Supplementary material

Dual-enzyme and NADPH co-embedded organic-inorganic hybrid nanoflowers prepared using biomimetic mineralization for the asymmetric synthesis of (*R*)-(-)-pantolactone

Author names and affiliations

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Table S1 Plasmids used in this study

Plasmid	Relevant genotype or characteristic	Reference or source
pET28a (+)	P_{T7lac}, Ori (ColE1), Kan^R	Novagen [a]
pET21a (+)	P_{T7lac}, Ori (ColE1), Amp^R	Novagen
pET28a-*Cdu*CPR	Expression vector, pET28a(+) derivative, Kan^R, containing the conjugated polyketone reductase gene from *C. dubliniensis* CD36 (*Cdu*CPR)	Cheng et al., 2019
pETgGDH	Expression vector, pET21a(+) derivative, Amp^R, containing the glucose dehydrogenase gene from *Themoproteus sp.* GDH-1 (TgGDH)	Aiba et al., 2015

[a] Merck KGaA, Darmstadt, Germany.

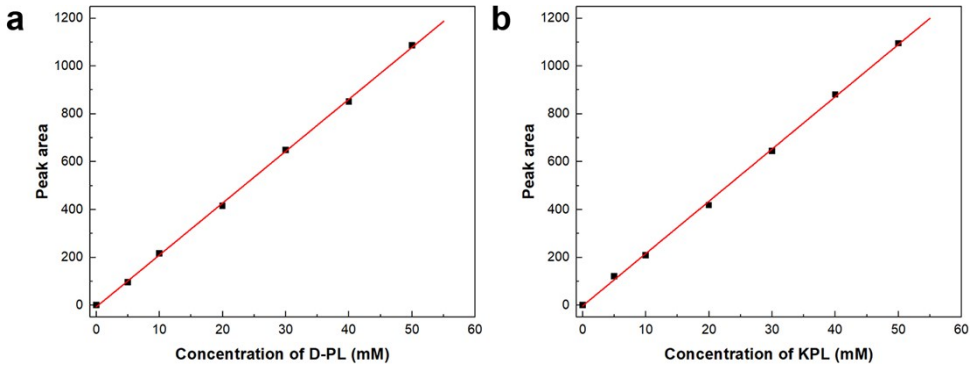

Fig. S1. The standard curves of (*R*)-PL (a) and KPL (b) by GC (external standard method).

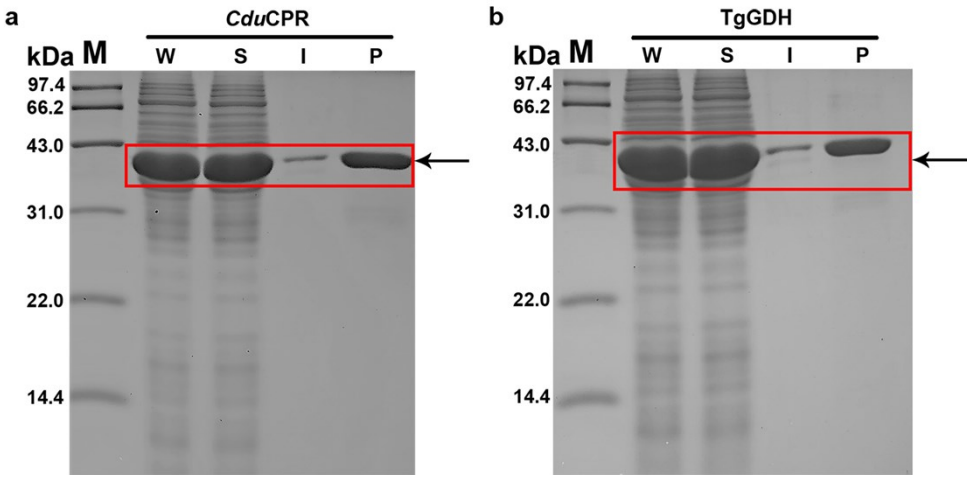

Fig. S2 The expression of *Cdu*CPR and TgGDH in *E. coli* BL21 (DE3) analyzed by SDS-PAGE. M: protein markers; W: whole cell proteins; S: soluble part; I: insoluble part of whole cell protein and P: purified protein.

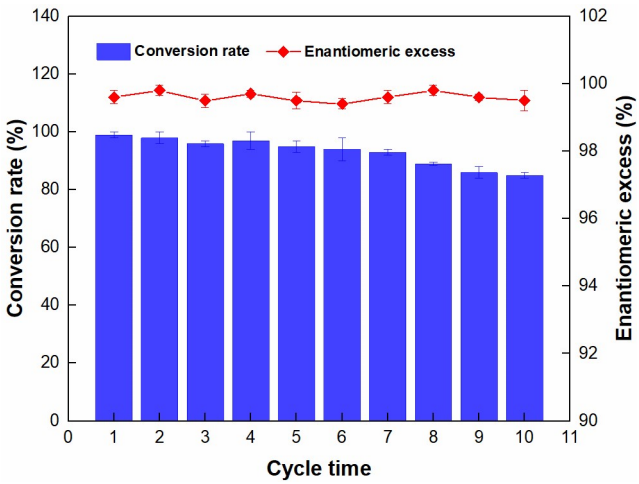

Fig. S3 Reusability of SA-$NADP^+$ in the dual-enzymatic synthesis of (*R*)-pantolactone.

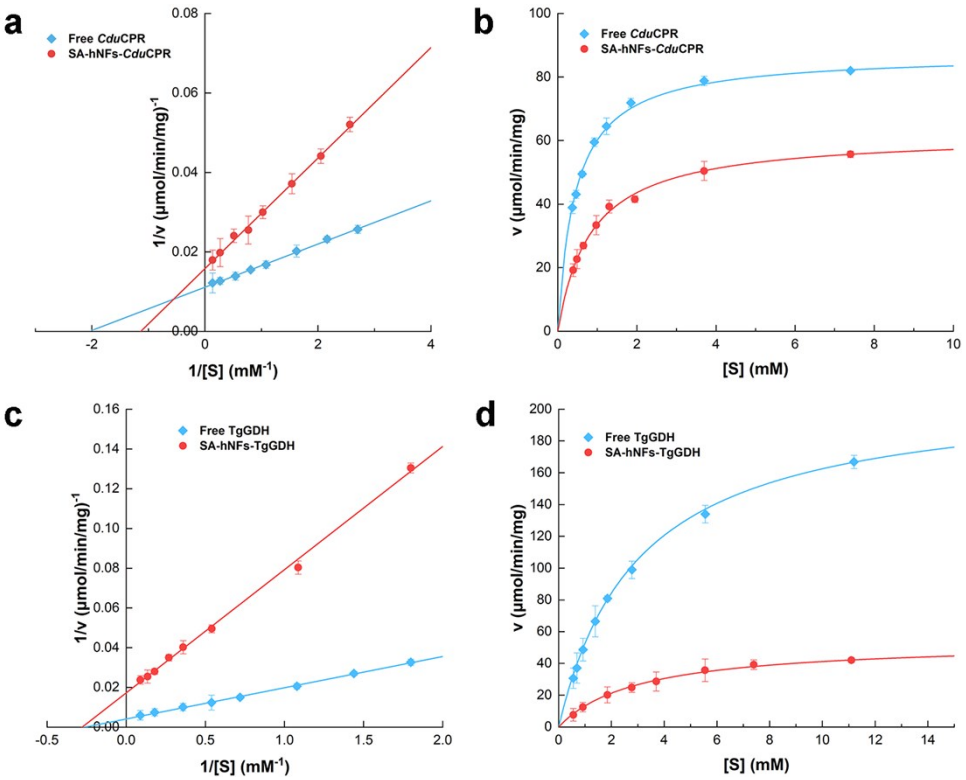

Fig. S4 Lineweaver-Burk Plots and substrate saturation plots for ketopantoyl lactone of *Cdu*CPR/TgGDH@$Ca_3(PO_4)_2$ hybrid composites with or without the SA coated.

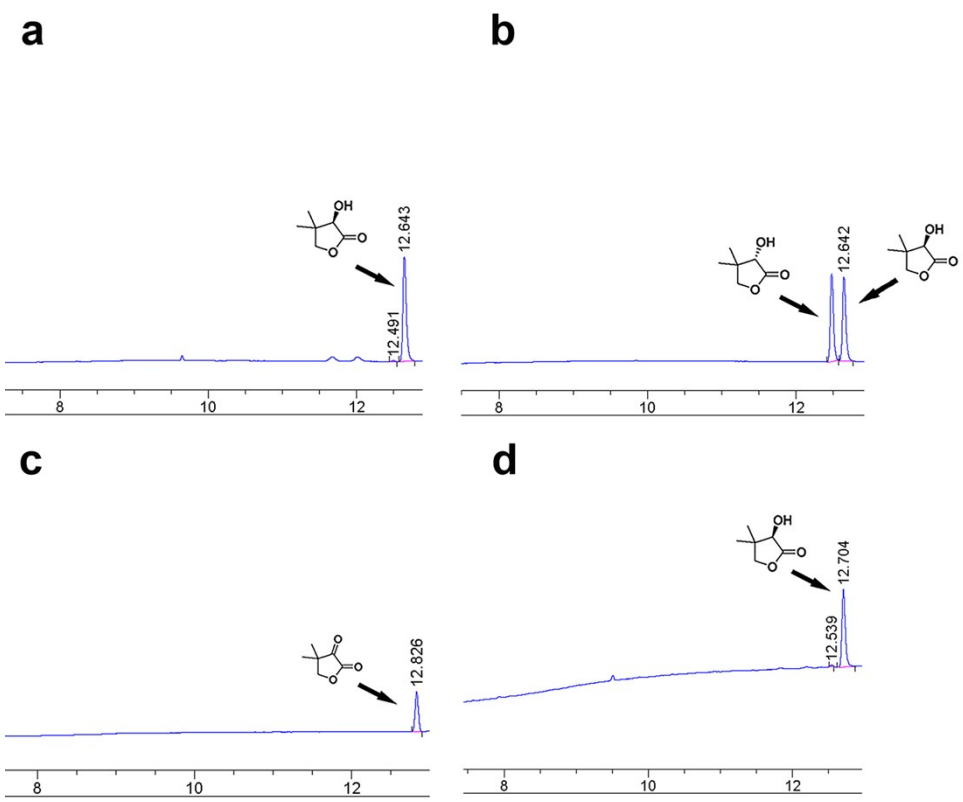

Fig. S5 GC analysis of biotransformation reaction. (a) (*R*)-PL reference standard; (b) (*RS*)-PL reference standard; (c) Ketopantoyl lactone reference standard; (d) The product with the SA-coated *Cdu*CPR/TgGDH@$Ca_3(PO_4)_2$.

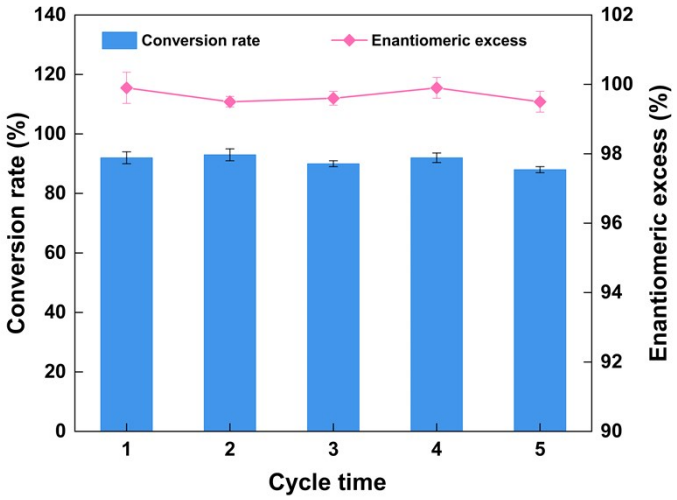

Fig. S6 Catalytic efficiency of mixed two different particles containing *Cdu*CPR and *Tg*GDH respectively.

The catalytic efficiency of mixed two different particles was performed under the optimum reaction condition. A total of 4 mL 100 mM potassium phosphate buffer (pH 7.0) contained 75 mM glucose, two different particles (containing 5 mg/mL of *Tg*GDH, 1 mg/mL of *Cdu*CPR) and 2.5 mg/mL SA-$NADP^+$. The substrate stock solution was prepared by dissolving 32 mg KPL in 1 mL acetic acid/sodium acetate (50 mM, pH 2.6). The stock solution of KPL was pumped into the reactor at 25 μL/min. The reaction pH was maintained at pH 7.0 by titration with 2 M Na_2CO_3. After the feeding was finished, the reaction was stirred at 30 °C for another 20 min. The concentration of (*R*)-PL and KPL in the reaction supernatant was determined by gas chromatography.

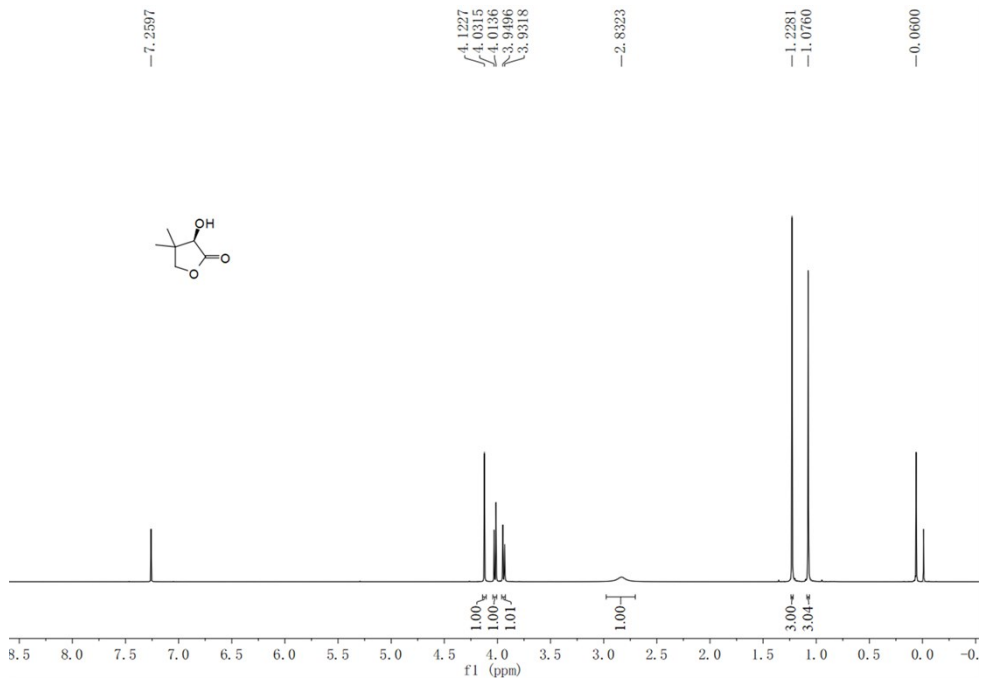

Fig. S7 ^{1}H NMR spectrum of the purified product (*R*)-PL catalyzed using SA- $NADP^{+}$ *Cdu*CPR/TgGDH@$Ca_3(PO_4)_2$. ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.12 (s, 1H), 4.02 (d, *J* = 8.9 Hz, 1H), 3.94 (d, *J* = 8.9 Hz, 1H), 2.83 (s, 1H), 1.23 (s, 3H), 1.08 (s, 3H).

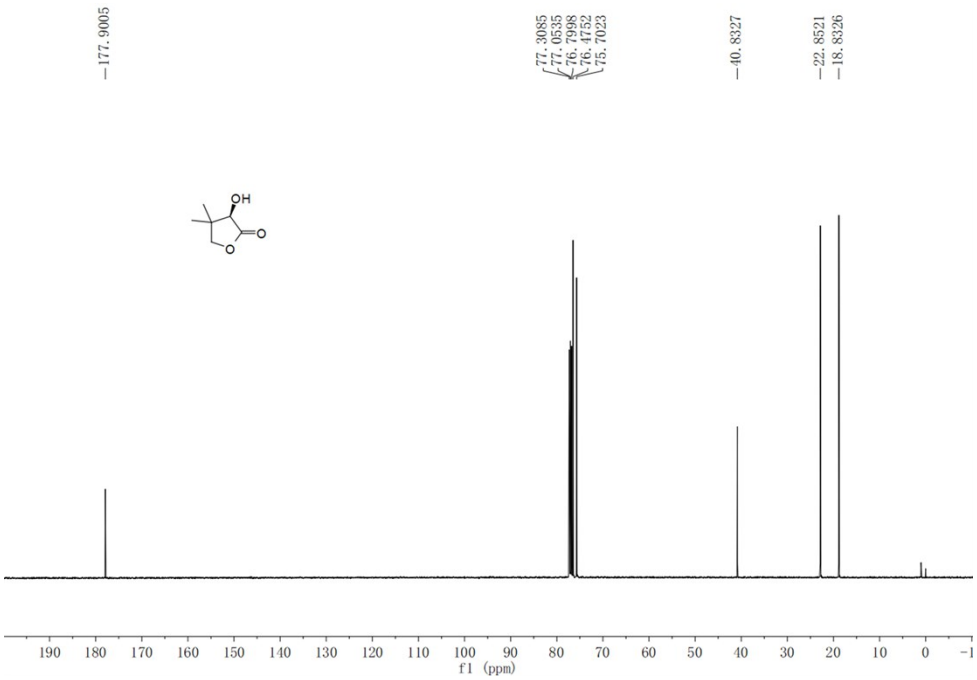

Fig. S8 ^{13}C NMR spectrum of the purified product (*R*)-PL catalyzed using SA- $NADP^+$ *Cdu*CPR/TgGDH@$Ca_3(PO_4)_2$. ^{13}C NMR (125 MHz, $CDCl_3$) δ 177.90 (s), 76.48 (s), 75.70 (s), 40.83 (s), 22.85 (s), 18.83 (s).