Supplementary Information

Bioconversion of crude glycerol into 1,3-propanediol(1,3-PDO) with bioelectrochemical system and zero-valent iron using *Klebsiella pneumoniae* L17

Da Seul Kong[1], Eun Joo Park[1], Sakuntala Mutyala[1], Minsoo Kim[1], Yunchul Cho[2], Sang-Eun Oh[3], Changman Kim[4,5*] and Jung Rae Kim[1,*]

Corresponding authors

Dr. **Changman Kim**

Advanced Biofuel and Bioproducts Process Development Unit,

Lawrence Berkeley National Laboratory, Emeryville, CA, 94608, USA

E-mail address: cmkim0408@gmail.com ; Phone: +82-10-4566-2661

Prof. **Jung Rae Kim**

School of Chemical Engineering,

Pusan National University, Busan 46241, Republic of Korea

E-mail address: j.kim@pusan.ac.kr; Phone: +82.51.510.2393, Fax: +82.51.512.8563

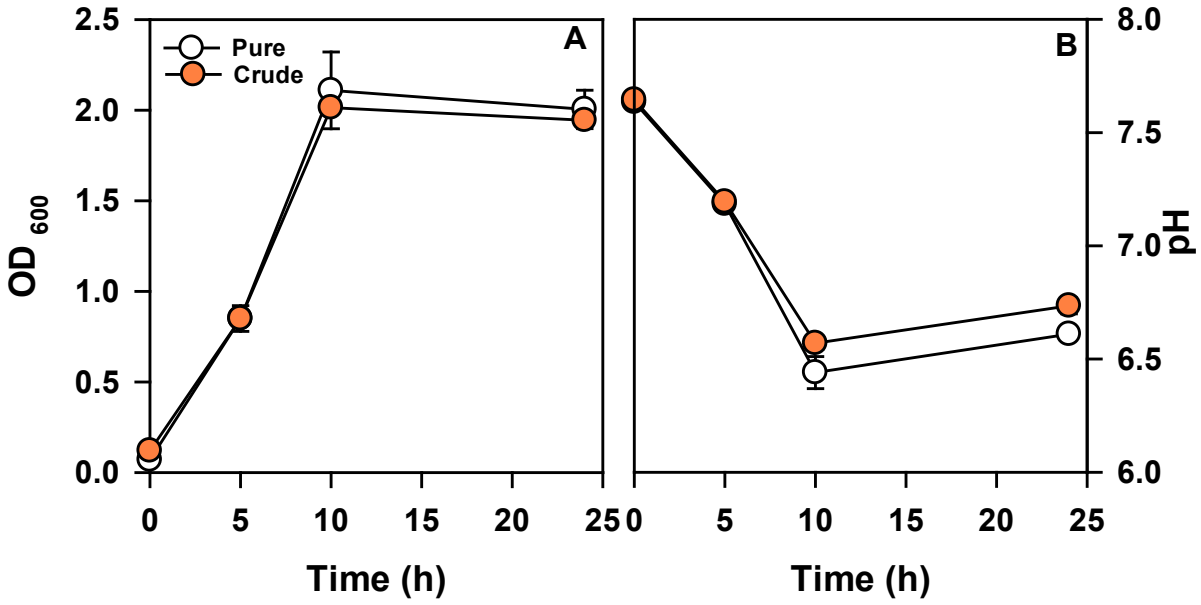

Figure S1. comparison OD and pH of pure and crude glycerol. (A) cell growth (OD) and (B) pH

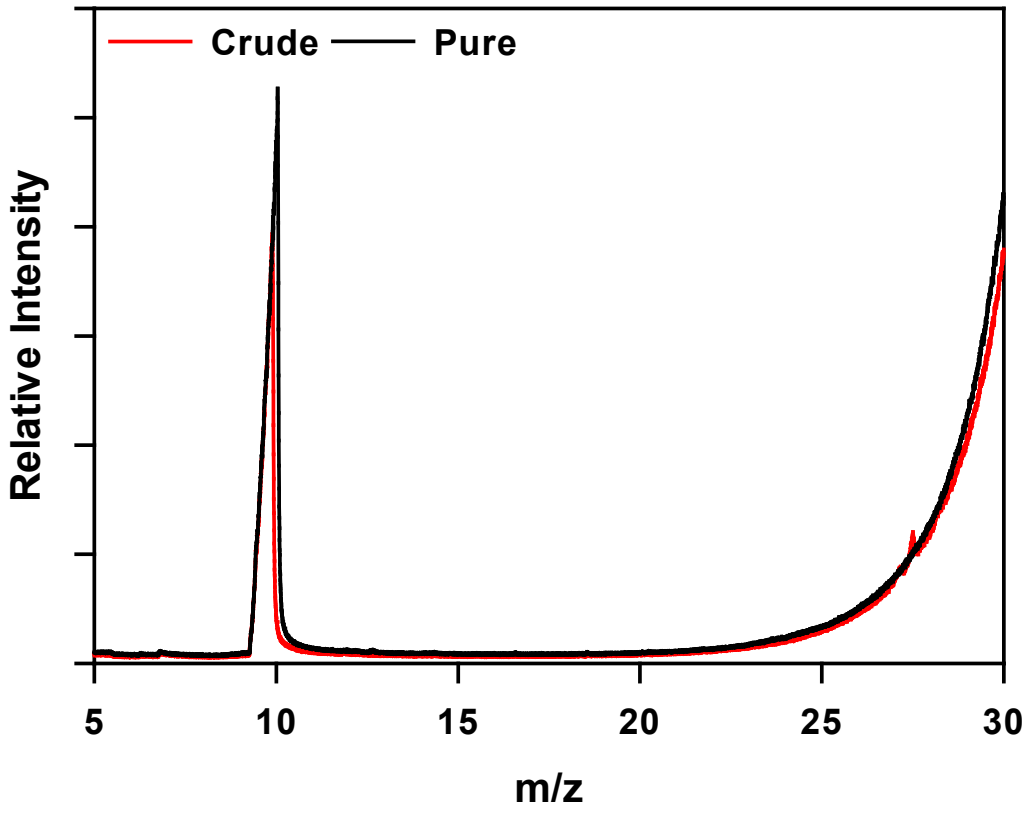

Figure S2. comparison of pure and crude glycerol in GC-MS. (A) cell growth (OD) and (B) pH

Table S1. The reactions and results of in silico metabolic flux analysis

Reaction No.	Reaction	Crude	Pure
Dipyr01	acetyl-CoA + 2 NADH -> Ethanol + 2 NAD + CoA	63.5148	74.884
Dipyr02	Pyruvate + Q + 2 H+ -> QH2 + Acetate	0	0
Dipyr03	acetyl-CoA + ADP -> Acetate + ATP + CoA	3.7404	4.6889
Dipyr04	Formate -> CO2 + H2	67.2552	79.5729
Dipyr05	NADH + Pyruvate <-> Lactate + NAD	0	0
Dipyr06	NADH + Oxaloacetate <-> Malate + NAD	0	0
Dipyr07	2 Pyruvate + NADH -> 2 CO2 + 2,3-butanediol + NAD	0	0
Dipyr08	Fumarate + NADH -> NAD + Succinate	0	0
Energy01	NADH + Q <-> NAD + QH2 + 2 H+	0	0
Energy03	NADPH + NAD -> NADP + NADH	33.6276	39.78645
Energy04	FADH + Q -> FAD + QH2	0	0
Energy05	NADP + NADH + 2 H+ -> NADPH + NAD	33.6276	39.78645
Energy06	ADP + Pi + 3 H+ <-> ATP	0	0
Energy07	ATP + AMP <-> 2 ADP	0	0
Energy08	ATP -> ADP + Pi	70.9956	84.2618
Energy09	Formate + Q <-> H+ + 2 QH2 + CO2	0	0
Energy10	H2 + Q -> QH2 + 2 H+	0	0
Energy11	ATP + NAD -> ADP + NADP	0	0
Energy12	Lactate + Q -> Pyruvate + QH2	0	0
Gly05	Glyceraldehyde-3-P <-> Dihydroxyacetone-P	-67.2552	-79.5729
Gly06	Glyceraldehyde-3-P + Pi + NAD <-> NADH + 1,3-biP-glycerate	67.2552	79.5729
Gly07	1,3-biP-glycerate + ADP <-> 3-P-glycerate + ATP	67.2552	79.5729
Gly08	3-P-glycerate <-> 2-P-glycerate	67.2552	79.5729
Gly09	2-P-glycerate <-> PEP	67.2552	79.5729
Gly10	PEP + ADP -> Pyruvate + ATP	67.2552	79.5729
Gly11	Pyruvate + ATP -> PEP + AMP + Pi	0	0
Gly12	Pyruvate + CoA + NAD -> NADH + CO2 + acetyl-CoA	0	0
Gly13	Oxaloacetate + ATP -> PEP + CO2 + ADP	0	0
Gly14	PEP + CO2 -> Oxaloacetate + Pi	0	0
Gly15	CoA + Pyruvate -> acetyl-CoA + Formate	67.2552	79.5729
GlyP-01	Glycerol + ATP -> Glycerol-3-P + ADP	0	0
GlyP-02	Glycerol-3-P + NAD <-> Dihydroxyacetone-P + NADH	0	0
GlyP-03	Glycerol + PEP -> Glycerol-3-P + Pyruvate	0	0
GlyP-04	Glycerol + NAD -> Dehydroxyacetone + NADH	67.2552	79.5729
GlyP-05	ATP + Dehydroxyacetone <-> ADP + Dihydroxyacetone-P	67.2552	79.5729
GlyRP-01	Glycerol -> 3-hydroxypropionaldehyde	40.4395	18.4513
GlyRP-02	3-hydroxypropionaldehyde + NADH <-> 1,3-propanediol + NAD	23.96015	13.91455
GlyRP-02-R	1,3-propanediol + NAD <-> 3-hydroxypropionaldehyde + NADH	0	0

GlyRP-03	3-hydroxypropionaldehyde + NAD -> 3-hydroxypropionate + NADH	16.47935	4.53675
GROWTH	41.3 ATP + 3.5 NAD + 18.2 NADPH + 0.1 Glyceraldehyde-3-P + 1.5 3-P-glycerate + 0.5 PEP + 2.8 Pyruvate + 3.7 acetyl-CoA + 1.8 Oxaloacetate + 1.1 α-ketoglutarate -> 41.3 ADP + 41.3 Pi + 3.5 NADH + 18.2 NADP + 3.7 CoA + BIOMASS	0	0
PDO	[1,3-propanediol] -> [1,3-PDO-ex]	15.3782	11.3689
TCA01	acetyl-CoA + Oxaloacetate -> CoA + Citrate	0	0
TCA02	Citrate <-> Isocitrate	0	0
TCA03	Isocitrate + NADP <-> CO2 + NADPH + α-ketoglutarate	0	0
TCA04	α-ketoglutarate + NAD + CoA -> CO2 + NADH + Succinyl-CoA	0	0
TCA05	Succinyl-CoA + ADP + Pi <-> ATP + CoA + Succinate	0	0
TCA06	Succinate + FAD -> FADH + Fumarate	0	0
TCA07	Fumarate + FADH -> Succinate + FAD	0	0
TCA08	Fumarate <-> Malate	0	0
TCA09	Malate + NAD <-> NADH + Oxaloacetate	0	0
TCA10	Isocitrate -> Glyoxylate + Succinate	0	0
TCA11	Glyoxylate + acetyl-CoA -> Malate + CoA	0	0
Trans03	Acetate <-> Acetate-ex	0	0
Trans04	Ethanol <-> Ethanol-ex + H+	3.7404	4.6889
Trans05	CO2 <-> CO2-ex	63.5148	74.884
Trans06	Pi <-> Pi-ex + H+	67.2552	79.5729
Trans08	H2 <-> H2-ex	3.7404	4.6889
Trans11	Lactate <-> Lactate-ex + H+	67.2552	79.5729
Trans12	2,3-butanediol <-> 2,3-butanediol-ex	0	0
Trans13	Glycerol-ex -> Glycerol	0	0