

# **Assembling Anthracene-Tailored Amphiphiles: Charge-Transfer Interactions Directed Hierarchical Nanofibers with Ameliorative Antibacterial Activity toward Plant Pathogens**

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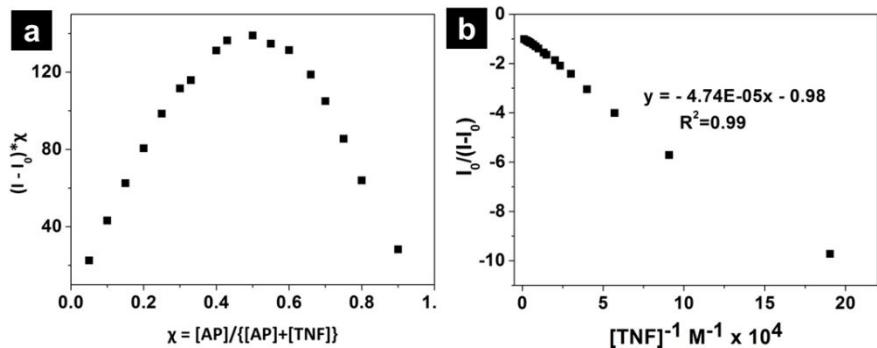
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## 1. The Job's plot experiment (Figure S1)



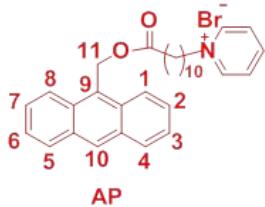
**Figure S1.** The Job's plot experiment (a) showed the 1:1 complex formation of AP and TNF (0.1 mM, molar ratio 1:1), with the binding constant  $2.06 \times 10^4 \text{ M}^{-1}$  (b).

## 2. Chemical shifts of TNF or AP before and after forming the CT complex



**Table S1.** Chemical shift of TNF before and after forming the CT complex.

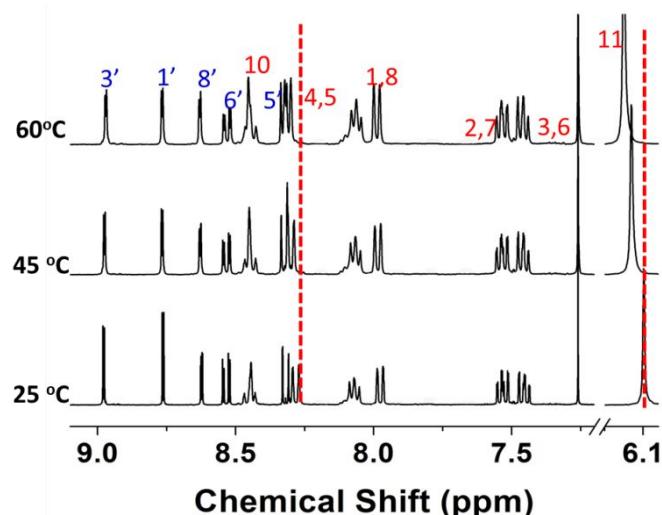
Chemical Shift	3'	1'	8'	6'	5'
TNF (ppm)	9.0255	8.8225	8.6735	8.5685	8.3645
Complex (ppm)	8.9760	8.7615	8.6220	8.5305	8.3165
Shift (ppm)	0.0495	0.0610	0.0515	0.0380	0.0480



**Table S2.** Chemical shift of AP before and after forming the CT complex.

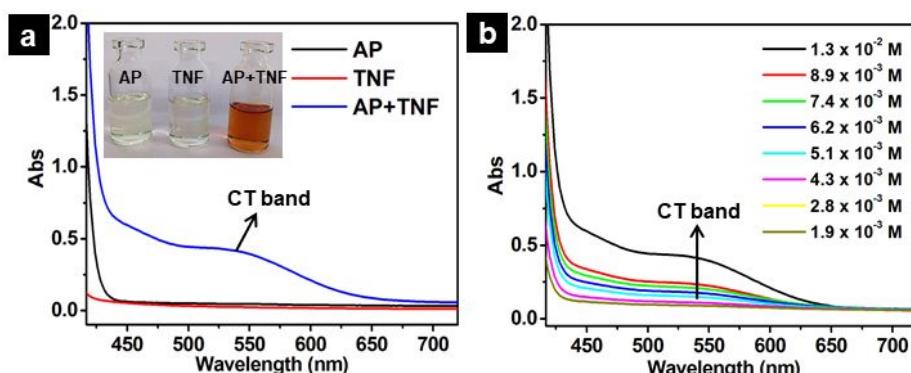
Chemical Shift	10	4, 5	1, 8	2, 7	3, 6
AP (ppm)	8.494	8.311	8.0165	7.553	7.4775
Complex (ppm)	8.446	8.279	7.9765	7.53	7.452
Shift (ppm)	0.048	0.032	0.04	0.023	0.0255

### 3. Temperature-dependent $^1\text{H}$ NMR spectra of complex AP-TNF (Figure S2)



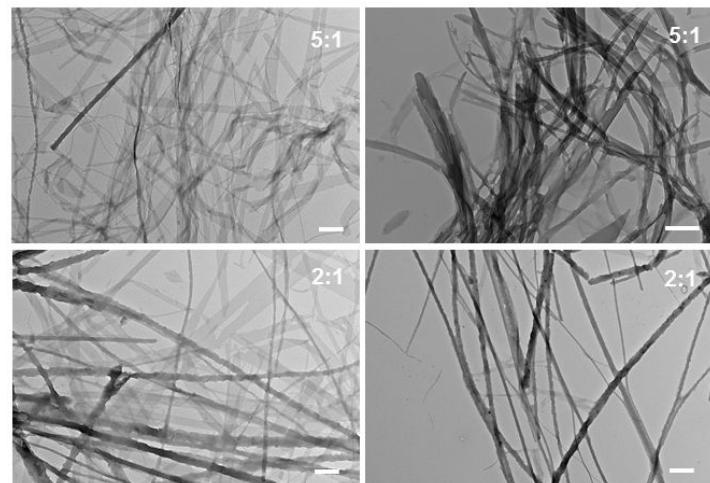
**Figure S2.** Temperature-dependent  $^1\text{H}$  NMR spectra of complex AP-TNF.

### 4. Photographs and UV-Vis spectra of AP, TNF and AP/TNF complex in $\text{CHCl}_3$ (Figure S3)



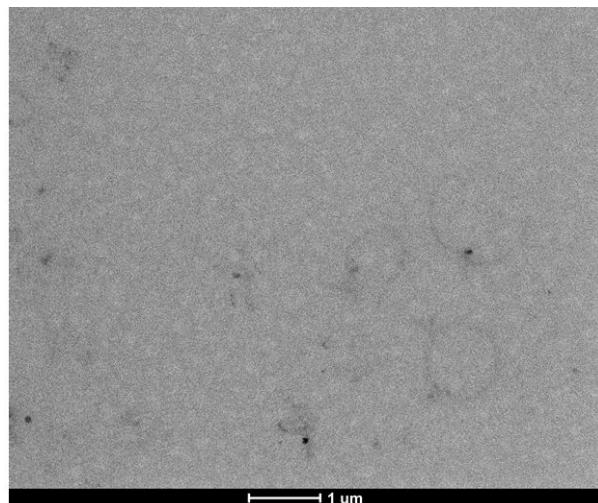
**Figure S3.** (a) Photographs and UV-Vis absorption spectra of AP, TNF and AP/TNF complex in  $\text{CHCl}_3$  ( $13.0 \text{ mM}$ , 1:1, molar ratio); (b) UV-Vis absorption spectra of AP/TNF complex with different concentrations in  $\text{CHCl}_3$  (1:1, molar ratio).

**5. TEM images of AP/TNF with different molar ratio (Figure S4)**



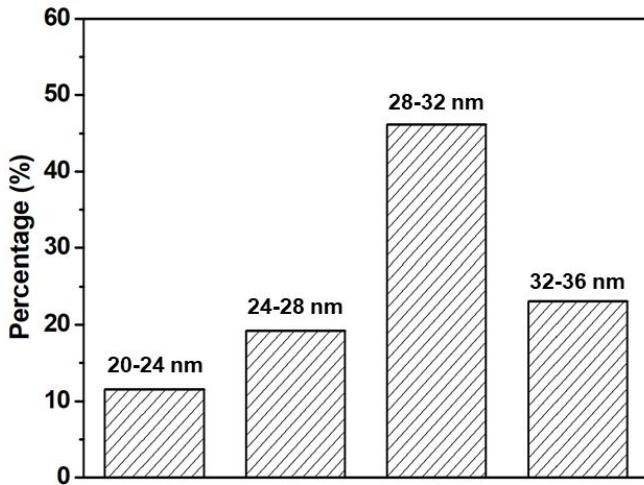
**Figure S4.** TEM images of AP/TNF with different molar ratio of 5:1 and 2:1, scale bars are 500 nm.

**6. The TEM image for just the NB medium (Figure S5)**



**Figure S5.** The TEM image for just the NB medium.

**7. Statistical analysis of the widths of AP-TNF nanofibers in screening medium (Figure S6)**



**Figure S6.** Statistical analysis of the widths of AP-TNF nanofibers in antibacterial screening medium.

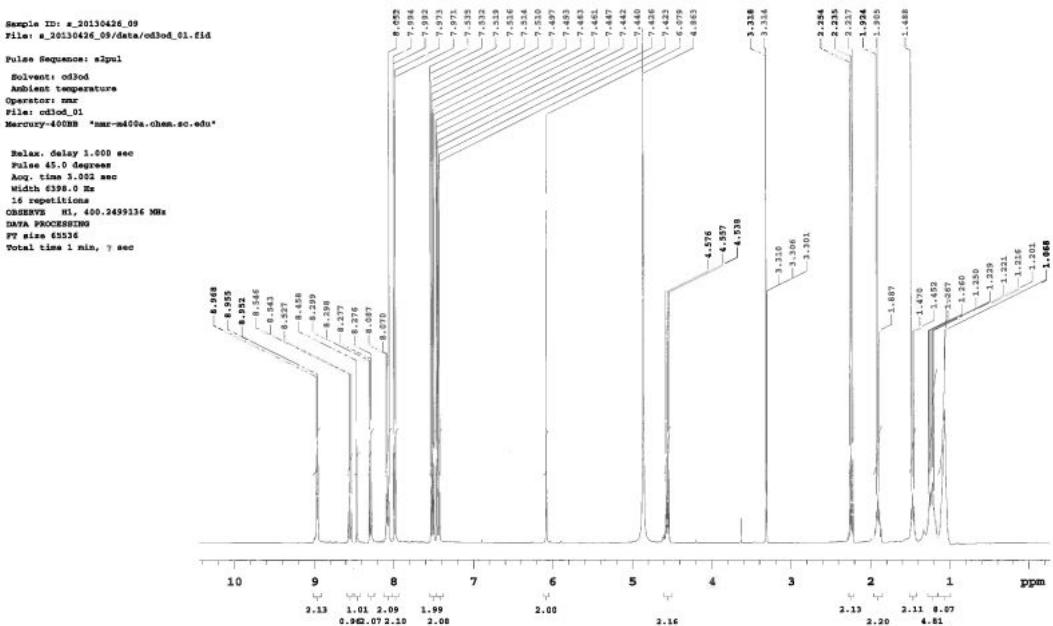
**8. Synthesis and NMR spectra of AP and TNF (Figures S7-S10)**

**Synthesis of 1-(11-(anthracen-9-ylmethoxy)-11-oxoundecyl) pyridinium bromide (AP)**

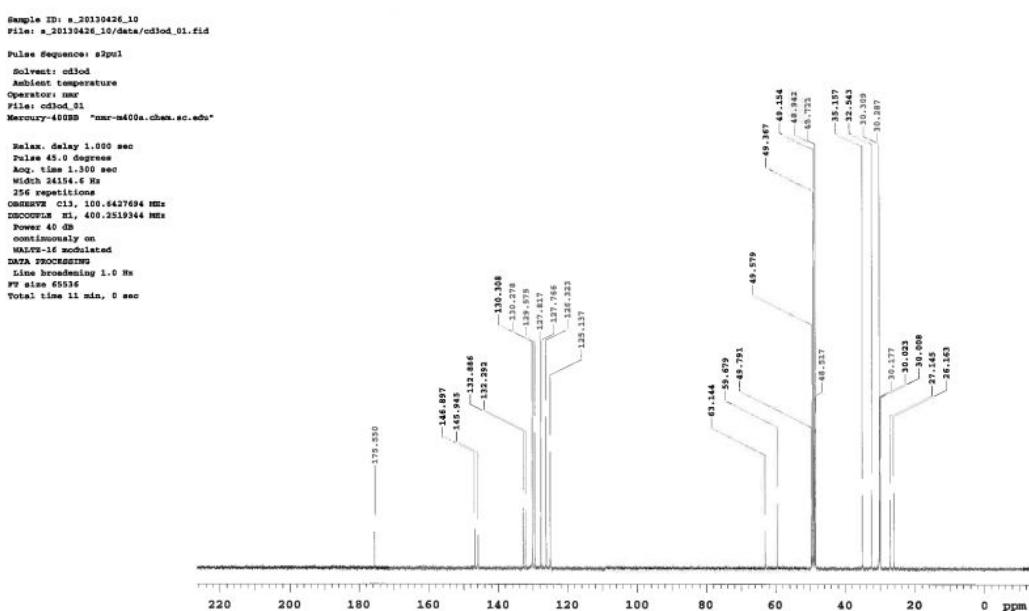
The synthesis of **AP** was carried out as previously described,<sup>[1]</sup> yield 66%; m. p. 96-98 °C; <sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD) δ 8.96 (2H, dd, *J* = 6.4, 1.2 Hz, pyridinium-H), 8.54 (1H, ddd, *J* = 7.2, 7.2, 1.2 Hz, pyridinium-H), 8.46 (1H, s, anthracene-H), 8.29 (2H, dd, *J* = 8.8, 0.4 Hz, anthracene-H), 8.07 (2H, t, *J* = 7.0 Hz, pyridinium-H), 7.98 (2H, dd, *J* = 8.4, 0.8 Hz, anthracene-H), 7.51 (2H, ddd, *J* = 8.8, 6.4, 0.8 Hz, anthracene-H), 7.44 (2H, ddd, *J* = 8.4, 6.4, 0.4 Hz, anthracene-H), 6.08 (2H, s, OCH<sub>2</sub>), 4.56 (2H, t, *J* = 7.6 Hz, NCH<sub>2</sub>), 2.24 (2H, t, *J* = 7.6 Hz, CH<sub>2</sub>CO), 1.91-1.30 (16H, m, CH<sub>2</sub>); <sup>13</sup>C NMR (100 MHz, CD<sub>3</sub>OD) δ 175.5 (C=O), 146.9, 145.9, 129.6, 132.9, 132.3, 130.3, 127.8, 126.3, 125.1, 63.1, 59.7, 35.2, 32.5, 30.3, 30.2, 30.0, 27.1, 26.2; MS-ESI (+) m/z: 454; HRMS (ESI): m/z calcd. for C<sub>31</sub>H<sub>36</sub>NO<sub>2</sub>: 454.2746, found: 454.2750.

**Synthesis of 2, 4, 7-trinitrofluorenone (TNF)**

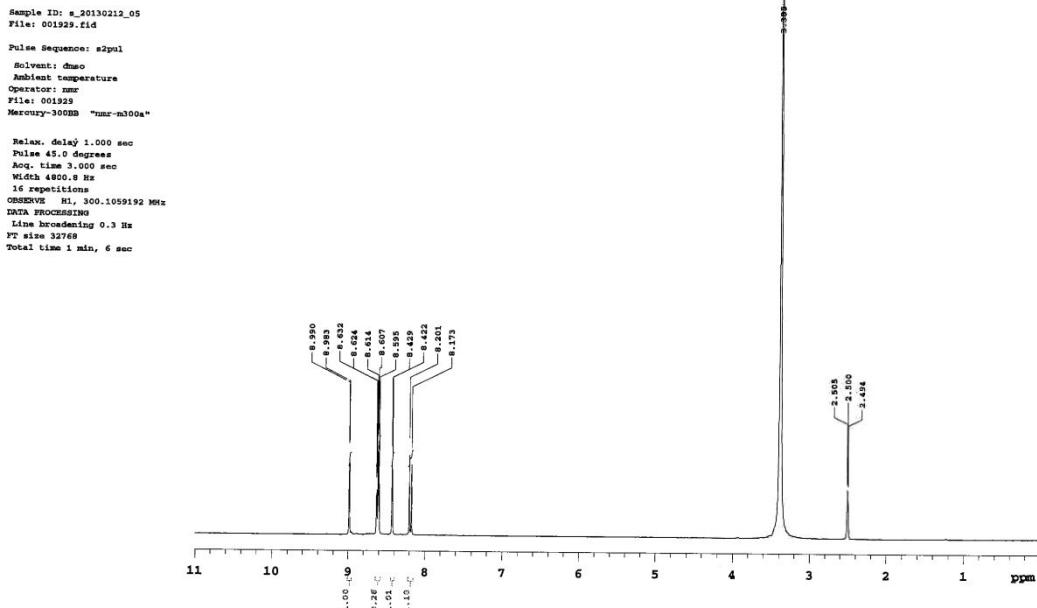
The synthesis of **TNF** was carried out as ref. [2]. m. p. 170-172 °C; <sup>1</sup>H NMR (300 MHz, DMSO-*d*<sub>6</sub>) δ 8.99 (1H, d, *J* = 2.1 Hz, 3-H), 8.63-8.59 (2H, m, 6-H, 7-H), 8.43 (1H, d, *J* = 2.1 Hz, 1-H), 8.19 (1H, d, *J* = 8.4 Hz, 5-H); <sup>13</sup>C NMR (75 MHz, DMSO-*d*<sub>6</sub>) δ 186.4, 149.7, 148.9, 144.8, 143.3, 138.8, 137.9, 136.2, 130.8, 128.0, 126.0, 122.2, 119.0; MS-EI (+) m/z: 315.



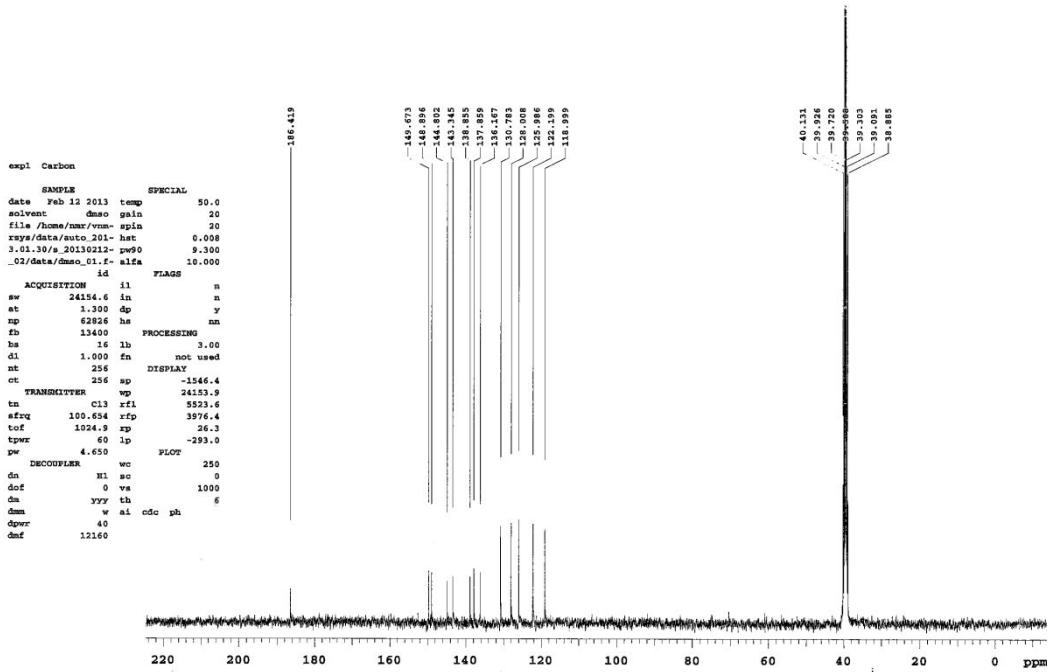
**Figure S7.**  $^1\text{H}$  NMR Spectrum (400MHz,CD<sub>3</sub>OD) of AP.



**Figure S8.**  $^{13}\text{C}$  NMR Spectrum (100MHz,  $\text{CD}_3\text{OD}$ ) of AP.



**Figure S9.**  $^1\text{H}$  NMR Spectrum (DMSO- $d_6$ , 300 MHz) of TNF



**Figure S10.**  $^{13}\text{C}$  NMR Spectrum (DMSO- $d_6$ , 75 MHz) of TNF.

## References

- [1] Wang, P. Y.; Hu, J.; Lin, Y.; Smith, M.; Yang, S.; Song, B. A.; Wang, Q. Microsheets assembled from pyridinium-tailored anthracenes. *Tetrahedron* **2014**, *70*, 6651–6655.
- [2] Hu, J.; Wu, J. D.; Wang, Q.; Ju, Y. Charge-transfer interaction mediated organogels from 18 $\beta$ -glycyrrhetic acid appended pyrene. *Beilstein J. Org. Chem.* **2013**, *9*, 2877–2885.