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Research Topic: Fluxomics and Metabolic Flux Analysis in Systems Biology

Flux Connections between Gluconate Pathway, Glycolysis, and Pentose-Phosphate Pathway during Carbohydrate Metabolism in *Bacillus Megaterium* QMB1551

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SUPPLEMENTARY MATERIAL

Fig. S1

Table S1

Table S2

Fig. S2

Fig. S3

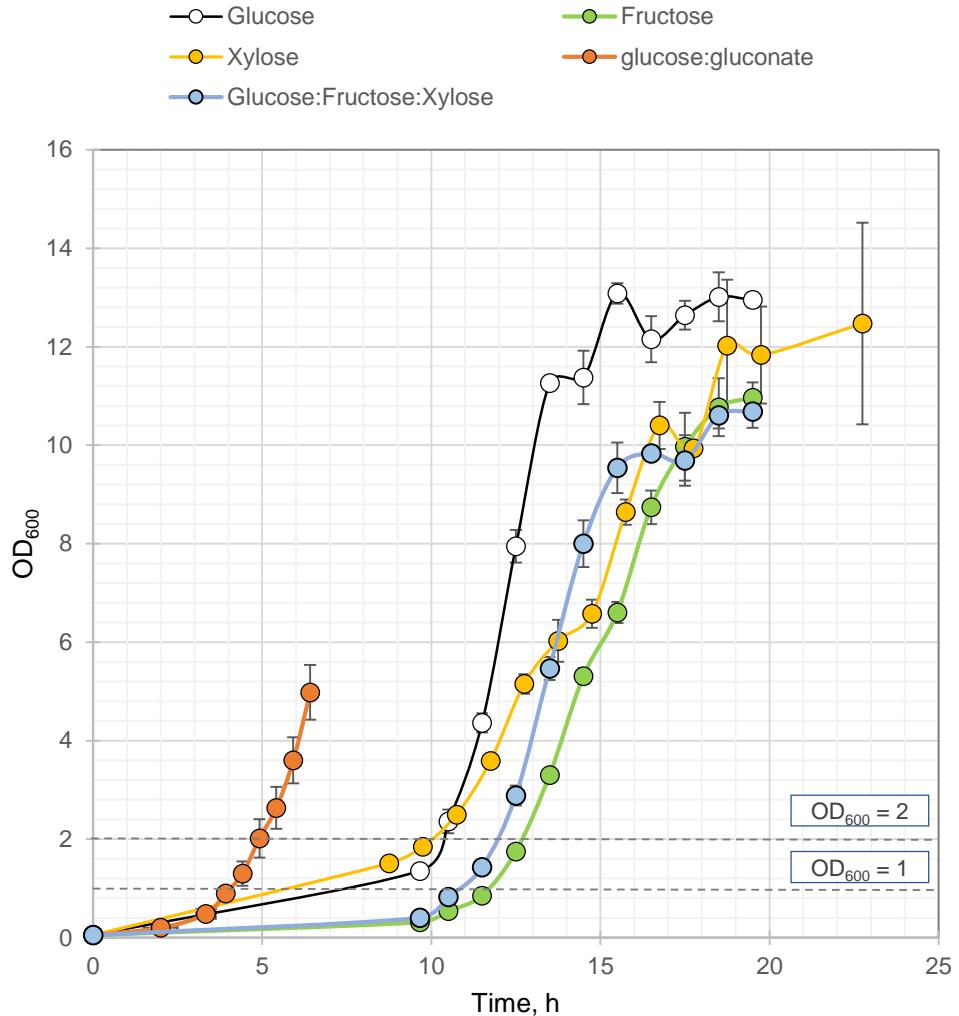


Fig. S1. Growth curves of *B. megaterium* QM B1551 grown on 330 mM total carbon of glucose alone (white circles), fructose alone (light green circles), xylose alone (yellow circles), glucose:gluconate mixture (orange circles), and equimolar mixture of glucose, fructose, and xylose (light blue circles). Data (average \pm standard deviation) were from three independent biological replicates.

Table S1. Growth parameters^a of *B. megaterium* QM B1551.

Growth Condition ^b	Glucose	Glucose:Fructose:Xylose
Growth Rate (hr⁻¹)	0.71 ± 0.04	0.57 ± 0.07
Uptake Rate (mmol gCDW⁻¹ hr⁻¹)	5.30 ± 1.61 ^c	Glucose: 0.28 ± 0.06 ^c
		Fructose: 0.13 ± 0.05
		Xylose: negligible
Gluconate Excretion rate (μmol gCDW⁻¹ hr⁻¹)	4.37 ± 1.76	2.30 ± 0.81

^aThe values in the table represent means ± standard deviation. Data were calculated from three independent biological replicates ($n = 3$).

^bThe total carbon-equivalent concentration of the growth substrates was 330 mM C.

^cUptake rate of glucose into the periplasm.

Table S2. Intracellular metabolic rates determined from quantitative flux modeling of the metabolism of [1,2-¹³C₂]-glucose in *B. megaterium* QM B1551 using the 13CFLUX2 software. These metabolic fluxes are illustrated in Fig. 7 in the main text, where they have been normalized to glucose uptake. Refer to the legends of Fig. 1 in the main text for the abbreviations of the metabolite names.

Reactions	[1,2- ¹³ C ₂]-glucose mmol gCDW ⁻¹ h ⁻¹	[1,2,3- ¹³ C ₃]-glucose, [1,6- ¹³ C ₂]-fructose, unlabeled xylose mmol gCDW ⁻¹ h ⁻¹
Gluc _{ext} -> Gluc _{peri}	5.30 ± 0.00	0.28 ± 0.00
Gluc _{peri} -> G6P	4.66 ± 0.09	0.21 ± 0.00
Gluc _{peri} -> Glucn _{peri}	0.64 ± 0.09	0.07 ± 0.00
Glucn _{peri} -> 6P-Glucn	0.64 ± 0.09	0.07 ± 0.00
G6P -> 6P-Glucn	1.97 ± 0.24	0.10 ± 0.01
GAP -> 3-PG	7.89 ± 0.16	0.61 ± 0.02
3-PG -> downstream processes	6.67 ± 0.12	0.52 ± 0.01
DHAP -> GAP	3.72 ± 0.11	0.30 ± 0.01
FBP -> DHAP + GAP	3.72 ± 0.11	0.30 ± 0.01
F6P -> FBP	3.72 ± 0.11	0.30 ± 0.01
G6P -> F6P	2.52 ± 0.17	0.09 ± 0.00
6P-Glucn -> Ru5P	2.60 ± 0.15	0.17 ± 0.00
Ru5P-> R5P	1.40 ± 0.09	0.10 ± 0.00
Ru5P -> Xu5P	1.20 ± 0.06	0.07 ± 0.00
Xu5P + R5P -> GAP + S7P	0.75 ± 0.01	0.05 ± 0.00
S7P + GAP -> E4P + F6P	0.75 ± 0.01	0.05 ± 0.00
E4P + Xu5P -> F6P + GAP	0.45 ± 0.05	0.02 ± 0.00
Fruc _{ext} -> F6P	--	0.14 ± 0.01
Fruc _{ext} -> FBP	--	0.00 ± 0.00
Xyl _{ext} -> Xyl	--	0.00 ± 0.00
E4P -> Biomass	0.30 ± 0.05	0.03 ± 0.00
G6P -> Biomass	0.17 ± 0.02	0.01 ± 0.00
3PG -> Biomass	1.22 ± 0.04	0.09 ± 0.00
R5P -> Biomass	0.65 ± 0.08	0.05 ± 0.00
Glucn _{in} -> Glucn _{ext}	0.1 ± 0.00	0.00 ± 0.00

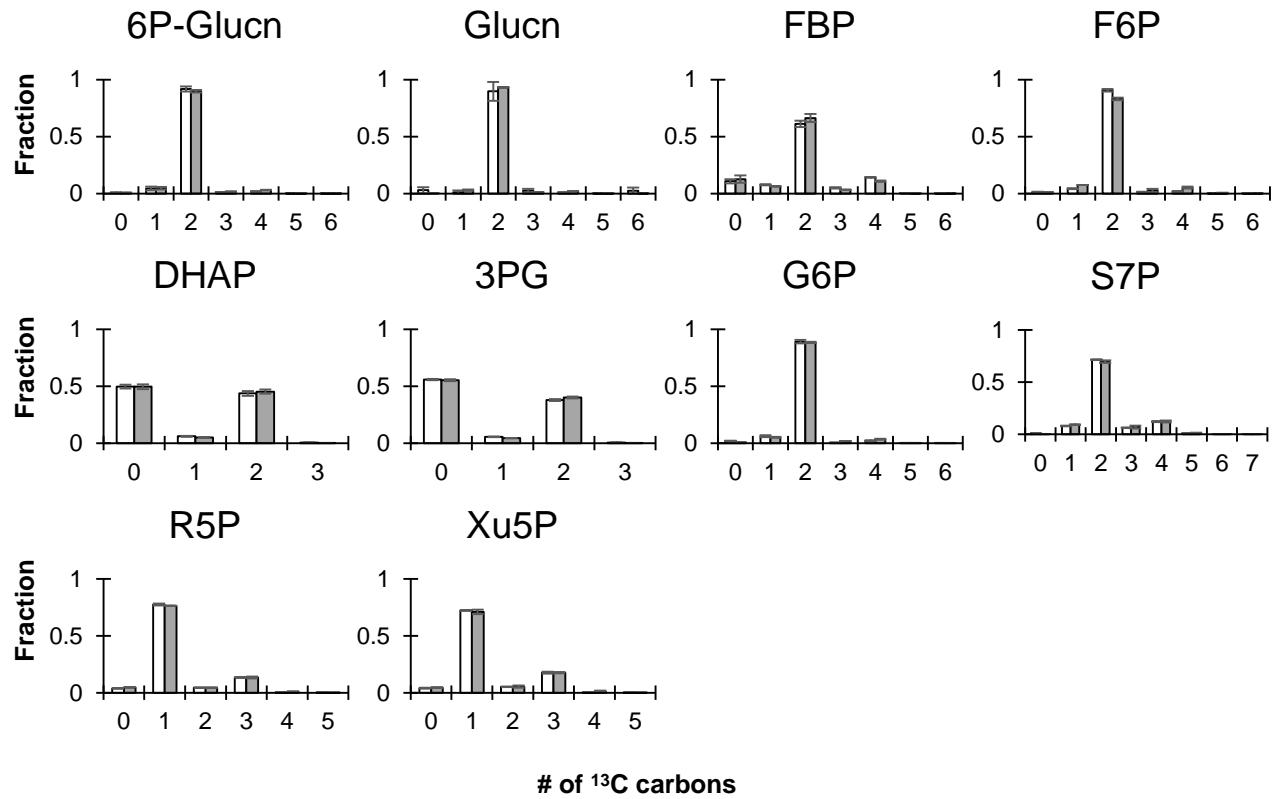


Fig. S2. Experimentally-determined (white bars) and model-estimated (grey bars) isotopomer distributions in the metabolite labeling patterns during *B. megaterium* QM B1551 growth on [1,2- $^{13}\text{C}_2$]-glucose. Data (average \pm standard deviation) were from optimizations of experimental data obtained from two independent biological replicates.

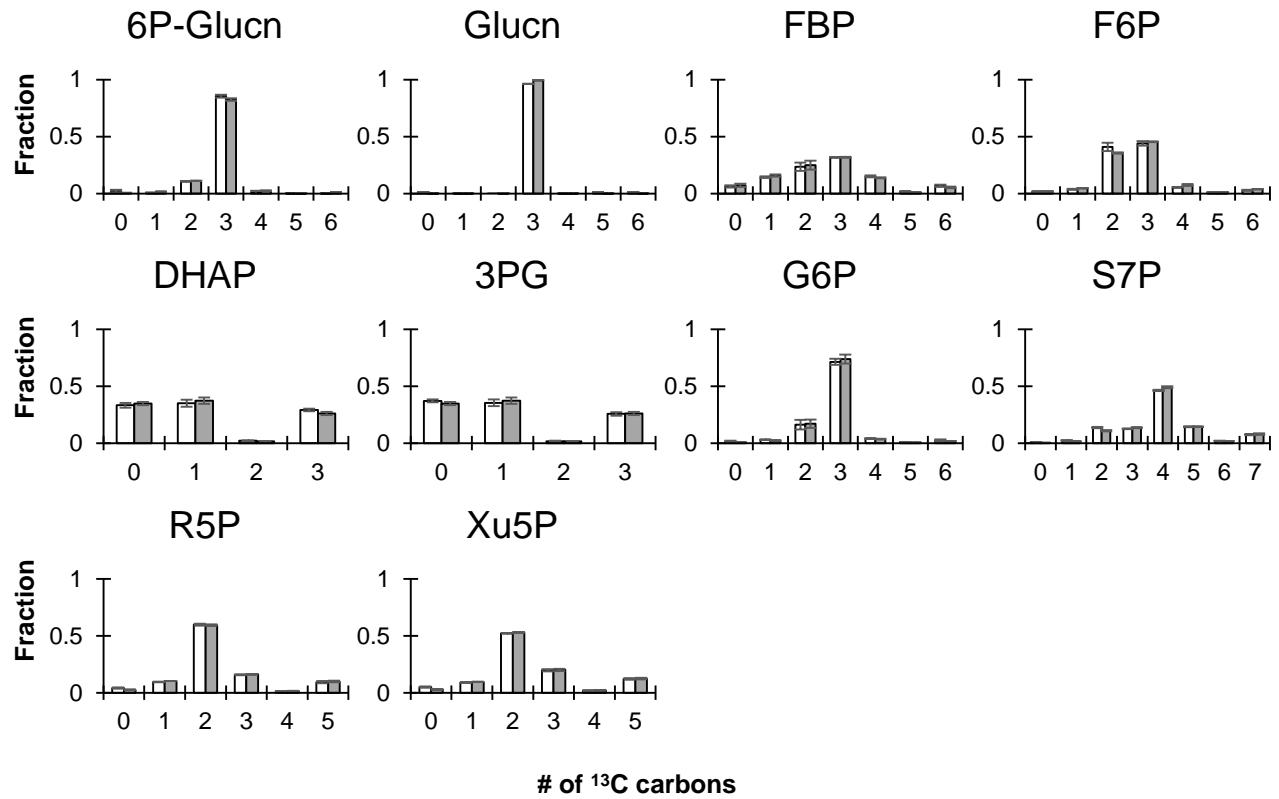


Fig. S3. Experimentally-determined (white bars) and model-estimated (grey bars) isotopomer distributions in the metabolite labeling patterns during *B. megaterium* QM growth on a mixture of [1,2,3- $^{13}\text{C}_3$]-glucose, [1,6- $^{13}\text{C}_2$]-fructose, and unlabeled xylose. Data (average \pm standard deviation) were from optimizations of experimental data obtained from two independent biological replicates.