Supplementary Materials: Highly Selective Oxidation of 5-Hydroxymethylfurfural to 5-Hydroxymethyl-2-Furancarboxylic Acid by a Robust Whole-Cell Biocatalyst

Ran Cang †, Li-Qun Shen †, Guang Yang, Zhi-Dong Zhang, He Huang *and Zhi-Gang Zhang *

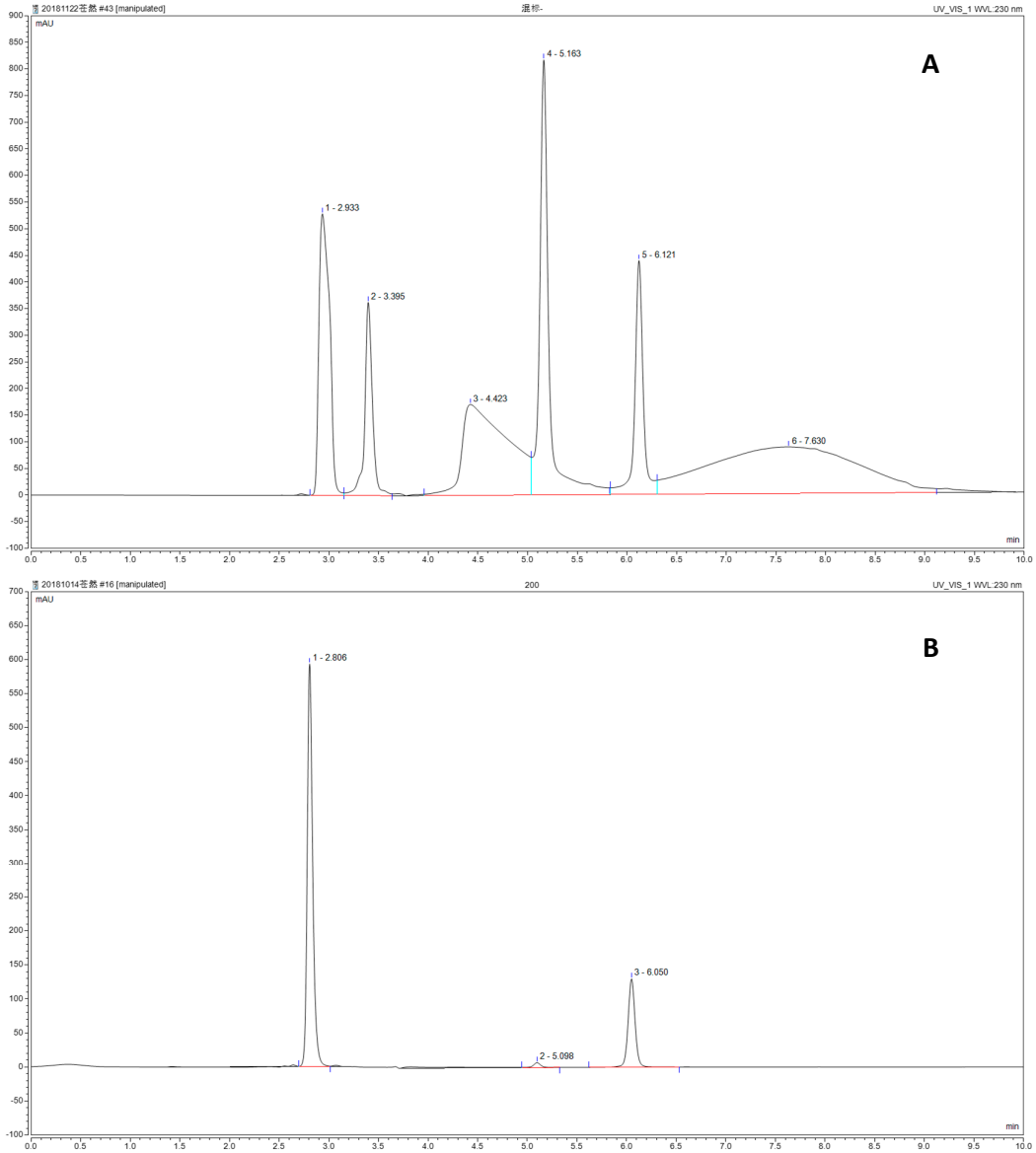


Figure S1. HPLC measurments: (**A**) HMF and its derivatives; (**B**) HMFCA, BHMF products and HMF substrate.

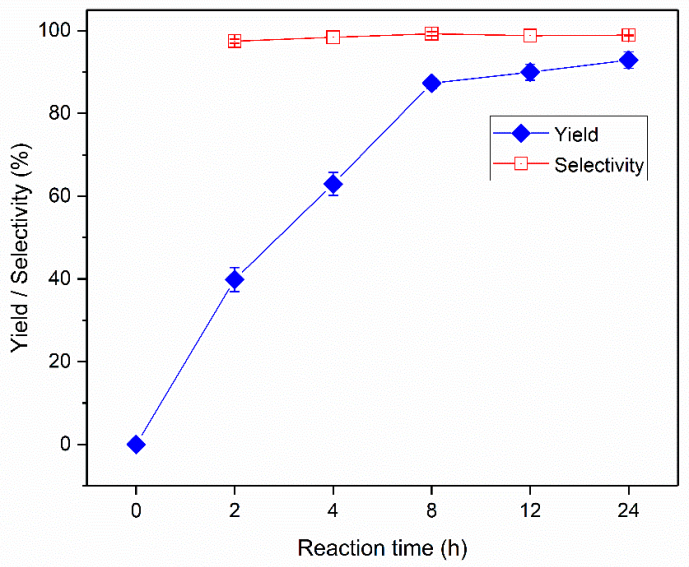


Figure S2. Effects of reaction time on HMFCA synthesis. 150 mM HMF, 0.12 g mL^{-1} microbial cells, 5 mL phosphate buffer (100 mM, pH 7.0), 30 °C, 850 rpm.

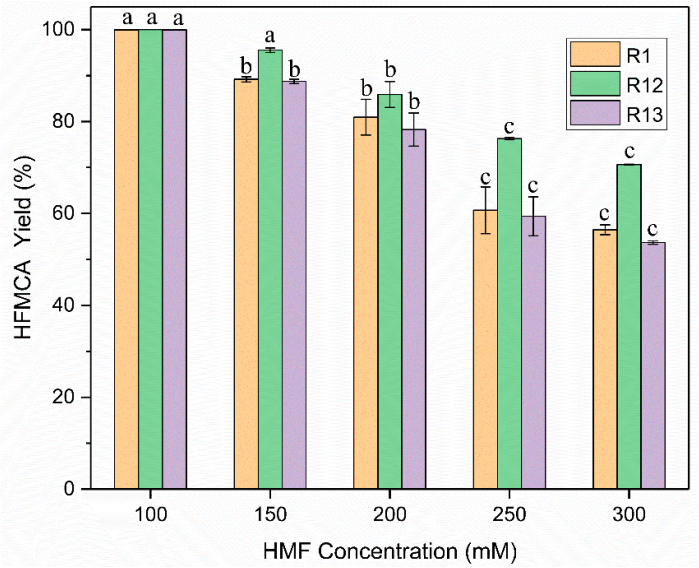


Figure S3. Biocatalytic oxidation of HMF to HMFCA by different *Deinococcus* strains. R1: *Deinococcus* radiodurans R1; R12: *Deinococcus wulumuqiensis* R12; R13: *Deinococcus xibeiensis* R13. Reaction conditions: 100 mM HMF, 0.12 g mL^{-1} microbial cells, 5 mL phosphate buffer (100 mM, pH 7.0), 30 °C, 850 rpm.

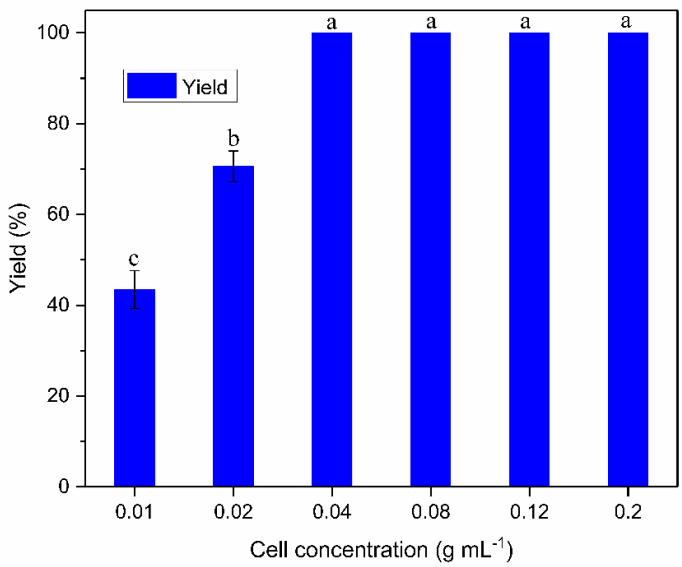
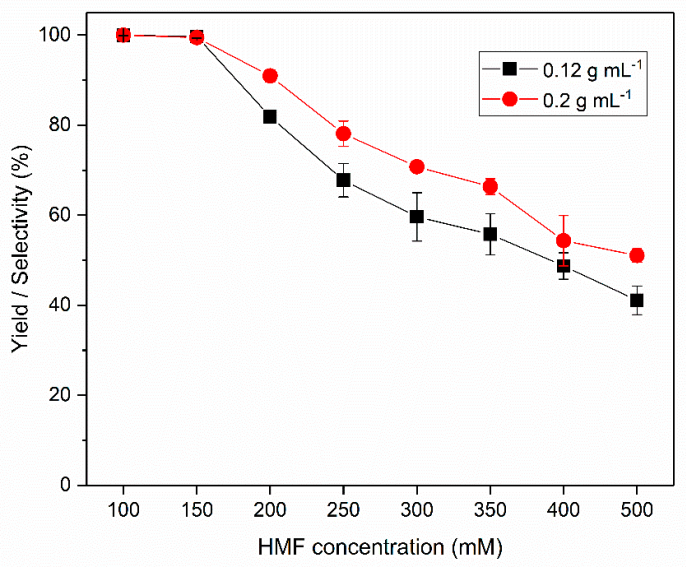
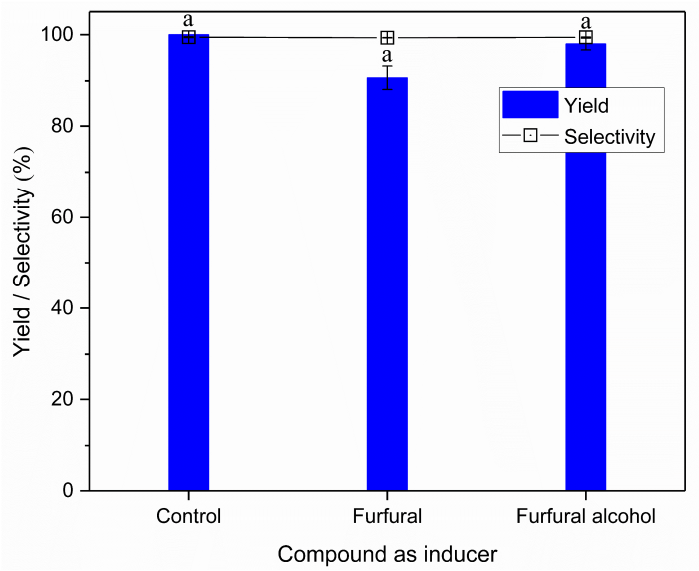


Figure S4. Effect of cell concentration. Reaction conditions: 40 mM HMF, 5 mL phosphate buffer (100 mM, pH 7.0), designated concentration of microbial cells, 850 rpm, 30 °C for 12 h.

a) Increasing biocatalyst dosage from 0.12 g mL^{-1} to 0.2 g mL^{-1}.



b) Using 5 mM of furfural and 5 mM of furfural alcohol respective induced D. *wulumuqiensis* R12 cell



c) Turning pH by $NaHCO_3$ / NaOH solution

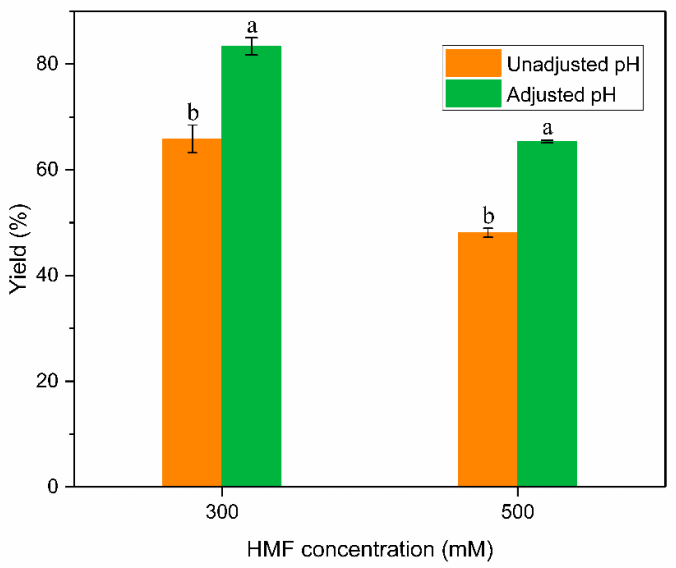


Figure S5. Optimizing reaction condition for HMFCA synthesis by using various strategies.

a) pH turning: add 20 μL of NaOH solution (1 M) carefully to the reaction system followed with rapid stir, meanwhile monitor the change of pH. Repeat the step until the pH go back to 7.0.
adjusting the pH of the reaction system to the range of 7.0 − 8.0 by using NaOH each 3 h for the first 12 h and each 12 h for the rest 36 h.

b) biocatalyst dosage: increasing microbial cells dosage from 0.12 g mL^{-1} to 0.2 g mL^{-1}, designated HMF concentration, 5 mL phosphate buffer (100 mM, pH 7.0), 850 rpm, 35 °C for 24 h.

c) Effect of induced R12 cells by furfural and furfural alcohol on HMFCA synthesis. Reaction condition: 100 mM HMF, 0.12 g mL^{-1} cells in 5 mL phosphate buffer (100 mM, pH 7.0) under 850 rpm, 30 °C for 8 h.