

1 **Design of Carboxylated Single-Walled Carbon Nanotube as High-**  
2 **Efficient Inhibitor against A $\beta$ 40 Fibrillation based on HyBER**  
3 **Mechanism**

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## 21 **Inductively coupled plasma-mass spectrometry (ICP-MS) analysis**

22 SWCNT-COOH with 4% carboxyl group ratio were mixed with metal ion solution at  
23 1:1 with the final concentration of 200 ppm. Then the mixture was cultured in shaker at 37  
24 °C for 1 h. The unchelated metal ions were removed by 8, 000 ×g centrifugation for 10 min  
25 and repeated three times. The final precipitate was nitrified and the chelating capacity of  
26 WWCNT-COOH were analyzed using a Thermo Fisher ICP-MS. The sample gas rate was  
27 0.75 mL min<sup>-1</sup>, and the additional gas rate was optimized for each run of analyses during  
28 tuning of the instrument (usually 0.12–0.14 mL min<sup>-1</sup>). Sample was pumped into the  
29 instrument at a rate of 120 μL min<sup>-1</sup>. Medium-resolution mode was used for <sup>56</sup>Fe, <sup>64</sup>Cu,  
30 and <sup>65</sup>Zn. Standard curve is the determination of different concentration gradient of the  
31 curve of the single ion solution. R<sup>2</sup> is greater than 99.999%. An E-HNO<sub>3</sub> acid blank and  
32 nitric acid standard were run after each sample on the ICP-MS as a quality control check  
33 of the data and to monitor the blanks associated with the ICP-MS over the course of the  
34 run.

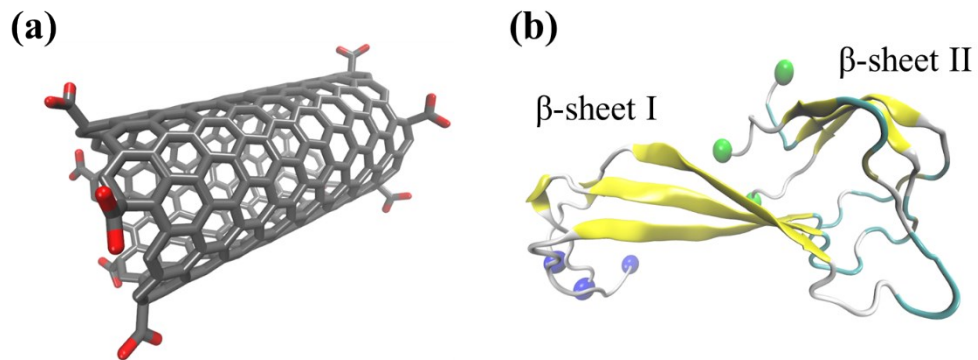
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36 **Table S1.** Chelating capacity of SWCNT-COOH with 4% carboxyl group

37 ratio for  $Zn^{2+}$ ,  $Cu^{2+}$  and  $Fe^{3+}$ .

Metal ions	Chelating capacity (mg/g)
$Zn^{2+}$	257.26
$Cu^{2+}$	27.75
$Fe^{3+}$	100.74

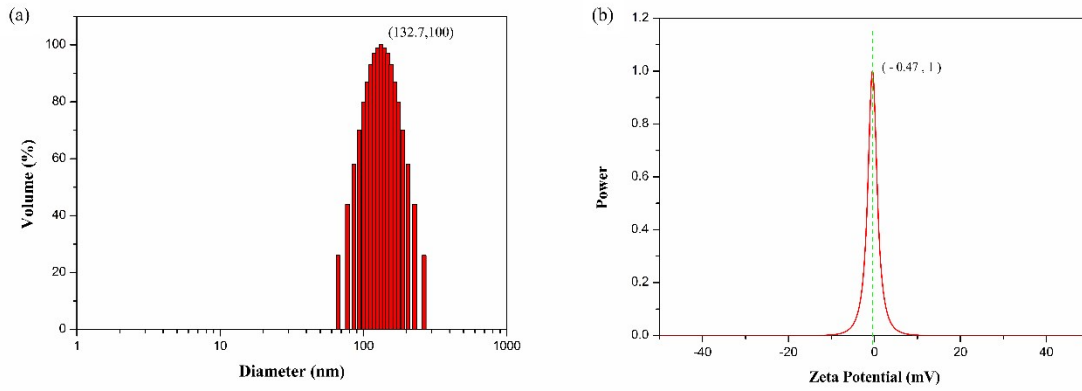
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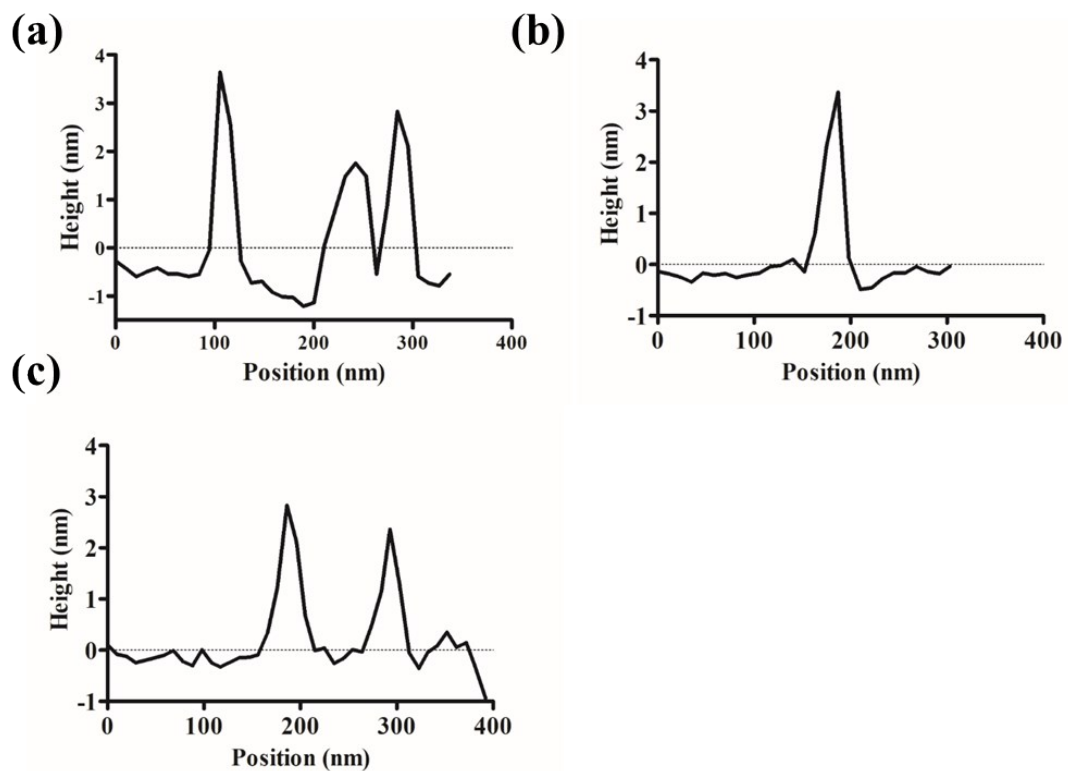
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40 **Fig.S1.** Three-dimensional structure of SWCNT-COOH (a). The carboxyl modification  
41 rate of the single-walled carbon nanotubes in this experiment was  $\sim 3.57\%$ ; The initial  
42 conformation of A $\beta$ 40 trimer (b), the conformation of amyloid protein is represented by  
43 the NewCartoon, and the blue and green sphere represent the N-terminal and C-terminal  
44 A $\beta$ 40 trimer, and the yellow area represents the amyloid  $\beta$ -sheet structure.

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46 **Fig. S2** Particle sizes (a) and Zeta potentials (b) of SWCNT-COOH with 4%  
47 carboxyl group ratio at 25 °C.  
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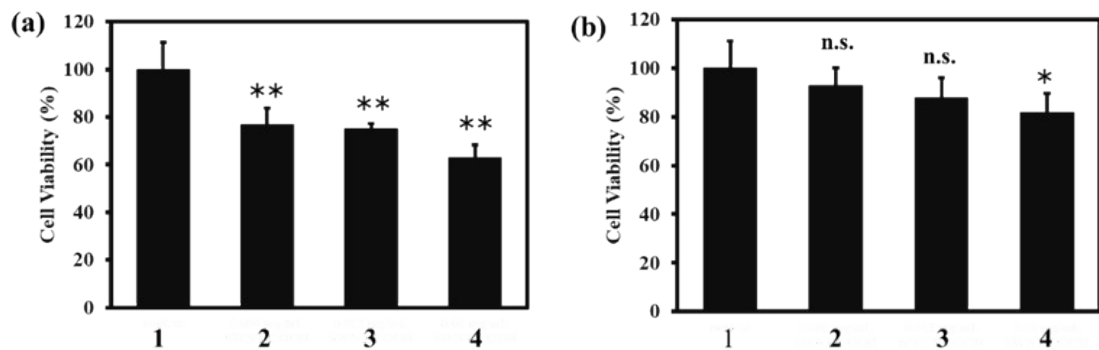
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50 **Fig.S3.** The corresponding height of the cross-sectional contours of the obtained A $\beta$ 40

51 species in Fig. 2a, 2b and 2c labeled by the black bars are shown in (a), (b) and (c),

52 respectively.

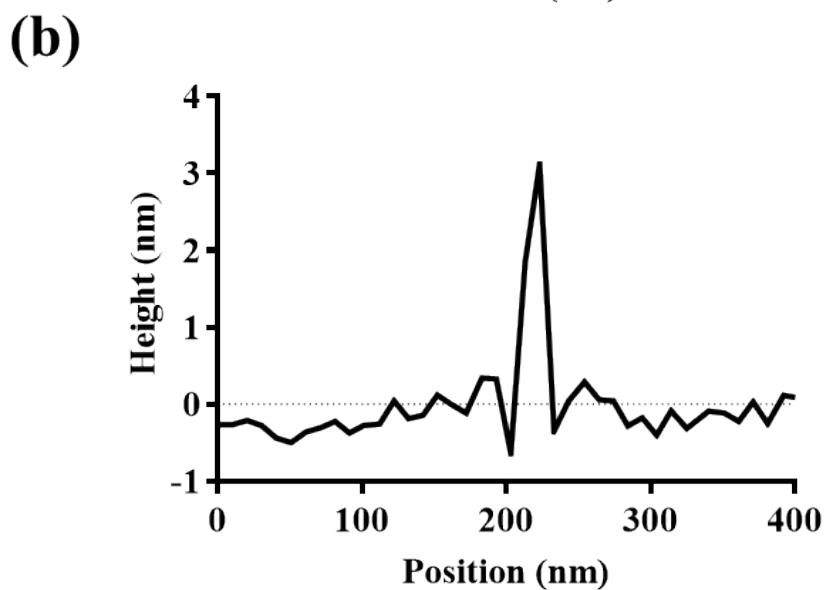
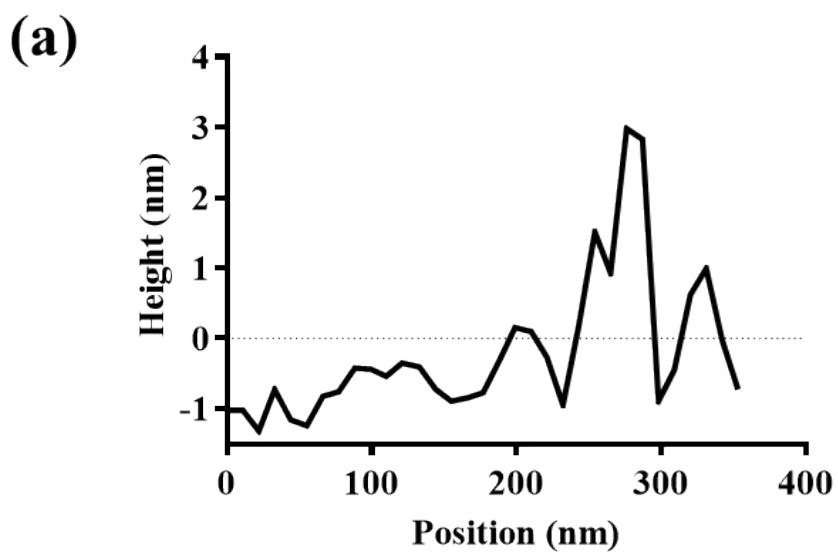
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55 **Fig. S4.** The effect of SWCNT-COOH with (a) 2% and (b) 4% carboxyl groups on the  
 56 cytotoxicity of PC12 cells. 1, 2, 3 and 4 represent the negative control (only PBS buffer,  
 57 0.0006 mg/mL SWCNT-COOH, 0.0012 mg/ml SWCNT-COOH, 0.006 mg/mL SWCNT-  
 58 COOH), respectively. The viability of cells treated with PBS buffer alone (negative  
 59 control) was set as 100%. All values represent means  $\pm$  s.d. (n=5). n.s. not significant; \*P  
 60 < 0.05; \*\*P < 0.01 compared to the control group.

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63 **Fig.S5.** The corresponding height of the cross-sectional contours of the obtained A $\beta$ 40

64 species in Fig. 4b and 4c labeled by the black bars are shown in (a) and (b), respectively.

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