Supplemental Information

Linking the *Salmonella enterica* 1,2-propanediol utilization bacterial microcompartment shell to the enzymatic core via the shell protein PduB

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Section A: Details of kinetic model of the 1,2-propanediol utilization (Pdu) pathway

The kinetic model for the 1,2-propanediol utilization (Pdu) pathway here was developed based on the original work of Jakobson et al. [1], with modifications described herein. Specifically, we assume in this model that the cytosol is well-mixed, such that we are working with a compartmental model. We also incorporate the effects of cell growth over time, and explicitly model the metabolite concentrations in the external media. This required several adjustments to the original model, which are outlined in detail below. We focus our analysis here on metabolite profiles over time in a batch reactor setting instead of at steady-state to best study the conditions under which we ran our growth curves.

A.1: Model assumptions

We assume the following in our model:

1. At time t, there are $N(t)$ identical, non-interacting cells in a well-mixed solution.
2. The substrates 1,2-propanediol, propionaldehyde, propionyl-CoA, propionate, and 1-propanol passively diffuse across the cell membrane at rates specified by permeability parameters.
3. The substrates 1,2-propanediol, propionaldehyde, propionyl-CoA, propionate, and 1-propanol passively diffuse across the microcompartment (MCP) shell or polar body surface at rates specified by permeability parameters.
4. There are n_{MCP} non-interacting MCPs or polar bodies in the cytosol of each cell.
5. Reactions catalyzed by PduCDE, PduP, and PduQ, forward or reverse, can only occur in the MCP or polar body.
6. Reactions catalyzed by PduL/W can only occur in the cytosol.
7. The external media, cytosol of the cell, and internal MCP volume are well-mixed such that the concentration in each compartment is assumed uniform at any given point in time.
8. The volume of the external media up to the leading order is the volume of the entire culture.
9. The volume of the cytosol up to the leading order is the volume of the cell.
10. All enzymes behave according to Michaelis-Menten kinetics.

A.2: Chemical reactions

The following reactions are considered in our model, with the assumptions described above:

$$1{,}2 - Propanediol \xrightarrow{\text{PduCDE}} Propionaldehyde$$

$$Propionaldehyde \xleftrightarrow{PduQ} 1 - Propanol$$

$$\text{Propionaldehyde} \xleftrightarrow{PduP} \text{Propionyl} - \text{CoA}$$

$$Propionyl - CoA \xrightarrow{PduLW} Propionate$$

A.3: Equations used in mathematical model

The differential equations described below were integrated forward in time from a starting condition of 55 mM 1,2-propanediol in the external media, the starting condition used in our growth curve experiments.

A.3.1: Variable definition

Concentrations of all substrates are defined by the following variables:

- P_i: 1,2-propanediol concentration in volume i (MCP/polar body, cytosol, or external media)
- A_i: Propionaldehyde concentration in volume i (MCP/polar body, cytosol, or external media)
- Pol_i: 1-Propanol concentration in volume i (MCP/polar body, cytosol, or external media)
- $PCoA_i$: Propionyl-CoA concentration in volume i (MCP/polar body, cytosol, or external media)
- $Pate_i$: Propionate concentration in volume i (MCP/polar body, cytosol, or external media)

Other constraints and variables used in the model are defined as follows:

- $V_{\text{compartment}}$: Volume of the compartment (MCP or polar body)
- $SA_{\text{compartment}}$: Surface area of the compartment (MCP or polar body)
- V_{cell}: Volume of the cell
- SA_{cell}: Surface area of the cell
- $Perm_i^j$: Permeability of substrate i at interface j (cell surface or MCP/polar body surface)
- $R_i(X_j)$: Reaction rate of enzyme i as a function of concentrations X in a given volume j (MCP/polar body, cytosol, or external media)
- $K_{\text{M}}^{i,j}$: Michaelis constant of enzyme i for substrate j

- $V_{\max}^{i,j}$: Maximum reaction velocity of enzyme i for substrate j
- $N(t)$: Number of cells at time t, calculated form the experimental growth profile
- PB: Refers to polar body
- MCP: Refers to MCP
- $n_{\mathrm{MCP/PB}}$: Number of MCPs/polar bodies per cell

A.3.2: Differential equations: MCP or polar body

The differential equations for the MCP or polar body volume were as follows:

$$\frac{dP_{\mathrm{MCP/PB}}}{dt} = -R_{\mathrm{PduCDE}}\left(X_{\mathrm{MCP/PB}}\right) + \frac{Perm_{\mathrm{MCP}/PB}^{\mathrm{P}} SA_{\mathrm{MCP/PB}}}{Vol_{\mathrm{MCP/PB}}}\left(P_{\mathrm{cytosol}} - P_{\mathrm{MCP/PB}}\right)$$

$$\begin{aligned}\frac{dA_{\mathrm{MCP/PB}}}{dt} = {} & R_{\mathrm{PduCDE}}\left(X_{\mathrm{MCP/PB}}\right) - R_{\mathrm{PduP},f}\left(X_{\mathrm{MCP/PB}}\right) + R_{\mathrm{PduP},r}\left(X_{\mathrm{MCP/PB}}\right) - R_{\mathrm{PduQ},f}\left(X_{\mathrm{MCP/PB}}\right) \\ & + R_{\mathrm{PduQ},r}\left(X_{\mathrm{MCP}/PB}\right) + \frac{Perm_{\mathrm{MCP}/PB}^{\mathrm{A}} SA_{\mathrm{MCP/PB}}}{Vol_{\mathrm{MCP/PB}}}\left(A_{\mathrm{cytosol}} - A_{\mathrm{MCP/PB}}\right)\end{aligned}$$

$$\begin{aligned}\frac{dPol_{\mathrm{MCP/PB}}}{dt} = {} & R_{\mathrm{PduQ},f}\left(X_{\mathrm{MCP}/PB}\right) - R_{\mathrm{PduQ},r}\left(X_{\mathrm{MCP}/PB}\right) \\ & + \frac{Perm_{\mathrm{MCP}/PB}^{Pol} SA_{\mathrm{MCP/PB}}}{Vol_{\mathrm{MCP/PB}}}\left(Pol_{\mathrm{cytosol}} - Pol_{\mathrm{MCP/PB}}\right)\end{aligned}$$

$$\begin{aligned}\frac{dPCoA_{\mathrm{MCP/PB}}}{dt} = {} & R_{\mathrm{PduP},f}\left(X_{\mathrm{MCP}/PB}\right) - R_{\mathrm{PduP},r}\left(X_{\mathrm{MCP}/PB}\right) \\ & + \frac{Perm_{\mathrm{MCP}/PB}^{PCoA} SA_{\mathrm{MCP/PB}}}{Vol_{\mathrm{MCP/PB}}}\left(PCoA_{\mathrm{cytosol}} - PCoA_{\mathrm{MCP/PB}}\right)\end{aligned}$$

$$\frac{dPate_{\mathrm{MCP/PB}}}{dt} = \frac{Perm_{\mathrm{MCP}/PB}^{Pate} SA_{\mathrm{MCP/PB}}}{Vol_{\mathrm{MCP/PB}}}\left(Pate_{\mathrm{cytosol}} - Pate_{\mathrm{MCP/PB}}\right)$$

A.3.3: Differential equations: cytosol

The differential equations for the cytosol of the cell were as follows:

$$\begin{aligned}\frac{dP_{\mathrm{cytosol}}}{dt} = {} & \frac{n_{\mathrm{MCP}} Perm_{\mathrm{MCP}/PB}^{\mathrm{P}} SA_{\mathrm{MCP/PB}}}{Vol_{\mathrm{cell}}}\left(P_{\mathrm{MCP/PB}} - P_{\mathrm{cytosol}}\right) \\ & + \frac{Perm_{\mathrm{cell}}^{\mathrm{P}} SA_{\mathrm{cell}}}{Vol_{\mathrm{cell}}}\left(P_{\mathrm{external}} - P_{\mathrm{cytosol}}\right)\end{aligned}$$

$$\frac{dA_{\text{cytosol}}}{dt} = \frac{n_{\text{MCP}} Perm_{\text{MCP}/PB}^{\text{A}} SA_{\text{MCP/PB}}}{Vol_{\text{cell}}} \left(A_{\text{MCP/PB}} - A_{\text{cytosol}}\right) + \frac{Perm_{\text{cell}}^{\text{A}} SA_{\text{cell}}}{Vol_{\text{cell}}} \left(A_{\text{external}} - A_{\text{cytosol}}\right)$$

$$\frac{dPol_{\text{cytosol}}}{dt} = \frac{n_{\text{MCP}} Perm_{\text{MCP}/PB}^{Pol} SA_{\text{MCP/PB}}}{Vol_{\text{cell}}} \left(Pol_{\text{MCP/PB}} - Pol_{\text{cytosol}}\right) + \frac{Perm_{\text{cell}}^{Pol} SA_{\text{cell}}}{Vol_{\text{cell}}} \left(Pol_{\text{external}} - Pol_{\text{cytosol}}\right)$$

$$\frac{dPCoA_{\text{cytosol}}}{dt} = -R_{\text{PduLW}}\left(X_{\text{cytosol}}\right) + \frac{n_{\text{MCP}} Perm_{\text{MCP}/PB}^{PCoA} SA_{\text{MCP/PB}}}{Vol_{\text{cell}}} \left(PCoA_{\text{MCP/PB}} - PCoA_{\text{cytosol}}\right) + \frac{Perm_{\text{cell}}^{PCoA} SA_{\text{cell}}}{Vol_{\text{cell}}} \left(PCoA_{\text{external}} - PCoA_{\text{cytosol}}\right)$$

$$\frac{dPate_{\text{cytosol}}}{dt} = R_{\text{PduLW}}\left(X_{\text{cytosol}}\right) + \frac{n_{\text{MCP}} Perm_{\text{MCP}/PB}^{Pate} SA_{\text{MCP/PB}}}{Vol_{\text{cell}}} \left(Pate_{\text{MCP/PB}} - Pate_{\text{cytosol}}\right) + \frac{Perm_{\text{cell}}^{Pate} SA_{\text{cell}}}{Vol_{\text{cell}}} \left(Pate_{\text{external}} - Pate_{\text{cytosol}}\right)$$

A.3.4: Differential equations: external media

The differential equations for the external media of the cell were as follows:

$$\frac{dP_{\text{external}}}{dt} = N(t) \frac{Perm_{\text{cell}}^{\text{P}} SA_{\text{cell}}}{Vol_{\text{external}}} \left(P_{\text{cytosol}} - P_{\text{external}}\right)$$

$$\frac{dA_{\text{external}}}{dt} = N(t) \frac{Perm_{\text{cell}}^{\text{A}} SA_{\text{cell}}}{Vol_{\text{external}}} \left(A_{\text{cytosol}} - A_{\text{external}}\right)$$

$$\frac{dPol_{\text{external}}}{dt} = N(t) \frac{Perm_{\text{cell}}^{Pol} SA_{\text{cell}}}{Vol_{\text{external}}} \left(Pol_{\text{cytosol}} - Pol_{\text{external}}\right)$$

$$\frac{dPCoA_{\text{external}}}{dt} = N(t) \frac{Perm_{\text{cell}}^{PCoA} SA_{\text{cell}}}{Vol_{\text{external}}} \left(PCoA_{\text{cytosol}} - PCoA_{\text{external}}\right)$$

$$\frac{dPate_{\text{external}}}{dt} = N(t) \frac{Perm_{\text{cell}}^{Pate} SA_{\text{cell}}}{Vol_{\text{external}}} \left(Pate_{\text{cytosol}} - Pate_{\text{external}}\right)$$

A.3.5: Definition of reaction rate

Reaction rates were assumed to follow Michaelis-Menten kinetics.

$$R_{\mathrm{PduCDE}} = V_{\mathrm{max}}^{\mathrm{PduCDE}} \frac{P_{\mathrm{MCP/PB}}}{K_{\mathrm{M}}^{\mathrm{PduCDE}} + P_{\mathrm{MCP/PB}}}$$

$$R_{\mathrm{PduP},f} = V_{\mathrm{max}}^{\mathrm{PduP},f} \frac{A_{\mathrm{MCP/PB}}}{K_{\mathrm{M}}^{\mathrm{PduP},f} + A_{\mathrm{MCP/PB}}}$$

$$R_{\mathrm{PduP},r} = V_{\mathrm{max}}^{\mathrm{PduP},r} \frac{PCoA_{\mathrm{MCP/PB}}}{K_{\mathrm{M}}^{\mathrm{PduP},r} + PCoA_{\mathrm{MCP/PB}}}$$

$$R_{\mathrm{PduQ},f} = V_{\mathrm{max}}^{\mathrm{PduQ},f} \frac{A_{\mathrm{MCP/PB}}}{K_{\mathrm{M}}^{\mathrm{PduQ},f} + A_{\mathrm{MCP/PB}}}$$

$$R_{\mathrm{PduQ},r} = V_{\mathrm{max}}^{\mathrm{PduQ},r} \frac{Pol_{\mathrm{MCP/PB}}}{K_{\mathrm{M}}^{\mathrm{PduQ},r} + Pol_{\mathrm{MCP/PB}}}$$

$$R_{\mathrm{PduLW}} = V_{\mathrm{max}}^{\mathrm{PduLW}} \frac{PCoA_{\mathrm{cytosol}}}{K_{\mathrm{M}}^{\mathrm{PduLW}} + PCoA_{\mathrm{cytosol}}}$$

Section B: Bioinformatic analysis of PduB homologs

The shell protein PduB from *Salmonella enterica* serovar Typhimurium LT2 is a circularly permutated trimeric shell protein that is critical for linking the enzymatic core of the 1,2-propanediol utilization (Pdu) microcompartment (MCP) to its shell. As described in detail in Lehman *et al*., this is likely mediated by an N-terminal extension that is hypothesized to interact with the enzymatic core [2]. To determine if this putative mechanism for enzyme encapsulation is broadly distributed across MCP types, we performed bioinformatic analyses on PduB homologs. These analyses are based on the in-depth studies published by Sutter *et al.* and Axen *et al.* [3, 4].

A list of 45 diverse PduB homologs was curated based on the comprehensive list available in Sutter *et al*. A representative from each of the subclades (designated based on the color palette available at https://xkcd.com/color/rgb/) of PduB homologs (including all BMC-T^P variants) was chosen from the full data set. The full set of sequences used for this analysis is available in **Table S5**. Of the 46 BMC-T^P homolog sequences analyzed, 20 contained N-terminal extensions (43%) (**Fig S4, Supplemental Alignment 1**). Within close PduB homologs (based on the distinction made in Sutter et al.), the N-terminal extension of PduB is not well conserved relative to other highly conserved motifs within PduB. The most highly conserved positions within the N-terminal extension are a leucine at position 6 (73% identical) and a valine at position 14 (77% identical). After position 19 conservation scores drop off rapidly, with no positions between 19 and 37 having greater than 30% conservation. By comparison, the conserved lysine residues at position 102 and 207 are 100% conserved among the PduB homologs analyzed. This implies that while this mechanism may be important for the close PduB homologs present in Pdu and GRM MCPs, other encapsulation mechanisms are likely present in Eut and SPU MCPs.

Section C: Supplemental Tables

Table S1. Strains used in this study.

Strain	Organism	Genotype
DTE003	*S. enterica* serovar Typhimurium LT2	Wild type
CMJS256	*S. enterica* serovar Typhimurium LT2	Δ*pocR*
TUC01 [5], [6]	*E. coli* W3110	*gal490 pglΔ8 λcI857 Δ(cro-bioA) int<>cat/sacB*
NWKs083	*S. enterica* serovar Typhimurium LT2	Δ*pduA* Δ*pduJ*
CEMS179	*S. enterica* serovar Typhimurium LT2	Δ*pduB*
NWKs365	*S. enterica* serovar Typhimurium LT2	Δ*pduB::pduB-K102A-K207A*
NWKs337	*S. enterica* serovar Typhimurium LT2	Δ*pduA::pduA-mCherry*
NWKs338	*S. enterica* serovar Typhimurium LT2	Δ*pduA::pduA-mCherry* Δ*pduB*
NWKs344	*S. enterica* serovar Typhimurium LT2	Δ*pduA::pduA-mCherry* Δ*pocR*
NWKs364	*S. enterica* serovar Typhimurium LT2	Δ*pduA::pduA-mCherry* Δ*pduB::pduB-K102A-K207A*
TMDS025	*S. enterica* serovar Typhimurium LT2	Δ*pduD::ssD-GFPmut2*
CEMS299	*S. enterica* serovar Typhimurium LT2	Δ*pocR* Δ*pduD::ssD-GFPmut2*
CEMS298	*S. enterica* serovar Typhimurium LT2	Δ*pduA* Δ*pduD::ssD-GFPmut2* Δ*pduJ*
CEMS218	*S. enterica* serovar Typhimurium LT2	Δ*pduB* Δ*pduD::ssD-GFPmut2*

CEMS296	*S. enterica* serovar Typhimurium LT2	Δ*pduB::pduB-K102A-K207A* Δ*pduD::ssD-GFPmut2*

Table S2. Plasmids used in this study.

Name	Plasmid	Origin	Resistance
CMJ069	pBAD33t-ssD-GFPmut2	p15A	Chloramphenicol
EYK208	pBAD33t-ssP-GFPmut2	p15A	Chloramphenicol
EYK193	pBAD33t-PduG-GFPmut2	p15A	Chloramphenicol
NWKp041	pBAD33t-PduO-GFPmut2	p15A	Chloramphenicol
NWKp042	pBAD33t-PduW-GFPmut2	p15A	Chloramphenicol
NWKp043	pBAD33t-ssL-GFPmut2	p15A	Chloramphenicol
CMJ140	pBAD33t-PduB-FLAG	p15A	Chloramphenicol
NWKp044	pBAD33t-PduB-K102A-K207A	p15A	Chloramphenicol
pSIM6 [6]	λ Red system repressed by cI857	pSC101 $repA^{ts}$	Ampicillin

Table S3. Primers used in this study.

Name	**Purpose**	**Description**	**Sequence***
NWKo493	Recombineering	Amplify *cat/sacB* with homology upstream of *pduB* For	gccctcacaccgatgtagaaaaaatcttaccgaagggaattagccaatgaTGTGACGGAAGATCACTTCG
NWKo494	Recombineering	Amplify *cat/sacB* with homology downstream of *pduB* Rev	ttcgccagtgcttcaaatcttttcgatctcatgaatcagcctcgtgggtaATCAAAGGGAAAACTGTCCATAT
NWKo517	Recombineering	Amplify *pduB-K102A-K207A* with homology upstream of *pduB* For	ccacgccctcacaccgatgtagaaaaaatcttaccgaagggaattagccaATGAGCAGCAATGAGCTGG
NWKo518	Recombineering	Amplify *pduB-K102A-K207A* with homology downstream of *pduB* Rev	gccagtgcttcaaatcttttcgatctcatgaatcagcctcgtgggtatcaGATGTAGGACGGACGATCG
NWKo499	Recombineering	Knockout *pduB*	cgcgtccgcacagcgatgttgaggccattttaccgaaatcagcctaatcgggcaagcgaggtgaagcgtaatggataaagagcttctgcaatcaacggtc
NWKo466	Sequencing	Amplify from upstream of *pduA*	CTGCGAACCTGTCTCC
NWKo467	Sequencing	Amplify from downstream of *pduA*	CGTCTCTCGTATAGGTTGG
NWKo501	Golden Gate cloning	Amplify *pduO* with GG overhang For	AttGGTCTCACATGGCGATTTATACCCGAAC
NWKo504	Golden Gate cloning	Amplify *pduO* with GG overhang and GS linker Rev	ATTGGTCTCAGCTGCCttgatgagttcccacgttaatag
NWKo502	Golden Gate cloning	Amplify *pduW* with GG overhang For	AttGGTCTCACATGTCTTACAAAATAATGGCCATTA

NWKo505	Golden Gate cloning	Amplify *pduW* with GG overhang and GS linker Rev	ATTGGTCTCAGCTGCCggctggtacacaaagcc
EYKP263	SacI cloning	Amplify *pduG* with SacI recognition For	TATTGAGCTCTTAAAGAGGAGAAAGGTCatgcgatatatagctggcattgacatc
EYKP264	XbaI cloning	Amplify *pduG* with XbaI recognition Rev	TATTTCTAGActgtccatgcgcaaactccttatg
NWKo506	Golden Gate cloning	Amplify *GFPmut2* with GG overhang and GS linker For	AttGGTCTCACAGCAgtaaaggagaagaacttttcactgg
NWKo507	Golden Gate cloning	Amplify *GFPmut2* with GG overhang Rev	ATTGGTCTCATTTAtttgtatagttcatccatgccatgtg
TMDP058	Golden Gate cloning	Amplify *ssL-GFPmut2* with GG overhang For	ATTGGTCTCACATGgataaagagcttctgcaatcaac
NWKo514	QuikChange	*PduB-K102A* For	ATGGCGGCGGACGAAGCGGTGGCGGCCACCAACACC
NWKo515	QuikChange	*PduB-K102A* Rev	CTGCTTCGCCACCGCCGGTGGTTGTGGCTTCACCAG
NWKo516	QuikChange	*PduB-K207A* For	ATACCGCGCTGGCGTCAGCCAACGTTGAAGTCG
NWKo517	QuikChange	*PduB-K207A* Rev	ACTACCGGCTATGGCGCGACCGCAGTCGGTTGC
MPV031	Sequencing	Sequence confirmation of *pduB* locus For	gccctcacaccgatgtagaaaaaatc
MPV030	Sequencing	Sequence confirmation of *pduB* locus Rev	tccatcgccatcacttcttcg
TMDP021	Sequencing, recombineering	Amplify from upstream of *pduD* locus For	ggcaacaggttatcgcctgc

TMD P022	Sequencing, recombineering	Amplify from downstream of *pduD* locus Rev	ccctgcaggctgttcatgc
TMD P072	Sequencing	Amplify from upstream of *pduD* locus For	catccagaaagccaagctaacc
TMD P073	Sequencing	Amplify from downstream of *pduD* locus Rev	cgtccagcgttttattggtgg
TMD P016	Recombineering	Amplify ssD-GFPmut2 with homology upstream of *pduD* For	TTGATCCCAACGAGATTGATTAAGGGGTGAGAAatggaaattaatgaaaaattgctgcgc
TMD P019	Recombineering	Amplify ssD-GFPmut2 with homology downstream of *pduD* Rev	ATTGCGTCGGTATTCATGGAGTTATCCTTTAttatttgtatagttcatccatgccatgtg

Table S4. Parameter values used in kinetic model of pathway performance in MCPs and polar bodies.

Parameter Name	MCP	Polar Body	Unit
CDE_con	0.462467024	0.462467024	mM
CDE_tot [7]	6000	6000	enzymes/cell
cell_length	2.47E-06	2.47E-06	m
cell_radius	3.75E-07	3.75E-07	m
cell_surface_area	5.82E-12	5.82E-12	m^2
cell_volume	9.81E-19	9.81E-19	m^3
external_volume	5.00E-05	5.00E-05	m^3
kcatCDE [8]	300	300	1/s
kcatL	100	100	1/s
kcatPf [9]	55	55	1/s
kcatPr [9]	6	6	1/s
kcatQf [10]	55	55	1/s
kcatQr [10]	6	6	1/s
L_con [11]	0.1	0.1	mM
mcp_surface_area	6.16E-14	3.75E-13	m^2/compartment
mcp_volume	1.44E-21	2.16E-20	m^3/compartment
Navogadro	6.02E+23	6.02E+23	molecules/mole
nmcp	15	1	MCPs/polar bodies per cell
P_con	0.693700536	0.693700536	mM
P_tot [7]	9000	9000	enzymes/cell
PermMCPNonPolar	3.98E-08	1.00E+01	m/s
PermMCPPolar	3.98E-08	1.00E+01	m/s
Q_con	0.520275402	0.520275402	mM
Q_tot [7]	6750	6750	enzymes/cell
radius_mcp [12]	7.00E-08	1.73E-07	m
VmaxCDEf	138.7401071	138.7401071	mM/s
VmaxLf	10	10	mM/s
VmaxPf	38.15352946	38.15352946	mM/s
VmaxPr	4.162203213	4.162203213	mM/s
VmaxQf	28.61514709	28.61514709	mM/s
VmaxQr	3.12165241	3.12165241	mM/s
KmCDEPropanediol [8]	0.5	0.5	mM
KmPfPropionaldehyde [9]	15	15	mM
KmPrPropionyl [9]	95	95	mM
KmQfPropionaldehyde [10]	15	15	mM
KmQrPropanol [10]	95	95	mM
KmLPropionyl	20	20	mM

PermCellPropanediol [13] [14] [15]	1.00E-04	1.00E-04	m/s
PermCellPropionaldehyde [13] [14] [15]	1.00E-02	1.00E-02	m/s
PermCellPropanol [13] [14] [15]	1.00E-04	1.00E-04	m/s
PermCellPropionyl [13] [14] [15]	1.00E-05	1.00E-05	m/s
PermCellPropionate [13] [14] [15]	1.00E-07	1.00E-07	m/s

Table S5. Sequences used for PduB phylogenetic tree and multiple sequence alignment (information obtained from Sutter et al. [3]).

Bacteria	BMC Type	Length	Accession Number (Uniprot)	Subclade Color Designation
Escherichia 9.0111 (Proteobacteria)	bmcType=PDU1AB (main)	277aa	[I2WHE2] pduB	greenishBeige0
Klebsiella PO552 (Proteobacteria)	bmcType=PDU1AB (main)	270aa	[A0A206YP55] pduB	greenishBeige1
Citrobacter MGH105 (Proteobacteria)	bmcType=GRM4 (main)	271aa	[A0A0J1LFA2] pduB	greenishBeige2
Listeria ATCC 33091 (Firmicutes)	bmcType=PDU1E (main)	267aa	[H1GCR5] pduB	sunYellow1
Enterococcus ATCC 43197 (Firmicutes)	bmcType=PDU1E (main)	269aa	[R2PCN6] pduB	sunYellow2
Lactobacillus DSM 20253 (Firmicutes)	bmcType=PDU1C (main)	263aa	[A0A0R2D124] pduB	sunYellow3
Clostridium ATCC 25763 (ADT22) (Firmicutes)	bmcType=MUF1 (main)	274aa	[A0A0L9YAN3] pduB	chartreuse1
unclassified-Eubacteriaceae CHKCI004 (Firmicutes)	bmcType=PDU1D (sat)	274aa	[A0A143XJ34] pduB	chartreuse2
Blautia MGS:257 (Firmicutes)	bmcType=PDU1D_GRM5 (sat)	274aa	[R5WST7] pduB	chartreuse3
Ruminococcus AM49-8 (Firmicutes)	bmcType=GRM5 (main)	242aa	[A0A373QR46] pduB	chartreuse4
Propionibacterium F0372 (Actinobacteria)	bmcType=PDU1D (main)	262aa	[S3X7K1] pduB	turquoiseBlue1
Romboutsia FRIFI (Firmicutes)	bmcType=PDU1D (main)	270aa	[A0A2P2BR70] pduB	turquoiseBlue2
Buttiauxella ATCC 51602 (Proteobacteria)	bmcType=GRM3B (main)	261aa	[A0A1B7IB09] pduB	turquoiseBlue3a
Azospirillum TSO35-2 (Proteobacteria)	bmcType=GRM3C (main)	275aa	[A0A2U1VFS1] pduB	turquoiseBlue3b
Quasibacillus SGZ-8 (QY95) (Firmicutes)	bmcType=PDU1D (main)	260aa	[A0A0F5HND3] pduB	lichen1
Fusobacterium 1_1_41FAA (Fusobacteria)	bmcType=PDU1F (main)	271aa	[D6LIA1] pduB	lichen2
Desulfofundulus DSM 16057 (Firmicutes)	bmcType=PDU1D (main)	274aa	[A0A1M6DW06] pduB	darkGrassGreen
Streptococcus NCTC13765 (Firmicutes)	bmcType=GRM3A (main)	261aa	[A0A380L0X7] pduB	aqua1
Megasphaera 28L (Firmicutes)	bmcType=GRM3A (main)	270aa	[D3LW76] pduB	aqua2
Pelosinus JBW45 (Firmicutes)	bmcType=PDU1D (main)	265aa	[I8TWY2] pduB	pistachio1
Paenibacillus KCTC 13049 (Firmicutes)	bmcType=GRM6 (main)	280aa	[A0A2Z2KG56] pduB	pistachio2
Morganella GCSL-Mp20 (AYY16) (Proteobacteria)	bmcType=EUT1 (main)	218aa	[A0A1B8H666] eutL	rosa
Photobacterium Gung47 (Proteobacteria)	bmcType=EUT1 (main)	218aa	[A0A0C5WBE8] eutL	darkLavender1
Pseudoflavonifractor ATCC 29799 (Firmicutes)	bmcType=EUT2G (main)	217aa	[A6NPH4] eutL	darkLavender2
Cellulosilyticum ATCC 49066 (Firmicutes)	bmcType=EUT2I (main)	217aa	[F2JLY6] eutL	darkPeach1
Brevibacillus LAK 1210 (EX87) (Firmicutes)	bmcType=EUT2I (main)	217aa	[A0A0F6Y0T9] eutL	darkPeach2
Bacillus 2046851 (Firmicutes)	bmcType=EUT2I (main)	217aa	[A0A268IB25] eutL	darkPeach3
Lachnoclostridium An196 (Firmicutes)	bmcType=EUT2B (main)	217aa	[A0A1Y4IQA1] eutL	mutedPink1
Dethiosulfovibrio peptidovorans (Synergistetes)	bmcType=EUT2B (main)	217aa	[A0A2G6M5H7] eutL	mutedPink2
Hathewaya DSM 3090 (Firmicutes)	bmcType=EUT2I (main)	218aa	[A0A1M6KC11] eutL	scarlet1
Fusobacterium ATCC 23726 (Fusobacteria)	bmcType=EUT2F (main)	221aa	[D5RF36] eutL	scarlet2
Halanaerobium sapolanicus (Firmicutes)	bmcType=PDU_EUT (sat)	217aa	[E4RJS6] eutL	scarlet3

Natronincola DSM 18979 (Firmicutes)	bmcType=EUT2B (main)	217aa	[A0A1I0EUU4] eutL	amethyst1
Fusicatenibacter (ERS852537) (Firmicutes)	bmcType=EUT2B (main)	218aa	[A0A174T4Q4] eutL	amethyst2
Vagococcus bH819 (Firmicutes)	bmcType=EUT2A (main)	218aa	[A0A1X6WPL8] eutL	amethyst3
Tepidanaerobacter JL (Firmicutes)	bmcType=EUT2B (main)	218aa	[A0A0U9HIK8] eutL	ceriseX
Sporomusa DSM 5090 (Firmicutes)	bmcType=UA (sat)	215aa	[A0A1W2F4B5] eutL	cerise1
Minicystis DSM 24000 (Proteobacteria)	bmcType=SPU3 (sat)	226aa	[A0A1L6L3A8] eutL	cerise2
Levilinea KIBI-1 (Chloroflexi)	bmcType=SPU6 (sat)	216aa	[A0A0P6XV62] eutL	cerise3
Alkalispirochaeta ASpG1 (Spirochaetes)	bmcType=EUT3 (main)	218aa	[A0A1N6TZP1] eutL	cerise4
Melghirimyces DSM 45787 (Firmicutes)	bmcType=EUT2C (main)	217aa	[A0A2T6C8Q0] eutL	orangePinkX
Brevibacillus AK1 (Firmicutes)	bmcType=EUT2E (main)	216aa	[M8D890] eutL	orangePink1
Fictibacillus ZFHKF-1 (Firmicutes)	bmcType=EUT2C (main)	217aa	[I8AM68] eutL	orangePink2
Salimicrobium WN024 (Firmicutes)	bmcType=EUT2C (main)	216aa	[A0A2A3A540] eutL	orangePink3
Domibacillus DSM 4337 (AWH48) (Firmicutes)	bmcType=EUT2C (main)	217aa	[A0A177KYD5] eutL	orangePink4

Section D: Supplemental Figures

Figure S1. Representative micrographs (top) and puncta quantification (bottom) for plasmid rescue experiments. PduB-WT and PduB-K102A-K207A were expressed from a pBAD33t plasmid in the PduB knockout strain (ΔB) to rescue MCP formation, visualized by the formation of fluorescent puncta. The ΔB strain contained significantly fewer puncta than the WT strain ($p < 0.0001$, one-tailed t-test). ΔB with the PduB-WT plasmid had significantly more puncta than the ΔB strain without a plasmid ($p < 0.0001$, one-tailed t-test). ΔB with PduB-K102A-K207A overexpressed did not have significantly different puncta counts (one-tailed t-test). Note that all strains contain ssD-GFP at the *pduD* locus to allow visualization of cargo location within the cell. Puncta were counted from three biological replicates and at least 85 puncta were counted in each condition. Scale bar = 1 μm.

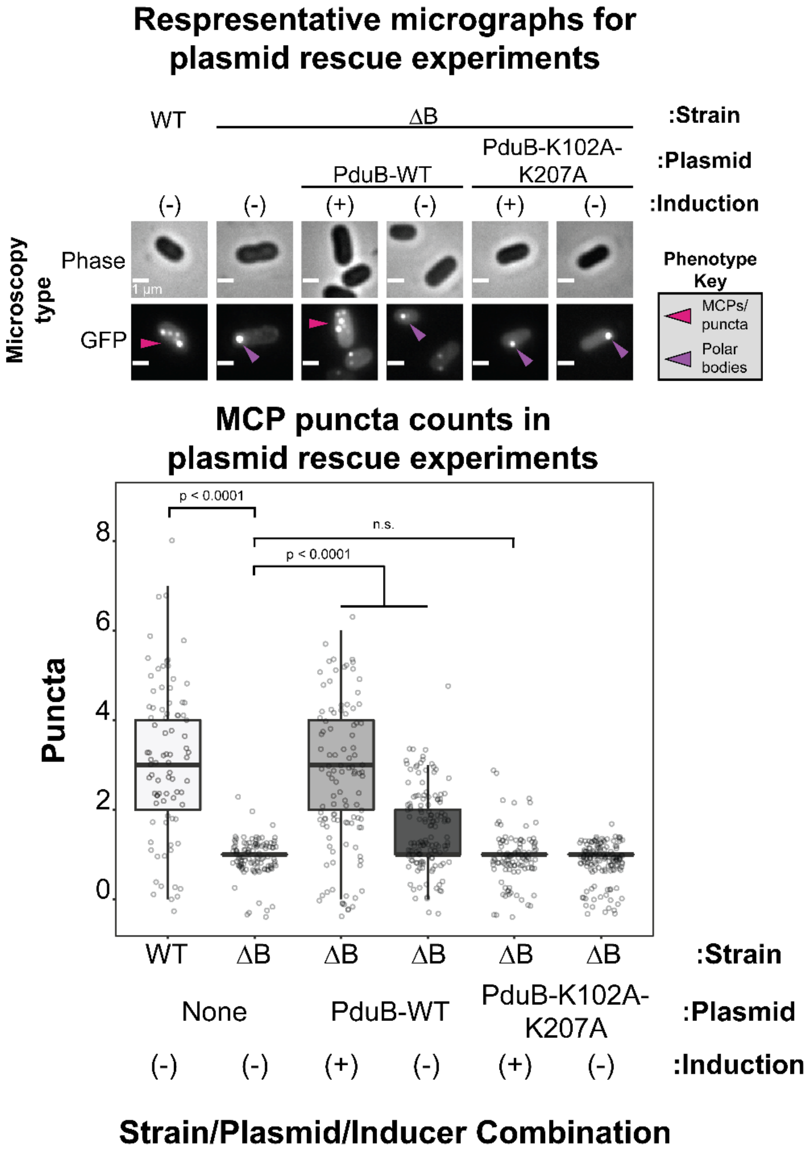


Figure S2. Tornado plot showing changes in maximum propionaldehyde level observed in MCP model with a 10% increase and decrease in the noted parameter.

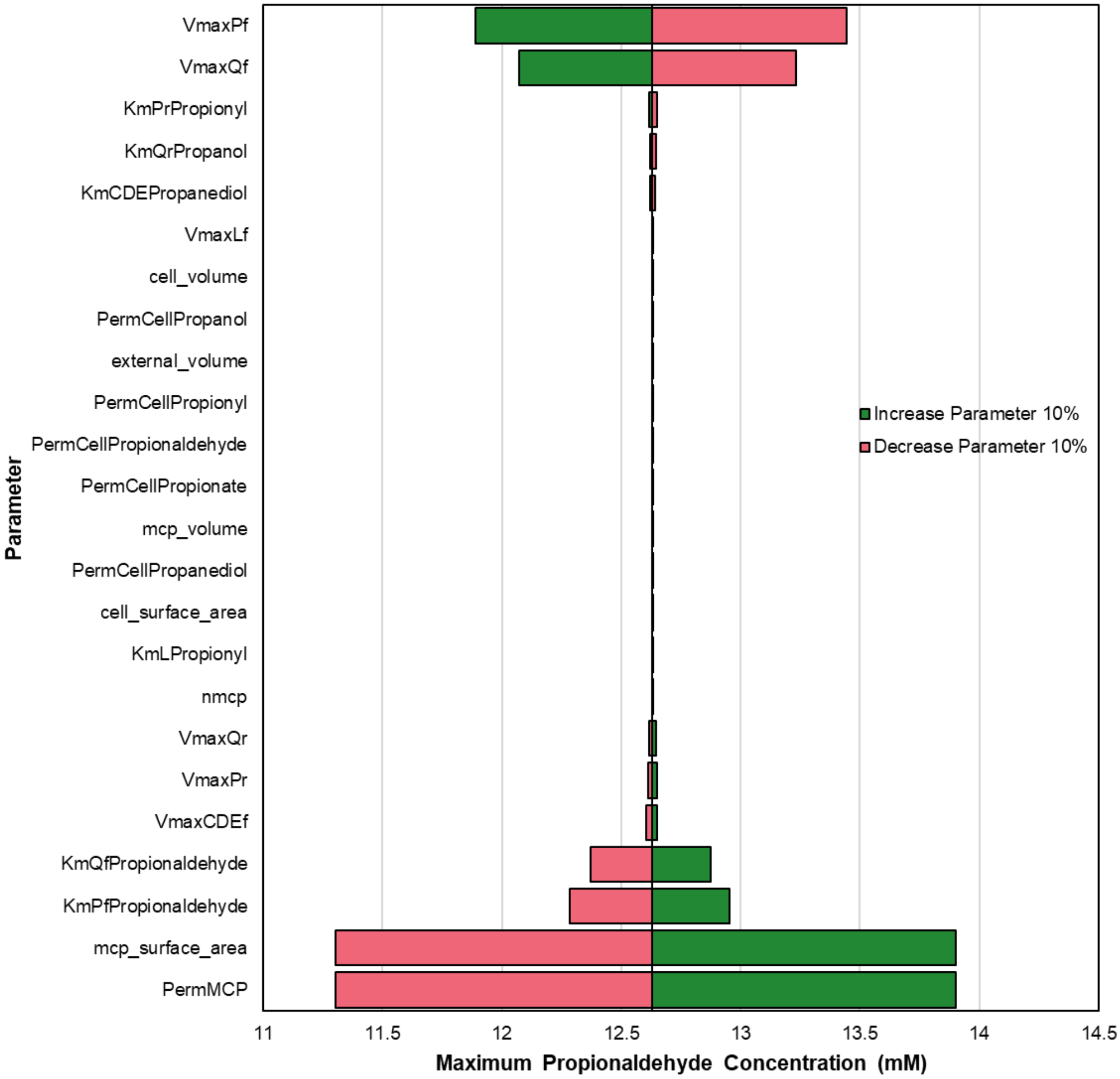


Figure S3. Tornado plot showing changes in maximum propionaldehyde level observed in polar body model with a 10% increase and decrease in the noted parameter.

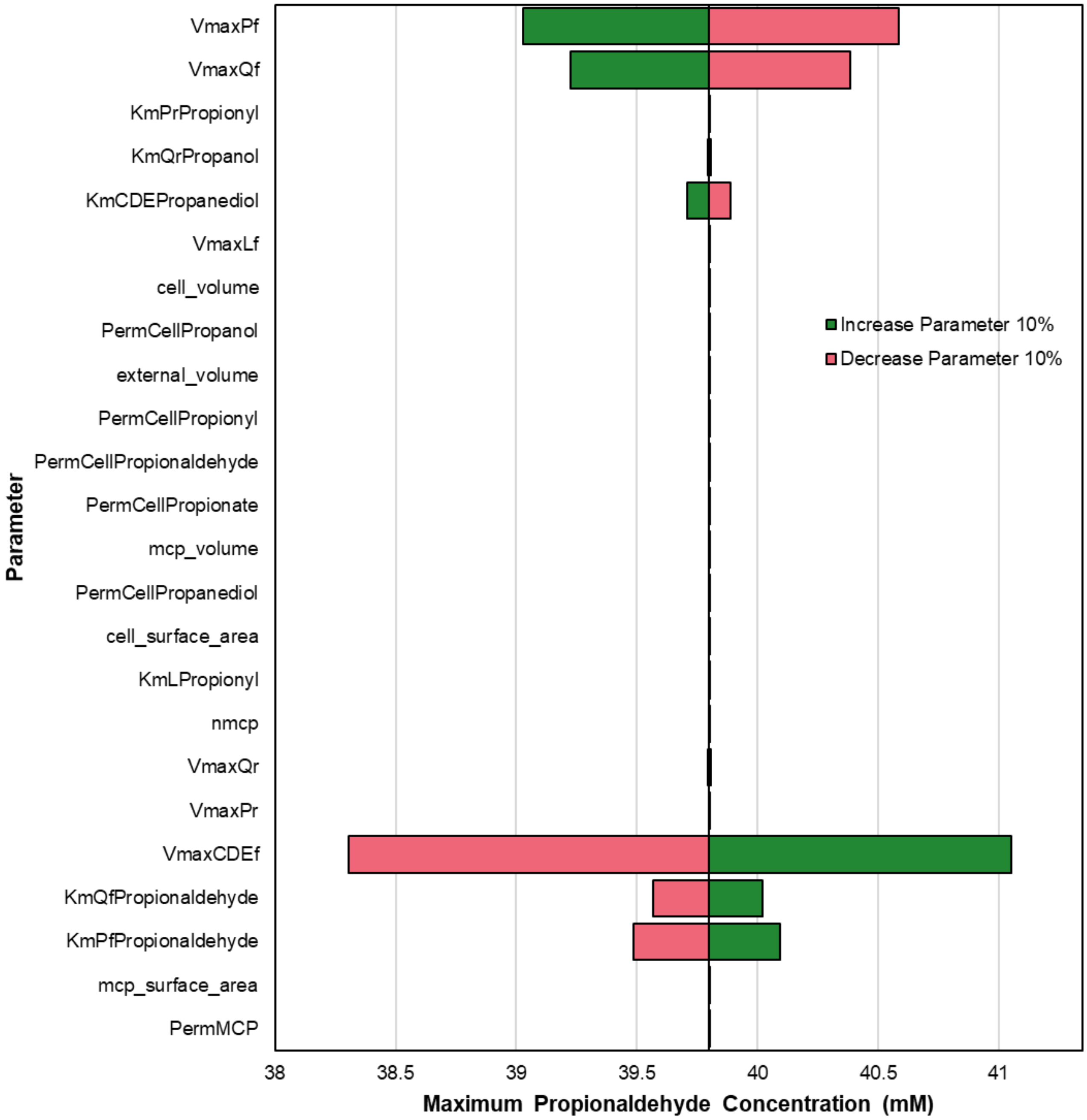
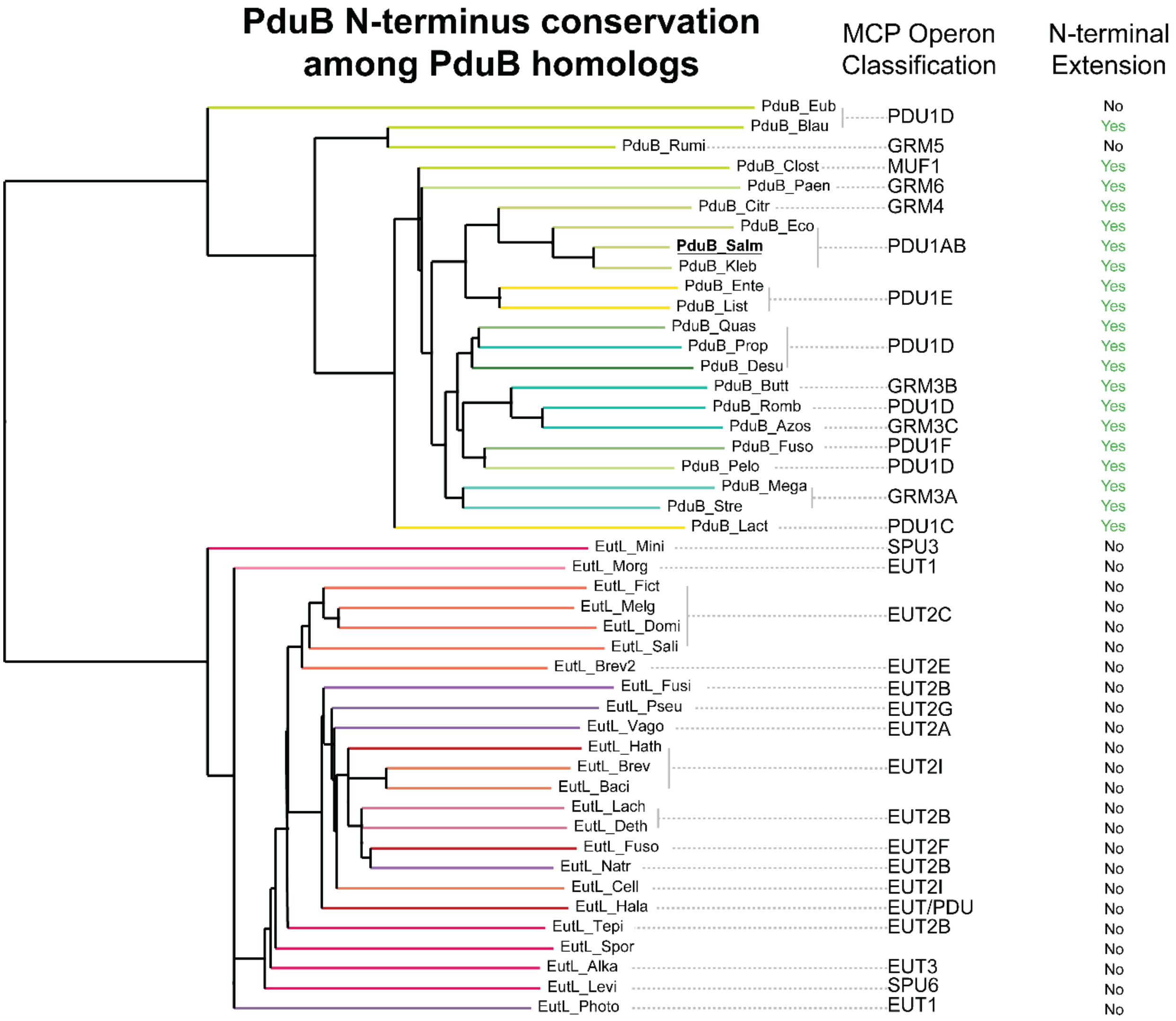


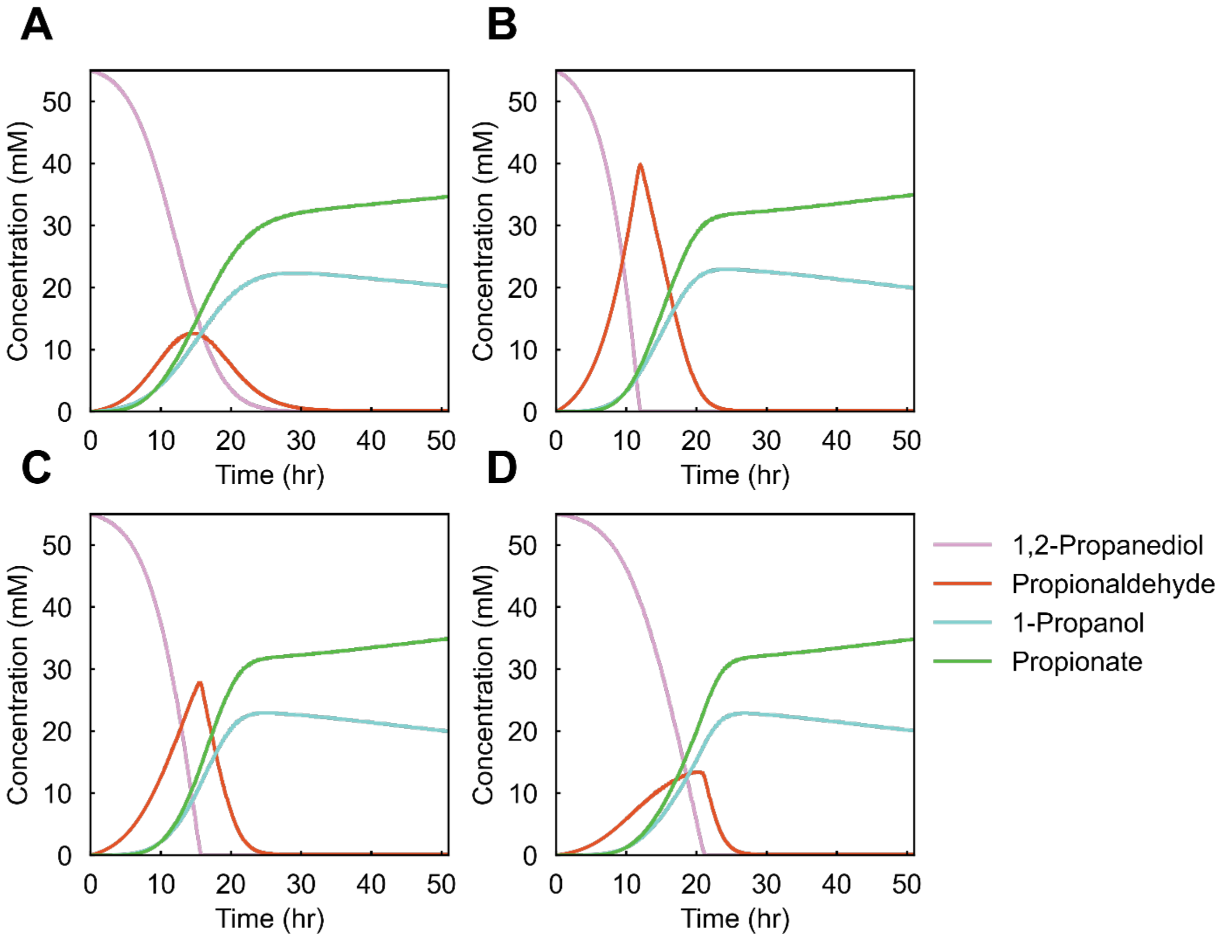
Figure S4. Phylogenetic tree of PduB homologs and their associated MCP types (information adapted from Sutter et al. [2]). The PduB sequence from *S. enterica* investigated in this work is underlined and bolded (PduB_Salm).



Acronym definitions

PDU	Propanediol utilization microcompartment
GRM	Glycyl radical enzyme containing microcompartment
MUF	Metabolosome microcompartment of unknown function
SPU	Sugar phosphate utilization micorcompartment
EUT	Ethanolamine utilization microcompartment

Figure S5. Full profiles of all metabolites for the kinetic model results shown in Figure 7. Profiles are shown for the (a) MCP model with 0.46 mM PduCDE and the polar body model with (b) 0.46 mM PduCDE, (c) 0.23 mM PduCDE, and (d) 0.12 mM PduCDE.



Section E: Supplemental Alignments

Supplemental Alignment S1. Multiple sequence alignment of PduB homologs.

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CLUSTAL O(1.2.4) multiple sequence alignment


EutL_Mini       -------------------------------------------------MSVLEPIIPKV 11
EutL_Morg       -------------------------------------------------MPVLDLIRPNI 11
EutL_Fict       --------------------------------------------------MSLRRIQTDI 10
EutL_Melg       --------------------------------------------------MDLQPVKAEI 10
EutL_Domi       --------------------------------------------------MTSQKIFAEL 10
EutL_Levi       ---------------------------------------------------MLDPIPANA 9
EutL_Sali       ---------------------------------------------------MIRPVYAEM 9
EutL_Photo      -------------------------------------------------MAILDKIQPAV 11
EutL_Alki       -------------------------------------------------MATLDPIKPTI 11
EutL_Spor       ---------------------------------------------------MIEPIKPKV 9
EutL_Brev2      ---------------------------------------------------MEKPIRATP 9
EutL_Fusi       --------------------------------------------------MTGDLIKAEI 10
EutL_Pseu       --------------------------------------------------MIDELIPVKV 10
EutL_Tepi       -------------------------------------------------MYGFKPIKAQV 11
EutL_Vago       --------------------------------------------------MINDSLGANV 10
EutL_Hath       --------------------------------------------------MIGEQIPVNI 10
EutL_Cell       --------------------------------------------------MKNDKVRANV 10
EutL_Hala       --------------------------------------------------MRDDPLRAEV 10
EutL_Brev       --------------------------------------------------MRNEPIYAKV 10
EutL_Baci       --------------------------------------------------MKNERLQANI 10
EutL_Lach       --------------------------------------------------MKRDPVRASV 10
EutL_Deth       --------------------------------------------------MKGDPLKTTL 10
EutL_Fuso       ---------------------------------------------ME-VKMINDPLRASV 14
EutL_Natr       --------------------------------------------------MRNDPIRAQV 10
PduB_Eub        -----------MGQV-------------------------------IQMADYFTPDAEQF 18
PduB_Blau       MFFLLK--------YVKTLSNTGKSIEIPQLLSYIKVTIPKGDFFMNVKDISTHCTRTEF 52
PduB_Rumi       -----------------------------------------MIDVHHIEQISQDCSLTEF 19
PduB_Clost      --MQEQLIRNIISEVLKNVENTIVANPNENKEE---LKN---IQNFQNNKISLENDIPEF 52
PduB_Paen       --MDEAILKQVIEAAVRAIPGGVPSSPAADAAAGLPLNNQQYTEKREQDVTTDYKAITEY 58
PduB_Lact       MKNENEIVDRVMSRILANKPTE--------------------AESGSNALKAKGQALTEF 40
PduB_Citr       -MSSDNLVENIIAEVLGKVGDLKTPSAASQP----------GISQQEPAIPRKLCGLTEF 49
PduB_Ente       MANTDQKIEEIMKRVLAKMETGNEL-----K----------TTNGGDHKMIEKQCALTEF 45
PduB_List       MSEQNKLIDEILKQVMETVNDAPEKIV---------------EDGGSRQMSEKAVQLTEF 45
PduB_Eco        -MSSNELVEQIMAQVIARVATPEHEVLP-ET----------THQTRETAMAEKSCTLTEF 48
PduB_Salm       -MSSNELVEQIMAQVIARVATPEQQAIP-GQ----------PQPIRETAMAEKSCSLTEF 48
PduB_Kleb       -MSSNELIDQIMTQVIARMAKPESNVIP-AP----------SHSTRETAMAEKNCSLTEF 48
PduB_Quas       --MREQLIEKIMEEVIKKVDAPATEEAP--------------------QAEKKHSSLTEF 38
PduB_Desu       --MDEQLVQKVLEQVMKKVGAASSSAAASSVPAS------SSPVAEQVAGRGLTSLPTEF 52
PduB_Prop       --MSNELVDQVMAEVLKKVGGSAPQAAPAAV------------------TPGVRPQSTEF 40
PduB_Butt       --MRDNLVEQIISEVMNKQTDVSA--------------------TGKNTANIPACGLTEF 38
PduB_Romb       --MKEDLMSKIMDEVMKKMGETPKLEVKEETA------------EEAKYEEPNSCSLTEF 46
PduB_Azos       --MKDELVEKIMGEVLRKMGGPDLLPAIPDSPRA------APPPSSSPSRSLGGCGLTEF 52
PduB_Mega       --MDQQLLEKVMKQVQHELESQVQVNTNGES----------IFPKEKEAGIKTMAGCTEF 48
PduB_Fuso       MSMQENLVQKMVAEVVEKLKDKGICETPKKV----------ESDCACASKND--CRLTEF 48
PduB_Stre       --MDQELLNKVVQGVRDELNKTT-----PTT----------SSDC----PINCATSITEF 39
PduB_Pelo       --MQEQLIDKVMDEIKKRMENHA-----PTA----------SQGVQEKPKASVNPGITEF 43
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EutL_Mini       LS--------VRRLPAADAALLRAYGADPERHTSLGLVTVDQDD-STYVALDEATKHAAV 62
EutL_Morg       TA--------MRLIANVQQDFCRELNLPK-HIRSLGLITVDSDD-VAYIAADEATKQAMV 61
EutL_Fict       LA--------VRLIPNADAALCEALHVPS-SFKSLGILTTTSDD-VGFTALDEATKQANV 60
EutL_Melg       LA--------AKMIPNVDAGLAESLALKP-HQRSIGILTTNIDD-VGYTALDAATKKADV 60
EutL_Domi       LA--------MKVIPNVDAGLAEKLKLKP-YQRSIGLFTSTIDD-VGYTAADEATKKADV 60
EutL_Levi       LA--------VRLIPSVAPEYARQLGLRP-DQRSLGLLTADNDD-ATYVSIDEATKMADV 59
EutL_Sali       LA--------TRIIPNVDKQLARQFGLGP-SHRSLGMFTVTLDD-VGVTALDEATKRADV 59
EutL_Photo      LA--------TRVIASVDPVYKEKMGLEP-HHNSIGLITADCDD-VTYCALDEATKAANV 61
EutL_Alki       LA--------VRLIPNVHTDFAKRLELRP-DQRSIAIITCDMDD-PLYVALDEATKMADV 61
EutL_Spor       LA--------VRLIPNVAPDLAAQLGLKD-YQRSIGMITSNMDD-PTYTALDEATKKAEV 59
EutL_Brev2      LA--------VRMIPNVDPRLAEKLNVAP-HIRSLGLLTSTIDD-VGYTAIDEATKKAAV 59
EutL_Fusi       LA--------AKIIPNVHPELAGKLKLGG-GSCSLGLLTCTSDD-VAYTALDEATKKADV 60
EutL_Pseu       LA--------THTIANVSEGLAKRLSLPD-GHRSIGILTTDCDD-MTYCALDEATKAAAV 60
EutL_Tepi       LA--------VKLIPNVNEYMKKELNLKP-EHRSIGMLTVTIDD-VGYTAVDEATKKADV 61
EutL_Vago       LS--------SKIISNIDPGLAKALNLDPVKHRSLGLVTGDCDD-VTYVALDEATKKAMV 61
EutL_Hath       LS--------VKMIPNVNPDMVKQFNLDP-NHKSIGMITADCDD-VTYTALDEATKASDV 60
EutL_Cell       LG--------VRVISNVSPELAAKLELGP-KHKSIGIITADSDD-VTYTALDEATKDADV 60
EutL_Hala       LS--------VQLIPNVNDALKEKLNLEA-GHRSIGLITCDIDD-VGYTALDEATKKASV 60
EutL_Brev       LG--------TKLISNVSPDMAEKLELKP-HHKSLGIITVDIDD-VTYTALDEATKAAEV 60
EutL_Baci       LS--------VKIISNISPDMAKELELKP-YHKSLGLITADTDD-VTYTALDEATKAADV 60
EutL_Lach       LA--------TKIIPNVSPDMAKEFNLDP-SMKSLALITADSDD-VTYTALDEATKKADV 60
EutL_Deth       LS--------IKIIPNVNPDLAASLGLRT-DQRSLGLVTADCDD-VTYTALDEATKKADV 60
EutL_Fuso       LS--------VKLIPNVDAKMAEELNLPN-GYRSIGIITADSDD-VTYTALDEATKMAEV 64
EutL_Natr       LS--------IKLIPNINPDMATELKLEK-QHRSIGIITTDIDD-VSYTALDEATKKADV 60
PduB_Eub        VGT-AAAHTIGLMIGNINGMVRLILDIPE-KYNALGIISSRTGTVAQAIAIDDAVKACNA 76
PduB_Blau       VGT-TVLDTIGLVISGIDHTLLQKMNIGT-KYYALGLFSSRTGAAGQLTAIDDAVKATNT 110
PduB_Rumi       VGT-TVLDTIGLVIPGIDPSLLEKMNLKK-PYKSLGLISSRTGAAGQINAADEAVKSTNT 77
PduB_Clost      VGS-AIGDTVGLVIANVNELLLNKMNVSK-KYRSIGIIGARTGASAQIISADEAVKGTNS 110
PduB_Paen       VGS-AMGDTVGLVIANLDRHLHESMGLDP-RYRSIGIISSRTGAGPHIMAADEAVKATNT 116
PduB_Lact       VGTAPIGDTIGLVIANVDANLAEKMNLDK-KYRSIGVISARTGASPQVMATDVAVKATNT 99
PduB_Citr       VGT-ATGDSIGLVIANVDSALLDAMHLEK-KYRSIGILGARTGAGPQIMAADEAVKATNT 107
PduB_Ente       VGATEFGDTIGLVIANVDSSLLETMKLEK-KYRSIGIVGARTGAGPHIMAADEAVKATNT 104
PduB_List       VGT-AIGDTIGLVIANVDGQLLEAMKLEK-SYRSIGILGARTGAGPHIMAADEAVKATNT 103
PduB_Eco        VGT-AIGDTVGLVIANVDSALLDAMKLEK-RYRSIGILGARIGAGPHIMAADEAVKATNT 106
PduB_Salm       VGT-AIGDTLGLVIANVDTALLDAMKLEK-RYRSIGILGARTGAGPHIMAADEAVKATNT 106
PduB_Kleb       VGT-AIGDTVGLVIANVDGALLEAMKLEK-RYRSIGILGARTGAGPHIMAADEAVKATNT 106
PduB_Quas       VGT-GLGDSIGLVIANVDHSIHEAMNLDK-KYRSIGILGARTGAGPQIMAADEAVKATNT 96
PduB_Desu       VGT-AMGDTIGLVIANVDPLLHEKMGLDS-RYRSIGILGGRTGAGPQIMAADEAVKATNT 110
PduB_Prop       VGT-GLGDTIGLVIANVDPALTEKMNIDP-KYRSIGIIGGRTGAGPQLFAADEAVKATNT 98
PduB_Butt       VGT-AMGHTIGLVIANVDNQLHEVMKIDK-KYRSIGILGARTGAGPHIFAADEAIKATNS 96
PduB_Romb       VGT-AIGNTIGLVIANVDYNLHELMNIDK-KYRSIGIVGGRTGAGPHIFAADEAVKATNS 104
PduB_Azos       VGT-AIGHTIGLVIANVDPLLHEKMKISP-KYRSIGIVGARTGAGPHIFAADEAVKATNS 110
PduB_Mega       VGT-AIGDTIGLVIAGVDPLLKDTMKLG--KFRSIGIIGGRIGAGPQIMAVDDAVKATNT 105
PduB_Fuso       VGLTTHGHGIGLVIANVDSALHEAMGLDK-KYRSIGIIGARTGAGPFIMAADEAVKATNT 107
PduB_Stre       VGT-AIGDTIGLVIANVDHELHEKMGIDP-KYRSIGIIGARVGAGPHIMAVDEAVKATNT 97
PduB_Pelo       VGT-AIGDTIGLVIANVDPMLHEKMKIDP-KYRSIGILGARTGAGPHIMAADEAVKATNT 101
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EutL_Fict       EVA---YAKSFYAGASHASGPLSGEFIGIVAGPTPDEVRSGIDAAIHTIEHEA-AFEALD 116
EutL_Melg       EVV---YGSSFYAGAAHASGPLSGEFIGILAGPTPAEVKSGMEVFCYTAENEA-WFYALD 116
EutL_Domi       EVV---YAKSFYAGAEHASGPLSGEFMAILAGPTSEEVKSALDAIQIKVESDA-YFEMIS 116
EutL_Levi       EVV---YAHSFYAGARHASGPLSGEIIALLAGPNPAEVRAGLDAALRYLSTRA-LWYSAN 115
EutL_Sali       DGV---YAASFYGGSDYPSGPLSGEFLGVLAGPDPEEVRSGMDAVKQMVESGA-HFEALD 115
EutL_Photo      DVV---YARSFYAGAAHSSGPTSGEVIGILAGACPADVIAGLERAKAFIEDEA-AFQCAD 117
EutL_Alki       EVV---YGQSFYAGSAHASGKLSGEVIGILAGNDPAEVRSGVNACVAYCEESA-WFYSAN 117
EutL_Spor       EVV---YAKSFYAGAAHASGPRSGEIIGILAAPTPAEISAGIDACINHLENEA-FFY-TC 114
EutL_Brev2      EVV---YARSFYAGSAHASGPLSGEFIGVIGGATPSEVESGLDAAIAFMANGA-CFYSLN 115
EutL_Fusi       KVV---YAKSLYAGSGNASTRFAGEVIGIIAGPDPEEVRSGLEACAEHIQNSA-FFHSAN 116
EutL_Pseu       EVV---YGRSLYAGAGNASTKLAGEVIGILAGPNPAEVQSGLRAAVAFLQEGG-GFRSAN 116
EutL_Tepi       EVV---YARSFYAGAAHASGPLSGEFIGILAGPNPAEVKSGLNAAIDCIENDA-CFWAAD 117
EutL_Vago       DVV---YARSLYAGAGSASTKLAGEVIGIIAGPNPAEVKSGLDVVVYEIENSP-GFVSAN 117
EutL_Hath       KVV---YARSFYGGAGNASTKLAGEVIGIISGPSPAEVRSGLNAIVDFIESGVATFRMAN 117
EutL_Cell       EVV---YARSMYAGAGNASTKLAGEVIGIIGGPSPAEVRSGLKAALDFFGSDA-CFISAN 116
EutL_Hala       DIV---YAKSFYAGADNATTKLAGEFIGIMAGPSPAEVNSGLDAAVDFIENGA-CFYSAN 116
EutL_Brev       DVV---YAKSMYAGSANASTKLAGEVIGIIAGPSPAEVKSGLSAAISYIEDSA-HFVGAN 116
EutL_Baci       EVV---YAKSLYAGSANASTKLAGEIIGILAGPSPAEVRSGLNAAVDFIENGA-HFISAN 116
EutL_Lach       KVV---YAKSFYAGAANANTKLAGEIIGILAGPNPAEVRSGLEAAVDMIENQA-YFISAN 116
EutL_Deth       KVV---YAKSFYGGAANANTKLAGEIIGILAGPNPAEVRSGLNALADFIENEA-WFISAN 116
EutL_Fuso       VIV---YAKSFYGGAANANTKLAGEVIGIMAGPNPAEVKSGLNAAIDFIENGG-CFYSAN 120
EutL_Natr       QVA---YAKSFYGGAANASTKLAGEFIGILAGPNPAEVRSGLNAAIEFIENGA-CFYSAN 116
PduB_Eub        KLLRFEMAIDAGRQCGQGC-------LFILGAETISDARKVVEESLHNID-YWSQCIYIN 128
PduB_Blau       EVLSIELPRDTKGWGGHGN-------YIVLGGNDVSDVRHAVQLALELTE-KYAGELYIS 162
PduB_Rumi       EIVSIELPRDTKGWGGHGC-------FIVIGGDNVSDVRRAVDITLEYIG-KYAGELYIS 129
PduB_Clost      EIIKVELARDTKGNAGHGV-------LIVFGAMDVSDVRQAVEITLNDLN-RTFGNLYIN 162
PduB_Paen       EVVSIEMARDTKGGAGHGC-------IIIFASEDVSDSRRAVEVVLKELP-RTFGDVYPC 168
PduB_Lact       AIISVEMPRDTKTGAGHGS-------LITIGGEDVSDVRRAVEVALAQTP-KMFGDIYTN 151
PduB_Citr       EVVAIELARDTKGGAGHGS-------LVLFGGQDVSDVKRAVEVALGELE-RTFGDIYAN 159
PduB_Ente       EVILIEMPRDTKGGAGHGS-------IVIFGGDDVSDVKRAVEVTLKEVDTRTFGDVYGN 157
PduB_List       EVVKIELPRDTKGGAGHGS-------LIIFGGDDVSDVKRAVEVALNELD-KTFGDVYGN 155
PduB_Eco        EVISIELPRDTKGGAGHGS-------LILLGGNDVSDVKRGIEVALKELD-RTFGDVYAN 158
PduB_Salm       EVVSIELPRDTKGGAGHGS-------LIILGGNDVSDVKRGIEVALKELD-RTFGDVYGN 158
PduB_Kleb       EVVSIELPRDTKGGPGHGS-------LIIIGGNDVSDVKRGIEVALKELD-RTFGDVYAN 158
PduB_Quas       EILAVELARDTKGGAGHGS-------LIIFGAEDVADARRAVEVALKELE-RTFGDVHAN 148
PduB_Desu       EVVAVELPRDTRGGAGHGS-------LIIFGAEEVSDARRAVEVALQELQ-RTFGDVYAN 162
PduB_Prop       EIVLAELPRDTKGGAGHGS-------LIVFAAEDVSDARRAVEVTLKELE-RTFGDVYGT 150
PduB_Butt       EILSIELARDTEGGGGHGC-------LIIFGATDVSDVRRAIEVALAEID-RTMGDVYGS 148
PduB_Romb       EILLIELPRDTEGGAGHGS-------LIIFGAEDVSDARRAVEVTLNELE-RTFGDVYGS 156
PduB_Azos       EVVLIELPRDTEGGAGHGC-------LILFGAEDVSDARRAVEVTLKEVE-RTMGDVYGT 162
PduB_Mega       EIISVELPRDTKGGAGHGS-------LILIGAEDVSDARRAVETALQVLP-KYFGDVYGN 157
PduB_Fuso       EVISIELPRDTEGGAGHGS-------LILFGAEDVSDVKRAVEVAINNVT-EKFGDVYAN 159
PduB_Stre       EVLSIELPRDTKGGAGHGS-------LIIIGSDDVSDARRGIEVALATLD-QTFGDVYSN 149
PduB_Pelo       EIISIELPRDTKGGAGHGS-------LILFGAEEVSDARRAIEVALKELD-RTFGDVYGN 153
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EutL_Mini       EKASVTVFPHVIASLGHYLSAQAGLAPGDTMAYLVAPP-IEATIALDHALKAADVRAVKV 177
EutL_Morg       DKEDTAFLAHLVSRTGSYLSGD-KIRAGDPIAYLVAPP-LEATFGIDAALKAADVQLATY 175
EutL_Fict       EEGNHALFAHVISRTGSYLSKVAGIAIGQPLAYLIAPP-LEAVVGLDYALKAADVQLATF 175
EutL_Melg       PEAKHTFYAHVISRTGSYLSEVAGIREGEPLAYLIAPP-LEAVMGLDAALKAADVRLVKF 175
EutL_Domi       GDPNHAFYAHTVSRTGSFLSKMAGIPEGEALAYLIAPP-LEATVGLDAALKAADVKLCEW 175
EutL_Levi       AEGTIAFFPHVISQTGRYLSQLCGVPVGSPIAYLIAPP-LEGVYGLDAALKAADVQLASY 174
EutL_Sali       ESEAHLLYAHVVSRSGTFLSKEAGVKEGEAIAYLIAPP-LESIYGVDAALKAAEVSMAVH 174
EutL_Photo      DNGDIAFFAHLVSSTGSYLSAEAGVEQGEALAYLIAPP-LEAMFALDAALKSADVRLVNL 176
EutL_Alki       DDDSIAFFPHTISRTGSFLSKMADIPLGTPLAYLIAPP-IESTFAIDAALKAADVEMKEW 176
EutL_Spor       DGGQTAWYPHTISRTGSYLSKIAGIQEGEPLAYLIAPP-IEAIYGIDAALKAAEVEMKAF 173
EutL_Brev2      EEGTHAYYAHVVSRTGSYLSQVAGIPEGEPLAYLIAPP-LEAMYGIDAALKAADVELKQF 174
EutL_Fusi       KDDSVIYYAQCISRTGSFLSKQAGIREGRSLAYLIAPP-LEAVYGLDAAMKAAQVKLCVF 175
EutL_Pseu       EDGSVVYFAHTVSRTGTYLSQTAGVAEGEALAYLIAPP-LEAMVGLDEALKAADVELVTL 175
EutL_Tepi       EEGQIAFYAQCISRTGSYLSKINNIPEGSPIAYLIAPP-IEAMYALDAAIKAAEVKLTSF 176
EutL_Vago       EDDSIPYYAHLVSRTGTHLSKEAGIKEGESLAYLIAPP-IEAMYALDAAIKAADVEVAAF 176
EutL_Hath       EDGSIPYYAYCVSRTGSYLSEQCGITEGEAIAYLIAPP-MEAMYALDAAMKAASVDMKCF 176
EutL_Cell       EDDSIVYYAHTVSRTGSYLSKVAGVEEGEPLAYLIAPP-MEAIYGLDAAMKAADVKLVEF 175
EutL_Hala       EDDSICYYNHCVSRTGSFLSAEAGVPKGQALAYLIAPP-IEALFALDAALKSANVELVTF 175
EutL_Brev       DDNSITYFAHCVSRTGSYLSQVANINEGEAIAYLIAPP-LEAMYALDAALKAADVSIGAF 175
EutL_Baci       DDNSIPYFAHCVSRTGSYLSQVAGIKEGEALAYLIAPP-LEAMYGLDAALKAANVTIAAF 175
EutL_Lach       EDDSIIYYAHCISRTGSYLSEGAGIQEGEALAYLIAPP-LEAMYGVDAALKAADVKMCVL 175
EutL_Deth       EDDTIPYYAHCISRTGSYLSETAGITEGEALAYLIAPP-LEAMYAVDAALKAADVRMATL 175
EutL_Fuso       EDDTIPYYAHCVSRTGSYLSKTAGVEEGAALAYLIAPP-LEAMYALDAALKAADVTLAAF 179
EutL_Natr       EDDSIAYYAHCISRSGSYLSDTAGIQEGEAIAYLIAPP-MEAMYALDAALKAADVRMAIF 175
PduB_Eub        EVGHME--SHVTPRAGEVLHEIFGTPVGRAFGVVGAAPAGVGIAAVDRAVKAAPVDIVWY 186
PduB_Blau       ESGHLE--FAYSASAGPALQKAFHAEPGQAFGFMAGSPAAIGLVMADTAMKASSVKIVSY 220
PduB_Rumi       QAGHLE--FTFSACADKALHMAFNAPIGKPFGFFCGSPAAIGLVMADLAVKSSPVEVIKY 187
PduB_Clost      ECGHLE--IQYTPRSSYACNKAFNAPIGTAFGVIVGAPAAIGLLMADSALKASNVDIIDH 220
PduB_Paen       DAGHVE--LHYTARASLALEKAFGAPAGKSFGILVGAPAAIGLLMADTALKTANVEIVTY 226
PduB_Lact       DAGDIE--MQYTARASFACQKAFGAPIGRAYGLVCGAPAGIGVIMADIAAKAANVDIIAY 209
PduB_Citr       AAGHVE--LQYTARASYALEKAFGAPLGRACGVIVGAPAAIGVLMADTAIKSANVDVVAY 217
PduB_Ente       EAGHIE--CQYTARASYACNKVFGAPVGKAFGILVGAPAAIGVVMADTALKSANVDVVSY 215
PduB_List       EAGHIE--LQYTARASHALNTAFGAPVGKAFGLMVGAPAGIGVVMADTAVKSANVDVVAY 213
PduB_Eco        EAGHLE--LQYTARASYALEKAFGAPLGRACGVIVGAPAAVGVLMADTALKSANVDVVAY 216
PduB_Salm       EAGHIE--LQYTARASYALEKAFGAPIGRACGIIVGAPASVGVLMADTALKSANVEVVAY 216
PduB_Kleb       EAGHIE--LQYTARASYALEKAFGAPVGRACGVIVGAPASVGVLMADTALKSANVEVVAY 216
PduB_Quas       EAGHLE--FQYTARASYACEKAFNAPIGKSFGLVVGAPAAIGIVLADTVVKAANVDVISY 206
PduB_Desu       DAGHLE--FQYTARASHALEKAFGAPLGRAFGLIVGAPAAIGVVCCDTAVKAAEVQVIGY 220
PduB_Prop       DAGHLE--FQYTARASYALNKVFGAPIGKAFGITVGAPAAIGIVLADTAVKASTIDVVSY 208
PduB_Butt       PAGHLE--FQYTARASHALNKAFGAPVGKSFGMTCACPAAIGVLIADAAAKSAIIEPIGY 206
PduB_Romb       SAGHLE--FQYTARASYALNKAFGAPIGKSFGITVGAPAAIGVLLADTAVKAANVDVVGY 214
PduB_Azos       PAGHLE--FQYTARASYALNKAFGAPIGQAFGITVGAPAAIGVLLADTAAKAATIDAVGY 220
PduB_Mega       EAGHLE--FQYSARASYCLEKALGAKFGKAFGMTCAGPAAIGVVLADTAVKAANVEVVSY 215
PduB_Fuso       SVGHIE--LQYTARASYAINKAFGAPLGKAFGLIVGAPAAIGVVIADIAVKAASVEVLAY 217
PduB_Stre       EAGHLE--FQYTARASYAINKAFGAPLGKSFGLICAGPAAIGVVLADTAVKAANVEVVSY 207
PduB_Pelo       DAGHIE--LQYTARASYAINKAFGAPVGKAFGLIVGAPAAIGVLMSDVAVKTANVEVVGY 211
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EutL_Mini       FPPPT-ETNFAAAW---LTGSLPACQAAAEAYAEAVVRIA----AE-PYE---------- 218
EutL_Morg       VAPPS-ETNYSAAF---LTGSQAACQAACNAFTEAVLDIA----RN-PIQ---------- 216
EutL_Fict       YGPPS-ETNYGGGL---VTGTESACRAAAEAFREAIISIA----KS-PRS---------- 216
EutL_Melg       YKPPS-ETNFGGGL---LTGSQSSCKSATQAFMDTVIRIA----EN-PKV---------- 216
EutL_Domi       FAPPS-ETNFSGGL---LTGSQSSCQAAADAFRQTILILT----AN-PKS---------- 216
EutL_Levi       TPPPS-ETNFMGAV---LTGTQSACQAAALAFQDAVLEVA----RR-PIE---------- 215
EutL_Sali       YGPPT-ETNFGGAL---LTGSQSACQAAADAFRDAVRSIA----DS-PLS---------- 215
EutL_Photo      FAPPS-ETNFGGGH---LAGSQAACRAACEAFQAAVLEVA----RN-PIA---------- 217
EutL_Alki       FKPPS-ETNFGGAL---MAGSQSACKAACQAFSDAVVEVA----AH-PLK---------- 217
EutL_Spor       YGPPT-ETNFGGAL---LTGSQSACRAACDAFQRAVIDVT----LN-ALK---------- 214
EutL_Brev2      FGPPT-ETNFGGAL---LTGSQSACSAAAEAFAEAVRSVA----AT-PVK---------- 215
EutL_Fusi       YGPPT-ETNFAGGL---LTGSQESCRAACDAFARAVEQTA----SE-PRD---------- 216
EutL_Pseu       YEPPS-ETNFGGGL---LTGTQSACNAACAAFAEAVKAIA----AR-PRE---------- 216
EutL_Tepi       FGPPS-ETNFAGGH---LTGSQSACKAACDAFAAAVMEVA----KY-PKR---------- 217
EutL_Vago       YGPPS-ETNFAGGL---LTGSQSACQAACDAFAQAVQSVA----AN-PKS---------- 217
EutL_Hath       FGPPS-ETNFGGAL---LTGSQSACKAACDAFADAVKFVA----AN-PTD---------- 217
EutL_Cell       FGPPS-ETNFGGGL---LTGTQSACHAACAAFAEAIKAVA----DN-PRD---------- 216
EutL_Hala       YGPPS-ETNFGGAL---LTGSQSACQAACNAFANAVKSVA----DK-PCN---------- 216
EutL_Brev       FGPPS-ETNFGGAL---LTGSQSACRAACDAFAAAVQFVA----DN-PTS---------- 216
EutL_Baci       YGPPS-ETNFGGGL---LTGSQSACKAACDAFAEAVQFVA----EN-PTN---------- 216
EutL_Lach       YAPPS-ETNFGGAL---LTGSQSACKAACDAFAAAVEFVA----DN-PKE---------- 216
EutL_Deth       FAPPS-ETNFAGGL---LTGSQSACKAACDAFAQAVIFVA----EN-PVL---------- 216
EutL_Fuso       FGPPS-ETNFGGGL---LTGSQSACKSACDAFAEAVKFVA----QN-PKK---------- 220
EutL_Natr       YGPPS-ETNFGGGL---LTGSQSACKAACDAFAAAVEYVA----DN-PTK---------- 216
PduB_Eub        GSPSH-NLRMMNEFVAGVTGDIAAVQKAMDVGKETGCQLLTALGIT-PISIQDVAEECGE 244
PduB_Blau       MTPDM-GTAHSNEVILALSGDAGAVKEAVLNARQIGLELLIAMGSY-PEIPGTP------ 272
PduB_Rumi       MTPDQ-GTSHSNEVIVAVTGDADAVKNAVLTARDLGLQLLVSMGSY-PESPATP------ 239
PduB_Clost      WSPAY-KTSYSNECVTTIYGDSEAVKQALITAREVGINVLSKIGST-PTSQSTP------ 272
PduB_Paen       ASPDK-GTARSNEIIVTITGDSGAVRQSVISARDVGVSVLRSMGHN-PVSMTQSN----- 279
PduB_Lact       ASPGK-GTSLTNEAMIHISGDSGAVRQAVVTARDVGIKLLSTLGSE-PKN-DYP------ 260
PduB_Citr       NSPAK-GTSFTNEVILIVSGDSGAVRQAVRSARDVGLTLLETMGGK-APSATTP------ 269
PduB_Ente       ATPQN-GQSFSNEVTMTITGDSGAVRQAIISARDIGCQLLGTMGST-PKN-DQP------ 266
PduB_List       SSPAD-GTSFSNEVILCISGDSGAVRQAVISAREIGKKLLGALGDE-PKN-DRP------ 264
PduB_Eco        SSPAQ-GTSYSNEVILIISGDSGAVARRSSPHAKSVKPCFRLSAIH-RKTIALPT----S 270
PduB_Salm       SSPAH-GTSFSNEAILVISGDSGAVRQAVTSAREIGKTVLATLGSE-PKN-DRP------ 267
PduB_Kleb       SSPAH-GTSFSNEAILVLSGDSGAVRQAVISAREIGKTILSTLGCE-PKN-DRP------ 267
PduB_Quas       SSPAK-GTSFTNEVILTFSGDSGAVRQALITAREVGLDLLGTLGGK-PASTTVP------ 258
PduB_Desu       ASPAK-GTSFTNEAILFISGDSGAVRQALIAAREVGIALLSTLGDK-PQSLTRP------ 272
PduB_Prop       ATPQH-GQSFSNEVTMTFSGDSGAVRQAVIAAREVGKTLLGAFGGD-VVSTTTP------ 260
PduB_Butt       ASPAN-GTSFSNEVIFTFAGDSGAVRQAVIAAREVGLQLLATLDPAPIQSATKP------ 259
PduB_Romb       STPGNGGTSYSNEVILTFSGDSGAVRQSIIAAREVGKQLLSTLSNEELKSSTIP------ 268
PduB_Azos       ASPGS-GTSYSNEVIFLFTGDSGAVRQAVIAAREVGKQVLATLDPAEIKSVTRP------ 273
PduB_Mega       ASPGNGKTSYSNEVILCFSGDSGAVRQAVKAAIVVGKKLLGALGDE-PKSTTTP------ 268
PduB_Fuso       SSPSKG-TSYSNEAILAICGDSGAVKQAVLAAKEVGVKLLEAMGGE-APSASHP------ 269
PduB_Stre       SSPSNG-TSYSNEVILTVTGDSGAVRQAVSAAREVGLNLLGSLGEQ-AVSTTKP------ 259
PduB_Pelo       GSPASG-TSYSNEVILQVTGDSGAVRQAVLAAKEVGVKLLEAMAGP-APSSTKP------ 263
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EutL_Mini       -RHFTAFSR---------------------     226
EutL_Morg       -RA---------------------------     218
EutL_Fict       -Y----------------------------     217
EutL_Melg       -Y----------------------------     217
EutL_Domi       -Y----------------------------     217
EutL_Levi       -Y----------------------------     216
EutL_Sali       -K----------------------------     216
EutL_Photo      -N----------------------------     218
EutL_Alki       -Y----------------------------     218
EutL_Spor       -F----------------------------     215
EutL_Brev2      -R----------------------------     216
EutL_Fusi       -II---------------------------     218
EutL_Pseu       -I----------------------------     217
EutL_Tepi       -Y----------------------------     218
EutL_Vago       -Y----------------------------     218
EutL_Hath       -F----------------------------     218
EutL_Cell       -Y----------------------------     217
EutL_Hala       -Y----------------------------     217
EutL_Brev       -Y----------------------------     217
EutL_Baci       -Y----------------------------     217
EutL_Lach       -E----------------------------     217
EutL_Deth       -Y----------------------------     217
EutL_Fuso       -I----------------------------     221
EutL_Natr       -F----------------------------     217
PduB_Eub        DYLKRNMSPAVCQEEKAASIHINKKCDEER     274
PduB_Blau       -YL---------------------------     274
PduB_Rumi       -YLQ--------------------------     242
PduB_Clost      -YI---------------------------     274
PduB_Paen       --L---------------------------     280
PduB_Lact       SYI---------------------------     263
PduB_Citr       -YI---------------------------     271
PduB_Ente       SYI---------------------------     269
PduB_List       SYI---------------------------     267
PduB_Eco        EFSEADL-----------------------     277
PduB_Salm       SYI---------------------------     270
PduB_Kleb       SYI---------------------------     270
PduB_Quas       -YI---------------------------     260
PduB_Desu       -YI---------------------------     274
PduB_Prop       -YI---------------------------     262
PduB_Butt       -YI---------------------------     261
PduB_Romb       -YI---------------------------     270
PduB_Azos       -YI---------------------------     275
PduB_Mega       -YI---------------------------     270
PduB_Fuso       -YI---------------------------     271
PduB_Stre       -YI---------------------------     261
PduB_Pelo       -YI---------------------------     265
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