

Supplementary Data

**Rational identification of target enzymes for starch improvement through system-level analysis of a potato tuber model**

**Chalothorn Liamwirat, Supapon Cheevadhanarak, Supatcharee Netrphan, Jeerayut Chaijaruwanich, Sakarindr Bhumiratana, and Asawin Meechai\***

**Supplementary Table 1.** Initial concentrations of all metabolites

Metabolite	Concentration (mM)	Reference
Suc_cyt	1	Arbitrarily
UDP_cyt	0.0524	Tiessen et al. (2002)
UDPglc_cyt	0.571	Tiessen et al. (2002)
Fru_cyt	1.37	Tiessen et al. (2002)
PP_cyt	0.012*	Tiessen et al. (2002)
G1P_cyt	0.0427	Tiessen et al. (2002)
UTP_cyt	0.238	Tiessen et al. (2002)
G6P_cyt	0.51	Tiessen et al. (2002)
ATP_cyt	0.292	Tiessen et al. (2002)
F6P_cyt	0.147	Tiessen et al. (2002)
ADP_cyt	0.0873	Tiessen et al. (2002)
Glc_cyt	10	Arbitrarily
Pi_cyt	2.4	Tiessen et al. (2002)
S6P_cyt	0	Arbitrarily
G6P_amp	0.379	Tiessen et al. (2002)
G1P_amp	0	Arbitrarily
ATP_amp	0.179	Tiessen et al. (2002)
ADPglc_amp	0	Arbitrarily
PP_amp	0.00236	Tiessen et al. (2002)
AL_amp	0	Arbitrarily
LG_amp	0	Arbitrarily
PG_amp	0	Arbitrarily
AP_amp	0	Arbitrarily
ADP_amp	0.149	Tiessen et al. (2002)
Pi_amp	0.87	Tiessen et al. (2002)
Suc_supply	300*	Kühn et al. (1999)
PGA3_amp	0.198*	Tiessen et al. (2002)
Glc_a	0	Arbitrarily
Glc_b	0	Arbitrarily

Note: \* is a constant during simulation. PGA3\_amp, Glc\_a, and Glc\_b are used in rate laws that are not shown in Fig. 1 in the main text.

**Supplementary Table 2.** Rate laws for enzymes, transporters and summarized reactions and the values of kinetic parameters used in the constructed model

Name	Reaction Rate																																				
ST	<p>An irreversible uni-uni Michaelis-Menten mechanism (Kühn et al., 1999).</p> $V1 = v_{\max} \frac{[Suc_{supply}]}{K_{m,Suc} + [Suc_{supply}]}$ <table border="1"> <thead> <tr> <th>Parameter</th> <th>Value</th> <th>Reference</th> <th>Parameter</th> <th>Value</th> <th>Reference</th> </tr> </thead> <tbody> <tr> <td><math>v_{\max}</math></td> <td>1.3833E-4</td> <td>Weise et al. (2000)</td> <td><math>K_{m,Suc}</math></td> <td>6</td> <td>Weise et al. (2000)</td> </tr> </tbody> </table>	Parameter	Value	Reference	Parameter	Value	Reference	$v_{\max}$	1.3833E-4	Weise et al. (2000)	$K_{m,Suc}$	6	Weise et al. (2000)																								
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SuSy EC 2.4.1.13	<p>A reversible ordered bi-reactant mechanism with UDP binding first and UDPglc dissociating last from the enzyme (Junker, 2004).</p> $V2 = v_f \frac{[UDP][Suc] - \frac{[Fru][UDPglc]}{K_{eq}}}{[UDP][Suc] \left(1 + \frac{[Fru]}{K_{i,Fru}}\right) + K_{m,Suc}([UDP] + K_{i,UDP}) + K_{m,UDP}[Suc] + \frac{v_f}{v_r K_{eq}} \times \left[ [Fru] K_{m,UDPglc} \left(1 + \frac{[UDP]}{K_{i,UDP}}\right) + [UDPglc] \left\{ K_{m,Fru} \left(1 + \frac{K_{m,UDP}[Suc]}{K_{i,UDP} K_{m,Suc}}\right) + [Fru] \left(1 + \frac{[Suc]}{K_{i,Suc}}\right) \right\} \right]}$ <table border="1"> <thead> <tr> <th>Parameter</th> <th>Value</th> <th>Reference</th> <th>Parameter</th> <th>Value</th> <th>Reference</th> </tr> </thead> <tbody> <tr> <td><math>v_f</math></td> <td>0.035</td> <td>Junker (2004)</td> <td><math>K_{m,Fru}</math></td> <td>7.8</td> <td>Junker (2004)</td> </tr> <tr> <td><math>v_r</math></td> <td>0.08</td> <td>"</td> <td><math>K_{m,UDPglc}</math></td> <td>0.076</td> <td>"</td> </tr> <tr> <td><math>K_{eq}</math></td> <td>0.36</td> <td>"</td> <td><math>K_{i,UDP}</math></td> <td>0.058</td> <td>"</td> </tr> <tr> <td><math>K_{m,Suc}</math></td> <td>50</td> <td>"</td> <td><math>K_{i,Fru}</math></td> <td>7.8</td> <td>"</td> </tr> <tr> <td><math>K_{m,UDP}</math></td> <td>0.058</td> <td>"</td> <td><math>K_{i,Suc}</math></td> <td>40</td> <td>"</td> </tr> </tbody> </table>	Parameter	Value	Reference	Parameter	Value	Reference	$v_f$	0.035	Junker (2004)	$K_{m,Fru}$	7.8	Junker (2004)	$v_r$	0.08	"	$K_{m,UDPglc}$	0.076	"	$K_{eq}$	0.36	"	$K_{i,UDP}$	0.058	"	$K_{m,Suc}$	50	"	$K_{i,Fru}$	7.8	"	$K_{m,UDP}$	0.058	"	$K_{i,Suc}$	40	"
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UGPase EC 2.7.7.9	<p>The "ordered Bi-Bi" kinetic type with UDPglc binding first and UTP dissociating last from the enzyme. No effectors are considered (Junker, 2004).</p> $V3 = v_f \frac{[UDPglc][PP] - \frac{[G1P][UTP]}{K_{eq}}}{[UDPglc][PP] \left(1 + \frac{[G1P]}{K_{i,G1P}}\right) + K_{m,PP}([UDPglc] + K_{i,UDPglc}) + K_{m,UDPglc}[PP] + \frac{v_f}{v_r K_{eq}} \left[ K_{m,UTP}[G1P] \left(1 + \frac{[UDPglc]}{K_{i,UDPglc}}\right) + [UTP] \left\{ K_{m,G1P} \left(1 + \frac{K_{m,UDPglc}[PP]}{K_{i,UDPglc} K_{m,PP}}\right) + [G1P] \left(1 + \frac{[PP]}{K_{i,PP}}\right) \right\} \right]}$ <table border="1"> <thead> <tr> <th>Parameter</th> <th>Value</th> <th>Reference</th> <th>Parameter</th> <th>Value</th> <th>Reference</th> </tr> </thead> <tbody> <tr> <td><math>v_f</math></td> <td>1.31</td> <td>Junker (2004)</td> <td><math>K_{m,G1P}</math></td> <td>0.16</td> <td>Junker (2004)</td> </tr> <tr> <td><math>v_r</math></td> <td>0.78</td> <td>"</td> <td><math>K_{m,UTP}</math></td> <td>0.142</td> <td>"</td> </tr> <tr> <td><math>K_{eq}</math></td> <td>3.2</td> <td>"</td> <td><math>K_{i,UDPglc}</math></td> <td>0.137</td> <td>"</td> </tr> <tr> <td><math>K_{m,UDPglc}</math></td> <td>0.137</td> <td>"</td> <td><math>K_{i,PP}</math></td> <td>0.127</td> <td>"</td> </tr> <tr> <td><math>K_{m,PP}</math></td> <td>0.127</td> <td>"</td> <td><math>K_{i,G1P}</math></td> <td>0.16</td> <td>"</td> </tr> </tbody> </table>	Parameter	Value	Reference	Parameter	Value	Reference	$v_f$	1.31	Junker (2004)	$K_{m,G1P}$	0.16	Junker (2004)	$v_r$	0.78	"	$K_{m,UTP}$	0.142	"	$K_{eq}$	3.2	"	$K_{i,UDPglc}$	0.137	"	$K_{m,UDPglc}$	0.137	"	$K_{i,PP}$	0.127	"	$K_{m,PP}$	0.127	"	$K_{i,G1P}$	0.16	"
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PGM EC 5.4.2.2	<p>"Uni-Uni" type reaction without inhibition (Junker, 2004).</p> $V4 = v_f \frac{[G1P] - \frac{[G6P]}{K_{eq}}}{[G1P] + K_{m,G1P} \left(1 + \frac{[G6P]}{K_{m,G6P}}\right)}$ <table border="1"> <thead> <tr> <th>Parameter</th> <th>Value</th> <th>Reference</th> <th>Parameter</th> <th>Value</th> <th>Reference</th> </tr> </thead> <tbody> <tr> <td><math>v_f</math></td> <td>0.023</td> <td>Junker (2004)</td> <td><math>K_{m,G1P}</math></td> <td>0.06</td> <td>Junker (2004)</td> </tr> <tr> <td><math>K_{eq}</math></td> <td>19</td> <td>"</td> <td><math>K_{m,G6P}</math></td> <td>0.5</td> <td>"</td> </tr> </tbody> </table>	Parameter	Value	Reference	Parameter	Value	Reference	$v_f$	0.023	Junker (2004)	$K_{m,G1P}$	0.06	Junker (2004)	$K_{eq}$	19	"	$K_{m,G6P}$	0.5	"																		
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INV EC 3.2.1.26	An irreversible Michaelis-Menten mechanism with competitive inhibition by fructose and non-competitive inhibition by glucose (Junker, 2004).	$V5 = \frac{v_{\max}}{1 + \frac{[Glc]}{K_{i,Glc}}} \times \frac{[Suc]}{K_{m,Suc} \left( 1 + \frac{[Fru]}{K_{i,Fru}} \right) + [Suc]}$	<table border="1"> <thead> <tr> <th>Parameter</th> <th>Value</th> <th>Reference</th> <th>Parameter</th> <th>Value</th> <th>Reference</th> </tr> </thead> <tbody> <tr> <td><math>v_{\max}</math></td> <td>0.015</td> <td>*</td> <td><math>K_{i,Glc}</math></td> <td>31</td> <td>Junker (2004)</td> </tr> <tr> <td><math>K_{m,Suc}</math></td> <td>41</td> <td>Junker (2004)</td> <td><math>K_{i,Fru}</math></td> <td>0.01</td> <td>''</td> </tr> </tbody> </table>	Parameter	Value	Reference	Parameter	Value	Reference	$v_{\max}$	0.015	*	$K_{i,Glc}$	31	Junker (2004)	$K_{m,Suc}$	41	Junker (2004)	$K_{i,Fru}$	0.01	''						
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HK EC 2.7.1.1	An irreversible random order bi-reactant mechanism (Junker, 2004).	$V6 = v_{\max} \frac{\frac{[Glc][ATP]}{K_{m,Glc} K_{m,ATP}}}{\left( 1 + \frac{[ATP]}{K_{m,ATP}} \right) \left( 1 + \frac{[Glc]}{K_{m,Glc}} + \frac{[Glc6P]}{K_{i,Glc6P}} \right)}$	<table border="1"> <thead> <tr> <th>Parameter</th> <th>Value</th> <th>Reference</th> <th>Parameter</th> <th>Value</th> <th>Reference</th> </tr> </thead> <tbody> <tr> <td><math>v_{\max}</math></td> <td>0.015</td> <td>Junker (2004)</td> <td><math>K_{m,ATP}</math></td> <td>0.185</td> <td>Junker (2004)</td> </tr> <tr> <td><math>K_{m,Glc}</math></td> <td>0.13</td> <td>''</td> <td><math>K_{i,G6P}</math></td> <td>4.1</td> <td>''</td> </tr> </tbody> </table>	Parameter	Value	Reference	Parameter	Value	Reference	$v_{\max}$	0.015	Junker (2004)	$K_{m,ATP}$	0.185	Junker (2004)	$K_{m,Glc}$	0.13	''	$K_{i,G6P}$	4.1	''						
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FK EC 2.7.1.4	Irreversible random-order bi-reactant kinetic, including competitive inhibition by ADP and non-competitive inhibition by Fru (Junker, 2004).	$V7 = \frac{v_{\max}}{1 + \frac{[Fru]}{K_{i,Fru}}} \times \frac{\frac{[Fru][ATP]}{K_{m,Fru} K_{m,ATP}}}{1 + \frac{[Fru]}{K_{m,Fru}} + \frac{[ATP]}{K_{m,ATP}} + \frac{[Fru][ATP]}{K_{m,Fru} K_{m,ATP}} + \frac{[ADP]}{K_{i,ADP}}}$	<table border="1"> <thead> <tr> <th>Parameter</th> <th>Value</th> <th>Reference</th> <th>Parameter</th> <th>Value</th> <th>Reference</th> </tr> </thead> <tbody> <tr> <td><math>V_{\max}</math></td> <td>0.058</td> <td>Junker (2004)</td> <td><math>K_{i,Fru}</math></td> <td>5.9</td> <td>Junker (2004)</td> </tr> <tr> <td><math>K_{m,Fru}</math></td> <td>0.077</td> <td>''</td> <td><math>K_{i,ADP}</math></td> <td>0.078</td> <td>''</td> </tr> <tr> <td><math>K_{m,ATP}</math></td> <td>0.026</td> <td>''</td> <td></td> <td></td> <td></td> </tr> </tbody> </table>	Parameter	Value	Reference	Parameter	Value	Reference	$V_{\max}$	0.058	Junker (2004)	$K_{i,Fru}$	5.9	Junker (2004)	$K_{m,Fru}$	0.077	''	$K_{i,ADP}$	0.078	''	$K_{m,ATP}$	0.026	''			
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bGly	A single reaction proceeding from Fru6P as an irreversible random order bi-reactant mechanism, including competitive inhibition by ATP (Junker, 2004).	$V9 = v_{\max} \frac{\frac{[Fru6P][ADP]}{K_{m,Fru6P} K_{m,ADP}}}{\left( 1 + \frac{[ADP]}{K_{m,ADP}} \right) \left( 1 + \frac{[Fru6P]}{K_{m,Fru6P}} + \frac{[ATP]}{K_{i,ATP}} \right)}$	<table border="1"> <thead> <tr> <th>Parameter</th> <th>Value</th> <th>Reference</th> <th>Parameter</th> <th>Value</th> <th>Reference</th> </tr> </thead> <tbody> <tr> <td><math>v_{\max}</math></td> <td>0.1</td> <td>*</td> <td><math>K_{m,ADP}</math></td> <td>0.018</td> <td>Junker (2004)</td> </tr> <tr> <td><math>K_{m,F6P}</math></td> <td>0.14</td> <td>Junker (2004)</td> <td><math>K_{i,ATP}</math></td> <td>0.21</td> <td>''</td> </tr> </tbody> </table>	Parameter	Value	Reference	Parameter	Value	Reference	$v_{\max}$	0.1	*	$K_{m,ADP}$	0.018	Junker (2004)	$K_{m,F6P}$	0.14	Junker (2004)	$K_{i,ATP}$	0.21	''						
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SPS EC 2.4.1.14	<p>A reversible ordered bi-reactant mechanism, with UDP-glucose binding first and UDP dissociating last from the enzyme; Pi was modeled as a competitive inhibitor with respect to Fru6P (Junker, 2004).</p>																																										
	$V10 = v_f \frac{[Fru6P][UDPglc] - \frac{[Suc6P][UDP]}{K_{eq}}}{[Fru6P][UDPglc] \left( 1 + \frac{[Suc6P]}{K_{i,Suc6P}} \right) + K_{m,Fru6P} \left( 1 + \frac{[Pi]}{K_{i,Pi}} \right) \left( [UDPglc] + K_{i,UDPglc} \right) + K_{m,UDPglc} [Fru6P] + \left[ \frac{v_f}{v_r K_{eq}} \times \left[ [UDP] \left\{ K_{m,Suc6P} \left( 1 + \frac{K_{m,UDPglc} [Fru6P]}{K_{i,UDPglc} K_{m,Fru6P} \left( 1 + \frac{[Pi]}{K_{i,Pi}} \right)} \right\} + [Suc6P] \left( 1 + \frac{[Fru6P]}{K_{i,Fru6P}} \right) \right] \right]}$																																										
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SPP EC 3.1.3.24	<p>An irreversible Michaelis-Menten mechanism with non-competitive inhibition by sucrose (Junker, 2004).</p>																																										
	$V11 = v_{max} \frac{[Suc6P]}{\left[ K_{m,Suc6P} \left( 1 + \frac{[Suc]}{K_{i,Suc}} \right) + [Suc6P] \left( 1 + \frac{[Suc]}{K_{i,Suc}} \right) \right]}$																																										
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$K_{m,S6P}$	0.1	"																																									
ATPcons	<p>Balancing Pi in cytosol</p> $V12 = 28V_{bGly} - V_{SPP} - V_{G6PT}$																																										
ATP:UDP phospho- transferase (EC 2.7.4.6)	<p>A reversible mass action (Assmus, 2005)</p> $V13 = v_{max} \left( k_f [ATP_{cyt}] [UDP_{cyt}] - k_r [ADP_{cyt}] [UTP_{cyt}] \right)$ <table border="1"> <thead> <tr> <th>Parameter</th> <th>Value</th> <th>Reference</th> <th>Parameter</th> <th>Value</th> <th>Reference</th> </tr> </thead> <tbody> <tr> <td><math>v_{max}</math></td> <td>1</td> <td>*</td> <td><math>k_r</math></td> <td>0.1</td> <td>*</td> </tr> <tr> <td><math>k_f</math></td> <td>0.1</td> <td>*</td> <td></td> <td></td> <td></td> </tr> </tbody> </table>	Parameter	Value	Reference	Parameter	Value	Reference	$v_{max}$	1	*	$k_r$	0.1	*	$k_f$	0.1	*																											
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$v_{max}$	1	*	$k_r$	0.1	*																																						
$k_f$	0.1	*																																									
G6PT	<p>A reversible mass action</p> $V14 = v_{max} \left( k_f [G6P_{cyt}] [Pi_{amp}] - k_r [G6P_{amp}] [Pi_{cyt}] \right)$ <table border="1"> <thead> <tr> <th>Parameter</th> <th>Value</th> <th>Reference</th> <th>Parameter</th> <th>Value</th> <th>Reference</th> </tr> </thead> <tbody> <tr> <td><math>v_{max}</math></td> <td>0.01</td> <td>Assmus (2005)</td> <td><math>k_r</math></td> <td>0.1</td> <td>Assmus (2005)</td> </tr> <tr> <td><math>k_f</math></td> <td>0.1</td> <td>"</td> <td></td> <td></td> <td></td> </tr> </tbody> </table>	Parameter	Value	Reference	Parameter	Value	Reference	$v_{max}$	0.01	Assmus (2005)	$k_r$	0.1	Assmus (2005)	$k_f$	0.1	"																											
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$k_f$	0.1	"																																									
pPGM EC 5.4.2.2	<p>“Uni-Uni” type reaction without inhibition</p> $V15 = v_f \frac{[G6P] - \frac{[G1P]}{K_{eq}}}{[G6P] + K_{m,G6P} \left( 1 + \frac{[G1P]}{K_{m,G1P}} \right)}$ <table border="1"> <thead> <tr> <th>Parameter</th> <th>Value</th> <th>Reference</th> <th>Parameter</th> <th>Value</th> <th>Reference</th> </tr> </thead> <tbody> <tr> <td><math>v_f</math></td> <td>0.023</td> <td>Junker (2004)</td> <td><math>K_{m,G6P}</math></td> <td>0.5</td> <td>Junker (2004)</td> </tr> <tr> <td><math>K_{eq}</math></td> <td>0.053</td> <td>Calculated by <math>1/K_{eq}^{PGM}</math></td> <td><math>K_{m,G1P}</math></td> <td>0.06</td> <td>"</td> </tr> </tbody> </table>	Parameter	Value	Reference	Parameter	Value	Reference	$v_f$	0.023	Junker (2004)	$K_{m,G6P}$	0.5	Junker (2004)	$K_{eq}$	0.053	Calculated by $1/K_{eq}^{PGM}$	$K_{m,G1P}$	0.06	"																								
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$v_f$	0.023	Junker (2004)	$K_{m,G6P}$	0.5	Junker (2004)																																						
$K_{eq}$	0.053	Calculated by $1/K_{eq}^{PGM}$	$K_{m,G1P}$	0.06	"																																						

The “ordered Bi-Bi” kinetic type with ATP binding first and ADPglc dissociating last from the enzyme with activation by 3-phosphoglyceric acid (3PGA) and inhibition by Pi (Kleczkowski et al., 1993; Assmus, 2005).

$$V16 = v_{app} \frac{[ATP][G1P] - \frac{[PP][ADPglc]}{K_{eq}}}{[ATP][G1P] \left( 1 + \frac{[PP]}{K_{i,PP}} \right) + K_{m,G1P} ([ATP] + K_{i,ATP}) + K_{m,ATP} [G1P] + \frac{v_f}{v_r K_{eq}} \left[ \frac{K_{m,ADPglc} [PP] \left( 1 + \frac{[ATP]}{K_{i,ATP}} \right) + [ADPglc] \left\{ K_{m,PP} \left( 1 + \frac{K_{m,ATP} [G1P]}{K_{i,ATP} K_{m,G1P}} \right) + [PP] \left( 1 + \frac{[G1P]}{K_{i,G1P}} \right) \right\}}{1 + \frac{3PGA}{K_{a,3PGA}}} \right]}$$

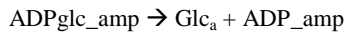
$$v_{app} = v_f \left( \frac{1 + \frac{3PGA}{K_{a,3PGA}}}{1 + \frac{Pi}{K_{i,Pi}}} \right)$$

AGPase  
EC 2.7.7.27

Parameter	Value	Reference	Parameter	Value	Reference
$v_f$	2.53E-6	Sowokinos and Preiss (1982)	$K_{i,G1P}$	0.14	*
$v_r$	3.24E-5	Sowokinos (1981)	$K_{m,G1P}$	0.14	Sowokinos and Preiss (1982)
$K_{eq}$	1	Assmus (2005)	$K_{m,PP}$	0.10	Sowokinos and Preiss (1982)
$K_{i,PP}$	0.00038	Amir and Cherry (1972)	$K_{i,ATP}$	0.19	
$K_{m,ADPglc}$	0.24	Sowokinos (1981)	$K_{a,3PGA}$	0.01	Assmus (2005)
$K_{m,ATP}$	0.19	Sowokinos and Preiss (1982)	$K_{i,Pi}$	0.16	Assmus (2005)

To represent GBSS reaction, there were two sub-reactions lumped together as follows:

i. ADP-Glc separation sub-reaction used an irreversible uni-uni Michaelis-Menten mechanism, where Glc<sub>a</sub> was Glc residue for GBSS reaction.

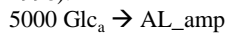


$$V17.1 = v_{max} \frac{[ADPglc]}{K_{m,ADPglc} + [ADPglc]}$$

GBSS  
EC  
2.4.1.242

Parameter	Value	Reference	Parameter	Value	Reference
$v_{max}$	6E-7	*	$K_{m,ADPglc}$	1.3	Edwards et al. (1999)

ii. Glc polymerization sub-reaction used a mass action law. The number of Glc residues (Glc<sub>a</sub>) used in the polymerization into AL\_AMP was assumed to be 5000, which was in the range of 1000 – 10,000 (Blennow et al., 1998).



$$V17.2 = kDP[Glc_a]$$

Parameter	Value	Reference
$kDP$	10	*

SS EC 2.4.1.21	To represent SS reaction, there were two sub-reactions lumped together as follows: i. ADP-Glc separation sub-reaction used an irreversible uni-uni Michaelis-Menten mechanism, where Glc <sub>b</sub> was Glc residue for SS reaction. ADPglc_amp → Glc <sub>b</sub> + ADP_amp $V18.1 = v_{\max} \frac{[ADPglc]}{K_{m,ADPglc} + [ADPglc]}$					
	Parameter	Value	Reference	Parameter	Value	Reference
	$v_{\max}$	1.75E-7	*	$K_{m,ADPglc}$	0.07	Edwards et al. (1999)
	ii. Glc polymerization sub-reaction used a mass action law. The number of Glc residues (Glc <sub>b</sub> ) used in the polymerization into LG_amp was assumed to be 21 that was in the range of 20 – 25 (Blennow et al., 1998). 21 Glc <sub>b</sub> → LG_amp $V18.2 = kDP[Glc_b]$					
	Parameter	Value	Reference			
	$kDP$	10	*			
SBE EC 2.4.1.18	An irreversible uni-uni Michaelis-Menten mechanism $V19 = v_{\max} \frac{[LG]}{K_{m,LG} + [LG]}$					
	Parameter	Value	Reference	Parameter	Value	Reference
	$v_{\max}$	6.2E-9	*	$K_{m,LG}$	0.13	Blennow et al. (1998)
DBE EC 3.2.1.41	An irreversible uni-uni Michaelis-Menten mechanism $V20 = v_{\max} \frac{[PG]}{K_{m,PG} + [PG]}$					
	Parameter	Value	Reference	Parameter	Value	Reference
	$v_{\max}$	1.868E-5	Hussain et al. (2003)	$K_{m,PG}$	0.37	Wu et al. (2002)
ATPT	A reversible mass action. $V21 = v_{\max} (k_f [ATP_{\text{cyt}}][ADP_{\text{amp}}] - k_r [ATP_{\text{amp}}][ADP_{\text{cyt}}])$					
	Parameter	Value	Reference	Parameter	Value	Reference
	$v_{\max}$	0.001	*	$k_r$	0.002	Assmus (2005)
	$k_f$	0.002	''			
iPPtase EC 3.6.1.1	A near-equilibrium (Assmus, 2005) $V22 = v_{\max} \left( 1 - \frac{[Pi]}{K_{eq} [PP]} \right)$					
	Parameter	Value	Reference	Parameter	Value	Reference
	$v_{\max}$	8.3333E-6	Assmus (2005)	$K_{eq}$	750000	Assmus (2005)
PiT	Balancing Pi in amyloplast $V23 = 2V_{iPPtase} - V_{G6PT}$					

Note: All  $v_{\max}$ ,  $v_f$ , and  $v_r$  are given in mM·sec<sup>-1</sup> and all  $K_m$  and  $K_i$  are given in mM.

\* The value of parameter was arbitrarily determined so that the simulation was compromised to reach the steady state and be closed to the literature data.

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**Supplementary Table 3.** Starch content and AC% from the perturbation of dual parameters

Dual parameter		starch content (mg/L)				AC% (% w/w)			
		from each cases of parameter change				from each case of parameter change			
		(-50%, -50%)	(-50%, 100%)	(100%, -50%)	(100%, 100%)	(-50%, -50%)	(-50%, 100%)	(100%, -50%)	(100%, 100%)
$V_{max}^{iPPtase}$	$K_{m,ADPglic}^{SS}$	245.53	239.56	394.68	354.45	18.70	26.01	21.45	31.35
$V_{max}^{iPPtase}$	$V_{max}^{SS}$	238.15	245.98	334.01	415.88	27.86	17.99	36.92	16.55
$V_{max}^{iPPtase}$	$K_{m,ADPglic}^{GBSS}$	244.08	242.24	393.52	361.24	26.27	18.64	33.36	19.99
$V_{max}^{iPPtase}$	$K_{a,PGA3}^{AGPase}$	247.92	238.59	390.27	346.09	21.84	21.70	26.67	24.53
$V_{max}^{iPPtase}$	$k_f^{ATPT}$	242.08	243.37	319.08	407.16	21.75	21.77	23.55	27.64
$V_{max}^{iPPtase}$	$V_{max}^{ATPT}$	242.09	243.36	319.19	407.05	21.75	21.77	23.56	27.64
$V_{max}^{iPPtase}$	$V_f^{AGPase}$	238.28	248.07	343.46	390.30	21.70	21.84	24.41	26.67
$V_{max}^{iPPtase}$	$K_{i,pi}^{AGPase}$	238.82	247.02	348.18	388.47	21.70	21.82	24.62	26.57
$V_{max}^{iPPtase}$	$k_f^{G6PT}$	240.36	244.74	345.65	393.05	21.71	21.80	24.51	26.82
$V_{max}^{iPPtase}$	$V_{max}^{GBSS}$	242.24	244.11	360.55	394.91	18.61	26.39	19.72	33.97
$K_{m,ADPglic}^{SS}$	$V_{max}^{SS}$	302.45	319.93	289.47	312.47	28.84	14.08	37.99	20.82
$K_{m,ADPglic}^{SS}$	$K_{m,ADPglic}^{GBSS}$	316.45	313.75	308.63	296.69	23.41	15.50	35.96	22.78
$K_{m,ADPglic}^{SS}$	$K_{a,PGA3}^{AGPase}$	320.20	305.38	306.86	293.50	18.82	18.55	28.97	28.35
$K_{m,ADPglic}^{SS}$	$k_f^{ATPT}$	308.73	316.11	290.83	305.16	18.61	18.73	28.21	28.89
$K_{m,ADPglic}^{SS}$	$V_{max}^{ATPT}$	308.79	316.10	290.92	305.14	18.61	18.73	28.22	28.89
$K_{m,ADPglic}^{SS}$	$V_f^{AGPase}$	304.37	320.32	292.56	306.92	18.54	18.82	28.30	28.97
$K_{m,ADPglic}^{SS}$	$K_{i,pi}^{AGPase}$	306.11	319.42	294.22	306.32	18.56	18.80	28.38	28.94
$K_{m,ADPglic}^{SS}$	$k_f^{G6PT}$	308.83	317.67	293.08	307.32	18.60	18.76	28.32	28.99
$K_{m,ADPglic}^{SS}$	$V_{max}^{GBSS}$	313.73	316.49	296.41	308.96	15.45	23.57	22.53	36.40
$V_{max}^{SS}$	$K_{m,ADPglic}^{GBSS}$	306.20	284.48	317.85	316.65	39.53	27.16	20.88	14.10
$V_{max}^{SS}$	$K_{a,PGA3}^{AGPase}$	300.36	287.94	322.92	307.28	33.53	32.33	16.64	16.78
$V_{max}^{SS}$	$k_f^{ATPT}$	283.65	299.56	311.84	318.08	31.89	33.47	16.73	16.67
$V_{max}^{SS}$	$V_{max}^{ATPT}$	283.73	299.54	311.89	318.07	31.90	33.47	16.73	16.67
$V_{max}^{SS}$	$V_f^{AGPase}$	287.08	300.41	306.25	323.06	32.25	33.54	16.79	16.64
$V_{max}^{SS}$	$K_{i,pi}^{AGPase}$	288.61	299.88	308.02	322.01	32.39	33.49	16.77	16.65
$V_{max}^{SS}$	$k_f^{G6PT}$	286.35	301.77	311.65	319.50	32.17	33.68	16.73	16.66
$V_{max}^{SS}$	$V_{max}^{GBSS}$	283.65	306.74	316.64	317.87	26.80	39.96	14.08	21.00
$K_{m,ADPglic}^{GBSS}$	$K_{a,PGA3}^{AGPase}$	317.95	303.34	311.17	297.86	29.50	28.80	18.62	18.45
$K_{m,ADPglic}^{GBSS}$	$k_f^{ATPT}$	305.52	314.33	297.26	308.86	28.90	29.32	18.45	18.59
$K_{m,ADPglic}^{GBSS}$	$V_{max}^{ATPT}$	305.60	314.31	297.35	308.84	28.91	29.32	18.45	18.59
$K_{m,ADPglic}^{GBSS}$	$V_f^{AGPase}$	302.33	318.06	296.91	311.24	28.75	29.51	18.44	18.62
$K_{m,ADPglic}^{GBSS}$	$K_{i,pi}^{AGPase}$	304.07	317.23	298.56	310.60	28.83	29.46	18.46	18.61
$K_{m,ADPglic}^{GBSS}$	$k_f^{G6PT}$	306.05	316.03	298.68	310.81	28.92	29.41	18.46	18.62
$K_{m,ADPglic}^{GBSS}$	$V_{max}^{GBSS}$	309.58	316.15	304.71	309.83	22.85	36.88	15.48	23.29
$K_{a,PGA3}^{AGPase}$	$k_f^{ATPT}$	306.04	316.20	289.80	302.80	23.03	23.36	22.56	22.92
$K_{a,PGA3}^{AGPase}$	$V_{max}^{ATPT}$	306.10	316.19	289.91	302.78	23.03	23.36	22.56	22.92
$K_{a,PGA3}^{AGPase}$	$V_f^{AGPase}$	309.55	316.98	275.54	310.12	23.14	23.39	22.21	23.16
$K_{a,PGA3}^{AGPase}$	$K_{i,pi}^{AGPase}$	310.27	316.56	279.46	308.78	23.16	23.37	22.30	23.11
$K_{a,PGA3}^{AGPase}$	$k_f^{G6PT}$	308.80	317.94	283.54	306.35	23.11	23.42	22.40	23.03
$K_{a,PGA3}^{AGPase}$	$V_{max}^{GBSS}$	311.08	318.11	297.80	303.46	18.49	29.81	18.35	29.06

$k_f^{ATPT}$	$v_{max}^{ATPT}$	261.40	309.71	309.77	312.05	22.09	23.14	23.14	23.22
$k_f^{ATPT}$	$v_f^{AGPase}$	288.68	306.10	301.91	316.31	22.53	23.03	22.90	23.36
$k_f^{ATPT}$	$K_{i,Pi}^{AGPase}$	290.65	305.41	303.45	315.51	22.58	23.01	22.94	23.34
$k_f^{ATPT}$	$k_f^{G6PT}$	289.15	307.42	305.40	314.27	22.54	23.07	23.00	23.29
$k_f^{ATPT}$	$v_{max}^{GBSS}$	297.17	305.71	308.78	314.45	18.34	29.18	18.47	29.62
$v_{max}^{ATPT}$	$v_f^{AGPase}$	288.79	306.17	301.89	316.29	22.53	23.03	22.90	23.36
$v_{max}^{ATPT}$	$K_{i,Pi}^{AGPase}$	290.75	305.48	303.43	315.49	22.58	23.01	22.94	23.34
$v_{max}^{ATPT}$	$k_f^{G6PT}$	289.28	307.47	305.37	314.26	22.55	23.07	23.00	23.29
$v_{max}^{ATPT}$	$v_{max}^{GBSS}$	297.25	305.78	308.76	314.44	18.34	29.18	18.47	29.62
$v_f^{AGPase}$	$K_{i,Pi}^{AGPase}$	277.27	308.31	310.42	316.62	22.25	23.10	23.17	23.38
$v_f^{AGPase}$	$k_f^{G6PT}$	281.52	305.69	308.89	318.06	22.35	23.01	23.12	23.43
$v_f^{AGPase}$	$v_{max}^{GBSS}$	296.85	302.44	311.15	318.22	18.34	29.01	18.50	29.82
$K_{i,Pi}^{AGPase}$	$k_f^{G6PT}$	285.04	306.82	308.00	317.21	22.43	23.05	23.09	23.40
$K_{i,Pi}^{AGPase}$	$v_{max}^{GBSS}$	298.50	304.19	310.51	317.38	18.36	29.10	18.49	29.77
$k_f^{G6PT}$	$v_{max}^{GBSS}$	298.59	306.21	310.73	316.14	18.36	29.20	18.49	29.71

Note: The highlighted cells in red and green represent the top three highest values and the bottom three lowest values, respectively.