Supporting Information

Photo-enzyme-coupled catalysis for selective oxidation of 2,5-diformylfuran into 2,5-furandicarboxylic acid

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Molecular docking simulations

The interaction between lipase and ethyl acetate was studied through molecular docking simulations. The lipase structure was obtained from the Protein Data Bank (PDB ID: 1IBS), and the ethyl acetate ligand was retrieved from PubChem. AutoDock 4.0 was employed for semi-flexible docking studies, while PyMOL 2.5.4 was used to analyze the active sites. Prior to docking, water molecules were removed and hydrogen atoms were added to both ethyl acetate and 1IBS, and the rotational bonds of the ethyl acetate molecule were set. A docking box of appropriate size was defined to fully encapsulate 1IBS for molecular docking, and the result with the lowest binding energy from 50 docking runs was selected. The docking result, with a binding energy of −2.44 Kcal/mol (less than −1.2 Kcal/mol), indicated a favorable docking outcome.

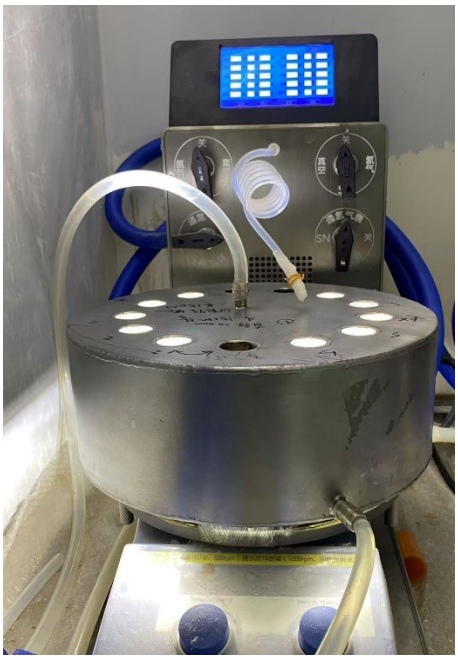

Fig.S1 Photochemical parallel reactor

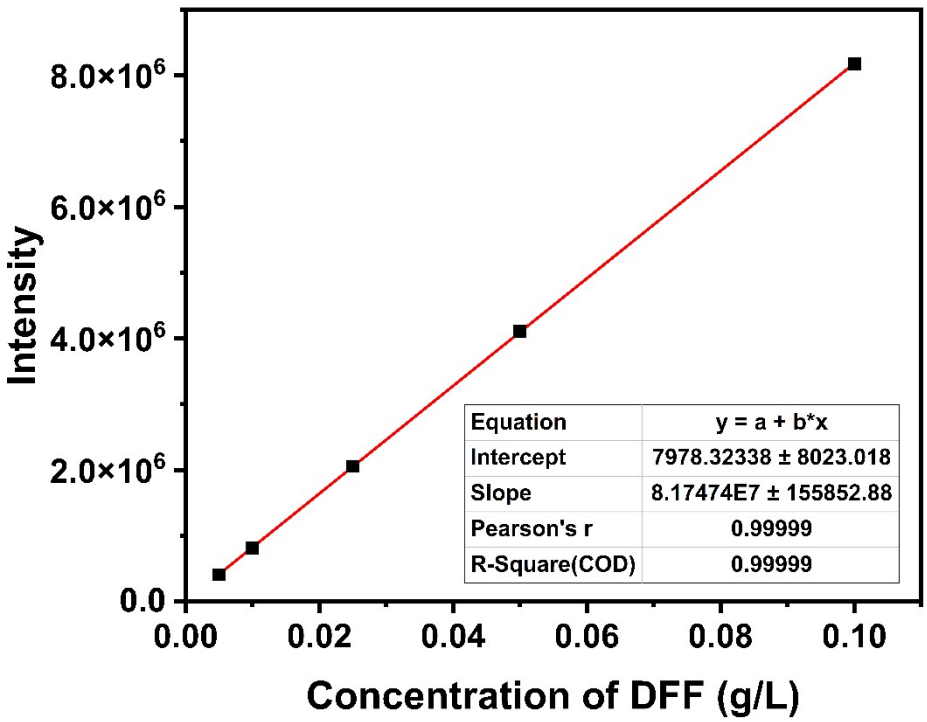

Fig.S2 Standard curves of DFF by HPLC.

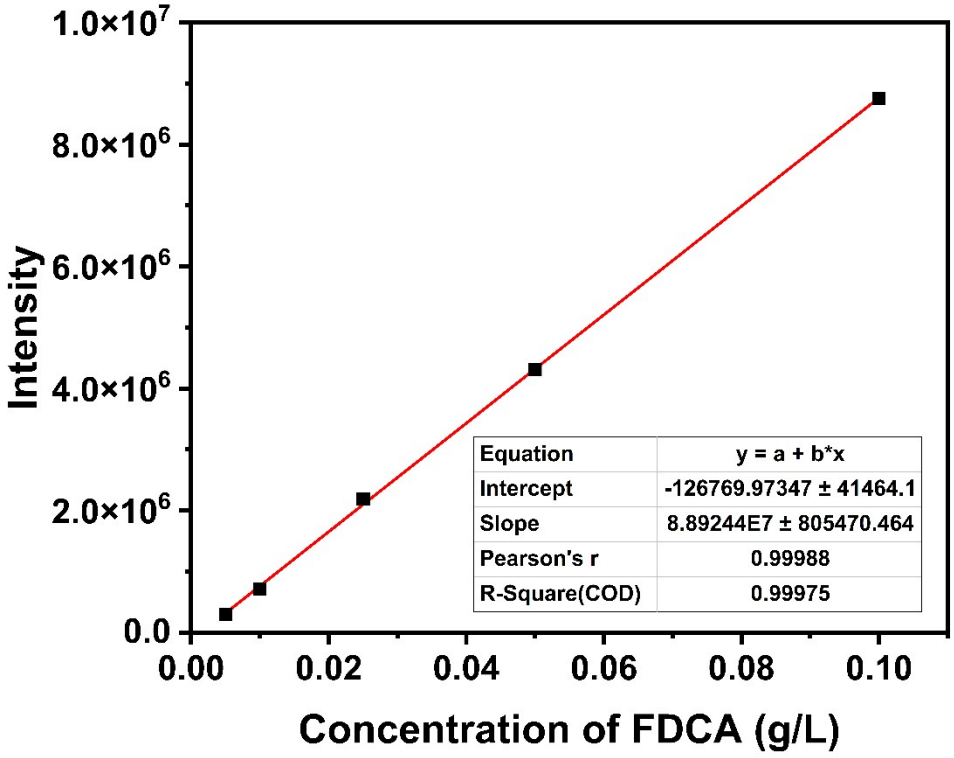

Fig.S3 Standard curves of FDCA by HPLC.

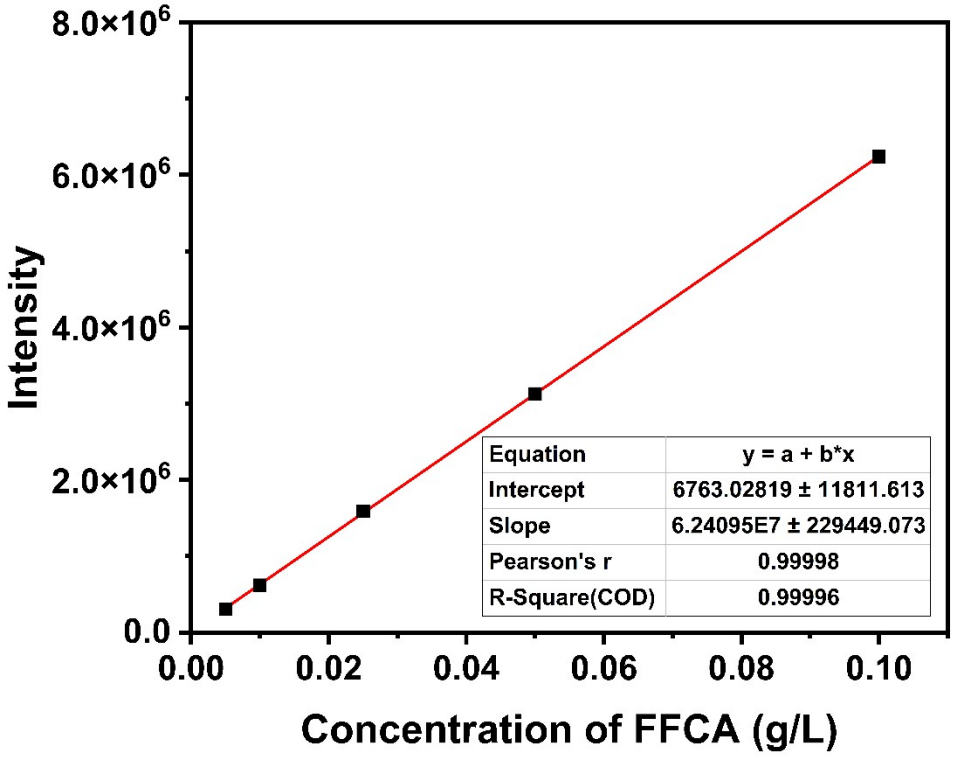

Fig.S4 Standard curves of FFCA by HPLC.

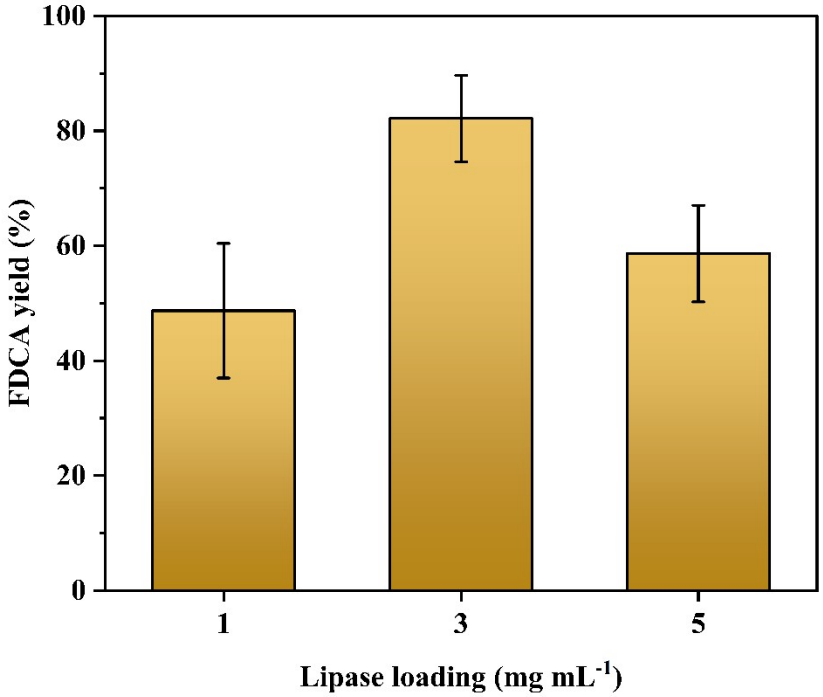

Fig.S5 Effect of lipase loading on FDCA yield.

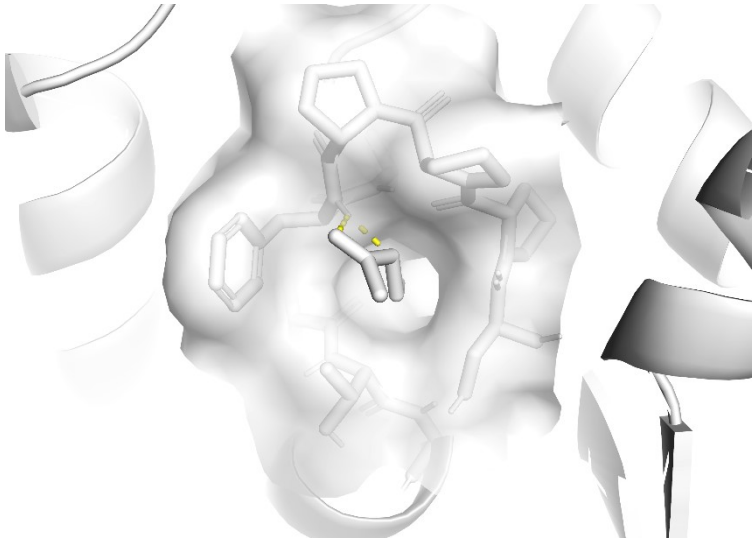

Fig.S6 Schematic representation of the active site pocket of Lipozyme 435 with ethyl acetate by molecular docking simulation.

Table S1 Organic elemental analysis

Lipozyme 435	Weight (mg)	N (wt%)	C (wt%)	H (wt%)	S (wt%)
Before	1.993	2.39	66.14	7.604	0.173
After	1.872	2.58	65.83	7.663	0.140