

## Supporting Information

### **A novel multiblock copolymer of CO<sub>2</sub>-based PPC-*mb*-PBS: from simulation to experiment**

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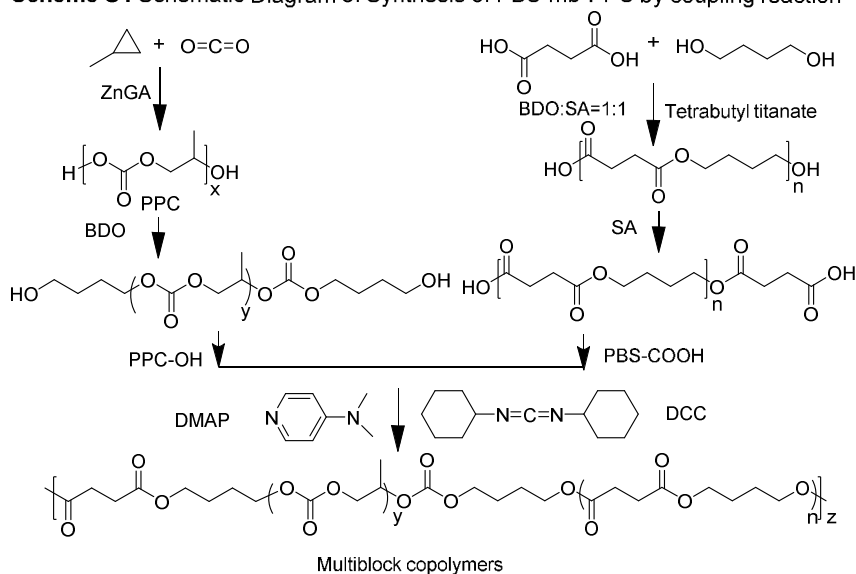
**5 pages, 2 schemes, 5 figures and 1 table**

**Measurement:**

$^1\text{H}$ -NMR spectra of the polyesters were recorded on a Bruker DRX-500 NMR spectrometer at room temperature. Deuterated chloroform ( $\text{CDCl}_3$ ) was used as solvent, chemical shifts were expressed in ppm with respect to tetramethylsilane (TMS). Diffusion ordered spectroscopy (DOSY) experiments were performed with a Bruker DRX-600 NMR spectrometer operating at 600 MHz, using  $\text{CDCl}_3$  as solvent. Number-average molecular mass ( $M_n$ ) and polydispersity index (PDI) of the resultant polymer product were measured using a gel permeation chromatography (GPC) system (Waters 515 HPLC Pump, Waters 2414 detector) with a set of three columns (Waters Styragel 500, 10,000, and 100,000 Å) and chloroform (HPLC grade) as eluent. The GPC system was calibrated by a series of poly-styrene standards with polydispersities of 1.02 standards. The glass transition temperature ( $T_g$ ) of the copolymers was measured by a DSC (Netzsch Model 204) and the measurements were carried out under nitrogen flow from  $-70$  to  $180$  °C at a heating rate of  $5$  °C/min.  $T_g$  of the samples was determined from the second run. The tensile tests were performed using a temperature-controlled tensile tester (New SANS, Shenzhen, China) at  $0$  and  $25$  °C with a crosshead speed of  $50$  mm/min. Five specimens of each sample were tested, and the average results were recorded.

**Film preparation:**

Prior to measurements of mechanical properties, the film samples of PPC, PBS and PPC-*mb*-PBSs copolymers (thickness  $\sim 0.2$  mm) were obtained by solution-cast method. The polyester was dissolved in chloroform (10 wt %) and then cast on a polytetrafluoroethylene (PTFE) dish, followed by evaporation of solvent at  $25$  °C for 24 h. The films were further dried at  $40$  °C in vacuum for 24 h.

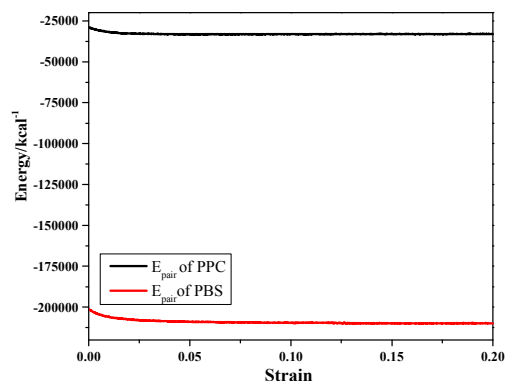
**Scheme S1** Schematic Diagram of Synthesis of PBS-*mb*-PPC by coupling reaction

$$\text{PBS-COOH} + \text{Cyclohexyl-N=N-Cyclohexyl} \longrightarrow \text{Cyclohexyl-N=N-Cyclohexyl-PBS-COO}^-$$

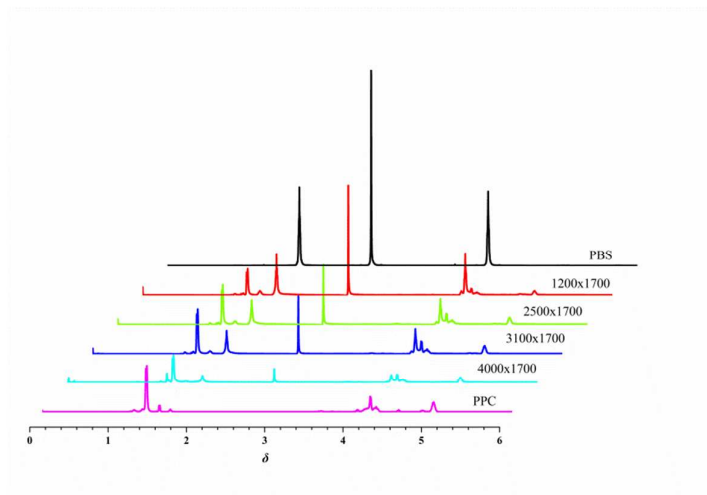
$$\text{PBS-CO-PPC} + \text{Cyclohexyl-NH-C(=O)-NH-Cyclohexyl} \longleftarrow \text{Cyclohexyl-NH-C(=O)-O-PBS-CO-PPC-OH}$$

$$\text{PBS-COOH} = \text{HO}-(\text{CH}_2)_2-\text{C}(=\text{O})-\text{CH}_2-\text{C}(=\text{O})-\text{O}-(\text{CH}_2)_6-\text{O}-(\text{CH}_2)_2-\text{C}(=\text{O})-\text{CH}_2-\text{C}(=\text{O})-\text{OH}$$

$$\text{PPC-OH} = \text{HO}-(\text{CH}_2)_6-\text{O}-(\text{CH}_2)_2-\text{C}(=\text{O})-\text{O}-(\text{CH}_2)_2-\text{C}(=\text{O})-\text{O}-(\text{CH}_2)_6-\text{OH}$$



$E_{\text{pair}}$  = Pairwise energy ( $E_{\text{vdwl}} + E_{\text{coul}} + E_{\text{long}}$ ),  $E_{\text{vdwl}}$  = Vander Waal pairwise energy (includes etail),  $E_{\text{coul}}$  = Coulombic pairwise energy,  $E_{\text{long}}$  = Long-range kspace energy



**Fig. S2**  $^1\text{H}$ -NMR spectra of PPC-mb-PBS copolyester:  $\delta(\text{PC}, \text{CH})=5.0$ ,  $\delta(\text{BS}, \text{CH}_2)=2.7$

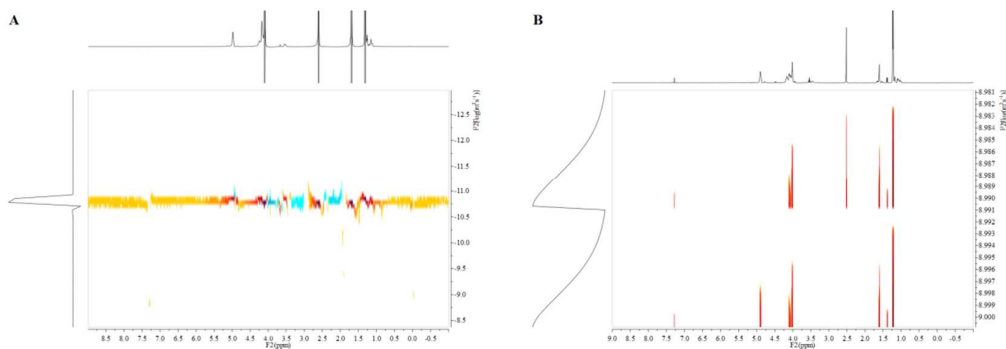


Fig. S3 DOSY spectrum of copolyester : (A) PPC-mb-PBS; (B) Mixture of PPC-OH and PBS-COOH

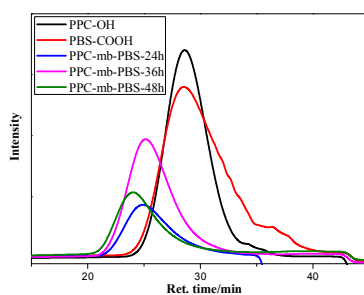


Fig. S4 GPC analysis of PPC-OH, PBS-COOH and multiblock copolymer

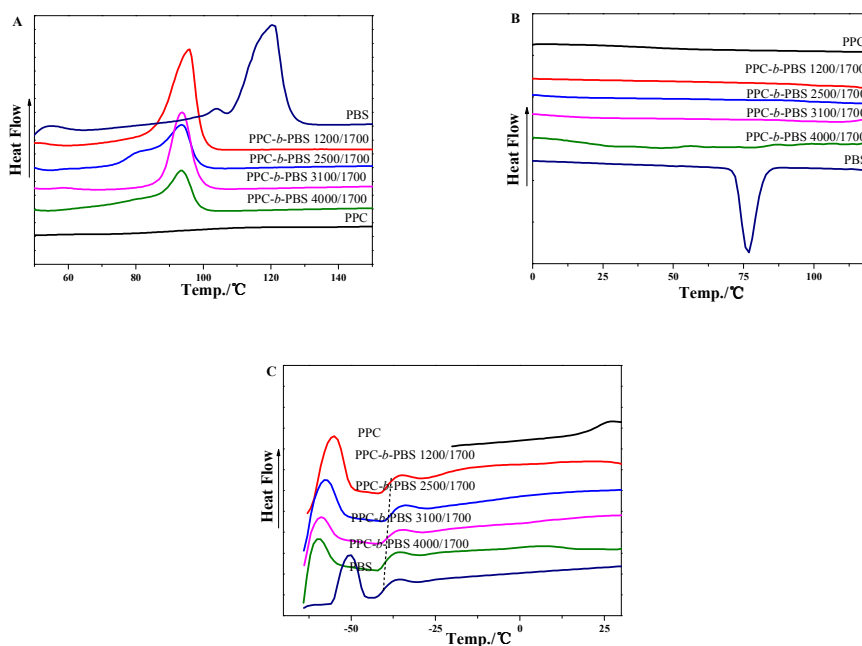


Fig. S5 DSC curves of PPC, PBS and PPC-*mb*-PBS: (A) first heating runs (B) cooling runs; (C) second heating runs

Tab. S1 Comparison of experimental results with calculation datas from simulations of different block sizes

Block length (PPC-b-PBS)	$T_g^a/^\circ\text{C}$	$T_g^b/^\circ\text{C}$	Deviation rate/%
PBS	-40.2	-42.0	4.5
1200/1700	-38.2	-39.1	2.3
2700/1700	-42.5	-38.1	11.5
3100/1700	-41.4	-39.0	6.2
4000/1700	-40.9	-39.9	2.5
PPC	-22.3	23.2	4.0

<sup>a</sup> Measured by DSC. <sup>b</sup> Calculated by molecular dynamic simulation.