

Supporting information

for

**Fabrication of color changeable CO<sub>2</sub> sensitive nanofibers**

by

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**1. Materials and Characterization**

**1.1 Materials.**

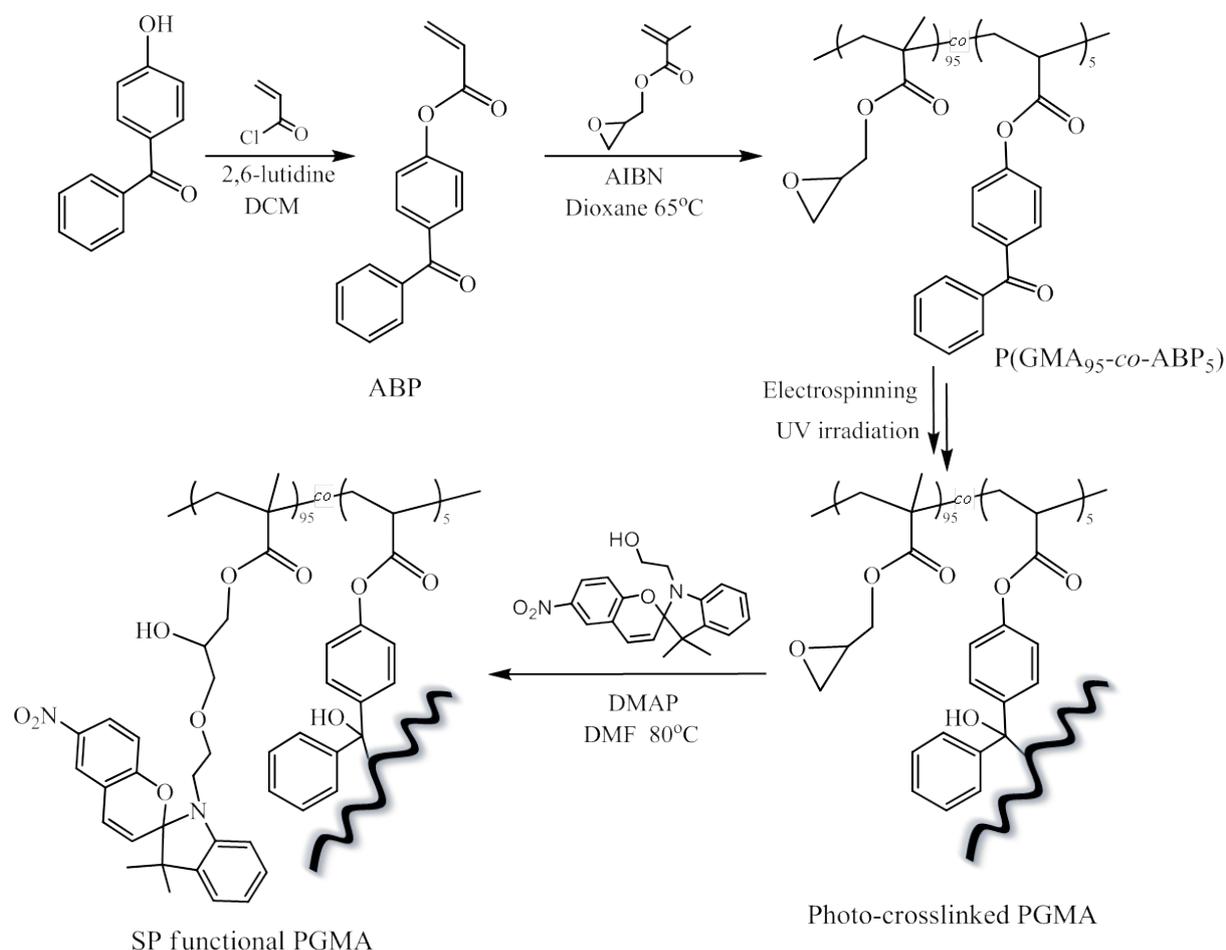
Glycidyl methacrylate (GMA) was purified by a neutral aluminum oxide column. 2,2'-azobisisobutyronitrole (AIBN) was recrystallized twice from methanol, 4-hydroxybenzophenone, 2,6-lutidine, acroloyl chloride and other materials were purchased from Sigma-Aldrich and used without further purification. 1'-(2-Hydroxyethyl)-3',3'-dimethyl-6-nitrospiro[1(2H)-benzopyran-2,2'-indoline] (SP-OH) is commercially available and was purchased from TCI.

**1.2 Characterization**

<sup>1</sup>H NMR spectra were recorded on a Bruker 400 MHz FT-NMR spectrometer in deuterated chloroform using tetramethylsilane as internal standard. FT-IR measurements were recorded on a Nicolet iS10 spectrometer from Thermo Scientific. SEC was performed at 60 °C with DMF as eluent, and the DMF system was equipped with an MZ-Gel SDplus linear 5 μm column, and their molecular weights and distributions were calculated against polystyrene

standards. Scanning electron microscopy (SEM) images were taken with a Zeiss EVO-MA 10 microscope operating at 5 kV. UV-vis absorption spectra were measured on a JASCO V-630 UV/Vis-photospectrometer from 200-800 nm. Water contact angle measurements were conducted using a DataPhysics OCA 20. As a general rule, a minimum of five data points on each sample were measured.

## 2 Synthesis of poly(glycidyl methacrylate-*co*-4-acryloylbenzophenone) P(GMA-*co*-ABP)



**Scheme S1.** Synthetic route of poly(glycidyl methacrylate-*co*-4-acryloylbenzophenone) copolymer P(GMA<sub>95</sub>-*co*-ABP<sub>5</sub>) and its post-modification

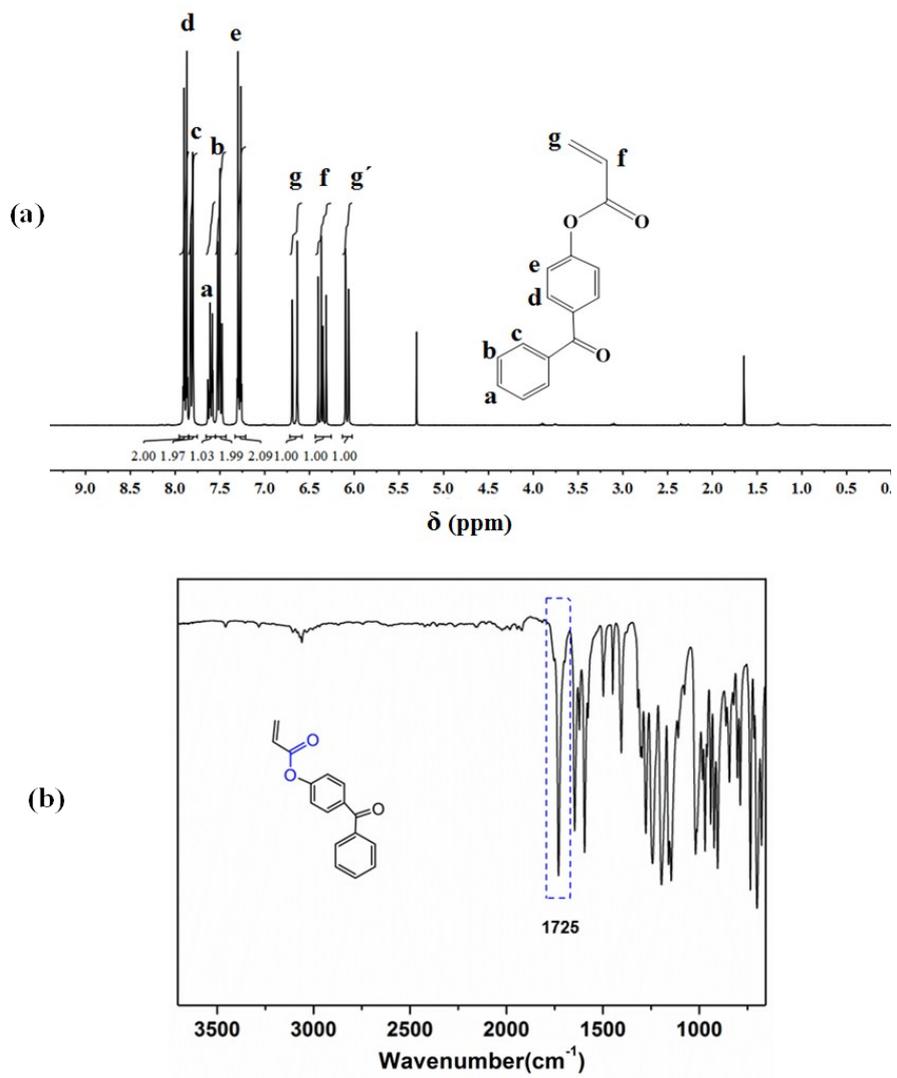
### 2.1 Synthesis of 4-acryloylbenzophenone (ABP)

4-Hydroxybenzophenone (10.00 g, 0.0504 mol) and 2,6-lutidine (6.50 mL, 0.0602 mol) were dissolved in 50mL of methylene chloride in a 100 mL flask, fitted with an overhead stirrer, a

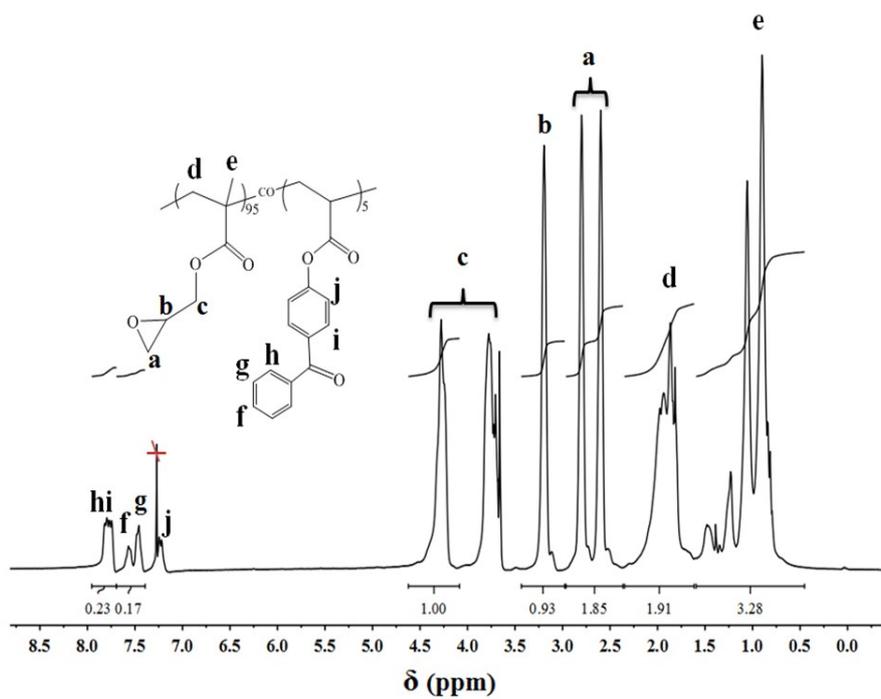
thermometer and an addition funnel. The apparatus was located in an ice bath and cooled to 0-5°C. Then acroloyl chloride (4.50 mL, 0.0555 mol) solution in 10 mL of methylene chloride was added dropwise over the funnel into the flask over a period of 1h. The reaction was kept for 3h. After the reaction was finished, the methylene chloride was removed using rotary evaporation and the solid substance thus obtained was washed with deionized water, DCM and a saturated solution of NaCl. The supernatant liquid was removed and dried over a subnatant liquid with Na<sub>2</sub>SO<sub>4</sub>. The solution was passed through a silica gel column with chloroform as eluent. Finally, 11.12 g (95%) of ABP was obtained. The structure of purified ABP was characterized via <sup>1</sup>H NMR and FT-IR (see Figure S1). <sup>1</sup>H NMR (300 MHz, Dichloromethane-*d*): δ 7.87 (s, 2H), 7.80 (s, 2H), 7.61 (s, 1H), 7.50 (s, 2H), 7.30 (s, 2H), 6.64 (s, 1H), 6.37 (s, 1H), 6.10 (s, 1H). FT-IR: 1725cm<sup>-1</sup>(C=O ester), 1638 cm<sup>-1</sup> (C=C).

## 2.2 Synthesis of P(GMA-*co*-ABP)

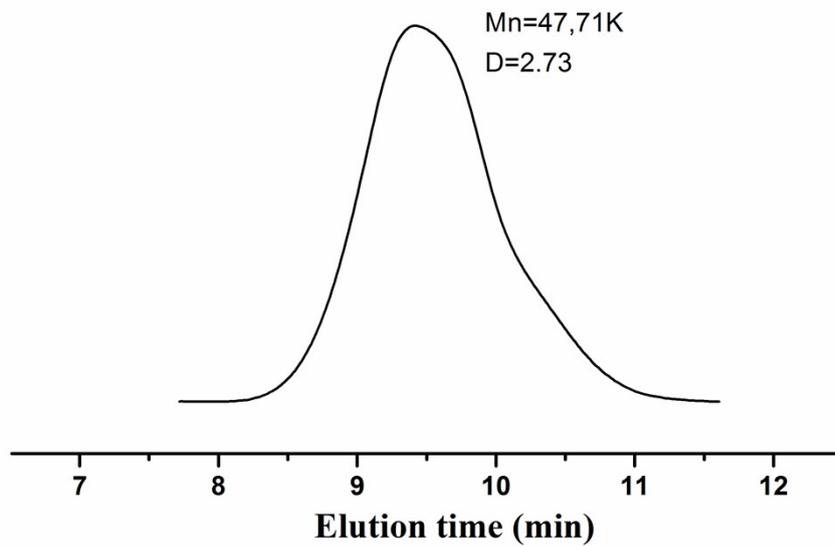
P(GMA-*co*-ABP) was synthesized via Free Radical Polymerization (FRP) using AIBN as an initiator. In a typical polymerization, first (2 g, 14.07 mmol) GMA, (0.187 g, 0.74 mmol) ABP and (0.024 g, 0.15 mmol) AIBN were dissolved in 5ml of 1,4-Dioxne in a 10ml reaction vial with mechanical stirring. Then, the reaction vial was purged with Argon for 30 min and then placed in a preheated oil bath at 70 °C for 8h. Next, the synthesized P(GMA-*co*-ABP) polymerization mixture was cooled down to room temperature and 750ml of methanol were used to precipitate the copolymer. Successively, the polymer was dried in a vacuum oven at 40 °C and the yield was calculated with 97.86 %. The chemical structure was characterized by <sup>1</sup>H NMR and FT-IR (see Figure S3). <sup>1</sup>H NMR (300 MHz, Chloroform-*d*): 5.49 – 5.05 (m, 3H); 4.11 (m, 4H); 2.53 (m, 1H); 1.61 (m, 4H); 1.51 (m, 2H); 1.25 (m, 36H); 0.86 (m, 6H). FT-IR (ATR mode, cm<sup>-1</sup>): 1725 cm<sup>-1</sup> (C=O ester), 904 cm<sup>-1</sup> and 845 cm<sup>-1</sup> (epoxy ring)



**Figure S1.**  $^1\text{H}$  NMR (a) and FT-IR (b) spectra of synthesized ABP



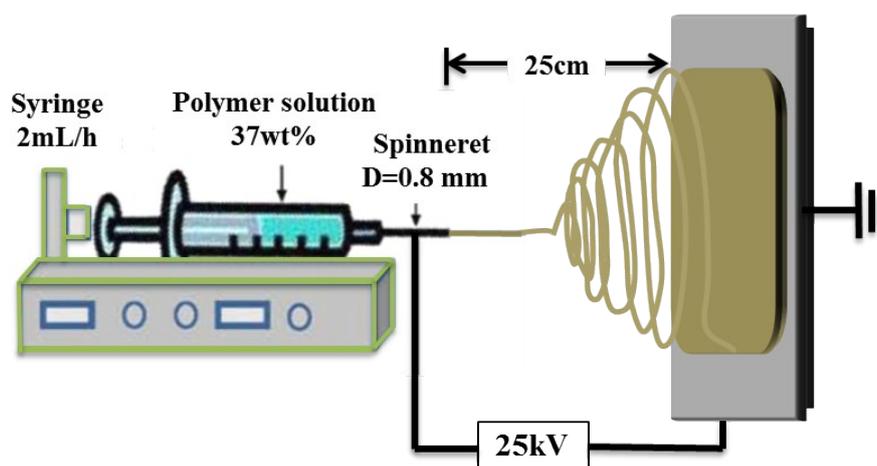
**Figure S2**  $^1\text{H}$  NMR spectrum of P(GMA-co-ABP) in  $\text{CDCl}_3$



**Figure S3.** SEC curve of P(GMA-co-ABP) copolymer in DMF

### 3. Preparation of P(GMA-co-ABP) nanofibers

Electrospinning was performed with 37wt% P(GMA-co-ABP) solution in a mixture of DMF: THF = 7:3 (v: v). The electrospinning apparatus was built with a horizontal alignment, as shown in Fig. S1. The voltage applied on a 0.8 mm diameter needle for electrospinning was 25 kV and the flow rate of the syringe pump was set to 2 mL/h for the experiment. The distance between the tip and the grounded collector was 25 cm. The spun nanofiber mats were dried in a vacuum oven at 40 °C overnight, and then an UV-A light ( $\lambda = 315\text{--}400\text{ nm}$ ) lamp irradiation was used to trigger crosslinking of the nanofiber for 2h. The crosslinked spun nanofiber was immersed in THF for 1 h, and then SEM was used for checking the morphology of nanofibers.



**Figure S4.** Illustration of the electrospinning setup in this work

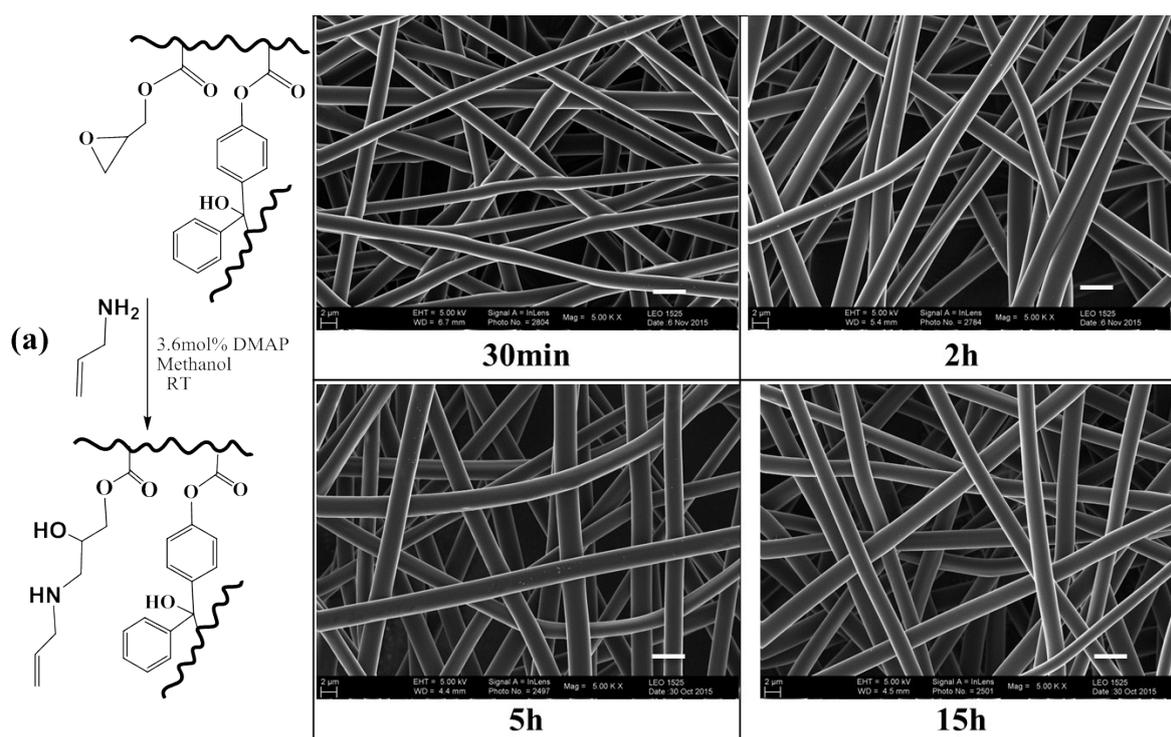
#### **4. General procedure for post-polymerization modification of a photo-crosslinked PGMA nanofibrous mat.**

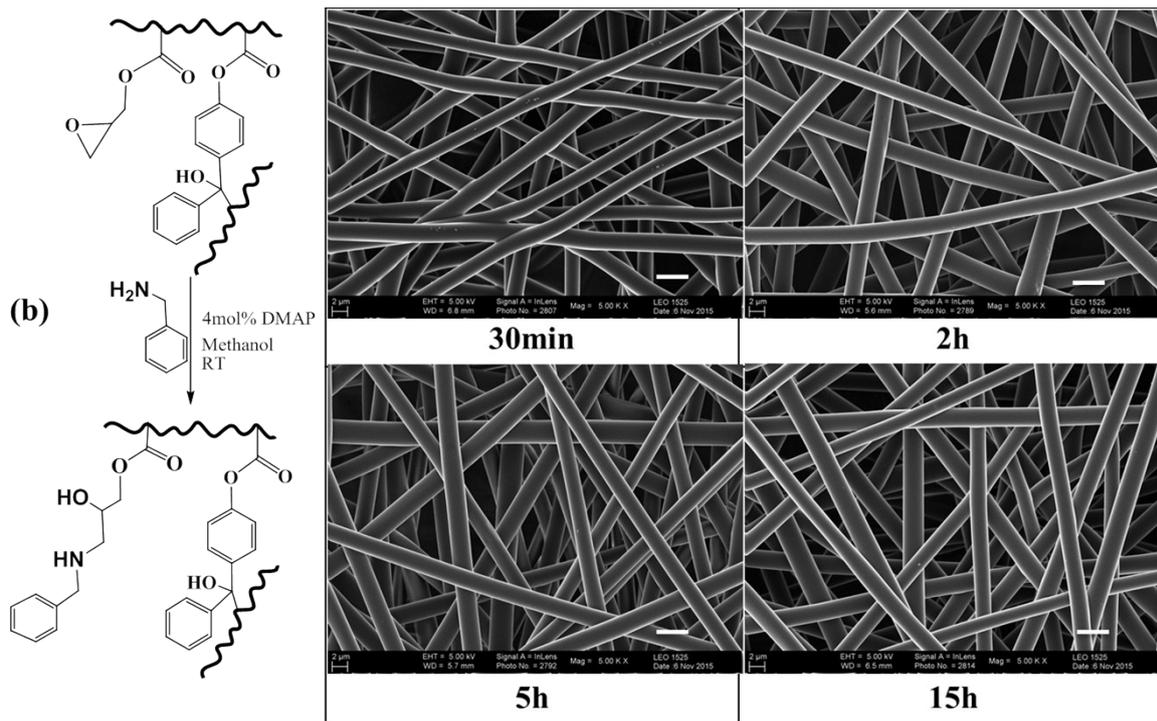
After successfully obtaining a photo-crosslinked nanofibrous mat, the post-polymerization modification of the versatile precursor nanofibers is expected to introduce the SP group on the surface of the nanofibers via the following procedure: The fixed nanofiber mats (1cm×1cm) were submerged in a solution of the respective amounts of SP-OH (10 wt%) and 3.5 mol% DMAP in 5 mL DMF at 80 °C overnight. Afterwards, the nanofibrous mat was kept at 25 °C

for a certain time and washed successively with water, THF and dichloromethane. The chemical structure and morphology of the SP functional nanofibrous mat were measured by FT-IR and SEM, respectively.

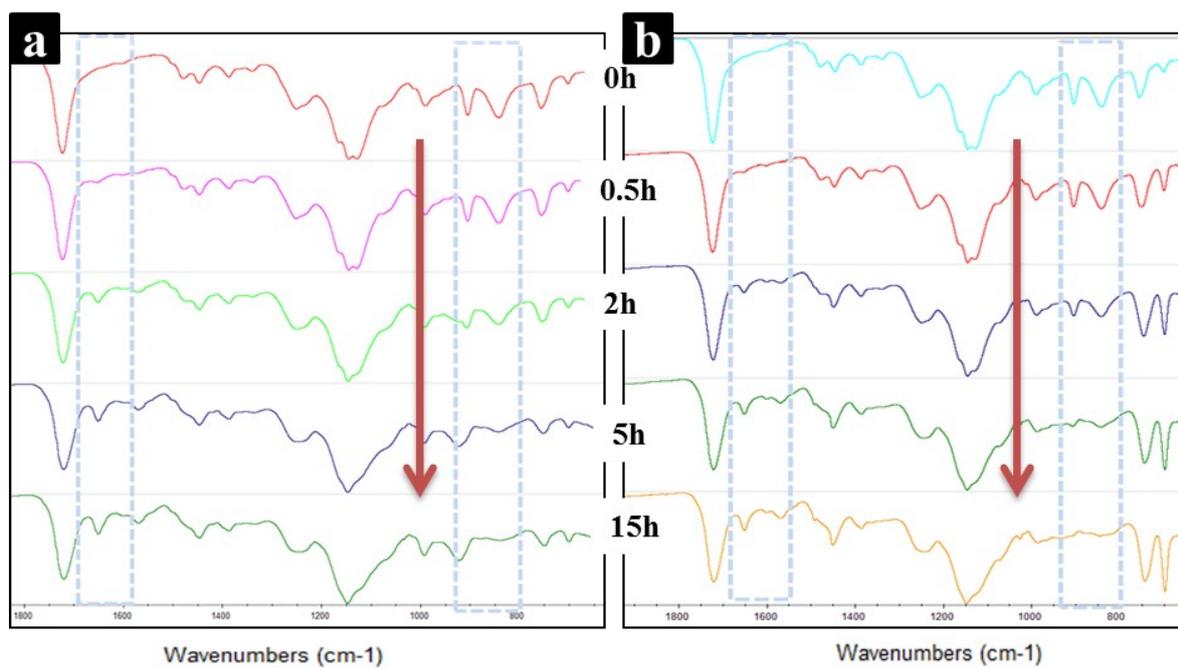
### 5 Additional figures about P(GMA-co-ABP) as an active precursor nanofiber mat after post-polymerization by amine and thiol compounds via $S_N2$ nucleophilic reaction.

Post-modified photo-crosslinked PGMA nanofibers by thiol and amine compounds were confirmed by FT-IR and SEM. As shown in Figures S6 and S8, compared to the precursor nanofibrous mat, the characteristic absorption bands belonging to the epoxide groups at  $824\text{ cm}^{-1}$  and  $905\text{ cm}^{-1}$  have completely disappeared after the post-polymerization modification, indicating the successful modification of PGMA nanofibers.





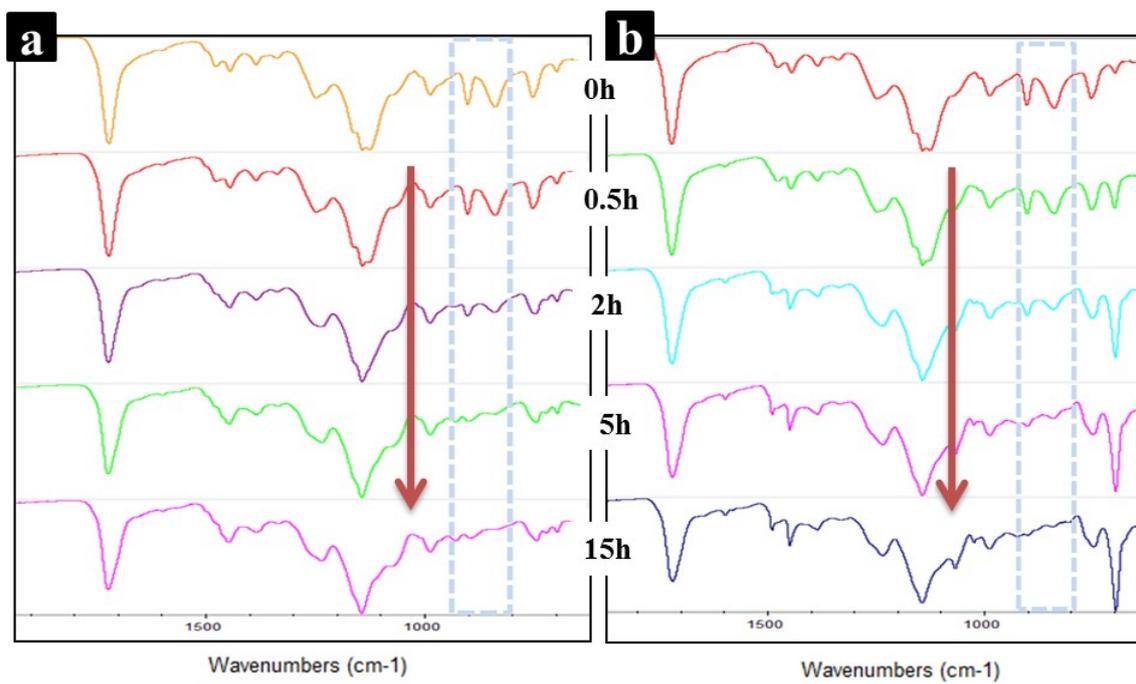
**Figure S5.** SEM images of nanofibrous morphologies of allylamine (a) and benzylamine (b) modified PGMA nanofibers for 30min, 2h, 5h and 15h, respectively. Scale bar =4μm



**Figure S6.** FT-IR spectra of allylamine (a) and benzylamine (b) modified PGMA nanofibers for 30min, 2h, 5h and 15h, respectively.



hexanethiol (a) and benzylthiol (b) for 30min, 2h, 5h and 15h, respectively. (Scale bar =4 $\mu$ m)



**Figure S8.** FT-IR spectra of post-modified nanofibers by 1-hexanethiol (a) and benzylthiol (b) for 30min, 2h, 5h and 15h, respectively.