}{\text{K}_{\text{adp}}} \right)^{\text{nHadp}-1} \cdot \left( \frac{[\text{BPG}] \cdot [\text{ADP}]}{\text{K}_{\text{bpg}} \cdot \text{K}_{\text{adp}}} - \frac{[\text{P3G}] \cdot [\text{ATP}]}{\text{K}_{\text{bpg}} \cdot \text{K}_{\text{adp}} \cdot \text{K}_{\text{eq}}} \right)}{\left( 1 + \frac{[\text{BPG}]}{\text{K}_{\text{bpg}}} + \frac{[\text{P3G}]}{\text{K}_{\text{p3g}}} \right) \cdot \left( 1 + \left( \frac{[\text{ADP}]}{\text{K}_{\text{adp}}} \right)^{\text{nHadp}} + \frac{[\text{ATP}]}{\text{K}_{\text{atp}}} \right)} \quad (30)$$

Table 57: Properties of each parameter.

| Id   | Name | SBO | Value    | Unit                   | Constant |
|------|------|-----|----------|------------------------|----------|
| kcat |      |     | 58.600   | s <sup>-1</sup>        | ✓        |
| Keq  |      |     | 3200.000 | dimensionless          | ✓        |
| Kp3g |      |     | 4.580    | mmol · l <sup>-1</sup> | ✓        |



| Id    | Name | SBO | Value | Unit                   | Constant                            |
|-------|------|-----|-------|------------------------|-------------------------------------|
| Katp  |      |     | 1.990 | mmol · l <sup>-1</sup> | <input checked="" type="checkbox"/> |
| Kbpg  |      |     | 0.003 | mmol · l <sup>-1</sup> | <input checked="" type="checkbox"/> |
| Kadp  |      |     | 0.200 | mmol · l <sup>-1</sup> | <input checked="" type="checkbox"/> |
| nHadp |      |     | 2.000 | dimensionless          | <input checked="" type="checkbox"/> |

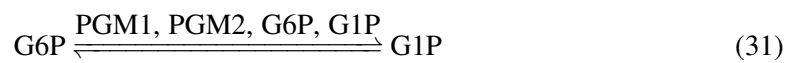
## 7.14 Reaction PGM

This is a reversible reaction of one reactant forming one product influenced by four modifiers.

**Name** PGM

**SBO:0000176** biochemical reaction

### Reaction equation



### Reactant

Table 58: Properties of each reactant.

| Id  | Name | SBO |
|-----|------|-----|
| G6P | G6P  |     |

### Modifiers

Table 59: Properties of each modifier.

| Id   | Name | SBO |
|------|------|-----|
| PGM1 | PGM1 |     |
| PGM2 | PGM2 |     |
| G6P  | G6P  |     |
| G1P  | G1P  |     |

### Product

Table 60: Properties of each product.

| Id  | Name | SBO |
|-----|------|-----|
| G1P | G1P  |     |

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{14} = \text{vol}(\text{cell}) \cdot \frac{V_{\max} \cdot \left( \frac{[\text{G6P}]}{K_{\text{g6p}}} - \frac{[\text{G1P}]}{K_{\text{g6p}} \cdot K_{\text{eq}}} \right)}{1 + \frac{[\text{G6P}]}{K_{\text{g6p}}} + \frac{[\text{G1P}]}{K_{\text{g1p}}}} \quad (32)$$

Table 61: Properties of each parameter.

| Id   | Name | SBO | Value | Unit  | Constant |
|------|------|-----|-------|---|----------|
| Vmax |      |     | 0.128 | $\text{mmol} \cdot \text{l}^{-1} \cdot \text{s}^{-1}$ | ✓        |
| Kg6p |      |     | 0.050 | $\text{mmol} \cdot \text{l}^{-1}$                     | ✓        |
| Kg1p |      |     | 0.023 | $\text{mmol} \cdot \text{l}^{-1}$                     | ✓        |
| Keq  |      |     | 0.167 | dimensionless   | ✓        |

## 7.15 Reaction PYK

This is a reversible reaction of two reactants forming two products influenced by eight modifiers.

**Name** PYK

**SBO:0000176** biochemical reaction

### Reaction equation



## Reactants

Table 62: Properties of each reactant.

| Id  | Name | SBO |
|-----|------|-----|
| ADP | ADP  |     |
| PEP | PEP  |     |

## Modifiers

Table 63: Properties of each modifier.

| Id    | Name  | SBO |
|-------|-------|-----|
| CDC19 | CDC19 |     |

| Id    | Name  | SBO |
|-------|-------|-----|
| F16bP | F16bP |     |
| CDC19 | CDC19 |     |
| PEP   | PEP   |     |
| ADP   | ADP   |     |
| PYR   | PYR   |     |
| ATP   | ATP   |     |
| F16bP | F16bP |     |

## Products

Table 64: Properties of each product.

| Id  | Name | SBO |
|-----|------|-----|
| ATP | ATP  |     |
| PYR | PYR  |     |

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{15} = \text{vol}(\text{cell}) \cdot \frac{[\text{CDC19}] \cdot k_{\text{cat}} \cdot \left( \frac{[\text{PEP}] \cdot [\text{ADP}] - \frac{[\text{PYR}] \cdot [\text{ATP}]}{K_{\text{eq}}}}{K_{\text{pep}} \cdot K_{\text{adp}}} \right)}{\left( 1 + \frac{[\text{PEP}]}{K_{\text{pep}}} + \frac{[\text{PYR}]}{K_{\text{pyr}}} + L_0 \cdot \frac{\frac{[\text{ATP}]}{K_{\text{iatp}}} + 1}{\frac{[\text{F16bP}]}{K_{\text{f16p}}} + 1} \right) \cdot \left( 1 + \frac{[\text{ADP}]}{K_{\text{adp}}} + \frac{[\text{ATP}]}{K_{\text{atp}}} \right)} \quad (34)$$

Table 65: Properties of each parameter.

| Id    | Name | SBO | Value    | Unit                   | Constant |
|-------|------|-----|----------|------------------------|----------|
| kcat  |      |     | 20.146   | s <sup>-1</sup>        | ✓        |
| Kpep  |      |     | 0.281    | mmol · l <sup>-1</sup> | ✓        |
| Kadp  |      |     | 0.243    | mmol · l <sup>-1</sup> | ✓        |
| Kpyr  |      |     | 21.000   | mmol · l <sup>-1</sup> | ✓        |
| Katp  |      |     | 1.500    | mmol · l <sup>-1</sup> | ✓        |
| Kiatp |      |     | 9.300    | mmol · l <sup>-1</sup> | ✓        |
| Kf16p |      |     | 0.200    | mmol · l <sup>-1</sup> | ✓        |
| L0    |      |     | 100.000  | dimensionless          | ✓        |
| Keq   |      |     | 6500.000 | dimensionless          | ✓        |

## 7.16 Reaction TDH

This is a reversible reaction of two reactants forming two products influenced by eight modifiers.

**Name** TDH

**SBO:0000176** biochemical reaction

### Reaction equation



### Reactants

Table 66: Properties of each reactant.

| Id  | Name | SBO |
|-----|------|-----|
| GAP | GAP  |     |
| NAD | NAD  |     |

### Modifiers

Table 67: Properties of each modifier.

| Id   | Name | SBO |
|------|------|-----|
| TDH1 | TDH1 |     |
| TDH3 | TDH3 |     |
| TDH1 | TDH1 |     |
| GAP  | GAP  |     |
| NAD  | NAD  |     |
| BPG  | BPG  |     |
| NADH | NADH |     |
| TDH3 | TDH3 |     |

### Products

Table 68: Properties of each product.

| Id   | Name | SBO |
|------|------|-----|
| BPG  | BPG  |     |
| NADH | NADH |     |

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{16} = \text{vol}(\text{cell}) \cdot \frac{[\text{TDH1}] \cdot \text{kcat\_TDH1} \cdot \left( \frac{[\text{GAP}] \cdot [\text{NAD}]}{\text{Kgap\_TDH1} \cdot \text{Knad\_TDH1}} - \frac{[\text{BPG}] \cdot [\text{NADH}]}{\text{Kgap\_TDH1} \cdot \text{Knad\_TDH1} \cdot \text{Keq}} \right)}{\left( 1 + \frac{[\text{GAP}]}{\text{Kgap\_TDH1}} + \frac{[\text{BPG}]}{\text{Kbpg\_TDH1}} \right) \cdot \left( 1 + \frac{[\text{NAD}]}{\text{Knad\_TDH1}} + \frac{[\text{NADH}]}{\text{Knadh\_TDH1}} \right)} + \text{vol}(\text{cell}) \cdot \frac{[\text{TDH3}] \cdot \text{kcat\_TDH3} \cdot \left( \frac{[\text{GAP}] \cdot [\text{NAD}]}{\text{Kgap\_TDH3} \cdot \text{Knad\_TDH3}} - \frac{[\text{BPG}] \cdot [\text{NADH}]}{\text{Kgap\_TDH3} \cdot \text{Knad\_TDH3} \cdot \text{Keq}} \right)}{\left( 1 + \frac{[\text{GAP}]}{\text{Kgap\_TDH3}} + \frac{[\text{BPG}]}{\text{Kbpg\_TDH3}} \right) \cdot \left( 1 + \frac{[\text{NAD}]}{\text{Knad\_TDH3}} + \frac{[\text{NADH}]}{\text{Knadh\_TDH3}} \right)} \quad (36)$$

Table 69: Properties of each parameter.

| Id         | Name | SBO | Value  | Unit                   | Constant |
|------------|------|-----|--------|------------------------|----------|
| kcat_TDH1  |      |     | 19.120 | s <sup>-1</sup>        | ✓        |
| Kgap_TDH1  |      |     | 0.495  | mmol · l <sup>-1</sup> | ✓        |
| Knad_TDH1  |      |     | 0.090  | mmol · l <sup>-1</sup> | ✓        |
| Kbpg_TDH1  |      |     | 0.010  | mmol · l <sup>-1</sup> | ✓        |
| Knadh_TDH1 |      |     | 0.060  | mmol · l <sup>-1</sup> | ✓        |
| kcat_TDH3  |      |     | 18.162 | s <sup>-1</sup>        | ✓        |
| Kgap_TDH3  |      |     | 0.423  | mmol · l <sup>-1</sup> | ✓        |
| Knad_TDH3  |      |     | 0.090  | mmol · l <sup>-1</sup> | ✓        |
| Kbpg_TDH3  |      |     | 0.909  | mmol · l <sup>-1</sup> | ✓        |
| Knadh_TDH3 |      |     | 0.060  | mmol · l <sup>-1</sup> | ✓        |
| Keq        |      |     | 0.005  | dimensionless          | ✓        |

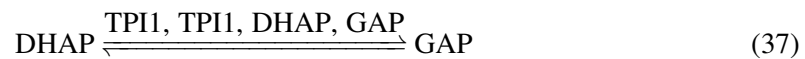
## 7.17 Reaction TPI

This is a reversible reaction of one reactant forming one product influenced by four modifiers.

**Name** TPI

**SBO:0000176** biochemical reaction

### Reaction equation



### Reactant

Table 70: Properties of each reactant.

| Id   | Name | SBO |
|------|------|-----|
| DHAP | DHAP |     |

Modifiers

Table 71: Properties of each modifier.

| Id   | Name | SBO |
|------|------|-----|
| TPI1 | TPI1 |     |
| TPI1 | TPI1 |     |
| DHAP | DHAP |     |
| GAP  | GAP  |     |

Product

Table 72: Properties of each product.

| Id  | Name | SBO |
|-----|------|-----|
| GAP | GAP  |     |

Kinetic Law

**Derived unit** contains undeclared units

$$v_{17} = \text{vol}(\text{cell}) \cdot \frac{\frac{[\text{TPI1}] \cdot k_{\text{cat}}}{K_{\text{dhap}}} \cdot \left( [\text{DHAP}] - \frac{[\text{GAP}]}{K_{\text{eq}}} \right)}{1 + \frac{[\text{DHAP}]}{K_{\text{dhap}}} + \frac{[\text{GAP}]}{K_{\text{gap}}} \cdot \left( 1 + \left( \frac{[\text{GAP}]}{K_{\text{igap}}} \right)^4 \right)}$$

(38)

Table 73: Properties of each parameter.

| Id    | Name | SBO | Value   | Unit                   | Constant |
|-------|------|-----|---------|------------------------|----------|
| kcat  |      |     | 564.380 | s <sup>-1</sup>        | ✓        |
| Kdhap |      |     | 6.454   | mmol · l <sup>-1</sup> | ✓        |
| Kgap  |      |     | 5.250   | mmol · l <sup>-1</sup> | ✓        |
| Kigap |      |     | 35.100  | mmol · l <sup>-1</sup> | ✓        |
| Keq   |      |     | 0.045   | dimensionless          | ✓        |

### 7.18 Reaction TPP

This is an irreversible reaction of one reactant forming one product influenced by three modifiers.

**Name** TPP

**SBO:0000176** biochemical reaction

#### Reaction equation



#### Reactant

Table 74: Properties of each reactant.

| Id  | Name | SBO |
|-----|------|-----|
| T6P | T6P  |     |

#### Modifiers

Table 75: Properties of each modifier.

| Id   | Name | SBO |
|------|------|-----|
| TPS1 | TPS1 |     |
| TPS2 | TPS2 |     |
| T6P  | T6P  |     |

#### Product

Table 76: Properties of each product.

| Id  | Name | SBO |
|-----|------|-----|
| TRH | TRH  |     |

#### Kinetic Law

**Derived unit** contains undeclared units

$$v_{18} = \text{vol}(\text{cell}) \cdot \frac{V_{\max} \cdot [\text{T6P}]}{K_{t6p} + [\text{T6P}]} \quad (40)$$

Table 77: Properties of each parameter.

| Id   | Name | SBO | Value | Unit  | Constant                            |
|------|------|-----|-------|---|-------------------------------------|
| Vmax |      |     | 2.340 | $\text{mmol} \cdot \text{l}^{-1} \cdot \text{s}^{-1}$ | <input checked="" type="checkbox"/> |
| Kt6p |      |     | 0.500 | $\text{mmol} \cdot \text{l}^{-1}$                     | <input checked="" type="checkbox"/> |

### 7.19 Reaction TPS

This is an irreversible reaction of two reactants forming two products influenced by four modifiers.

**Name** TPS

**SBO:0000176** biochemical reaction

#### Reaction equation



#### Reactants

Table 78: Properties of each reactant.

| Id  | Name | SBO |
|-----|------|-----|
| G6P | G6P  |     |
| UDG | UDG  |     |

#### Modifiers

Table 79: Properties of each modifier.

| Id   | Name | SBO |
|------|------|-----|
| TPS1 | TPS1 |     |
| TPS2 | TPS2 |     |
| G6P  | G6P  |     |
| UDG  | UDG  |     |

#### Products



Table 80: Properties of each product.

| Id  | Name | SBO |
|-----|------|-----|
| T6P | T6P  |     |
| UDP | UDP  |     |

### Kinetic Law

**Derived unit** contains undeclared units

$$v_{19} = \text{vol}(\text{cell}) \cdot \frac{\frac{V_{\max} \cdot [\text{G6P}] \cdot [\text{UDG}]}{K_{\text{g6p}} \cdot K_{\text{udg}}}}{\left(1 + \frac{[\text{G6P}]}{K_{\text{g6p}}}\right) \cdot \left(1 + \frac{[\text{UDG}]}{K_{\text{udg}}}\right)} \quad (42)$$

Table 81: Properties of each parameter.

| Id   | Name | SBO | Value | Unit  | Constant |
|------|------|-----|-------|---|----------|
| Vmax |      |     | 0.494 | $\text{mmol} \cdot \text{l}^{-1} \cdot \text{s}^{-1}$ | ✓        |
| Kg6p |      |     | 3.800 | $\text{mmol} \cdot \text{l}^{-1}$                     | ✓        |
| Kudg |      |     | 0.886 | $\text{mmol} \cdot \text{l}^{-1}$                     | ✓        |

### 7.20 Reaction UGP

This is an irreversible reaction of two reactants forming one product influenced by four modifiers.

**Name** UGP

**SBO:0000176** biochemical reaction

### Reaction equation



### Reactants

Table 82: Properties of each reactant.

| Id  | Name | SBO |
|-----|------|-----|
| G1P | G1P  |     |
| UTP | UTP  |     |

## Modifiers

Table 83: Properties of each modifier.

| Id   | Name | SBO |
|------|------|-----|
| UGP1 | UGP1 |     |
| UTP  | UTP  |     |
| G1P  | G1P  |     |
| UDG  | UDG  |     |

## Product

Table 84: Properties of each product.

| Id  | Name | SBO |
|-----|------|-----|
| UDG | UDG  |     |

## Kinetic Law

**Derived unit** 0.0010000000000000013 mol · s<sup>-1</sup>

$$v_{20} = \text{vol}(\text{cell}) \cdot \frac{V_{\max} \cdot [\text{UTP}] \cdot [\text{G1P}]}{K_{\text{utp}} \cdot K_{\text{g1p}} + \frac{K_{\text{utp}}}{K_{\text{utp}}} + \frac{[\text{UTP}]}{K_{\text{utp}}} + \frac{[\text{G1P}]}{K_{\text{g1p}}} + \frac{[\text{UTP}] \cdot [\text{G1P}]}{K_{\text{utp}} \cdot K_{\text{g1p}}} + \frac{K_{\text{utp}} \cdot [\text{UDG}]}{K_{\text{udg}}} + \frac{[\text{G1P}] \cdot [\text{UDG}]}{K_{\text{g1p}} \cdot K_{\text{udg}}}} \quad (44)$$

Table 85: Properties of each parameter.

| Id    | Name | SBO | Value  | Unit                                     | Constant |
|-------|------|-----|--------|--|----------|
| Vmax  |      |     | 13.255 | mmol · l <sup>-1</sup> · s <sup>-1</sup> | ✓        |
| Kutp  |      |     | 0.110  | mmol · l <sup>-1</sup>                   | ✓        |
| Kiutp |      |     | 0.110  | mmol · l <sup>-1</sup>                   | ✓        |
| Kg1p  |      |     | 0.320  | mmol · l <sup>-1</sup>                   | ✓        |
| Kiudg |      |     | 0.004  | mmol · l <sup>-1</sup>                   | ✓        |

### 7.21 Reaction acetate\_branch

This is an irreversible reaction of two reactants forming two products influenced by two modifiers.

**Name** acetate\_branch

**SBO:0000176** biochemical reaction

### Reaction equation



### Reactants

Table 86: Properties of each reactant.

| Id    | Name  | SBO |
|-------|-------|-----|
| AcAld | AcAld |     |
| NAD   | NAD   |     |

### Modifiers

Table 87: Properties of each modifier.

| Id    | Name  | SBO |
|-------|-------|-----|
| AcAld | AcAld |     |
| NAD   | NAD   |     |

### Products

Table 88: Properties of each product.

| Id   | Name | SBO |
|------|------|-----|
| ACE  | ACE  |     |
| NADH | NADH |     |

### Kinetic Law

**Derived unit**  $\text{s}^{-1} \cdot \text{mmol}$

$$v_{21} = \text{vol}(\text{cell}) \cdot k \cdot [\text{AcAld}] \cdot [\text{NAD}] \quad (46)$$

Table 89: Properties of each parameter.

| Id | Name | SBO | Value | Unit  | Constant                            |
|----|------|-----|-------|---|-------------------------------------|
| k  |      |     | 0.006 | $\text{mmol}^{-1} \cdot \text{l} \cdot \text{s}^{-1}$ | <input checked="" type="checkbox"/> |

## 7.22 Reaction `udp_to_utp`

This is an irreversible reaction of two reactants forming two products influenced by two modifiers.

**Name** `udp_to_utp`

**SBO:0000176** biochemical reaction

### Reaction equation



### Reactants

Table 90: Properties of each reactant.

| Id  | Name | SBO |
|-----|------|-----|
| UDP | UDP  |     |
| ATP | ATP  |     |

### Modifiers

Table 91: Properties of each modifier.

| Id  | Name | SBO |
|-----|------|-----|
| UDP | UDP  |     |
| ATP | ATP  |     |

### Products

Table 92: Properties of each product.

| Id  | Name | SBO |
|-----|------|-----|
| UTP | UTP  |     |
| ADP | ADP  |     |

### Kinetic Law

**Derived unit**  $\text{s}^{-1} \cdot \text{mmol}$

$$v_{22} = \text{vol}(\text{cell}) \cdot k \cdot [\text{UDP}] \cdot [\text{ATP}] \quad (48)$$

Table 93: Properties of each parameter.

| Id | Name | SBO | Value | Unit  | Constant                            |
|----|------|-----|-------|---|-------------------------------------|
| k  |      |     | 0.075 | $\text{mmol}^{-1} \cdot \text{l} \cdot \text{s}^{-1}$ | <input checked="" type="checkbox"/> |

### 7.23 Reaction HXT

This is a reversible reaction of one reactant forming one product influenced by two modifiers.

**Name** HXT

**SBO:0000185** transport reaction

#### Reaction equation



#### Reactant

Table 94: Properties of each reactant.

| Id   | Name | SBO |
|------|------|-----|
| GLCx | GLCx |     |

#### Modifiers

Table 95: Properties of each modifier.

| Id   | Name | SBO |
|------|------|-----|
| GLCx | GLCx |     |
| GLC  | GLC  |     |

#### Product

Table 96: Properties of each product.

| Id  | Name | SBO |
|-----|------|-----|
| GLC | GLC  |     |

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{23} = \text{vol}(\text{cell}) \cdot \frac{V_{\max} \cdot ([\text{GLC}_x] - [\text{GLC}])}{K_{\text{glc}} \left( 1 + \frac{[\text{GLC}_x]}{K_{\text{glc}}} + \frac{[\text{GLC}]}{K_{\text{glc}}} + \frac{K_i \cdot [\text{GLC}_x]}{K_{\text{glc}}} \cdot [\text{GLC}] \right)} \quad (50)$$

Table 97: Properties of each parameter.

| Id   | Name | SBO | Value | Unit                                     | Constant                            |
|------|------|-----|-------|--|-------------------------------------|
| Vmax |      |     | 3.35  | mmol · l <sup>-1</sup> · s <sup>-1</sup> | <input checked="" type="checkbox"/> |
| Kglc |      |     | 0.90  | mmol · l <sup>-1</sup>                   | <input checked="" type="checkbox"/> |
| Ki   |      |     | 0.91  | dimensionless                            | <input checked="" type="checkbox"/> |

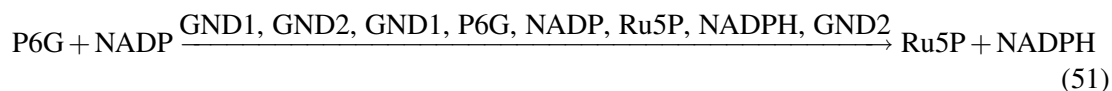
## 7.24 Reaction GND

This is an irreversible reaction of two reactants forming two products influenced by eight modifiers.

**Name** GND

**SBO:0000176** biochemical reaction

## Reaction equation



## Reactants

Table 98: Properties of each reactant.

| Id   | Name | SBO |
|------|------|-----|
| P6G  | P6G  |     |
| NADP | NADP |     |

## Modifiers

Table 99: Properties of each modifier.

| Id    | Name  | SBO |
|-------|-------|-----|
| GND1  | GND1  |     |
| GND2  | GND2  |     |
| GND1  | GND1  |     |
| P6G   | P6G   |     |
| NADP  | NADP  |     |
| Ru5P  | Ru5P  |     |
| NADPH | NADPH |     |
| GND2  | GND2  |     |

## Products

Table 100: Properties of each product.

| Id    | Name  | SBO |
|-------|-------|-----|
| Ru5P  | Ru5P  |     |
| NADPH | NADPH |     |

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{24} = \text{vol}(\text{cell}) \cdot \left( \frac{[\text{GND1}] \cdot \text{kcat\_GND1} \cdot [\text{P6G}] \cdot [\text{NADP}]}{\text{Kp6g\_GND1} \cdot \text{Knadp\_GND1}} \right. \\ \left. + \frac{[\text{GND2}] \cdot \text{kcat\_GND2} \cdot [\text{P6G}] \cdot [\text{NADP}]}{\left(1 + \frac{[\text{P6G}]}{\text{Kp6g\_GND2}} + \frac{[\text{Ru5P}]}{\text{Kru5p\_GND2}}\right) \cdot \left(1 + \frac{[\text{NADP}]}{\text{Knadp\_GND2}} + \frac{[\text{NADPH}]}{\text{Knadph\_GND2}}\right)} \right) \quad (52)$$

Table 101: Properties of each parameter.

| Id          | Name | SBO | Value  | Unit                   | Constant |
|-------------|------|-----|--------|------------------------|----------|
| kcat_GND1   |      |     | 28.000 | s <sup>-1</sup>        | ✓        |
| Kp6g_GND1   |      |     | 0.062  | mmol · l <sup>-1</sup> | ✓        |
| Knadp_GND1  |      |     | 0.094  | mmol · l <sup>-1</sup> | ✓        |
| Kru5p_GND1  |      |     | 0.100  | mmol · l <sup>-1</sup> | ✓        |
| Knadph_GND1 |      |     | 0.055  | mmol · l <sup>-1</sup> | ✓        |
| kcat_GND2   |      |     | 27.300 | s <sup>-1</sup>        | ✓        |

| Id          | Name | SBO | Value | Unit                   | Constant                            |
|-------------|------|-----|-------|------------------------|-------------------------------------|
| Kp6g_GND2   |      |     | 0.115 | mmol · l <sup>-1</sup> | <input checked="" type="checkbox"/> |
| Knadp_GND2  |      |     | 0.094 | mmol · l <sup>-1</sup> | <input checked="" type="checkbox"/> |
| Kru5p_GND2  |      |     | 0.100 | mmol · l <sup>-1</sup> | <input checked="" type="checkbox"/> |
| Knadph_GND2 |      |     | 0.055 | mmol · l <sup>-1</sup> | <input checked="" type="checkbox"/> |

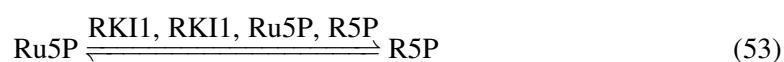
## 7.25 Reaction RKI

This is a reversible reaction of one reactant forming one product influenced by four modifiers.

**Name** RKI

**SBO:0000176** biochemical reaction

### Reaction equation



### Reactant

Table 102: Properties of each reactant.

| Id   | Name | SBO |
|------|------|-----|
| Ru5P | Ru5P |     |

### Modifiers

Table 103: Properties of each modifier.

| Id   | Name | SBO |
|------|------|-----|
| RKI1 | RKI1 |     |
| RKI1 | RKI1 |     |
| Ru5P | Ru5P |     |
| R5P  | R5P  |     |

### Product

Table 104: Properties of each product.

| Id  | Name | SBO |
|-----|------|-----|
| R5P | R5P  |     |



## Kinetic Law

**Derived unit** contains undeclared units

$$v_{25} = \frac{\text{vol}(\text{cell}) \cdot [\text{RKI1}] \cdot \text{kcat} \cdot \left( [\text{Ru5P}] - \frac{[\text{R5P}]}{\text{K}_{\text{eq}}} \right)}{\text{K}_{\text{ru5p}} + \frac{[\text{Ru5P}]}{\text{K}_{\text{ru5p}}} + \frac{[\text{R5P}]}{\text{K}_{\text{r5p}}}} \quad (54)$$

Table 105: Properties of each parameter.

| Id     | Name | SBO | Value  | Unit                   | Constant                            |
|--------|------|-----|--------|------------------------|-------------------------------------|
| kcat   |      |     | 335.00 | s <sup>-1</sup>        | <input checked="" type="checkbox"/> |
| Kru5p  |      |     | 2.47   | mmol · l <sup>-1</sup> | <input checked="" type="checkbox"/> |
| Kr5p   |      |     | 5.70   | mmol · l <sup>-1</sup> | <input checked="" type="checkbox"/> |
| Kiru5p |      |     | 9.88   | mmol · l <sup>-1</sup> | <input checked="" type="checkbox"/> |
| Keq    |      |     | 4.00   | dimensionless          | <input checked="" type="checkbox"/> |

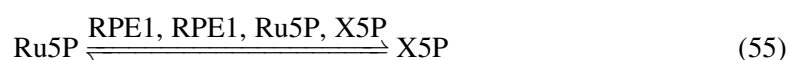
## 7.26 Reaction RPE

This is a reversible reaction of one reactant forming one product influenced by four modifiers.

**Name** RPE

**SBO:0000176** biochemical reaction

## Reaction equation



## Reactant

Table 106: Properties of each reactant.

| Id   | Name | SBO |
|------|------|-----|
| Ru5P | Ru5P |     |

## Modifiers

Table 107: Properties of each modifier.

| Id   | Name | SBO |
|------|------|-----|
| RPE1 | RPE1 |     |
| RPE1 | RPE1 |     |
| Ru5P | Ru5P |     |
| X5P  | X5P  |     |

## Product

Table 108: Properties of each product.

| Id  | Name | SBO |
|-----|------|-----|
| X5P | X5P  |     |

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{26} = \frac{\text{vol}(\text{cell}) \cdot [\text{RPE1}] \cdot \text{kcat} \cdot \left( [\text{Ru5P}] - \frac{[\text{X5P}]}{K_{\text{eq}}} \right)}{1 + \frac{[\text{Ru5P}]}{K_{\text{ru5p}}} + \frac{[\text{X5P}]}{K_{\text{x5p}}}} \quad (56)$$

Table 109: Properties of each parameter.

| Id    | Name | SBO | Value   | Unit                   | Constant |
|-------|------|-----|---------|------------------------|----------|
| kcat  |      |     | 4020.00 | s <sup>-1</sup>        | ✓        |
| Kru5p |      |     | 5.97    | mmol · l <sup>-1</sup> | ✓        |
| Kx5p  |      |     | 7.70    | mmol · l <sup>-1</sup> | ✓        |
| Keq   |      |     | 1.40    | dimensionless          | ✓        |

## 7.27 Reaction SOL

This is an irreversible reaction of one reactant forming one product influenced by four modifiers.

**Name** SOL

**SBO:0000176** biochemical reaction

## Reaction equation



## Reactant

Table 110: Properties of each reactant.

| Id  | Name | SBO |
|-----|------|-----|
| G6L | G6L  |     |

## Modifiers

Table 111: Properties of each modifier.

| Id   | Name | SBO |
|------|------|-----|
| SOL3 | SOL3 |     |
| SOL3 | SOL3 |     |
| G6L  | G6L  |     |
| P6G  | P6G  |     |

## Product

Table 112: Properties of each product.

| Id  | Name | SBO |
|-----|------|-----|
| P6G | P6G  |     |

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{27} = \frac{\text{vol}(\text{cell}) \cdot [\text{SOL3}] \cdot \text{kcat} \cdot [\text{G6L}]}{1 + \frac{[\text{G6L}]}{\text{Kg6l}} + \frac{[\text{P6G}]}{\text{Kp6g}}} \quad (58)$$

Table 113: Properties of each parameter.

| Id   | Name | SBO | Value | Unit                   | Constant |
|------|------|-----|-------|------------------------|----------|
| kcat |      |     | 4.3   | s <sup>-1</sup>        | ✓        |
| Kg6l |      |     | 0.8   | mmol · l <sup>-1</sup> | ✓        |
| Kp6g |      |     | 0.5   | mmol · l <sup>-1</sup> | ✓        |

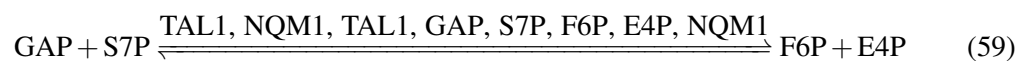
## 7.28 Reaction TAL

This is a reversible reaction of two reactants forming two products influenced by eight modifiers.

**Name** TAL

**SBO:0000176** biochemical reaction

### Reaction equation



### Reactants

Table 114: Properties of each reactant.

| Id  | Name | SBO |
|-----|------|-----|
| GAP | GAP  |     |
| S7P | S7P  |     |

### Modifiers

Table 115: Properties of each modifier.

| Id   | Name | SBO |
|------|------|-----|
| TAL1 | TAL1 |     |
| NQM1 | NQM1 |     |
| TAL1 | TAL1 |     |
| GAP  | GAP  |     |
| S7P  | S7P  |     |
| F6P  | F6P  |     |
| E4P  | E4P  |     |
| NQM1 | NQM1 |     |

### Products

Table 116: Properties of each product.

| Id  | Name | SBO |
|-----|------|-----|
| F6P | F6P  |     |
| E4P | E4P  |     |

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{28} = \text{vol}(\text{cell}) \cdot \left( \frac{\frac{[\text{TAL1}] \cdot \text{kcat\_TAL1} \cdot \left( [\text{GAP}] \cdot [\text{S7P}] - \frac{[\text{F6P}] \cdot [\text{E4P}]}{\text{Keq}} \right)}{\text{Kgap\_TAL1} \cdot \text{Ks7p\_TAL1}}}{\left( 1 + \frac{[\text{GAP}]}{\text{Kgap\_TAL1}} + \frac{[\text{F6P}]}{\text{Kf6p\_TAL1}} \right) \cdot \left( 1 + \frac{[\text{S7P}]}{\text{Ks7p\_TAL1}} + \frac{[\text{E4P}]}{\text{Ke4p\_TAL1}} \right)} + \frac{\frac{[\text{NQM1}] \cdot \text{kcat\_NQM1} \cdot \left( [\text{GAP}] \cdot [\text{S7P}] - \frac{[\text{F6P}] \cdot [\text{E4P}]}{\text{Keq}} \right)}{\text{Kgap\_NQM1} \cdot \text{Ks7p\_NQM1}}}{\left( 1 + \frac{[\text{GAP}]}{\text{Kgap\_NQM1}} + \frac{[\text{F6P}]}{\text{Kf6p\_NQM1}} \right) \cdot \left( 1 + \frac{[\text{S7P}]}{\text{Ks7p\_NQM1}} + \frac{[\text{E4P}]}{\text{Ke4p\_NQM1}} \right)} \right) \quad (60)$$

Table 117: Properties of each parameter.

| Id        | Name | SBO | Value | Unit                   | Constant |
|-----------|------|-----|-------|------------------------|----------|
| kcat_TAL1 |      |     | 0.694 | s <sup>-1</sup>        | ✓        |
| Kgap_TAL1 |      |     | 0.272 | mmol · l <sup>-1</sup> | ✓        |
| Ks7p_TAL1 |      |     | 0.786 | mmol · l <sup>-1</sup> | ✓        |
| Kf6p_TAL1 |      |     | 1.440 | mmol · l <sup>-1</sup> | ✓        |
| Ke4p_TAL1 |      |     | 0.362 | mmol · l <sup>-1</sup> | ✓        |
| kcat_NQM1 |      |     | 0.694 | s <sup>-1</sup>        | ✓        |
| Kgap_NQM1 |      |     | 0.272 | mmol · l <sup>-1</sup> | ✓        |
| Ks7p_NQM1 |      |     | 0.786 | mmol · l <sup>-1</sup> | ✓        |
| Kf6p_NQM1 |      |     | 1.040 | mmol · l <sup>-1</sup> | ✓        |
| Ke4p_NQM1 |      |     | 0.305 | mmol · l <sup>-1</sup> | ✓        |
| Keq       |      |     | 1.050 | dimensionless          | ✓        |

## 7.29 Reaction TKL\_E4P

This is a reversible reaction of two reactants forming two products influenced by ten modifiers.

**Name** TKL (E4P:F6P)

**SBO:0000176** biochemical reaction

### Reaction equation



### Reactants

Table 118: Properties of each reactant.

| Id  | Name | SBO |
|-----|------|-----|
| X5P | X5P  |     |
| E4P | E4P  |     |

## Modifiers

Table 119: Properties of each modifier.

| Id   | Name | SBO |
|------|------|-----|
| TKL1 | TKL1 |     |
| R5P  | R5P  |     |
| S7P  | S7P  |     |
| TKL1 | TKL1 |     |
| X5P  | X5P  |     |
| E4P  | E4P  |     |
| GAP  | GAP  |     |
| F6P  | F6P  |     |
| R5P  | R5P  |     |
| S7P  | S7P  |     |

## Products

Table 120: Properties of each product.

| Id  | Name | SBO |
|-----|------|-----|
| GAP | GAP  |     |
| F6P | F6P  |     |

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{29} = \frac{\text{vol}(\text{cell}) \cdot [\text{TKL1}] \cdot \text{kat} \cdot \left( [\text{X5P}] \cdot [\text{E4P}] - \frac{[\text{GAP}] \cdot [\text{F6P}]}{K_{\text{eq}}} \right)}{K_{\text{x5p\_TAL}} \cdot K_{\text{e4p\_TAL}}} \cdot \left( 1 + \frac{[\text{X5P}]}{K_{\text{x5p\_TAL}}} + \frac{[\text{GAP}]}{K_{\text{gap\_TAL}}} \right) \cdot \left( 1 + \frac{[\text{E4P}]}{K_{\text{e4p\_TAL}}} + \frac{[\text{F6P}]}{K_{\text{f6p\_TAL}}} + \frac{[\text{R5P}]}{K_{\text{r5p\_TAL}}} + \frac{[\text{S7P}]}{K_{\text{s7p\_TAL}}} \right) \quad (62)$$

Table 121: Properties of each parameter.

| Id   | Name | SBO | Value | Unit            | Constant                            |
|------|------|-----|-------|-----------------|-------------------------------------|
| kcat |      |     | 47.1  | s <sup>-1</sup> | <input checked="" type="checkbox"/> |
| Keq  |      |     | 10.0  | dimensionless   | <input checked="" type="checkbox"/> |

### 7.30 Reaction TKL\_R5P

This is a reversible reaction of two reactants forming two products influenced by ten modifiers.

**Name** TKL (R5P:S7P)

**SBO:0000176** biochemical reaction

#### Reaction equation



#### Reactants

Table 122: Properties of each reactant.

| Id  | Name | SBO |
|-----|------|-----|
| X5P | X5P  |     |
| R5P | R5P  |     |

#### Modifiers

Table 123: Properties of each modifier.

| Id   | Name | SBO |
|------|------|-----|
| TKL1 | TKL1 |     |
| E4P  | E4P  |     |
| F6P  | F6P  |     |
| TKL1 | TKL1 |     |
| X5P  | X5P  |     |
| R5P  | R5P  |     |
| GAP  | GAP  |     |
| S7P  | S7P  |     |
| E4P  | E4P  |     |
| F6P  | F6P  |     |

## Products

Table 124: Properties of each product.

| Id  | Name | SBO |
|-----|------|-----|
| GAP | GAP  |     |
| S7P | S7P  |     |

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{30} = \frac{\text{vol}(\text{cell}) \cdot [\text{TKL1}] \cdot \text{kcat} \cdot \left( \frac{[\text{X5P}] \cdot [\text{R5P}] - \frac{[\text{GAP}] \cdot [\text{S7P}]}{\text{Keq}}}{\text{Kx5p\_TAL} \cdot \text{Kr5p\_TAL}} \right)}{\left( 1 + \frac{[\text{X5P}]}{\text{Kx5p\_TAL}} + \frac{[\text{GAP}]}{\text{Kgap\_TAL}} \right) \cdot \left( 1 + \frac{[\text{E4P}]}{\text{Ke4p\_TAL}} + \frac{[\text{F6P}]}{\text{Kf6p\_TAL}} + \frac{[\text{R5P}]}{\text{Kr5p\_TAL}} + \frac{[\text{S7P}]}{\text{Ks7p\_TAL}} \right)} \quad (64)$$

Table 125: Properties of each parameter.

| Id   | Name | SBO | Value | Unit            | Constant                            |
|------|------|-----|-------|-----------------|-------------------------------------|
| kcat |      |     | 40.5  | s <sup>-1</sup> | <input checked="" type="checkbox"/> |
| Keq  |      |     | 1.2   | dimensionless   | <input checked="" type="checkbox"/> |

## 7.31 Reaction ZWF

This is an irreversible reaction of two reactants forming two products influenced by six modifiers.

**Name** ZWF

**SBO:0000176** biochemical reaction

## Reaction equation



## Reactants

Table 126: Properties of each reactant.

| Id   | Name | SBO |
|------|------|-----|
| G6P  | G6P  |     |
| NADP | NADP |     |



## Modifiers

Table 127: Properties of each modifier.

| Id    | Name  | SBO |
|-------|-------|-----|
| ZWF1  | ZWF1  |     |
| ZWF1  | ZWF1  |     |
| G6P   | G6P   |     |
| NADP  | NADP  |     |
| G6L   | G6L   |     |
| NADPH | NADPH |     |

## Products

Table 128: Properties of each product.

| Id    | Name  | SBO |
|-------|-------|-----|
| G6L   | G6L   |     |
| NADPH | NADPH |     |

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{31} = \frac{\text{vol}(\text{cell}) \cdot [\text{ZWF1}] \cdot \text{kcat} \cdot [\text{G6P}] \cdot [\text{NADP}]}{\text{Kg6p} \cdot \text{Knadp}} \cdot \left( 1 + \frac{[\text{G6P}]}{\text{Kg6p}} + \frac{[\text{G6L}]}{\text{Kg6l}} \right) \cdot \left( 1 + \frac{[\text{NADP}]}{\text{Knadp}} + \frac{[\text{NADPH}]}{\text{Knadph}} \right) \quad (66)$$

Table 129: Properties of each parameter.

| Id     | Name | SBO | Value   | Unit                   | Constant |
|--------|------|-----|---------|------------------------|----------|
| kcat   |      |     | 189.000 | s <sup>-1</sup>        | ✓        |
| Kg6p   |      |     | 0.042   | mmol · l <sup>-1</sup> | ✓        |
| Knadp  |      |     | 0.045   | mmol · l <sup>-1</sup> | ✓        |
| Kg6l   |      |     | 0.010   | mmol · l <sup>-1</sup> | ✓        |
| Knadph |      |     | 0.017   | mmol · l <sup>-1</sup> | ✓        |

### 7.32 Reaction NADPH\_oxidase

This is an irreversible reaction of one reactant forming one product influenced by one modifier.

**Name** NADPH oxidase

**SBO:0000176** biochemical reaction

### Reaction equation



### Reactant

Table 130: Properties of each reactant.

| Id    | Name  | SBO |
|-------|-------|-----|
| NADPH | NADPH |     |

### Modifier

Table 131: Properties of each modifier.

| Id    | Name  | SBO |
|-------|-------|-----|
| NADPH | NADPH |     |

### Product

Table 132: Properties of each product.

| Id   | Name | SBO |
|------|------|-----|
| NADP | NADP |     |

### Kinetic Law

**Derived unit**  $\text{s}^{-1} \cdot \text{mmol}$

$$v_{32} = \text{vol}(\text{cell}) \cdot k \cdot [\text{NADPH}] \quad (68)$$

Table 133: Properties of each parameter.

| Id | Name | SBO | Value | Unit            | Constant                            |
|----|------|-----|-------|-----------------|-------------------------------------|
| k  |      |     | 1.0   | $\text{s}^{-1}$ | <input checked="" type="checkbox"/> |

### 7.33 Reaction E4P\_sink

This is an irreversible reaction of one reactant forming no product influenced by one modifier.

**Name** E4P sink

**SBO:0000176** biochemical reaction

#### Reaction equation



#### Reactant

Table 134: Properties of each reactant.

| Id  | Name | SBO |
|-----|------|-----|
| E4P | E4P  |     |

#### Modifier

Table 135: Properties of each modifier.

| Id  | Name | SBO |
|-----|------|-----|
| E4P | E4P  |     |

#### Kinetic Law

**Derived unit**  $\text{s}^{-1} \cdot \text{mmol}$

$$v_{33} = \text{vol}(\text{cell}) \cdot k \cdot [\text{E4P}] \quad (70)$$

Table 136: Properties of each parameter.

| Id | Name | SBO | Value | Unit            | Constant                            |
|----|------|-----|-------|-----------------|-------------------------------------|
| k  |      |     | 1.0   | $\text{s}^{-1}$ | <input checked="" type="checkbox"/> |

### 7.34 Reaction R5P\_sink

This is an irreversible reaction of one reactant forming no product influenced by one modifier.

**Name** R5P sink

**SBO:0000176** biochemical reaction

### Reaction equation



### Reactant

Table 137: Properties of each reactant.

| Id  | Name | SBO |
|-----|------|-----|
| R5P | R5P  |     |

### Modifier

Table 138: Properties of each modifier.

| Id  | Name | SBO |
|-----|------|-----|
| R5P | R5P  |     |

### Kinetic Law

**Derived unit**  $\text{s}^{-1} \cdot \text{mmol}$

$$v_{34} = \text{vol}(\text{cell}) \cdot k \cdot [\text{R5P}] \quad (72)$$

Table 139: Properties of each parameter.

| Id | Name | SBO | Value | Unit            | Constant                            |
|----|------|-----|-------|-----------------|-------------------------------------|
| k  |      |     | 1.0   | $\text{s}^{-1}$ | <input checked="" type="checkbox"/> |

## 8 Derived Rate Equations

When interpreted as an ordinary differential equation framework, this model implies the following set of equations for the rates of change of each species.

Identifiers for kinetic laws highlighted in gray cannot be verified to evaluate to units of SBML substance per time. As a result, some SBML interpreters may not be able to verify the consistency of the units on quantities in the model. Please check if

- parameters without an unit definition are involved or

- volume correction is necessary because the `hasOnlySubstanceUnits` flag may be set to `false` and `spacialDimensions > 0` for certain species.

## 8.1 Species ADP

**Name** ADP

**SBO:0000247** simple chemical

**Initial concentration**  $1.29 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in 14 reactions (as a reactant in [AK](#), [PGK](#), [PYK](#) and as a product in [ATPase](#), [HXX](#), [PFK](#), [udp\\_to\\_otp](#) and as a modifier in [AK](#), [GPD](#), [GPD](#), [HXX](#), [PFK](#), [PGK](#), [PYK](#)).

$$\frac{d}{dt}\text{ADP} = v_3 + v_9 + v_{11} + v_{22} - 2v_2 - v_{13} - v_{15} \quad (73)$$

## 8.2 Species ATP

**Name** ATP

**SBO:0000247** simple chemical

**Initial concentration**  $4.29 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in 16 reactions (as a reactant in [ATPase](#), [HXX](#), [PFK](#), [udp\\_to\\_otp](#) and as a product in [AK](#), [PGK](#), [PYK](#) and as a modifier in [AK](#), [ATPase](#), [GPD](#), [GPD](#), [HXX](#), [PFK](#), [PGK](#), [PYK](#), [udp\\_to\\_otp](#)).

$$\frac{d}{dt}\text{ATP} = v_2 + v_{13} + v_{15} - v_3 - v_9 - v_{11} - v_{22} \quad (74)$$

## 8.3 Species AcAld

**Name** AcAld

**SBO:0000247** simple chemical

**Initial concentration**  $0.178140579850657 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in five reactions (as a reactant in [ADH](#), [acetate\\_branch](#) and as a product in [PDC](#) and as a modifier in [ADH](#), [acetate\\_branch](#)).

$$\frac{d}{dt}\text{AcAld} = v_{10} - v_1 - v_{21} \quad (75)$$

## 8.4 Species BPG

**Name** BPG

**SBO:0000247** simple chemical

**Initial concentration**  $7.36873499865602 \cdot 10^{-4} \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in [PGK](#) and as a product in [TDH](#) and as a modifier in [PGK](#), [TDH](#)).

$$\frac{d}{dt}\text{BPG} = v_{16} - v_{13} \quad (76)$$

## 8.5 Species DHAP

**Name** DHAP

**SBO:0000247** simple chemical

**Initial concentration**  $1.1613768527467 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in six reactions (as a reactant in [GPD](#), [TPI](#) and as a product in [FBA](#) and as a modifier in [FBA](#), [GPD](#), [TPI](#)).

$$\frac{d}{dt}\text{DHAP} = v_5 - v_6 - v_{17} \quad (77)$$

## 8.6 Species F16bP

**Name** F16bP

**SBO:0000247** simple chemical

**Initial concentration**  $4.58321859006931 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in eight reactions (as a reactant in [FBA](#) and as a product in [PFK](#) and as a modifier in [FBA](#), [GPD](#), [GPD](#), [PFK](#), [PYK](#), [PYK](#)).

$$\frac{d}{dt}\text{F16bP} = v_{11} - v_5 \quad (78)$$

## 8.7 Species F6P

**Name** F6P

**SBO:0000247** simple chemical

**Initial concentration**  $0.235441221891221 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in ten reactions (as a reactant in [PFK](#) and as a product in [PGI](#), [TAL](#), [TKL\\_E4P](#) and as a modifier in [PFK](#), [PGI](#), [TAL](#), [TKL\\_E4P](#), [TKL\\_R5P](#), [TKL\\_R5P](#)).

$$\frac{d}{dt}\text{F6P} = v_{12} + v_{28} + v_{29} - v_{11} \quad (79)$$

## 8.8 Species G1P

**Name** G1P

**SBO:0000247** simple chemical

**Initial concentration** 0.539248506344921 mmol · l<sup>-1</sup>

This species takes part in four reactions (as a reactant in [UGP](#) and as a product in [PGM](#) and as a modifier in [PGM](#), [UGP](#)).

$$\frac{d}{dt}G1P = v_{14} - v_{20} \quad (80)$$

## 8.9 Species G3P

**Name** G3P

**SBO:0000247** simple chemical

**Initial concentration** 0.274002929191284 mmol · l<sup>-1</sup>

This species takes part in four reactions (as a reactant in [GPP](#) and as a product in [GPD](#) and as a modifier in [GPD](#), [GPP](#)).

$$\frac{d}{dt}G3P = v_6 - v_8 \quad (81)$$

## 8.10 Species G6P

**Name** G6P

**SBO:0000247** simple chemical

**Initial concentration** 0.772483203645216 mmol · l<sup>-1</sup>

This species takes part in ten reactions (as a reactant in [PGI](#), [PGM](#), [TPS](#), [ZWF](#) and as a product in [H XK](#) and as a modifier in [H XK](#), [PGI](#), [PGM](#), [TPS](#), [ZWF](#)).

$$\frac{d}{dt}G6P = v_9 - v_{12} - v_{14} - v_{19} - v_{31} \quad (82)$$

## 8.11 Species GAP

**Name** GAP

**SBO:0000247** simple chemical

**Initial concentration** 0.315891028770503 mmol · l<sup>-1</sup>

This species takes part in twelve reactions (as a reactant in [TDH](#), [TAL](#) and as a product in [FBA](#), [TPI](#), [TKL\\_E4P](#), [TKL\\_R5P](#) and as a modifier in [FBA](#), [TDH](#), [TPI](#), [TAL](#), [TKL\\_E4P](#), [TKL\\_R5P](#)).

$$\frac{d}{dt}GAP = v_5 + v_{17} + v_{29} + v_{30} - v_{16} - v_{28} \quad (83)$$

### 8.12 Species GLC

**Name** GLC

**SBO:0000247** simple chemical

**Initial concentration** 6.28000179338242 mmol · l<sup>-1</sup>

This species takes part in four reactions (as a reactant in [HXX](#) and as a product in [HXT](#) and as a modifier in [HXX](#), [HXT](#)).

$$\frac{d}{dt}\text{GLC} = v_{23} - v_9 \quad (84)$$

### 8.13 Species NAD

**Name** NAD

**SBO:0000247** simple chemical

**Initial concentration** 1.50329030201531 mmol · l<sup>-1</sup>

This species takes part in eight reactions (as a reactant in [TDH](#), [acetate\\_branch](#) and as a product in [ADH](#), [GPD](#) and as a modifier in [ADH](#), [GPD](#), [TDH](#), [acetate\\_branch](#)).

$$\frac{d}{dt}\text{NAD} = v_1 + v_6 - v_{16} - v_{21} \quad (85)$$

### 8.14 Species P2G

**Name** P2G

**SBO:0000247** simple chemical

**Initial concentration** 0.0677379081099344 mmol · l<sup>-1</sup>

This species takes part in four reactions (as a reactant in [ENO](#) and as a product in [GPM](#) and as a modifier in [ENO](#), [GPM](#)).

$$\frac{d}{dt}\text{P2G} = v_7 - v_4 \quad (86)$$

### 8.15 Species P3G

**Name** P3G

**SBO:0000247** simple chemical

**Initial concentration** 0.469825011134444 mmol · l<sup>-1</sup>

This species takes part in four reactions (as a reactant in [GPM](#) and as a product in [PGK](#) and as a modifier in [GPM](#), [PGK](#)).

$$\frac{d}{dt}\text{P3G} = v_{13} - v_7 \quad (87)$$



### 8.16 Species PEP

**Name** PEP

**SBO:0000247** simple chemical

**Initial concentration**  $0.610005413358042 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in [PYK](#) and as a product in [ENO](#) and as a modifier in [ENO](#), [PYK](#)).

$$\frac{d}{dt}\text{PEP} = v_4 - v_{15} \quad (88)$$

### 8.17 Species PYR

**Name** PYR

**SBO:0000247** simple chemical

**Initial concentration**  $2.10847140717419 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in [PDC](#) and as a product in [PYK](#) and as a modifier in [PDC](#), [PYK](#)).

$$\frac{d}{dt}\text{PYR} = v_{15} - v_{10} \quad (89)$$

### 8.18 Species T6P

**Name** T6P

**SBO:0000247** simple chemical

**Initial concentration**  $0.02 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in five reactions (as a reactant in [TPP](#) and as a product in [TPS](#) and as a modifier in [HXK](#), [HXK](#), [TPP](#)).

$$\frac{d}{dt}\text{T6P} = v_{19} - v_{18} \quad (90)$$

### 8.19 Species UDP

**Name** UDP

**SBO:0000247** simple chemical

**Initial concentration**  $0.2815 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in [udp\\_to\\_utp](#) and as a product in [TPS](#) and as a modifier in [udp\\_to\\_utp](#)).

$$\frac{d}{dt}\text{UDP} = v_{19} - v_{22} \quad (91)$$

## 8.20 Species UTP

**Name** UTP

**SBO:0000247** simple chemical

**Initial concentration**  $0.6491 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in [UGP](#) and as a product in [udp\\_to\\_utp](#) and as a modifier in [UGP](#)).

$$\frac{d}{dt}\text{UTP} = v_{22} - v_{20} \quad (92)$$

## 8.21 Species AMP

**Name** AMP

**SBO:0000247** simple chemical

**Initial concentration**  $0.44 \text{ mmol} \cdot \text{l}^{-1}$

**Involved in rule** [AMP](#)

This species takes part in four reactions (as a product in [AK](#) and as a modifier in [AK](#), [PFK](#), [PFK](#)). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

## 8.22 Species NADH

**Name** NADH

**SBO:0000247** simple chemical

**Initial concentration**  $0.0867096979846952 \text{ mmol} \cdot \text{l}^{-1}$

**Involved in rule** [NADH](#)

This species takes part in seven reactions (as a reactant in [ADH](#), [GPD](#) and as a product in [TDH](#), [acetate\\_branch](#) and as a modifier in [ADH](#), [GPD](#), [TDH](#)). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

## 8.23 Species UDG

**Name** UDG

**SBO:0000247** simple chemical

**Initial concentration**  $0.467246194874247 \text{ mmol} \cdot \text{l}^{-1}$

Involved in rule [UDG](#)

This species takes part in four reactions (as a reactant in [TPS](#) and as a product in [UGP](#) and as a modifier in [TPS](#), [UGP](#)). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

## 8.24 Species [ACE](#)

**Name** ACE

**SBO:0000247** simple chemical

**Initial concentration** 223.000253398294 mmol · l<sup>-1</sup>

This species takes part in one reaction (as a product in [acetate.branch](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}ACE = 0 \quad (93)$$

## 8.25 Species [EtOH](#)

**Name** EtOH

**SBO:0000247** simple chemical

**Initial concentration** 221.890311417536 mmol · l<sup>-1</sup>

This species takes part in two reactions (as a product in [ADH](#) and as a modifier in [ADH](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}EtOH = 0 \quad (94)$$

## 8.26 Species [F26bP](#)

**Name** F26bP

**SBO:0000247** simple chemical

**Initial concentration** 0.0030 mmol · l<sup>-1</sup>

This species takes part in two reactions (as a modifier in [PFK](#), [PFK](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}F26bP = 0 \quad (95)$$

### 8.27 Species GLCx

**Name** GLCx

**SBO:0000247** simple chemical

**Initial concentration**  $74 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in [HXT](#) and as a modifier in [HXT](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{GLCx} = 0 \quad (96)$$

### 8.28 Species GLY

**Name** GLY

**SBO:0000247** simple chemical

**Initial concentration**  $0.15 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in [GPP](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{GLY} = 0 \quad (97)$$

### 8.29 Species SUC

**Name** SUC

**SBO:0000247** simple chemical

**Initial concentration**  $0 \text{ mmol} \cdot \text{l}^{-1}$

$$\frac{d}{dt} \text{SUC} = 0 \quad (98)$$

### 8.30 Species TRH

**Name** TRH

**SBO:0000247** simple chemical

**Initial concentration**  $0.0153878853696526 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in [TPP](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{TRH} = 0 \quad (99)$$

### 8.31 Species ADH1

**Name** ADH1

**SBO:0000252** polypeptide chain

**Initial concentration** 0.163908510928009 mmol · l<sup>-1</sup>

This species takes part in two reactions (as a modifier in [ADH](#), [ADH](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}ADH1 = 0 \quad (100)$$

### 8.32 Species CDC19

**Name** CDC19

**SBO:0000252** polypeptide chain

**Initial concentration** 2.0483901071712 mmol · l<sup>-1</sup>

This species takes part in two reactions (as a modifier in [PYK](#), [PYK](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}CDC19 = 0 \quad (101)$$

### 8.33 Species ENO1

**Name** ENO1

**SBO:0000252** polypeptide chain

**Initial concentration** 0.686371954155832 mmol · l<sup>-1</sup>

This species takes part in two reactions (as a modifier in [ENO](#), [ENO](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}ENO1 = 0 \quad (102)$$

### 8.34 Species ENO2

**Name** ENO2

**SBO:0000252** polypeptide chain

**Initial concentration** 1.97444629317817 mmol · l<sup>-1</sup>

This species takes part in two reactions (as a modifier in [ENO](#), [ENO](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}ENO2 = 0 \quad (103)$$

### 8.35 Species FBA1

**Name** FBA1

**SBO:0000252** polypeptide chain

**Initial concentration**  $1.33839465704882 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a modifier in [FBA](#), [FBA](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{FBA1} = 0 \quad (104)$$

### 8.36 Species GLK1

**Name** GLK1

**SBO:0000252** polypeptide chain

**Initial concentration**  $0.0450869624419226 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a modifier in [HXX](#), [HXX](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{GLK1} = 0 \quad (105)$$

### 8.37 Species GPD1

**Name** GPD1

**SBO:0000252** polypeptide chain

**Initial concentration**  $0.00683511177089872 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a modifier in [GPD](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{GPD1} = 0 \quad (106)$$

### 8.38 Species GPD2

**Name** GPD2

**SBO:0000252** polypeptide chain

**Initial concentration**  $7.93405666424228 \cdot 10^{-4} \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a modifier in [GPD](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{GPD2} = 0 \quad (107)$$

### 8.39 Species GPM1

**Name** GPM1

**SBO:0000252** polypeptide chain

**Initial concentration** 0.73000029889707 mmol · l<sup>-1</sup>

This species takes part in two reactions (as a modifier in [GPM](#), [GPM](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{GPM1} = 0 \quad (108)$$

### 8.40 Species HOR2

**Name** HOR2

**SBO:0000252** polypeptide chain

**Initial concentration** 0.0054734695639756 mmol · l<sup>-1</sup>

This species takes part in one reaction (as a modifier in [GPP](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{HOR2} = 0 \quad (109)$$

### 8.41 Species HXK1

**Name** HXK1

**SBO:0000252** polypeptide chain

**Initial concentration** 0.0167807457149784 mmol · l<sup>-1</sup>

This species takes part in two reactions (as a modifier in [HXK](#), [HXK](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{HXK1} = 0 \quad (110)$$

### 8.42 Species HXK2

**Name** HXK2

**SBO:0000252** polypeptide chain

**Initial concentration** 0.0613313539705155 mmol · l<sup>-1</sup>

This species takes part in two reactions (as a modifier in [HXK](#), [HXK](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{HXK2} = 0 \quad (111)$$

### 8.43 Species PDC1

**Name** PDC1

**SBO:0000252** polypeptide chain

**Initial concentration** 1.06781077822834 mmol · l<sup>-1</sup>

This species takes part in two reactions (as a modifier in [PDC](#), [PDC](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}PDC1 = 0 \quad (112)$$

### 8.44 Species PDC5

**Name** PDC5

**SBO:0000252** polypeptide chain

**Initial concentration** 0.0123547443267676 mmol · l<sup>-1</sup>

This species takes part in two reactions (as a modifier in [PDC](#), [PDC](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}PDC5 = 0 \quad (113)$$

### 8.45 Species PDC6

**Name** PDC6

**SBO:0000252** polypeptide chain

**Initial concentration** 0.00654086421106118 mmol · l<sup>-1</sup>

This species takes part in two reactions (as a modifier in [PDC](#), [PDC](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}PDC6 = 0 \quad (114)$$

### 8.46 Species PFK1

**Name** PFK1

**SBO:0000252** polypeptide chain

**Initial concentration** 0.0467850299063124 mmol · l<sup>-1</sup>

This species takes part in one reaction (as a modifier in [PFK](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}PFK1 = 0 \quad (115)$$



#### 8.47 Species PFK2

**Name** PFK2

**SBO:0000252** polypeptide chain

**Initial concentration** 0.0390366215332091 mmol · l<sup>-1</sup>

This species takes part in two reactions (as a modifier in [PFK](#), [PFK](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{PFK2} = 0 \quad (116)$$

#### 8.48 Species PGI1

**Name** PGI1

**SBO:0000252** polypeptide chain

**Initial concentration** 0.1382907072901 mmol · l<sup>-1</sup>

This species takes part in two reactions (as a modifier in [PGI](#), [PGI](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{PGI1} = 0 \quad (117)$$

#### 8.49 Species PGK1

**Name** PGK1

**SBO:0000252** polypeptide chain

**Initial concentration** 0.257656912658955 mmol · l<sup>-1</sup>

This species takes part in two reactions (as a modifier in [PGK](#), [PGK](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{PGK1} = 0 \quad (118)$$

#### 8.50 Species PGM1

**Name** PGM1

**SBO:0000252** polypeptide chain

**Initial concentration** 0.00326229546307459 mmol · l<sup>-1</sup>

This species takes part in one reaction (as a modifier in [PGM](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{PGM1} = 0 \quad (119)$$

### 8.51 Species PGM2

**Name** PGM2

**SBO:0000252** polypeptide chain

**Initial concentration** 0.00125868877176552 mmol · l<sup>-1</sup>

This species takes part in one reaction (as a modifier in [PGM](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{PGM2} = 0 \quad (120)$$

### 8.52 Species RHR2

**Name** RHR2

**SBO:0000252** polypeptide chain

**Initial concentration** 0.0511804773718313 mmol · l<sup>-1</sup>

This species takes part in one reaction (as a modifier in [GPP](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{RHR2} = 0 \quad (121)$$

### 8.53 Species TDH1

**Name** TDH1

**SBO:0000252** polypeptide chain

**Initial concentration** 0.350864642801396 mmol · l<sup>-1</sup>

This species takes part in two reactions (as a modifier in [TDH](#), [TDH](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{TDH1} = 0 \quad (122)$$

### 8.54 Species TDH3

**Name** TDH3

**SBO:0000252** polypeptide chain

**Initial concentration** 4.20440474648547 mmol · l<sup>-1</sup>

This species takes part in two reactions (as a modifier in [TDH](#), [TDH](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{TDH3} = 0 \quad (123)$$

### 8.55 Species TPI1

**Name** TPI1

**SBO:0000252** polypeptide chain

**Initial concentration** 0.294357819645508 mmol · l<sup>-1</sup>

This species takes part in two reactions (as a modifier in [TPI](#), [TPI](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{TPI1} = 0 \quad (124)$$

### 8.56 Species TPS1

**Name** TPS1

**SBO:0000252** polypeptide chain

**Initial concentration** 0.00339248174237065 mmol · l<sup>-1</sup>

This species takes part in two reactions (as a modifier in [TPP](#), [TPS](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{TPS1} = 0 \quad (125)$$

### 8.57 Species TPS2

**Name** TPS2

**SBO:0000252** polypeptide chain

**Initial concentration** 0.00265985181347494 mmol · l<sup>-1</sup>

This species takes part in two reactions (as a modifier in [TPP](#), [TPS](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{TPS2} = 0 \quad (126)$$

### 8.58 Species UGP1

**Name** UGP1

**SBO:0000252** polypeptide chain

**Initial concentration** 0.00620211419860714 mmol · l<sup>-1</sup>

This species takes part in one reaction (as a modifier in [UGP](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{UGP1} = 0 \quad (127)$$

### 8.59 Species E4P

**Name** E4P

**SBO:0000247** simple chemical

**Initial concentration**  $0.029 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in eight reactions (as a reactant in [TKL\\_E4P](#), [E4P\\_sink](#) and as a product in [TAL](#) and as a modifier in [TAL](#), [TKL\\_E4P](#), [TKL\\_R5P](#), [TKL\\_R5P](#), [E4P\\_sink](#)).

$$\frac{d}{dt}E4P = v_{28} - v_{29} - v_{33} \quad (128)$$

### 8.60 Species G6L

**Name** G6L

**SBO:0000247** simple chemical

**Initial concentration**  $0.1 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in [SOL](#) and as a product in [ZWF](#) and as a modifier in [SOL](#), [ZWF](#)).

$$\frac{d}{dt}G6L = v_{31} - v_{27} \quad (129)$$

### 8.61 Species NADPH

**Name** NADPH

**SBO:0000247** simple chemical

**Initial concentration**  $0.16 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in six reactions (as a reactant in [NADPH\\_oxidase](#) and as a product in [GND](#), [ZWF](#) and as a modifier in [GND](#), [ZWF](#), [NADPH\\_oxidase](#)).

$$\frac{d}{dt}NADPH = v_{24} + v_{31} - v_{32} \quad (130)$$

### 8.62 Species P6G

**Name** P6G

**SBO:0000247** simple chemical

**Initial concentration**  $0.25 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in [GND](#) and as a product in [SOL](#) and as a modifier in [GND](#), [SOL](#)).

$$\frac{d}{dt}P6G = v_{27} - v_{24} \quad (131)$$

### 8.63 Species R5P

**Name** R5P

**SBO:0000247** simple chemical

**Initial concentration**  $0.118 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in eight reactions (as a reactant in [TKL\\_R5P](#), [R5P\\_sink](#) and as a product in [RKI](#) and as a modifier in [RKI](#), [TKL\\_E4P](#), [TKL\\_E4P](#), [TKL\\_R5P](#), [R5P\\_sink](#)).

$$\frac{d}{dt}R5P = v_{25} - v_{30} - v_{34} \quad (132)$$

### 8.64 Species Ru5P

**Name** Ru5P

**SBO:0000247** simple chemical

**Initial concentration**  $0.033 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in six reactions (as a reactant in [RKI](#), [RPE](#) and as a product in [GND](#) and as a modifier in [GND](#), [RKI](#), [RPE](#)).

$$\frac{d}{dt}Ru5P = v_{24} - v_{25} - v_{26} \quad (133)$$

### 8.65 Species S7P

**Name** S7P

**SBO:0000247** simple chemical

**Initial concentration**  $0.082 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in six reactions (as a reactant in [TAL](#) and as a product in [TKL\\_R5P](#) and as a modifier in [TAL](#), [TKL\\_E4P](#), [TKL\\_E4P](#), [TKL\\_R5P](#)).

$$\frac{d}{dt}S7P = v_{30} - v_{28} \quad (134)$$

### 8.66 Species X5P

**Name** X5P

**SBO:0000247** simple chemical

**Initial concentration**  $0.041 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in six reactions (as a reactant in [TKL\\_E4P](#), [TKL\\_R5P](#) and as a product in [RPE](#) and as a modifier in [RPE](#), [TKL\\_E4P](#), [TKL\\_R5P](#)).

$$\frac{d}{dt}X5P = v_{26} - v_{29} - v_{30} \quad (135)$$

### 8.67 Species NADP

**Name** NADP

**SBO:0000247** simple chemical

**Initial concentration**  $0.17 \text{ mmol} \cdot \text{l}^{-1}$

**Involved in rule** NADP

This species takes part in five reactions (as a reactant in GND, ZWF and as a product in NADPH-oxidase and as a modifier in GND, ZWF). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

### 8.68 Species GND1

**Name** GND1

**SBO:0000252** polypeptide chain

**Initial concentration**  $0.013 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a modifier in GND, GND), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{GND1} = 0 \quad (136)$$

### 8.69 Species GND2

**Name** GND2

**SBO:0000252** polypeptide chain

**Initial concentration**  $0.0030 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a modifier in GND, GND), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{GND2} = 0 \quad (137)$$

### 8.70 Species NQM1

**Name** NQM1

**SBO:0000252** polypeptide chain

**Initial concentration**  $0.02 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a modifier in [TAL](#), [TAL](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{NQM1} = 0 \quad (138)$$

### 8.71 Species [RKI1](#)

**Name** RKI1

**SBO:0000252** polypeptide chain

**Initial concentration**  $0.05 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a modifier in [RKI](#), [RKI](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{RKI1} = 0 \quad (139)$$

### 8.72 Species [RPE1](#)

**Name** RPE1

**SBO:0000252** polypeptide chain

**Initial concentration**  $0.03 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a modifier in [RPE](#), [RPE](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{RPE1} = 0 \quad (140)$$

### 8.73 Species [SOL3](#)

**Name** SOL3

**SBO:0000252** polypeptide chain

**Initial concentration**  $0.0296 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a modifier in [SOL](#), [SOL](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{SOL3} = 0 \quad (141)$$

### 8.74 Species TAL1

**Name** TAL1

**SBO:0000252** polypeptide chain

**Initial concentration**  $0.144 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a modifier in [TAL](#), [TAL](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{TAL1} = 0 \quad (142)$$

### 8.75 Species TKL1

**Name** TKL1

**SBO:0000252** polypeptide chain

**Initial concentration**  $0.455 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a modifier in [TKL\\_E4P](#), [TKL\\_E4P](#), [TKL\\_R5P](#), [TKL\\_R5P](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{TKL1} = 0 \quad (143)$$

### 8.76 Species ZWF1

**Name** ZWF1

**SBO:0000252** polypeptide chain

**Initial concentration**  $0.02 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a modifier in [ZWF](#), [ZWF](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{ZWF1} = 0 \quad (144)$$

## A Glossary of Systems Biology Ontology Terms

**SBO:0000176 biochemical reaction:** An event involving one or more chemical entities that modifies the electrochemical structure of at least one of the participants.

**SBO:0000185 transport reaction:** Movement of a physical entity without modification of the structure of the entity



**SBO:0000247 simple chemical:** Simple, non-repetitive chemical entity

**SBO:0000252 polypeptide chain:** Naturally occurring macromolecule formed by the repetition of amino-acid residues linked by peptidic bonds. A polypeptide chain is synthesized by the ribosome. CHEBI:1654

SBML<sup>2</sup>TeX was developed by Andreas Dräger<sup>a</sup>, Hannes Planatscher<sup>a</sup>, Dieudonné M Wouamba<sup>a</sup>, Adrian Schröder<sup>a</sup>, Michael Hucka<sup>b</sup>, Lukas Endler<sup>c</sup>, Martin Golebiewski<sup>d</sup> and Andreas Zell<sup>a</sup>. Please see <http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX> for more information.

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