SUPPORTING INFORMATION

Dynameric host frameworks for the activation of lipase through H-bond and interfacial encapsulation

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1. General methods

Reagents were obtained from Manchester organics (trialdehyde**1**) and Sigma Aldrich (compounds **2-5**) and used as received. ^{1}H-NMR spectra were recorded on an ARX 300 MHz Bruker. Chemical shifts are reported as δ values (ppm) with $CDCl_3$ (^{1}H-NMR δ 7.26) as an internal standard. Fluorescence spectra were recorded in Perkin Elmer LS-55, using a quartz cuvette (2 ml), with excitation and emission slit width at 8. UV-vis spectra were obtained from Shimadzu UV-2401PC, using a quartz cuvette (1 ml).

2.Typical synthesis of the dynamic dynamers

Benzene-1,3,5-tricarbaldehyde (**1**, 0.1 mmol) or isopthalaldehyde (**5**, 0.1 mmol) was added into a flask with 0.1 mmol poly(ethylene glycol) bis(3-aminopropyl) terminated (**2**,Mn~1500) and 5 mL solvent MeOH, together with 0.1 mmol corresponding amide functionalized amine*N*-(2-aminoethyl)acetamide (**3**) or dendrimer PAMAM (**4**, ethylenediamine core, generation 1.0). The reaction mixture was stirred at 60°C for 3-4 days, and monitored by ^{1}H-NMR until the equilibrium was reached. The solvent was thereafter removed and 10 mL mini-Q H_2O was subsequently added to prepare the stock solution for further analysis.

3. Fluorescence studies ofthe binding between dynamers 6-8 and lipase

Stock solution of lipase (45.5 μM) was prepared by adding 9 mg of lipase powder (molecular mass 33 kDa) into 6 mL of PBS buffer solution (100 mM, pH 7.0). Stock solution of dynamer/monomer (10 mM) was prepared by adding 0.01 mmol of chemicals into 1 mL mini-Q H_2O.

The procedure was started by adding 500 μL of lipase stock solution to 1.5 mL of PBS buffer (100 mM, pH 7.0) in a 2 mL quartz cuvette. The initial fluorescence of lipase alone was firstly recorded at λ_{exc} =

280 nm and λ_{em} from 290 to 500 nm. Then increasing amount of dynamer/monomer solution was added into the same cuvette to measure the intensity change.

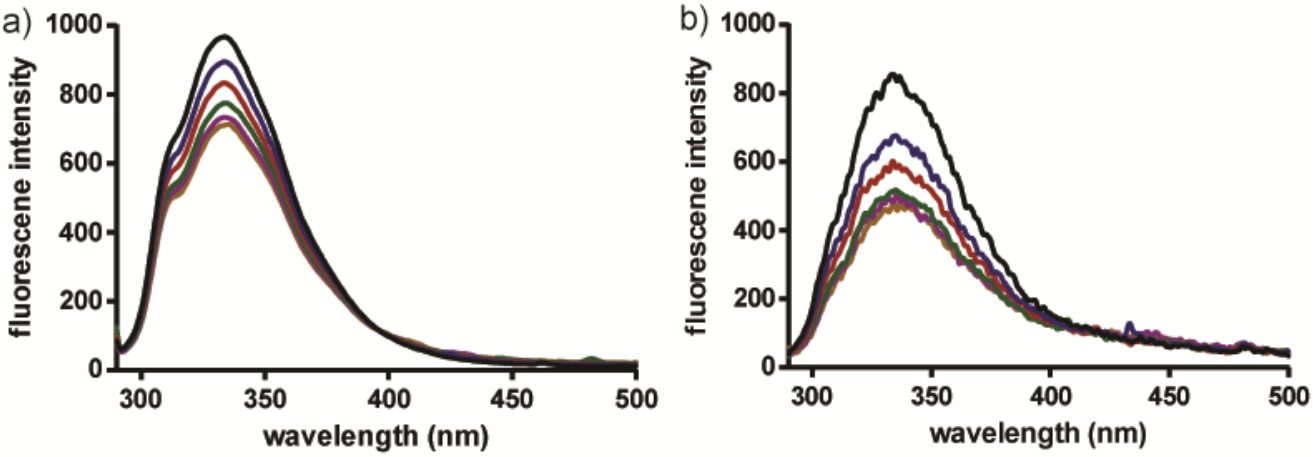


Figure S1. Fluorescence quenching of lipase upon addition of increasing amount of a) amide **3**; b) dendrimer **4**. The concentrations of dynamers are 0 mM, 0.01 mM, 0.025 mM, 0.05 mM, 0.10 mM, 0.15 mM and 0.20 mM respectively from top to bottom.

To calculate the association constant (K_a), the highest fluorescence intensityat 343 nm was used and applied into the plot of Stern-Volmer relation ($I_0/I = 1+K_a$ [P]), where I_0 is the initial fluorescence intensity of lipase alone; I is the intensity of lipase with the presence of dynamers (**6**-**8**) or monomers (**3**-**4**); [P] is the concentration of added dynamers or monomers. For **3** and **4**, the Stern-Volmer relation does not fit well the experimental data.

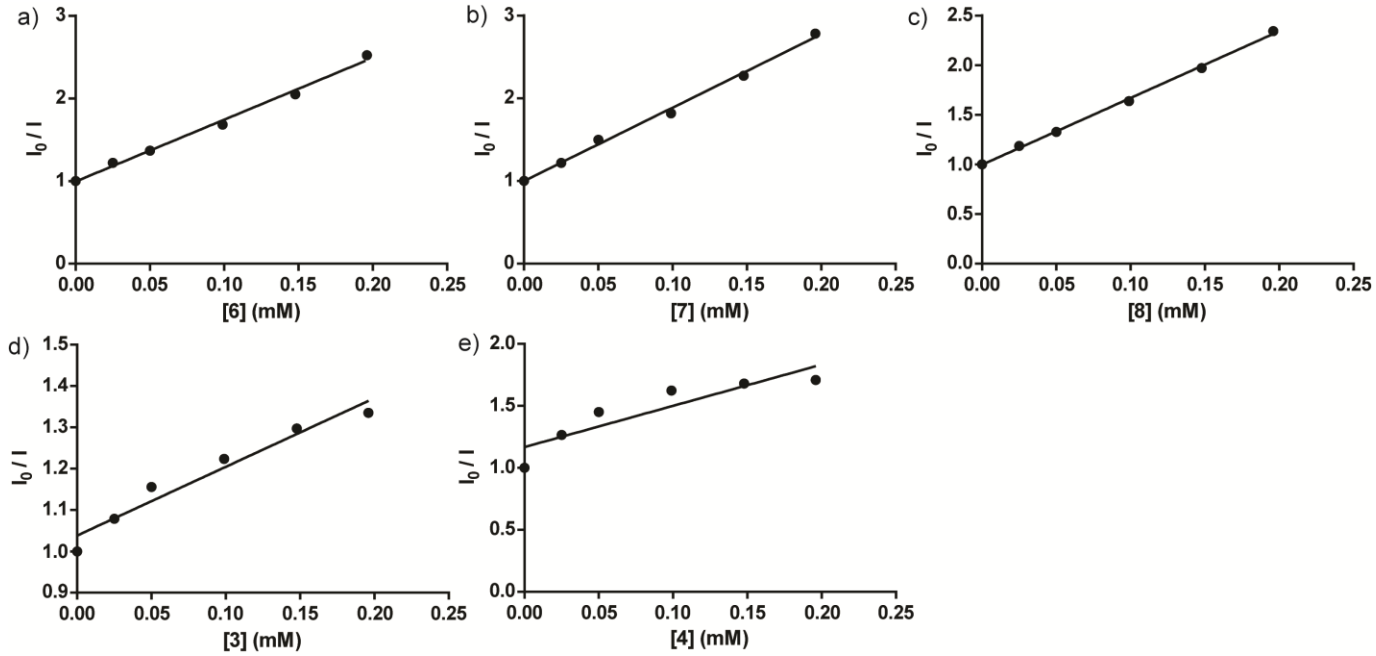
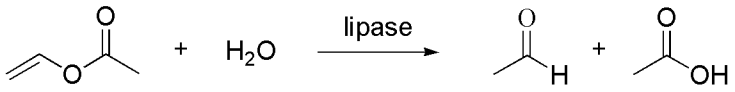


Figure S2. Plots of Stern-Volmer relation for the determination of association constant between lipase and a) dynamer **6**; b) dynamer **7**; c) dynamer **8**; d) monoamide **3**; e) monodendrimer **4**.

4. ^{1}H-NMR studies of the activation effects of the dynamers

The catalytic reactivity of lipase was studied using ^{1}H-NMR spectroscopy, based on the hydrolysis reaction of vinyl acetate (Scheme S1). The formation of product acetaldehyde was followed by ^{1}H-NMR with the time interval of 10 min. The conversions were calculated through the integrations of methyl group in vinyl acetate and methyl group in acetic acid.



Scheme S1. Hydrolysis reaction of vinyl acetate catalyzed by lipase.

The same stock solutions of dynamers/monomers used for for fluorescence were also used in this NMR study. Stock solution of lipase used here was prepared by adding 50 mg of lipase powder into 0.5 mL H_2O. The hydrolysis reaction was initiated by adding 0.1mmol of vinyl acetate (8.6 mg) into the NMR tube containing 10 µL lipase solution, 1 mL D_2O and increasing amount of dynamer/monomer solutions. Control experiments without the presence of lipase were also carried out to check the hydrolysis ability of the dynamers/monomers alone.

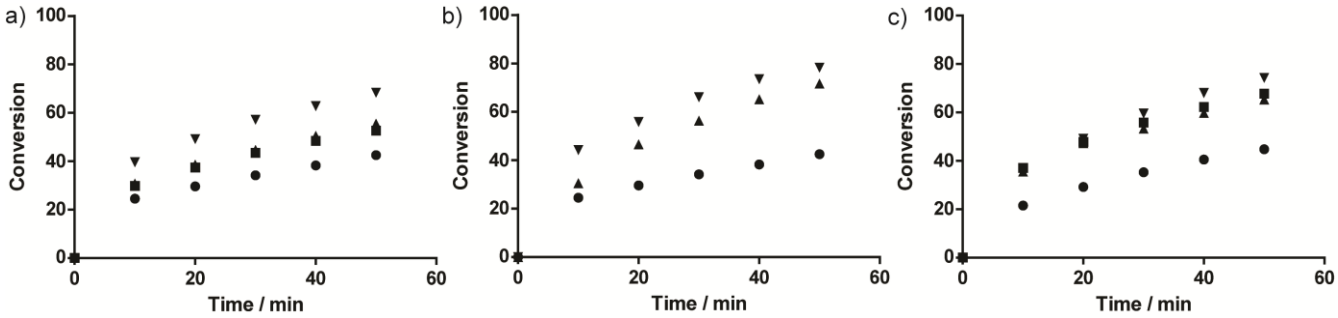


Figure S3. Activity change of lipase on hydrolysis reaction of vinyl acetate, with the gradual addition of a) monoamide **3**; b) dynamer **8**; c) dendrimer **4**, followed ^{1}H-NMR spectroscopy. For a) and b), the added concentrations are 0 (●), 1 (▲), 2 (■) and 3 (▼) mM. For c), the added concentrations are 0 (●), 0.01 (▲), 0.1 (■) and 0.2 (▼) mM.

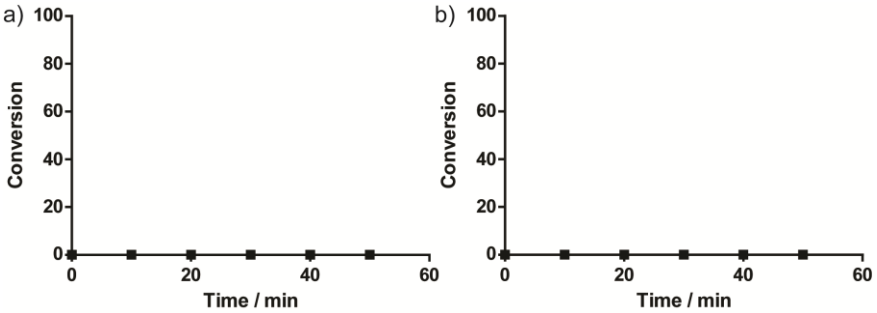


Figure S4. Control experiments of hydrolysis reaction of vinyl acetate in the absence of lipase, with the addition of a) 3 mM of dynamer **6** (●) and monoamide (■); b) 0.3 mM of dynamer **7** (●) and monodendrimer (■), followed ^{1}H-NMR spectroscopy.