## SBML Model Report

# Model name: "Nag2011_ChloroplasticStarchDegradation"

May 6, 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[1] and Ambarish Nag[2] at November first 2010 at no o' clock in the morning. and last time modified at April first 2014 at 1:29 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 | 7 |
| species types | 0 | species | 28 |
| events | 0 | constraints | 0 |
| reactions | 9 | function definitions | 0 |
| global parameters | 62 | unit definitions | 10 |
| rules | 3 | initial assignments | 4 |

### Model Notes

This model is from the article:
**Kinetic modeling and exploratory numerical simulation of chloroplastic starch degradation.**
Nag A, Lunacek M, Graf PA, Chang CH. BMC Syst Biol.2011 Jun 18;5:94. 21682905,

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**Abstract:**
BACKGROUND:Higher plants and algae are able to fix atmospheric carbon dioxide through photosynthesis and store this fixed carbon in large quantities as starch, which can be hydrolyzed into sugars serving as feedstock for fermentation to biofuels and precursors. Rational engineering of carbon flow in plant cells requires a greater understanding of how starch breakdown fluxes respond to variations in enzyme concentrations, kinetic parameters, and metabolite concentrations. We have therefore developed and simulated a detailed kinetic ordinary differential equation model of the degradation pathways for starch synthesized in plants and green algae, which to our knowledge is the most complete such model reported to date.RESULTS:Simulation with 9 internal metabolites and 8 external metabolites, the concentrations of the latter fixed at reasonable biochemical values, leads to a single reference solution showing -amylase activity to be the rate-limiting step in carbon flow from starch degradation. Additionally, the response coefficients for stromal glucose to the glucose transporter kcat and KM are substantial, whereas those for cytosolic glucose are not, consistent with a kinetic bottleneck due to transport. Response coefficient norms show stromal maltopentaose and cytosolic glucosylated arabinogalactan to be the most and least globally sensitive metabolites, respectively, and -amylase kcat and KM for starch to be the kinetic parameters with the largest aggregate effect on metabolite concentrations as a whole. The latter kinetic parameters, together with those for glucose transport, have the greatest effect on stromal glucose, which is a precursor for biofuel synthetic pathways. Exploration of the steady-state solution space with respect to concentrations of 6 external metabolites and 8 dynamic metabolite concentrations show that stromal metabolism is strongly coupled to starch levels, and that transport between compartments serves to lower coupling between metabolic subsystems in different compartments.CONCLUSIONS:We find that in the reference steady state, starch cleavage is the most significant determinant of carbon flux, with turnover of oligosaccharides playing a secondary role. Independence of stationary point with respect to initial dynamic variable values confirms a unique stationary point in the phase space of dynamically varying concentrations of the model network. Stromal maltooligosaccharide metabolism was highly coupled to the available starch concentration. From the most highly converged trajectories, distances between unique fixed points of phase spaces show that cytosolic maltose levels depend on the total concentrations of arabinogalactan and glucose present in the cytosol. In addition, cellular compartmentalization serves to dampen much, but not all, of the effects of one subnetwork on another, such that kinetic modeling of single compartments would likely capture most dynamics that are fast on the timescale of the transport reactions.

## 2 Unit Definitions

This is an overview of 13 unit definitions of which three are predefined by SBML and not mentioned in the model.

### 2.1 Unit per_s

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

### 2.2 Unit volume

**Definition** $\mathrm{l}$

### 2.3 Unit area

**Definition** $\mu\mathrm{m}^{2}$

### 2.4 Unit umole

**Definition** $\mu\mathrm{mol}$

### 2.5 Unit uM

**Definition** $\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$

### 2.6 Unit uM_per_s

**Definition** $\mu\mathrm{mol} \cdot \mathrm{l}^{-1} \cdot \mathrm{s}^{-1}$

### 2.7 Unit per_uM_per_s

**Definition** $\mu\mathrm{mol}^{-1} \cdot \mathrm{l} \cdot \mathrm{s}^{-1}$

### 2.8 Unit gm_per_L

**Definition** $\mathrm{g} \cdot \mathrm{l}^{-1}$

### 2.9 Unit gm_per_L_2

**Definition** $\mathrm{g}^{2} \cdot \mathrm{l}^{-2}$

### 2.10 Unit gm_per_umole

**Definition** $\mathrm{g} \cdot \mu\mathrm{mol}^{-1}$

## 2.11 Unit `substance`

**Notes** Mole is the predefined SBML unit for `substance`.

**Definition** mol

## 2.12 Unit `length`

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

**Definition** m

## 2.13 Unit `time`

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

**Definition** s

# 3 Compartments

This model contains seven compartments.

Table 2: Properties of all compartments.

| Id | Name | SBO | Spatial Dimensions | Size |
|---|---|---|---|---|
| `Cell` | Cell | 0000290 | 3 | $3.534 \cdot 10^{-}$ |
| `Cytosol` | Cytosol | 0000290 | 3 | 1 |
| `Chloroplast` | Chloroplast | 0000290 | 3 | 1 |
| `ChloroplastOuterMembrane` | Chloroplast Outer Membrane | 0000290 | 2 | 1000 |
| `ChloroplastIntermembraneSpace` | Chloroplast Intermembrane Space | 0000290 | 3 | 1 |
| `ChloroplastInnerMembrane` | Chloroplast Inner Membrane | 0000290 | 2 | 1000 |
| `ChloroplastStroma` | Chloroplast Stroma | 0000290 | 3 | 1 |

## 3.1 Compartment `Cell`

This is a three dimensional compartment with a constant size of $3.534 \cdot 10^{-12}$ litre.

**Name** Cell

**SBO:0000290** physical compartment

## 3.2 Compartment `Cytosol`

This is a three dimensional compartment with a not constant size of one litre, which is surrounded by `Cell` (Cell).

**Name** Cytosol

**SBO:0000290** physical compartment

## 3.3 Compartment `Chloroplast`

This is a three dimensional compartment with a not constant size of one litre, which is surrounded by `Cytosol` (Cytosol).

**Name** Chloroplast

**SBO:0000290** physical compartment

## 3.4 Compartment `ChloroplastOuterMembrane`

This is a two dimensional compartment with a constant size of 1000 $\mu m^2$, which is surrounded by `Cytosol` (Cytosol).

**Name** Chloroplast Outer Membrane

**SBO:0000290** physical compartment

## 3.5 Compartment `ChloroplastIntermembraneSpace`

This is a three dimensional compartment with a constant size of one litre, which is surrounded by `ChloroplastOuterMembrane` (Chloroplast Outer Membrane).

**Name** Chloroplast Intermembrane Space

**SBO:0000290** physical compartment

## 3.6 Compartment `ChloroplastInnerMembrane`

This is a two dimensional compartment with a constant size of 1000 $\mu m^2$, which is surrounded by `ChloroplastIntermembraneSpace` (Chloroplast Intermembrane Space).

**Name** Chloroplast Inner Membrane

**SBO:0000290** physical compartment

## 3.7 Compartment `ChloroplastStroma`

This is a three dimensional compartment with a constant size of one litre, which is surrounded by `ChloroplastInnerMembrane` (Chloroplast Inner Membrane).

**Name** Chloroplast Stroma

**SBO:0000290** physical compartment

## 4 Species

This model contains 28 species. The boundary condition of seven of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 9 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 |
|---|---|---|---|---|---|
| cpd_C00080_CY | H+ | Cytosol | $\mu mol \cdot l^{-1}$ | ☐ | ☑ |
| cpd_C00369_CS | Starch | ChloroplastStroma | $g \cdot l^{-1}$ | ☐ | ☐ |
| cpd_C00369Glc_CS | Starch Glucosyl unit | ChloroplastStroma | $\mu mol \cdot l^{-1}$ | ☐ | ☑ |
| cpd_C00369db_CS | Starch exposed to Beta Amylase due to action of Isoamylase (Starch DB) | ChloroplastStroma | $g \cdot l^{-1}$ | ☐ | ☐ |
| cpd_C00208_CY | Maltose | Cytosol | $\mu mol \cdot l^{-1}$ | ☐ | ☐ |
| cpd_C00208_CS | Maltose | ChloroplastStroma | $\mu mol \cdot l^{-1}$ | ☐ | ☐ |
| cpd_C01835_CS | Maltotriose | ChloroplastStroma | $\mu mol \cdot l^{-1}$ | ☐ | ☐ |
| cpd_G00343_CS | Maltopentaose | ChloroplastStroma | $\mu mol \cdot l^{-1}$ | ☐ | ☐ |
| cpd_C00031_CS | (D)-Glucose | ChloroplastStroma | $\mu mol \cdot l^{-1}$ | ☐ | ☐ |
| cpd_C00031_CY | (D)-Glucose | Cytosol | $\mu mol \cdot l^{-1}$ | ☐ | ☐ |
| cpd_C00569_CY | Arabinogalactan (AG) | Cytosol | $\mu mol \cdot l^{-1}$ | ☐ | ☐ |
| cpd_C00569Glc_CY | Glucosyl Arabinogalactan (GlcAG) | Cytosol | $\mu mol \cdot l^{-1}$ | ☐ | ☐ |
| cpd_C00002tot_CY | ATP pool | Cytosol | $\mu mol \cdot l^{-1}$ | ☐ | ☑ |
| cpd_C00008tot_CY | ADP pool | Cytosol | $\mu mol \cdot l^{-1}$ | ☐ | ☑ |
| cpd_C00009tot_CY | Orthophosphate(HPi) pool | Cytosol | $\mu mol \cdot l^{-1}$ | ☐ | ☑ |
| cpd_C00051_CY | Glutathione (reduced) | Cytosol | $\mu mol \cdot l^{-1}$ | ☐ | ☐ |
| cpd_C00660tot_CY | (D)-Glucose-1,6-bisphosphate pool | Cytosol | $\mu mol \cdot l^{-1}$ | ☐ | ☐ |
| cpd_C03339tot_CY | 2,3-Bisphosphoglycerate pool | Cytosol | $\mu mol \cdot l^{-1}$ | ☐ | ☐ |
| cpd_C00103tot_CY | G1P pool | Cytosol | $\mu mol \cdot l^{-1}$ | ☐ | ☑ |
| cpd_C00092tot_CY | G6P pool | Cytosol | $\mu mol \cdot l^{-1}$ | ☐ | ☑ |

| Id | Name | Compartment | Derived Unit | Constant | Boundary Condition |
| --- | --- | --- | --- | --- | --- |
| ec_3_2_1_2_CS | Beta amylase | ChloroplastStroma | $g \cdot l^{-1}$ | ⊟ | ⊟ |
| ec_3_2_1_68_CS | Isoamylase | ChloroplastStroma | $g \cdot l^{-1}$ | ⊟ | ⊟ |
| ec_2_4_1_25_CS | Disproportionating enzyme 1(DPE1) | ChloroplastStroma | $\mu mol \cdot l^{-1}$ | ⊟ | ⊟ |
| ec_2_4_1_25_CY | Disproportionating enzyme 2(DPE2) | Cytosol | $\mu mol \cdot l^{-1}$ | ⊟ | ⊟ |
| ec_2_4_1_1_CY | Cytosolic Glucan phosphorylase | Cytosol | $\mu mol \cdot l^{-1}$ | ⊟ | ⊟ |
| ec_2_7_1_1_CY | Hexokinase | Cytosol | $\mu mol \cdot l^{-1}$ | ⊟ | ⊟ |
| tc_2_A_84_1_2_CIMS | Maltose exporter (MEX) | ChloroplastIntermembraneSpace | $\mu mol \cdot l^{-1}$ | ⊟ | ⊟ |
| tc_2_A_1_1_17_CIMS | Glucose transporter (pGlcT) | ChloroplastIntermembraneSpace | $\mu mol \cdot l^{-1}$ | ⊟ | ⊟ |

# 5 Parameters

This model contains 62 global parameters.

Table 4: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| C00369_MW | Starch Mol. Wt. | 0000504 | 0.270 | $g \cdot \mu mol^{-1}$ | ☑ |
| N_Glc_Starch | Number of Glucosyl units in a Starch molecule | 0000503 | 1667.000 | dimensionless | ☑ |
| f_bamylase | Fraction of Starch amenable to degradation by Beta Amylase only | 0000540 | 0.582 | dimensionless | ☑ |
| f_G2 | Fraction of starch degraded to Maltose | 0000540 | 0.870 | dimensionless | ☑ |
| f_G3 | Fraction of starch degraded to Maltotriose | 0000540 | 0.130 | dimensionless | ☑ |
| conv_gm_umole | Unit conversion factor to meet SBML standards | 0000565 | 1.000 | $g \cdot \mu mol^{-1}$ | ☑ |
| ec_3_2_1_2_MW | Beta amylase molecular weight | 0000504 | 0.206 | $g \cdot \mu mol^{-1}$ | ☑ |
| G00343_MW | Maltopentaose Mol. Wt. | 0000504 | $8.28 \cdot 10^{-4}$ | $g \cdot \mu mol^{-1}$ | ☑ |
| C01835_MW | Maltotriose Mol. Wt. | 0000504 | $5.04 \cdot 10^{-4}$ | $g \cdot \mu mol^{-1}$ | ☑ |
| C00208_MW | Maltose Mol. Wt. | 0000504 | $3.42 \cdot 10^{-4}$ | $g \cdot \mu mol^{-1}$ | ☑ |
| R05196CS_kcat | DPE1 kcat | 0000025 | 50.000 | $s^{-1}$ | ☑ |
| R05196CS_Keq | DPE1 Keq | 0000281 | 1.000 | dimensionless | ☑ |
| R05196CS_G3_KM | DPE1 G3 KM | 0000027 | 3300.000 | $\mu mol \cdot l^{-1}$ | ☑ |
| R05196CS_Glc_KM | DPE1 Glc KM | 0000027 | 11700.000 | $\mu mol \cdot l^{-1}$ | ☑ |
| R05196CS_G5_KM | DPE1 G5 KM | 0000027 | 210.000 | $\mu mol \cdot l^{-1}$ | ☑ |
| R05196CS_G3_Ki | DPE1 G3 Ki | 0000009 | 746.420 | $\mu mol \cdot l^{-1}$ | ☑ |
| R05196CS_Glc_Ki | DPE1 Glc Ki | 0000009 | 5571.429 | $\mu mol \cdot l^{-1}$ | ☑ |

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| R05196CS_G5-_Ki | DPE1 G5 Ki | 0000009 | 100.000 | $\mu mol \cdot l^{-1}$ | ☑ |
| AT2G40840CY-_kcat | DPE2 kcat | 0000025 | 50.000 | $s^{-1}$ | ☑ |
| AT2G40840CY-_Keq | DPE2 Keq | 0000281 | 1.000 | dimensionless | ☑ |
| AT2G40840CY-_Glc_KM | DPE2 Glc KM | 0000027 | 11700.000 | $\mu mol \cdot l^{-1}$ | ☑ |
| AT2G40840CY-_G2_KM | DPE2 Maltose KM | 0000027 | 4600.000 | $\mu mol \cdot l^{-1}$ | ☑ |
| AT2G40840CY-_AG_KM | DPE2 AG KM | 0000027 | 1100.000 | $\mu mol \cdot l^{-1}$ | ☑ |
| AT2G40840CY-_GlcAG_KM | DPE2 GlcAG KM | 0000027 | 1100.000 | $\mu mol \cdot l^{-1}$ | ☑ |
| AT2G40840CY-_Glc_Ki | DPE2 Glc Ki | 0000009 | 5571.429 | $\mu mol \cdot l^{-1}$ | ☑ |
| AT2G40840CY-_G2_Ki | DPE2 Maltose Ki | 0000009 | 2190.476 | $\mu mol \cdot l^{-1}$ | ☑ |
| AT2G40840CY-_AG_Ki | DPE2 AG Ki | 0000009 | 1000.000 | $\mu mol \cdot l^{-1}$ | ☑ |
| AT2G40840CY-_GlcAG_Ki | DPE2 GlcAG Ki | 0000009 | 1000.000 | $\mu mol \cdot l^{-1}$ | ☑ |
| R06050CY-_kcat | Cytosolic glucan phosphorylase kcat | 0000025 | 50.000 | $s^{-1}$ | ☑ |
| R06050CY-_GlcAG_KM | Cytosolic glucan phosphorylase Glucosyl Arabinogalactan KM | 0000027 | 2100.000 | $\mu mol \cdot l^{-1}$ | ☑ |
| R06050CY-_GlcAG_Ki | Cytosolic glucan phosphorylase Glucosyl Arabinogalactan Ki | 0000009 | 3800.000 | $\mu mol \cdot l^{-1}$ | ☑ |
| R06050CY_AG-_KM | Cytosolic glucan phosphorylase Arabinogalactan KM | 0000027 | 3800.000 | $\mu mol \cdot l^{-1}$ | ☑ |
| R06050CY_Pi-_KM | Cytosolic glucan phosphorylase Pi KM | 0000027 | 5900.000 | $\mu mol \cdot l^{-1}$ | ☑ |
| R06050CY-_G1P_KM | Cytosolic glucan phosphorylase G1P KM | 0000027 | 2000.000 | $\mu mol \cdot l^{-1}$ | ☑ |

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| R06050CY_G1P_Ki | Cytosolic glucan phosphorylase G1P Ki | 0000009 | 3100.000 | $\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$ | ☑ |
| R06050CY_Keq | Cytosolic glucan phosphorylase Keq | 0000281 | $6.15 \cdot 10^{-4}$ | dimensionless | ☑ |
| TC_2_A_84_1_2_kcat | Maltose exporter (MEX) kcat | 0000025 | 5.963 | $\mathrm{s}^{-1}$ | ☑ |
| TC_2_A_84_1_2_KM | Maltose exporter (MEX) KM | 0000027 | 4000.000 | $\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$ | ☑ |
| TC_2_A_1_1_17_kcat | Glucose transporter (pGlcT) kcat | 0000025 | 240.278 | $\mathrm{s}^{-1}$ | ☑ |
| TC_2_A_1_1_17_KM | Glucose transporter (pGlcT) KM | 0000027 | 19300.000 | $\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$ | ☑ |
| R02112CS_Gn_KM | Beta Amylase KM for Starch | 0000027 | 0.500 | $\mathrm{g} \cdot \mathrm{l}^{-1}$ | ☑ |
| R02112CS_G5_KM | Beta Amylase KM for Maltopentaose | 0000027 | 1.460 | $\mathrm{g} \cdot \mathrm{l}^{-1}$ | ☑ |
| R02112CS_G2C_KM | Beta Amylase KM for Maltose condensation | 0000027 | 4.190 | $\mathrm{g}^{2} \cdot \mathrm{l}^{-2}$ | ☑ |
| R02112CS_Keq | Keq for Maltotetraose degradation | 0000281 | 18800.000 | $\mathrm{g} \cdot \mathrm{l}^{-1}$ | ☑ |
| R02112CS_Gn_kcat | kcat_betaamylase_Starch | 0000025 | 0.073 | $\mathrm{s}^{-1}$ | ☑ |
| R02112CS_G5_kcat | kcat_betaamylase_Maltopentaose | 0000025 | 0.091 | $\mathrm{s}^{-1}$ | ☑ |
| ec_3_2_1_68_CS_kcat | Isoamylase kcat | 0000025 | 0.020 | $\mathrm{s}^{-1}$ | ☑ |
| R00299CY_kfor | Hexokinase kcat,forward | 0000320 | 180.000 | $\mathrm{s}^{-1}$ | ☑ |
| R00299CY_krev | Hexokinase kcat,reverse | 0000321 | 0.000 | $\mathrm{s}^{-1}$ | ⊟ |
| R00299CY_Keq | Hexokinase Keq | 0000281 | 155.000 | dimensionless | ☑ |
| R00299CY_MgATP_KM | Hexokinase KM(MgATP) | 0000027 | 1000.000 | $\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$ | ☑ |
| R00299CY_MgATP_Ki | Hexokinase Ki(MgATP) | 0000009 | 1000.000 | $\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$ | ☑ |
| R00299CY_Glc_KM | Hexokinase KM(glucose) | 0000027 | 47.000 | $\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$ | ☑ |

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| R00299CY-_Glc_Ki | Hexokinase Ki(glucose) | 0000009 | 47.000 | $\mu mol \cdot l^{-1}$ | ☑ |
| R00299CY-_G6P_KM | Hexokinase KM(G6P) | 0000027 | 47.000 | $\mu mol \cdot l^{-1}$ | ☑ |
| R00299CY-_G6P_Ki | Hexokinase Ki(G6P) | 0000009 | 47.000 | $\mu mol \cdot l^{-1}$ | ☑ |
| R00299CY-_MgADP_KM | Hexokinase KM(MgADP) | 0000027 | 1000.000 | $\mu mol \cdot l^{-1}$ | ☑ |
| R00299CY-_MgADP_Ki | Hexokinase Ki(MgADP) | 0000009 | 1000.000 | $\mu mol \cdot l^{-1}$ | ☑ |
| R00299CY-_G6P_Kip | Hexokinase Ki(G6P),2 | 0000009 | 10.000 | $\mu mol \cdot l^{-1}$ | ☑ |
| R00299CY-_BPG_Kip | Hexokinase Ki(2,3-bisphosphoglycerate) | 0000009 | 4000.000 | $\mu mol \cdot l^{-1}$ | ☑ |
| R00299CY-_G16P_Kip | Hexokinase Ki(glucose 1,6-bisphosphate | 0000009 | 30.000 | $\mu mol \cdot l^{-1}$ | ☑ |
| R00299CY-_GSH_Kip | Hexokinase Ki(glutathione) | 0000009 | 3000.000 | $\mu mol \cdot l^{-1}$ | ☑ |

# 6 Initialassignments

This is an overview of four initialassignments.

## 6.1 Initialassignment `Cytosol`

**Derived unit** contains undeclared units

**Math** $0.447 \cdot \mathrm{vol}\,(\mathrm{Cell})$

## 6.2 Initialassignment `ChloroplastIntermembraneSpace`

**Derived unit** contains undeclared units

**Math** $0.01 \cdot \mathrm{vol}\,(\mathrm{Chloroplast})$

## 6.3 Initialassignment `Chloroplast`

**Derived unit** contains undeclared units

**Math** $0.2 \cdot \mathrm{vol}\,(\mathrm{Cell})$

### 6.4 Initialassignment ChloroplastStroma

**Derived unit** contains undeclared units

**Math** $0.5 \cdot \mathrm{vol}\left(\mathrm{Chloroplast}\right)$

# 7 Rules

This is an overview of three rules.

## 7.1 Rule R00299CY_krev

Rule R00299CY_krev is an assignment rule for parameter R00299CY_krev:

$$\mathrm{R00299CY\_krev} = \frac{\mathrm{R00299CY\_kfor} \cdot \mathrm{R00299CY\_MgADP\_Ki} \cdot \mathrm{R00299CY\_G6P\_KM}}{\mathrm{R00299CY\_Keq} \cdot \mathrm{R00299CY\_Glc\_Ki} \cdot \mathrm{R00299CY\_MgATP\_KM}} \tag{1}$$

**Derived unit** $\mathrm{s}^{-1}$

## 7.2 Rule cpd_C00369_CS

Rule cpd_C00369_CS is an assignment rule for species cpd_C00369_CS:

$$\mathrm{cpd\_C00369\_CS} = \frac{[\mathrm{cpd\_C00369Glc\_CS}] \cdot \mathrm{C00369\_MW}}{\mathrm{N\_Glc\_Starch}} \tag{2}$$

**Derived unit** $\mathrm{l}^{-1} \cdot \mathrm{g}$

## 7.3 Rule cpd_C00369db_CS

Rule cpd_C00369db_CS is a rate rule for species cpd_C00369db_CS:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cpd\_C00369db\_CS} = {} & [\mathrm{ec\_3\_2\_1\_68\_CS}] \cdot \mathrm{ec\_3\_2\_1\_68\_CS\_kcat} \\ & \cdot \left(1 - \frac{1}{1 + \exp\left(-100 \cdot \left(\frac{[\mathrm{cpd\_C00369db\_CS}]}{[\mathrm{cpd\_C00369\_CS}] \cdot (1 - \mathrm{f\_bamylase})} - 0.3\right)\right)} \right. \\ & + \frac{1}{1 + \exp\left(-100 \cdot \left(\frac{[\mathrm{cpd\_C00369db\_CS}]}{[\mathrm{cpd\_C00369\_CS}] \cdot (1 - \mathrm{f\_bamylase})} - 0.3\right)\right)} \\ & \left. \cdot \left(1 - 1.429 \cdot \left(\frac{[\mathrm{cpd\_C00369db\_CS}]}{[\mathrm{cpd\_C00369\_CS}] \cdot (1 - \mathrm{f\_bamylase})} - 0.3\right)\right)\right)\end{aligned} \tag{3}$$

# 8 Reactions

This model contains nine 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

| № | Id | Name | Reaction Equation | SBO |
|---|---|---|---|---|
| 1 | `rn_R02112CS_G2` | Maltose formation from Starch | 12345 · 7 cpd_C00369Glc_CS $\xrightleftharpoons{\text{ec\_3\_2\_1\_2\_CS, cpd\_C00369\_CS, cpd\_C00369db\_CS}}$ 29 | 0000393 |
| 2 | `rn_R02112CS_G3` | Maltotriose formation from Starch | 18518 · 5 cpd_C00369Glc_CS $\xrightarrow{\text{ec\_3\_2\_1\_2\_CS, cpd\_C00369\_CS, cpd\_C00369db\_CS}}$ 198 | 0000393 |
| 3 | `rn_R02112CS_G5` | Maltopentaose degradation | 1207 · 73 cpd_G00343_CS $\xrightarrow{\text{ec\_3\_2\_1\_2\_CS}}$ 2923 · 98 cpd_C00208_CS + 1984 · 13 cpd_C01835_CS | 0000179 |
| 4 | `tr_TC_2_A_84_1_2` | Maltose exporter | cpd_C00208_CS $\xrightarrow{\text{tc\_2\_A\_84\_1\_2\_CIMS}}$ cpd_C00208_CY | 0000185 |
| 5 | `tr_TC_2_A_1_1_17` | Plastidic Glucose transporter | cpd_C00031_CS $\xrightarrow{\text{tc\_2\_A\_1\_1\_17\_CIMS}}$ cpd_C00031_CY | 0000185 |
| 6 | `rn_R00299CY` | Hexokinase | cpd_C00002tot_CY + cpd_C00031_CY $\xrightleftharpoons{\text{ec\_2\_7\_1\_1\_CY, cpd\_C00051\_CY, cpd\_C00660tot\_CY, cpd\_C03339tc}}$ cpd_C00008tot_CY + cpd_C00080_CY | 0000559 |
| 7 | `rn_R06050CY` | Cytosolic glucan phosphorylase | cpd_C00569Glc_CY + cpd_C00009tot_CY $\xrightleftharpoons{\text{ec\_2\_4\_1\_1\_CY}}$ cpd_C00103tot_CY + cpd_C00569_CY | 0000559 |
| 8 | `rn_AT2G40840CY` | DPE2 | cpd_C00208_CY + cpd_C00569_CY $\xrightleftharpoons{\text{ec\_2\_4\_1\_25\_CY}}$ cpd_C00031_CY + cpd_C00569Glc_CY | 0000559 |
| 9 | `rn_R05196CS` | DPE1 | 2 cpd_C01835_CS $\xrightleftharpoons{\text{ec\_2\_4\_1\_25\_CS}}$ cpd_C00031_CS + cpd_G00343_CS | 0000559 |

## 8.1 Reaction rn_R02112CS_G2

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

**Name** Maltose formation from Starch

**SBO:0000393** production

### Reaction equation

$$12345 \cdot 7\, \text{cpd\_C00369Glc\_CS} \xrightleftharpoons{\text{ec\_3\_2\_1\_2\_CS, cpd\_C00369\_CS, cpd\_C00369db\_CS}} 2923 \cdot 98\, \text{cpd\_C00208\_CS} \tag{4}$$

### Reactant

Table 6: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| cpd_C00369Glc_CS | Starch Glucosyl unit | |

### Modifiers

Table 7: Properties of each modifier.

| Id | Name | SBO |
|---|---|---|
| ec_3_2_1_2_CS | beta amylase | |
| cpd_C00369_CS | Starch | |
| cpd_C00369db_CS | Starch DB | |

### Product

Table 8: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| cpd_C00208_CS | Maltose | |

### Kinetic Law

**Derived unit** contains undeclared units

$$v_1 = \frac{\mathrm{vol}\left(\mathrm{ChloroplastStroma}\right) \cdot \mathrm{R02112CS\_Gn\_kcat} \cdot [\mathrm{ec\_3\_2\_1\_2\_CS}] \cdot \Big(\mathrm{f\_G2} \cdot (\mathrm{f\_bamylase} \cdot [\mathrm{cpd\_C00369\_CS}] + [\mathrm{cpd}}{\mathrm{conv\_gm\_umole} \cdot \Big(\mathrm{f\_G2} \cdot (\mathrm{f\_bamylase} \cdot [\mathrm{cpd\_C00369\_CS}] + [\mathrm{cpd\_C00369db\_CS}]) + \mathrm{R02112CS\_Gn\_KM}} \quad (5)$$

## 8.2 Reaction `rn_R02112CS_G3`

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

**Name** Maltotriose formation from Starch

**SBO:0000393** production

### Reaction equation

$$18518 \cdot 5\,\mathrm{cpd\_C00369Glc\_CS} \xrightarrow{\mathrm{ec\_3\_2\_1\_2\_CS},\ \mathrm{cpd\_C00369\_CS},\ \mathrm{cpd\_C00369db\_CS}} 1984 \cdot 13\,\mathrm{cpd\_C01835\_CS} \quad (6)$$

### Reactant

Table 9: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| `cpd_C00369Glc_CS` | Starch Glucosyl unit | |

### Modifiers

Table 10: Properties of each modifier.

| Id | Name | SBO |
|---|---|---|
| `ec_3_2_1_2_CS` | beta amylase | |
| `cpd_C00369_CS` | Starch | |
| `cpd_C00369db_CS` | Starch DB | |

### Product

Table 11: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| `cpd_C01835_CS` | Maltotriose | |

### Kinetic Law

**Derived unit** $\mathrm{s}^{-1} \cdot \mu\mathrm{mol}$

$$v_2 = \frac{\mathrm{vol}\left(\mathrm{ChloroplastStroma}\right) \cdot \mathrm{R02112CS\_Gn\_kcat} \cdot [\mathrm{ec\_3\_2\_1\_2\_CS}] \cdot \mathrm{f\_G3} \cdot \left(\mathrm{f\_bamylase} \cdot [\mathrm{cpd\_C00369\_CS}] + [\mathrm{cpd\_C}\right.}{\mathrm{conv\_gm\_umole} \cdot \left(\mathrm{f\_G3} \cdot \left(\mathrm{f\_bamylase} \cdot [\mathrm{cpd\_C00369\_CS}] + [\mathrm{cpd\_C00369db\_CS}]\right) + \mathrm{R02112CS\_Gn\_K}\right.} \quad (7)$$

## 8.3 Reaction `rn_R02112CS_G5`

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

**Name** Maltopentaose degradation

**SBO:0000179** degradation

### Reaction equation

$$1207 \cdot 73\,\mathrm{cpd\_G00343\_CS} \xrightarrow{\mathrm{ec\_3\_2\_1\_2\_CS}} 2923 \cdot 98\,\mathrm{cpd\_C00208\_CS} + 1984 \cdot 13\,\mathrm{cpd\_C01835\_CS} \quad (8)$$

### Reactant

Table 12: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| `cpd_G00343_CS` | Maltopentaose | |

### Modifier

Table 13: Properties of each modifier.

| Id | Name | SBO |
|---|---|---|
| `ec_3_2_1_2_CS` | beta amylase | |

### Products

Table 14: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| `cpd_C00208_CS` | Maltose | |
| `cpd_C01835_CS` | Maltotriose | |

### Kinetic Law

**Derived unit** $\mathrm{s}^{-1} \cdot \mu\mathrm{mol}$

$$v_3 = \frac{\mathrm{vol}\left(\mathrm{ChloroplastStroma}\right) \cdot \mathrm{R02112CS\_G5\_kcat} \cdot [\mathrm{ec\_3\_2\_1\_2\_CS}] \cdot [\mathrm{cpd\_G00343\_CS}] \cdot \mathrm{G00343\_MW}}{\mathrm{conv\_gm\_umole} \cdot \left([\mathrm{cpd\_G00343\_CS}] \cdot \mathrm{G00343\_MW} + \mathrm{R02112CS\_G5\_KM}\right)} \quad (9)$$

## 8.4 Reaction `tr_TC_2_A_84_1_2`

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

**Name** Maltose exporter

**SBO:0000185** transport reaction

### Reaction equation

$$\mathrm{cpd\_C00208\_CS} \xrightarrow{\mathrm{tc\_2\_A\_84\_1\_2\_CIMS}} \mathrm{cpd\_C00208\_CY} \quad (10)$$

### Reactant

Table 15: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| `cpd_C00208_CS` | Maltose | |

### Modifier

Table 16: Properties of each modifier.

| Id | Name | SBO |
|---|---|---|
| `tc_2_A_84_1_2_CIMS` | Maltose exporter(MEX) | |

### Product

Table 17: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| `cpd_C00208_CY` | Maltose | |

### Kinetic Law

**Derived unit** $\mathrm{s}^{-1} \cdot 10^{-6}\ \mathrm{mol}$

$$v_4 = \frac{\mathrm{vol}\left(\mathrm{ChloroplastStroma}\right) \cdot \mathrm{TC\_2\_A\_84\_1\_2\_kcat} \cdot [\mathrm{tc\_2\_A\_84\_1\_2\_CIMS}] \cdot [\mathrm{cpd\_C00208\_CS}]}{\mathrm{TC\_2\_A\_84\_1\_2\_KM} + [\mathrm{cpd\_C00208\_CS}]} \tag{11}$$

## 8.5 Reaction `tr_TC_2_A_1_1_17`

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

**Name** Plastidic Glucose transporter

**SBO:0000185** transport reaction

### Reaction equation

$$\mathrm{cpd\_C00031\_CS} \xrightarrow{\mathrm{tc\_2\_A\_1\_1\_17\_CIMS}} \mathrm{cpd\_C00031\_CY} \tag{12}$$

### Reactant

Table 18: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| `cpd_C00031_CS` | Glucose | |

### Modifier

Table 19: Properties of each modifier.

| Id | Name | SBO |
|---|---|---|
| `tc_2_A_1_1_17_CIMS` | Glucose transporter(pGlcT) | |

### Product

Table 20: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| `cpd_C00031_CY` | Glucose | |

### Kinetic Law

**Derived unit** $\mathrm{s}^{-1} \cdot 10^{-6}\ \mathrm{mol}$

$$v_5 = \frac{\mathrm{vol}\left(\mathrm{ChloroplastStroma}\right) \cdot \mathrm{TC\_2\_A\_1\_1\_17\_kcat} \cdot [\mathrm{tc\_2\_A\_1\_1\_17\_CIMS}] \cdot [\mathrm{cpd\_C00031\_CS}]}{\mathrm{TC\_2\_A\_1\_1\_17\_KM} + [\mathrm{cpd\_C00031\_CS}]} \tag{13}$$

## 8.6 Reaction `rn_R00299CY`

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

**Name** Hexokinase

**SBO:0000559** enzyme activity

**Notes** Kinetics reversible random sequential bi-bi.

### Reaction equation

$$\mathrm{cpd\_C00002tot\_CY} + \mathrm{cpd\_C00031\_CY} \xrightleftharpoons{\mathrm{ec\_2\_7\_1\_1\_CY},\ \mathrm{cpd\_C00051\_CY},\ \mathrm{cpd\_C00660tot\_CY},\ \mathrm{cpd\_C03339tot\_CY}} \mathrm{c} \tag{14}$$

### Reactants

Table 21: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| `cpd_C00002tot_CY` | ATP pool | |
| `cpd_C00031_CY` | Glucose | |

### Modifiers

Table 22: Properties of each modifier.

| Id | Name | SBO |
|---|---|---|
| `ec_2_7_1_1_CY` | Hexokinase (cytosolic) | |
| `cpd_C00051_CY` | Reduced glutathione | |
| `cpd_C00660tot_CY` | (D)-Glucose-1,6-bisphosphate pool | |
| `cpd_C03339tot_CY` | 2,3-Bisphosphoglycerate pool | |

### Products

Table 23: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| cpd_C00092tot_CY | G6P pool | |
| cpd_C00008tot_CY | ADP pool | |
| cpd_C00080_CY | H+ | |

### Kinetic Law

**Derived unit** contains undeclared units

$$v_6 = \frac{[\mathrm{ec\_2\_7\_1\_1\_CY}] \cdot \mathrm{vol}(\mathrm{Cytosol}) \cdot \left(\frac{\mathrm{R00299CY\_kfor} \cdot [\mathrm{cpd\_C0000}}{\mathrm{R00299CY\_Glc\_Ki} \cdot \mathrm{R00}}\right.}{1 + \frac{[\mathrm{cpd\_C00002tot\_CY}]}{\mathrm{R00299CY\_MgATP\_Ki}} + \frac{[\mathrm{cpd\_C00031\_CY}]}{\mathrm{R00299CY\_Glc\_Ki}} \cdot \left(1 + \frac{[\mathrm{cpd\_C00092tot\_CY}]}{\mathrm{R00299CY\_G6P\_Kip}} + \frac{[\mathrm{cpd\_C00660tot\_CY}]}{\mathrm{R00299CY\_G16P\_Kip}} + \frac{[\mathrm{cpd\_C03339tot\_CY}]}{\mathrm{R00299CY\_BPG\_Kip}} + \frac{[\mathrm{cpd\_C}}{\mathrm{R00299C}}\right.} \quad (15)$$

## 8.7 Reaction rn_R06050CY

This is a reversible reaction of two reactants forming two products influenced by one modifier.

**Name** Cytosolic glucan phosphorylase

**SBO:0000559** enzyme activity

### Reaction equation

$$\mathrm{cpd\_C00569Glc\_CY} + \mathrm{cpd\_C00009tot\_CY} \xrightleftharpoons{\mathrm{ec\_2\_4\_1\_1\_CY}} \mathrm{cpd\_C00103tot\_CY} + \mathrm{cpd\_C00569\_CY} \quad (16)$$

### Reactants

Table 24: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| cpd_C00569Glc_CY | Glucosyl Arabinogalactan | |
| cpd_C00009tot_CY | HPi | |

### Modifier

Table 25: Properties of each modifier.

| Id | Name | SBO |
|---|---|---|
| ec_2_4_1_1_CY | Cytosolic glucan phosphorylase | |

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

### Products

Table 26: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| cpd_C00103tot_CY | G1P pool | |
| cpd_C00569_CY | Arabinogalactan | |

### Kinetic Law

**Derived unit** $\mathrm{s}^{-1} \cdot 1.0000000000000024 \cdot 10^{-6}\ \mathrm{mol}$

$$v_7 \tag{17}$$

$$= \frac{}{\mathrm{R06050CY\_GlcAG\_Ki} \cdot \mathrm{R06050CY\_Pi\_KM} + \mathrm{R06050CY\_Pi\_KM} \cdot [\mathrm{cpd\_C00569Glc\_CY}] + \mathrm{R06050CY\_GlcAG\_}}$$

## 8.8 Reaction rn_AT2G40840CY

This is a reversible reaction of two reactants forming two products influenced by one modifier.

**Name** DPE2

**SBO:0000559** enzyme activity

### Reaction equation

$$\mathrm{cpd\_C00208\_CY} + \mathrm{cpd\_C00569\_CY} \xrightleftharpoons{\mathrm{ec\_2\_4\_1\_25\_CY}} \mathrm{cpd\_C00031\_CY} + \mathrm{cpd\_C00569Glc\_CY} \tag{18}$$

### Reactants

Table 27: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| cpd_C00208_CY | Maltose | |
| cpd_C00569_CY | AG | |

### Modifier

Table 28: Properties of each modifier.

| Id | Name | SBO |
|---|---|---|
| ec_2_4_1_25_CY | DPE2 | |

### Products

Table 29: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| cpd_C00031_CY | Glucose | |
| cpd_C00569Glc_CY | GlcAG | |

### Kinetic Law

**Derived unit** contains undeclared units

$$v_8 \tag{19}$$

$$= \frac{}{\mathrm{AT2G40840CY\_AG\_KM} \cdot [\mathrm{cpd\_C00208\_CY}] + \mathrm{AT2G40840CY\_G2\_KM} \cdot [\mathrm{cpd\_C00569\_CY}] + [\mathrm{cpd\_C00208\_CY}}$$

## 8.9 Reaction rn_R05196CS

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

**Name** DPE1

**SBO:0000559** enzyme activity

### Reaction equation

$$2\,\mathrm{cpd\_C01835\_CS} \xrightleftharpoons{\mathrm{ec\_2\_4\_1\_25\_CS}} \mathrm{cpd\_C00031\_CS} + \mathrm{cpd\_G00343\_CS} \tag{20}$$

### Reactant

Table 30: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| cpd_C01835_CS | Maltotriose | |

### Modifier

Table 31: Properties of each modifier.

| Id | Name | SBO |
|---|---|---|
| ec_2_4_1_25_CS | DPE1 | |

### Products

Table 32: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| cpd_C00031_CS | D-Glucose | |
| cpd_G00343_CS | Maltopentaose | |

### Kinetic Law

**Derived unit** contains undeclared units

$$v_9 \tag{21}$$

$$= \frac{\mathrm{vol}\,(\mathrm{ChloroplastStroma}) \cdot \mathrm{R05196CS}}{\mathrm{R05196CS\_G3\_KM} \cdot [\mathrm{cpd\_C01835\_CS}] + [\mathrm{cpd\_C01835\_CS}]^2 + \frac{\mathrm{R05196CS\_G3\_KM} \cdot \mathrm{R05196CS\_G3\_Ki}}{\mathrm{R05196CS\_Glc\_KM} \cdot \mathrm{R05196CS\_G5\_Ki}} \cdot \left(\mathrm{R05196CS\_G5\_I}\right.}$$

## 9 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.

### 9.1 Species cpd_C00080_CY

**Name** H+

**SBO:0000327** non-macromolecular ion

**Initial concentration** $0.1\ \mu\mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in one reaction (as a product in rn_R00299CY), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cpd\_C00080\_CY} = 0 \tag{22}$$

### 9.2 Species cpd_C00369_CS

**Name** Starch

**SBO:0000247** simple chemical

**Involved in rule** cpd_C00369_CS

This species takes part in two reactions (as a modifier in rn_R02112CS_G2, rn_R02112CS_G3) and is also involved in one rule which determines this species' quantity.

### 9.3 Species cpd_C00369Glc_CS

**Name** Starch Glucosyl unit

**SBO:0000247** simple chemical

**Initial concentration** $1000\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in two reactions (as a reactant in rn_R02112CS_G2, rn_R02112CS_G3), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{cpd\_C00369Glc\_CS} = 0 \tag{23}$$

### 9.4 Species cpd_C00369db_CS

**Name** Starch exposed to Beta Amylase due to action of Isoamylase (Starch DB)

**SBO:0000247** simple chemical

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

**Involved in rule** cpd_C00369db_CS

This species takes part in two reactions (as a modifier in rn_R02112CS_G2, rn_R02112CS_G3) and is also involved in one rule which determines this species' quantity.

### 9.5 Species cpd_C00208_CY

**Name** Maltose

**SBO:0000247** simple chemical

**Initial concentration** $10\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in two reactions (as a reactant in rn_AT2G40840CY and as a product in tr_TC_2_A_84_1_2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{cpd\_C00208\_CY} = v_4 - v_8 \tag{24}$$

## 9.6 Species cpd_C00208_CS

**Name** Maltose

**SBO:0000247** simple chemical

**Initial concentration** $10\ \mu mol \cdot l^{-1}$

This species takes part in three reactions (as a reactant in tr_TC_2_A_84_1_2 and as a product in rn_R02112CS_G2, rn_R02112CS_G5).

$$\frac{d}{dt}\text{cpd\_C00208\_CS} = 2923.98v_1 + 2923.98v_3 - v_4 \tag{25}$$

## 9.7 Species cpd_C01835_CS

**Name** Maltotriose

**SBO:0000247** simple chemical

**Initial concentration** $100\ \mu mol \cdot l^{-1}$

This species takes part in three reactions (as a reactant in rn_R05196CS and as a product in rn_R02112CS_G3, rn_R02112CS_G5).

$$\frac{d}{dt}\text{cpd\_C01835\_CS} = 1984.13v_2 + 1984.13v_3 - 2v_9 \tag{26}$$

## 9.8 Species cpd_G00343_CS

**Name** Maltopentaose

**SBO:0000247** simple chemical

**Initial concentration** $1000\ \mu mol \cdot l^{-1}$

This species takes part in two reactions (as a reactant in rn_R02112CS_G5 and as a product in rn_R05196CS).

$$\frac{d}{dt}\text{cpd\_G00343\_CS} = v_9 - 1207.73v_3 \tag{27}$$

## 9.9 Species cpd_C00031_CS

**Name** (D)-Glucose

**SBO:0000247** simple chemical

**Initial concentration** $10\ \mu mol \cdot l^{-1}$

This species takes part in two reactions (as a reactant in tr_TC_2_A_1_1_17 and as a product in rn_R05196CS).

$$\frac{d}{dt}\text{cpd\_C00031\_CS} = v_9 - v_5 \tag{28}$$

### 9.10 Species cpd_C00031_CY

**Name** (D)-Glucose

**SBO:0000247** simple chemical

**Initial concentration** $10\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in three reactions (as a reactant in rn_R00299CY and as a product in tr_TC_2_A_1_1_17, rn_AT2G40840CY).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{cpd\_C00031\_CY} = v_5 + v_8 - v_6 \tag{29}$$

### 9.11 Species cpd_C00569_CY

**Name** Arabinogalactan (AG)

**SBO:0000247** simple chemical

**Initial concentration** $10000\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in two reactions (as a reactant in rn_AT2G40840CY and as a product in rn_R06050CY).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{cpd\_C00569\_CY} = v_7 - v_8 \tag{30}$$

### 9.12 Species cpd_C00569Glc_CY

**Name** Glucosyl Arabinogalactan (GlcAG)

**SBO:0000247** simple chemical

**Initial concentration** $10000\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in two reactions (as a reactant in rn_R06050CY and as a product in rn_AT2G40840CY).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{cpd\_C00569Glc\_CY} = v_8 - v_7 \tag{31}$$

### 9.13 Species cpd_C00002tot_CY

**Name** ATP pool

**SBO:0000247** simple chemical

**Initial concentration** $10000\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in one reaction (as a reactant in rn_R00299CY), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{cpd\_C00002tot\_CY} = 0 \tag{32}$$

## 9.14 Species cpd_C00008tot_CY

**Name** ADP pool

**SBO:0000247** simple chemical

**Initial concentration** $10000\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in rn_R00299CY), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cpd\_C00008tot\_CY} = 0 \tag{33}$$

## 9.15 Species cpd_C00009tot_CY

**Name** Orthophosphate(HPi) pool

**SBO:0000247** simple chemical

**Initial concentration** $10000\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a reactant in rn_R06050CY), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cpd\_C00009tot\_CY} = 0 \tag{34}$$

## 9.16 Species cpd_C00051_CY

**Name** Glutathione (reduced)

**SBO:0000247** simple chemical

**Initial concentration** $1000\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a modifier in rn_R00299CY).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cpd\_C00051\_CY} = 0 \tag{35}$$

## 9.17 Species cpd_C00660tot_CY

**Name** (D)-Glucose-1,6-bisphosphate pool

**SBO:0000247** simple chemical

**Initial concentration** $10000\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a modifier in rn_R00299CY).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cpd\_C00660tot\_CY} = 0 \tag{36}$$

### 9.18 Species cpd_C03339tot_CY

**Name** 2,3-Bisphosphoglycerate pool

**SBO:0000247** simple chemical

**Initial concentration** $10000\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a modifier in rn_R00299CY).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{cpd\_C03339tot\_CY} = 0 \tag{37}$$

### 9.19 Species cpd_C00103tot_CY

**Name** G1P pool

**SBO:0000247** simple chemical

**Initial concentration** $10000\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in rn_R06050CY), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{cpd\_C00103tot\_CY} = 0 \tag{38}$$

### 9.20 Species cpd_C00092tot_CY

**Name** G6P pool

**SBO:0000247** simple chemical

**Initial concentration** $10000\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in rn_R00299CY), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{cpd\_C00092tot\_CY} = 0 \tag{39}$$

### 9.21 Species ec_3_2_1_2_CS

**Name** Beta amylase

**SBO:0000014** enzyme

**Initial concentration** $0.00783\ \text{g} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a modifier in rn_R02112CS_G2, rn_R02112CS_G3, rn_R02112CS_G5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{ec\_3\_2\_1\_2\_CS} = 0 \tag{40}$$

## 9.22 Species ec_3_2_1_68_CS

**Name** Isoamylase

**SBO:0000014** enzyme

**Initial concentration** $0.0118\ \mathrm{g} \cdot \mathrm{l}^{-1}$

This species does not take part in any reactions. Its quantity does hence not change over time:

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{ec\_3\_2\_1\_68\_CS} = 0 \tag{41}$$

## 9.23 Species ec_2_4_1_25_CS

**Name** Disproportionating enzyme 1(DPE1)

**SBO:0000014** enzyme

**Initial concentration** $2\ \mu\mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in one reaction (as a modifier in rn_R05196CS).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{ec\_2\_4\_1\_25\_CS} = 0 \tag{42}$$

## 9.24 Species ec_2_4_1_25_CY

**Name** Disproportionating enzyme 2(DPE2)

**SBO:0000014** enzyme

**Initial concentration** $2\ \mu\mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in one reaction (as a modifier in rn_AT2G40840CY).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{ec\_2\_4\_1\_25\_CY} = 0 \tag{43}$$

## 9.25 Species ec_2_4_1_1_CY

**Name** Cytosolic Glucan phosphorylase

**SBO:0000014** enzyme

**Initial concentration** $2\ \mu\mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in one reaction (as a modifier in rn_R06050CY).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{ec\_2\_4\_1\_1\_CY} = 0 \tag{44}$$

## 9.26 Species ec_2_7_1_1_CY

**Name** Hexokinase

**SBO:0000014** enzyme

**Initial concentration** $10\ \mu\mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in one reaction (as a modifier in rn_R00299CY).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ec\_2\_7\_1\_1\_CY} = 0 \tag{45}$$

## 9.27 Species tc_2_A_84_1_2_CIMS

**Name** Maltose exporter (MEX)

**SBO:0000284** transporter

**Initial concentration** $2\ \mu\mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in one reaction (as a modifier in tr_TC_2_A_84_1_2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{tc\_2\_A\_84\_1\_2\_CIMS} = 0 \tag{46}$$

## 9.28 Species tc_2_A_1_1_17_CIMS

**Name** Glucose transporter (pGlcT)

**SBO:0000284** transporter

**Initial concentration** $20\ \mu\mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in one reaction (as a modifier in tr_TC_2_A_1_1_17).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{tc\_2\_A\_1\_1\_17\_CIMS} = 0 \tag{47}$$

# A Glossary of Systems Biology Ontology Terms

**SBO:0000009 kinetic constant:** Numerical parameter that quantifies the velocity of a chemical reaction

**SBO:0000014 enzyme:** A protein that catalyzes a chemical reaction. The word comes from en “a” or“i”) and simo “leave” or“yeas”)

**SBO:0000025 catalytic rate constant:** Numerical parameter that quantifies the velocity of an enzymatic reaction

**SBO:0000027 Michaelis constant:** Substrate concentration at which the velocity of reaction is half its maximum. Michaelis constant is an experimental parameter. According to the underlying molecular mechanism it can be interpreted differently in terms of microscopic constants

**SBO:0000179 degradation:** Complete disappearance of a physical entity

**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:0000281 equilibrium constant:** Quantity characterizing a chemical equilibrium in a chemical reaction, which is a useful tool to determine the concentration of various reactants or products in a system where chemical equilibrium occurs

**SBO:0000284 transporter:** Participating entity that facilitates the movement of another physical entity from a defined subset of the physical environment (for instance a cellular compartment) to another.

**SBO:0000290 physical compartment:** Specific location of space, that can be bounded or not. A physical compartment can have 1, 2 or 3 dimensions

**SBO:0000320 product catalytic rate constant:** Numerical parameter that quantifies the velocity of product creation by a reversible enzymatic reaction.

**SBO:0000321 substrate catalytic rate constant:** Numerical parameter that quantifies the velocity of substrate creation by a reversible enzymatic reaction.

**SBO:0000327 non-macromolecular ion:** Chemical entity having a net electric charge

**SBO:0000393 production:** Generation of a material or conceptual entity.

**SBO:0000503 number of entity pool constituents:** The numerical quantification of an entity pool. This may be expressed as, for example, the number of molecules or the number of moles of identical entities of which an specific entity pool is comprised

**SBO:0000504 mass of an entity pool:** The mass that comprises an entity pool

**SBO:0000540 fraction of an entity pool:** A ratio that represents the quantity of a defined constituent entity over the total number of all constituent entities present.

**SBO:0000559 enzyme activity:** A measure of the amount of active enzyme present, expressed under specified conditions. This is often expressed as micromol per min (also known as enzyme unit, U), rather than the less practical official SI unit, Katal (1 mol per second). Enzyme activity normally refers to the natural substrate for the enzyme, but can also be given for standardised substrates such as gelatin, where it is then referred to as GDU (Gelatin Digesting Units)

**SBO:0000565 systems description constant:** A physical constant that is required in the calculation of a system parameter.

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