

# ***Supporting Information***

## **A Supramolecular Polyethylenimine-cored Carbazole Dendritic Polymer with Dual Applications**

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### Calculation of the carbazole groups per complex

Take the PEI-G0 for example:

Molar extinction coefficient ( $\epsilon$ )= $4.046 \times 10^3$  (mol/L·cm)<sup>-1</sup> at the absorption peak of 343 nm.

The PEI-G0 was diluted 100 times for UV-vis spectrum measurement.

$$c(\text{carbazole}) = 100 \times \frac{A}{\epsilon l} = 100 \times \frac{1.19}{4.064 \times 1000 \times 1} = 0.0293 \text{ mol/L} = 29.3 \text{ mol/L}$$

For G0-COOH, the concentration of COOH group =  $c(\text{carbazole}) = 29.3 \text{ mol/L}$

$$c(\text{PEI}) = 20 \times \frac{1.43}{10.86} = 2.63 \text{ mg/mL} = 0.263 \text{ mmol/L}.$$

The concentration of amine groups =  $230 \times 0.263 \text{ mmol/L} = 60.5 \text{ mmol/L}$ . ( $c(\text{NH}_2^-) = 20.0 \text{ mmol/L}$ ,  $c(\text{NH}^-) = 24.2 \text{ mmol/L}$ ,  $c(\text{N}^-) = 16.3 \text{ mmol/L}$ )

$$\text{The carbazole per PEI molecule } N = \frac{c(\text{carbazole})}{c(\text{PEI})} = \frac{29.3}{0.263} = 111$$

Therefore, the G0-COOH dendron per PEI molecule is 111.

Similarly, for complex PEI-G1, the carbazole per PEI molecule was calculated to be 79.4.

Therefore, the G1-COOH dendron per PEI molecules is 40.

For complex PEI-G2, the carbazole per PEI molecule was calculated to be 81.2.

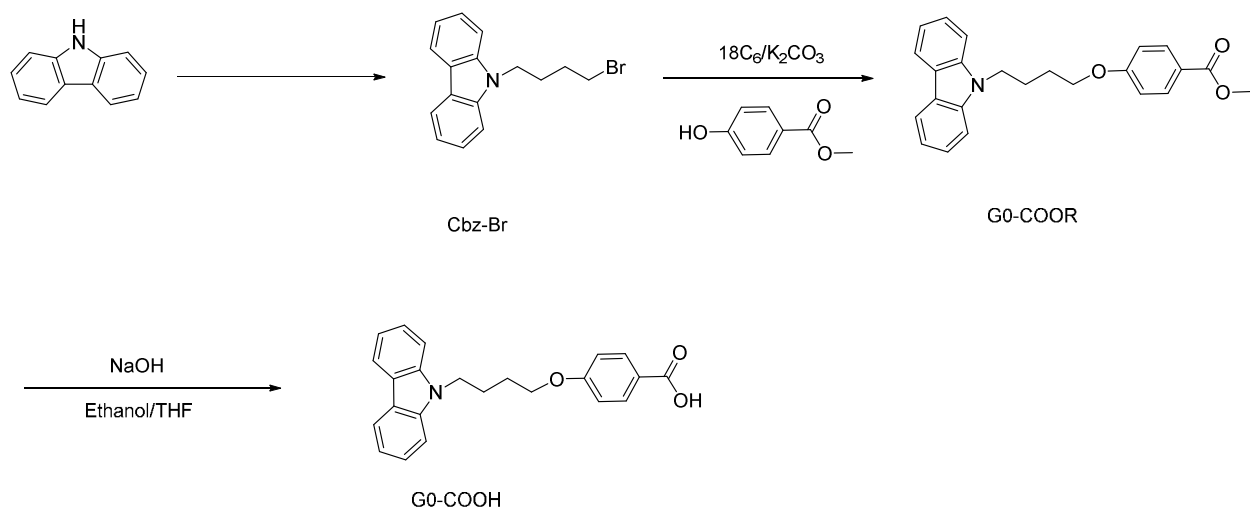
Therefore, the G2-COOH dendron per PEI molecules is 20.

### Calculation of the molecular weight of the complex

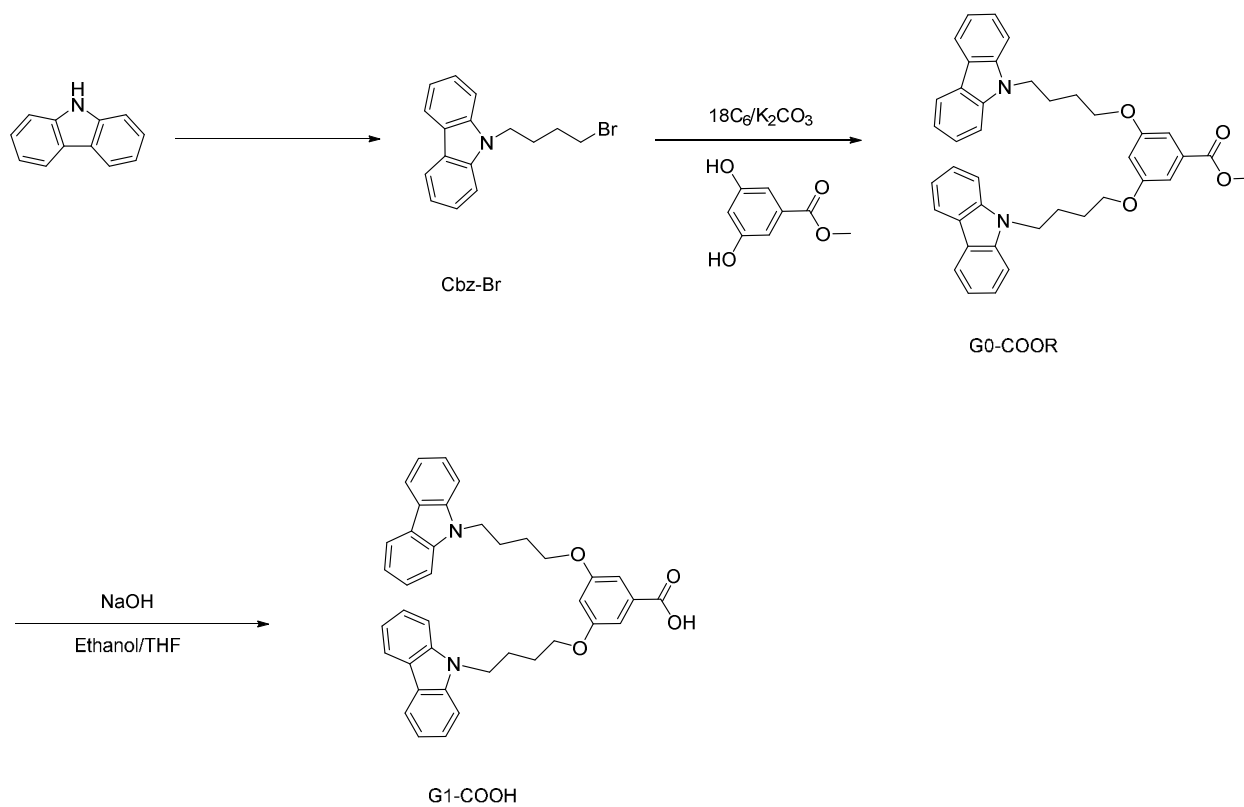
$$\text{Mw (PEI-G0 complex)} = \text{Mw (PEI)} + N1 \times \text{Mw(G0-COOH)} = 10,000 + 111 \times 359.43 = 49.8 \text{ kDa}$$

$$\text{Mw (PE-G1 complex)} = \text{Mw (PEI)} + N2 \times \text{Mw(G1-COOH)} = 10,000 + 39.7 \times 596.73 = 33.7 \text{ kDa}$$

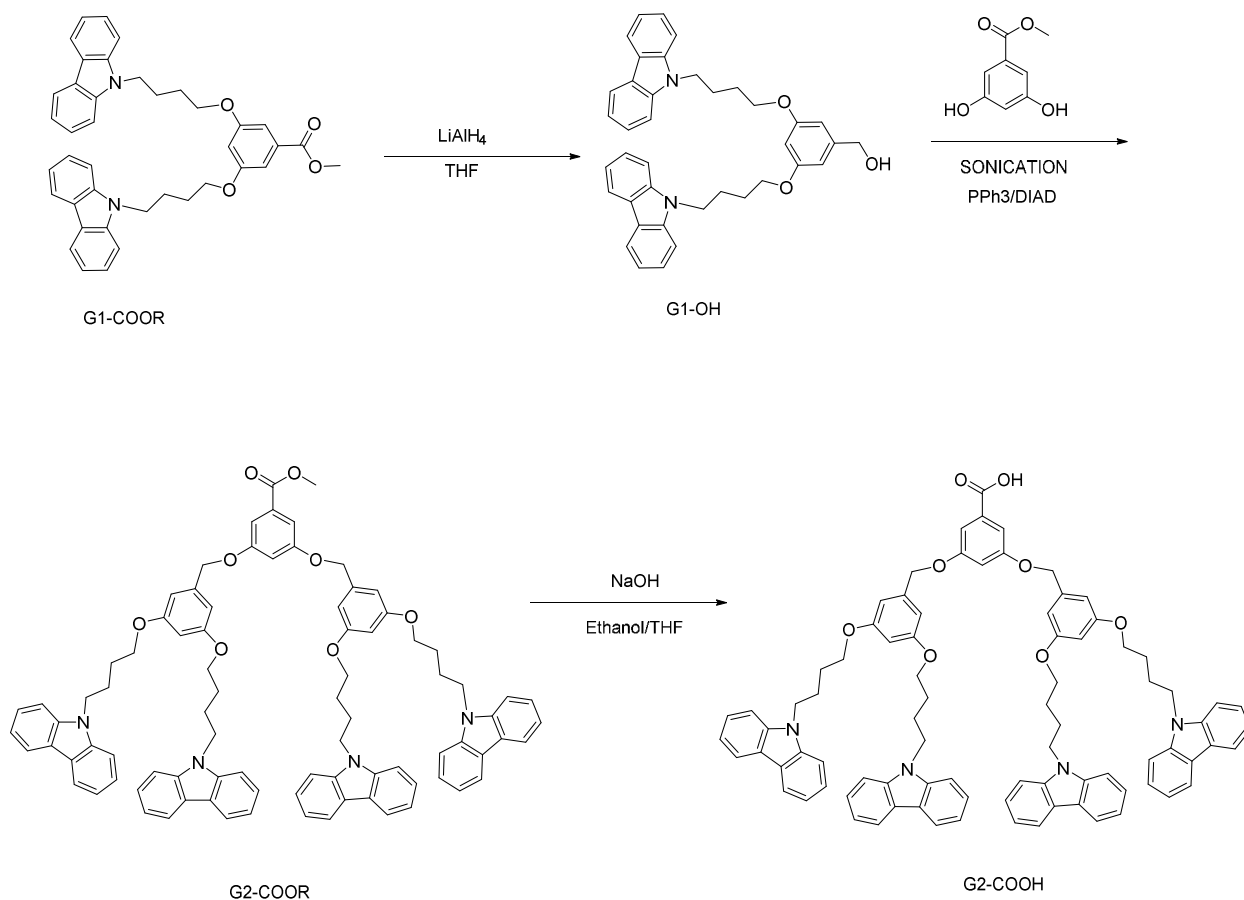
$$\text{Mw (PE-G2 complex)} = \text{Mw (PEI)} + N3 \times \text{Mw(G2-COOH)} = 10,000 + 20.3 \times 1283.58 = 36.1 \text{ kDa}$$



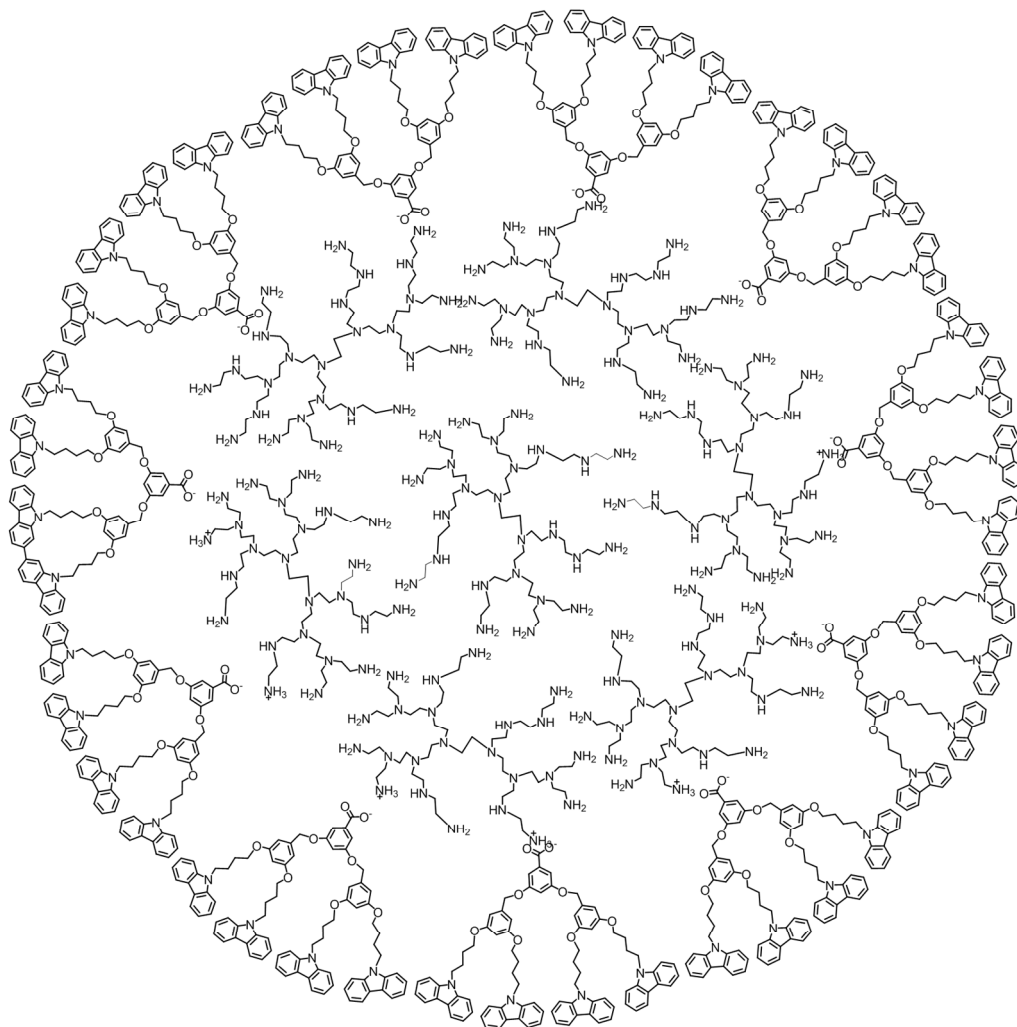
**Scheme S1.** Synthesis of G0-COOH



**Scheme S2.** Synthesis of G1-COOH



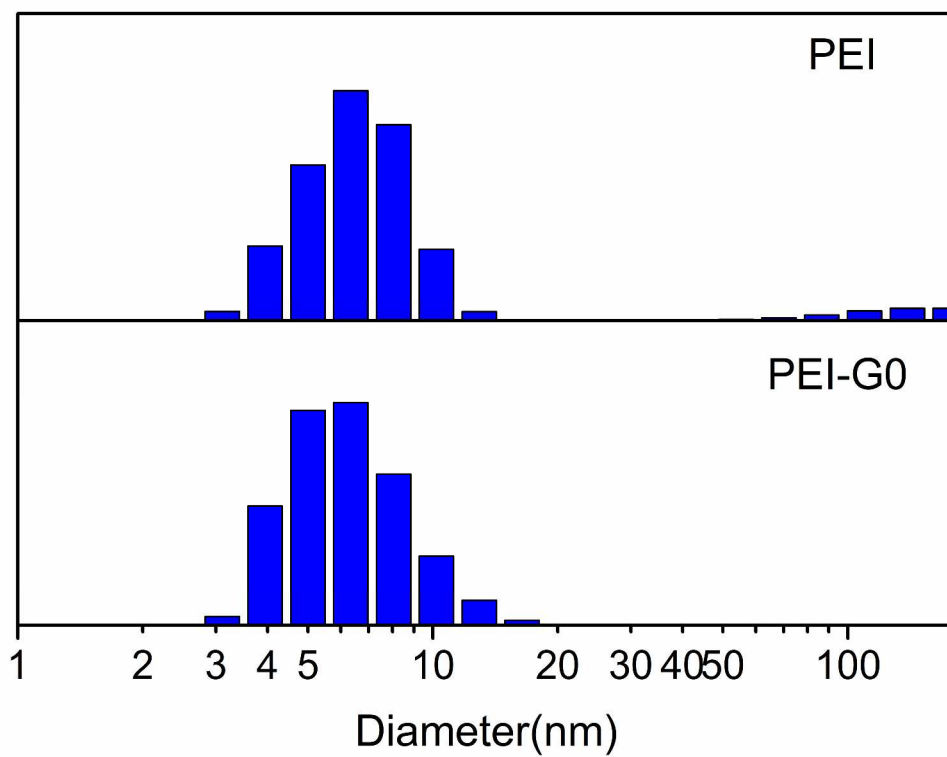
**Scheme S3.** Synthesis of G2-COOH



**Scheme S4.** Demonstration of the supramolecular dendritic multilarm polymer (SDMPs) based on high-generation carbazole dendron.

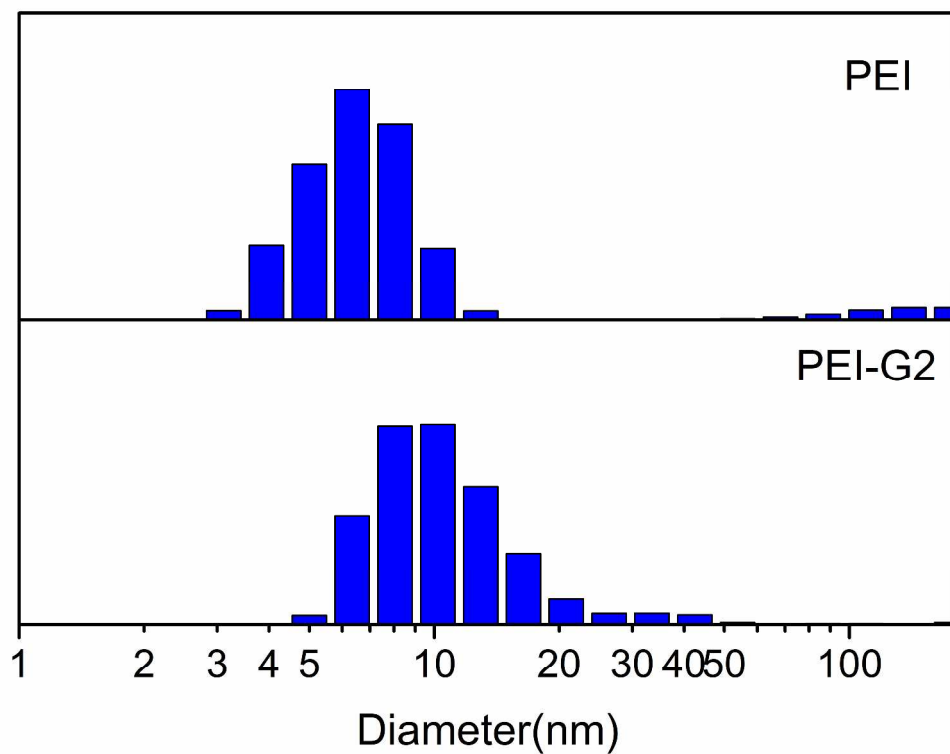
**Table S1.** Comparative ratio of carboxylic acid (-COOH) to amines for nanocomplexes with different carbazole generations. The listed numbers are based on one PEI molecule.

|                | <b>Amines</b> | <b>Primary amines</b> | <b>Secondary amines</b> | <b>Tertiary amines</b> | <b>-COOH</b> | <b>-COOH/amines</b> |
|----------------|---------------|-----------------------|-------------------------|------------------------|--------------|---------------------|
| <b>G0-COOH</b> | 230           | 76                    | 92                      | 62                     | 111          | 0.483               |
| <b>G1-COOH</b> | 230           | 76                    | 92                      | 62                     | 40           | 0.174               |
| <b>G2-COOH</b> | 230           | 76                    | 92                      | 62                     | 21           | 0.091               |

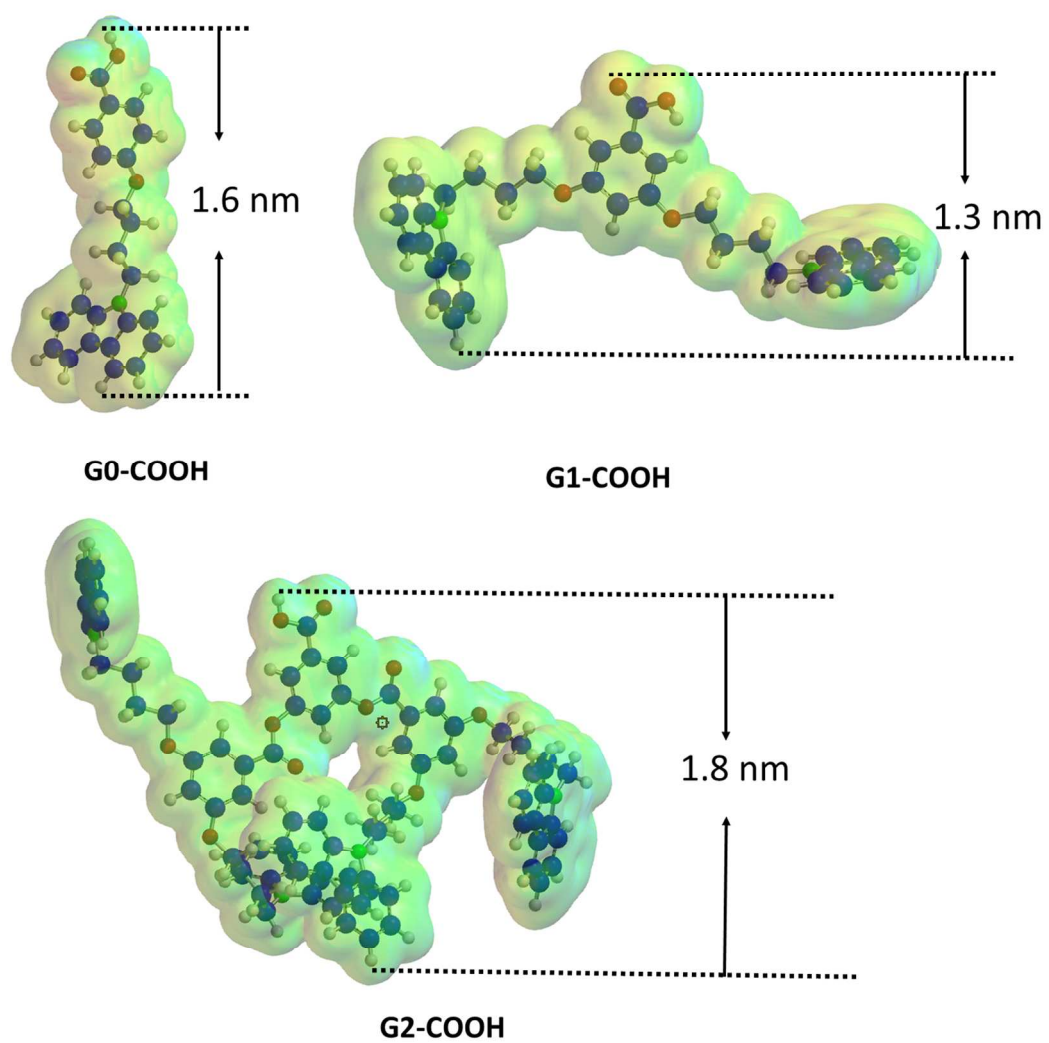


**Figure S1.** Comparative DLS analysis of PEI and PEI-G0 complex

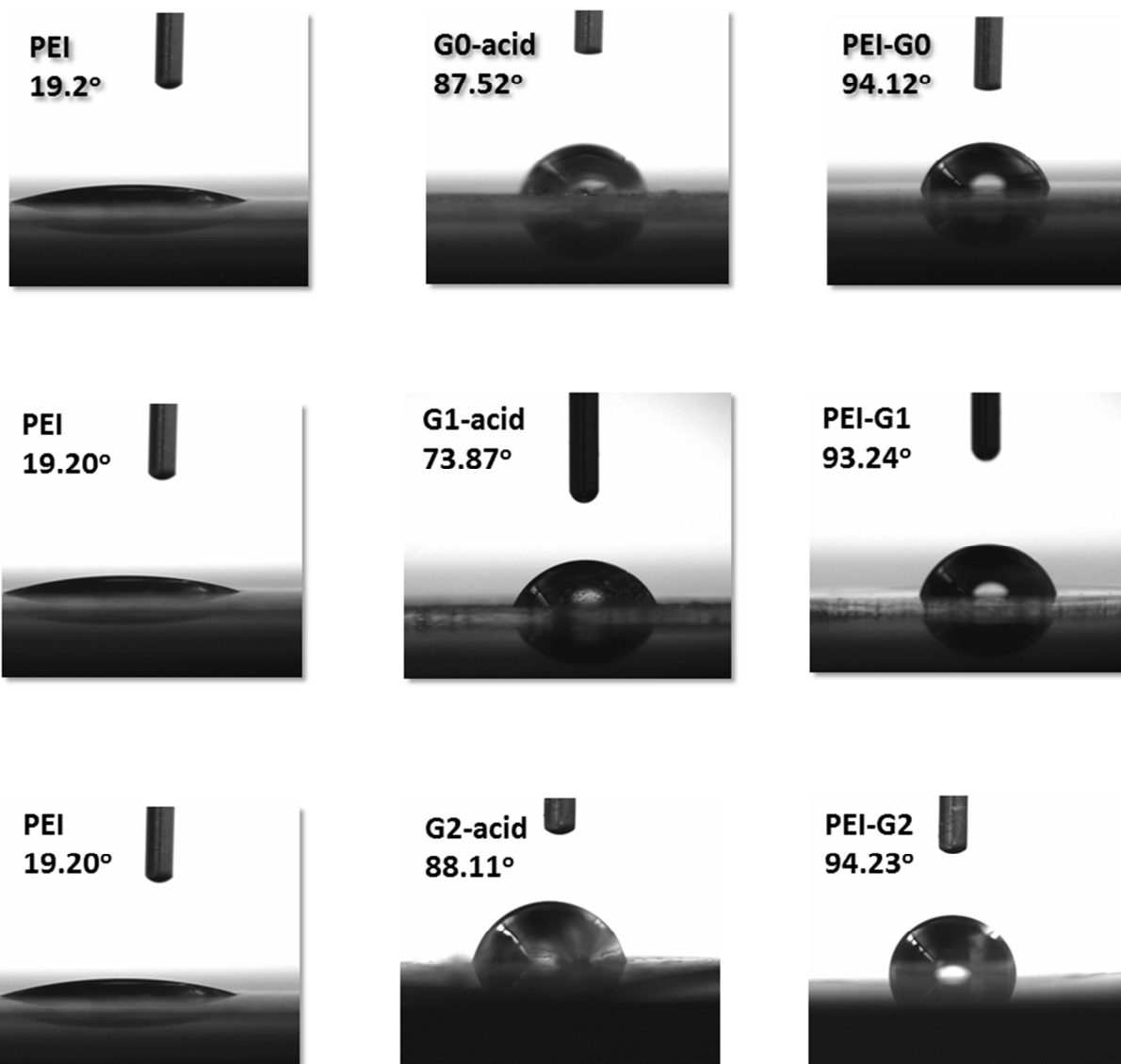




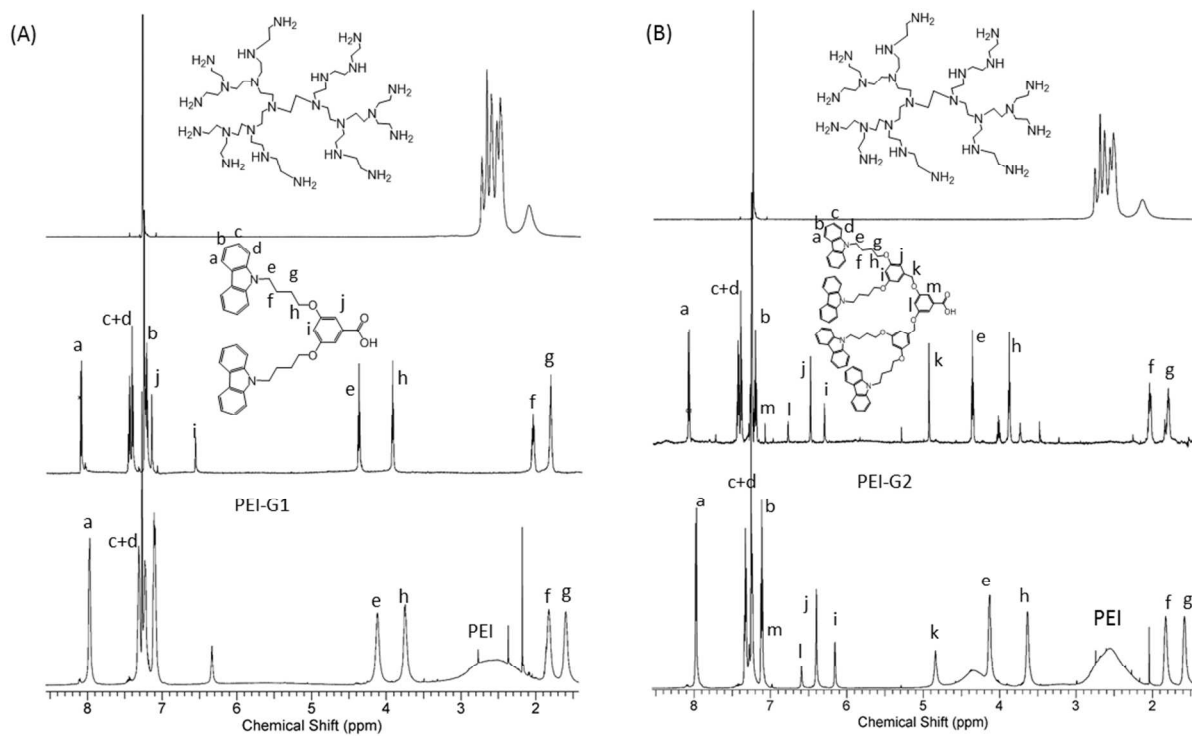
**Figure S2.** Comparative DLS analysis of PEI and PEI-G2 complex



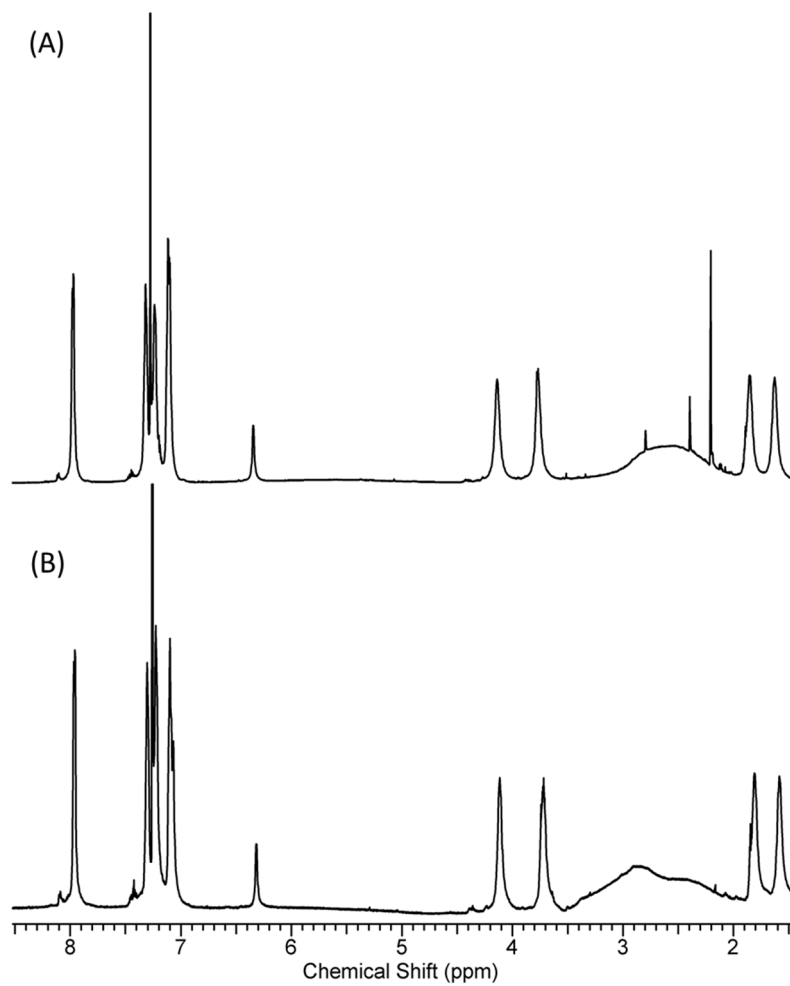
**Figure S3.** Molecular modelling of the G0-COOH, G1-COOH and G2-COOH by Spantan.



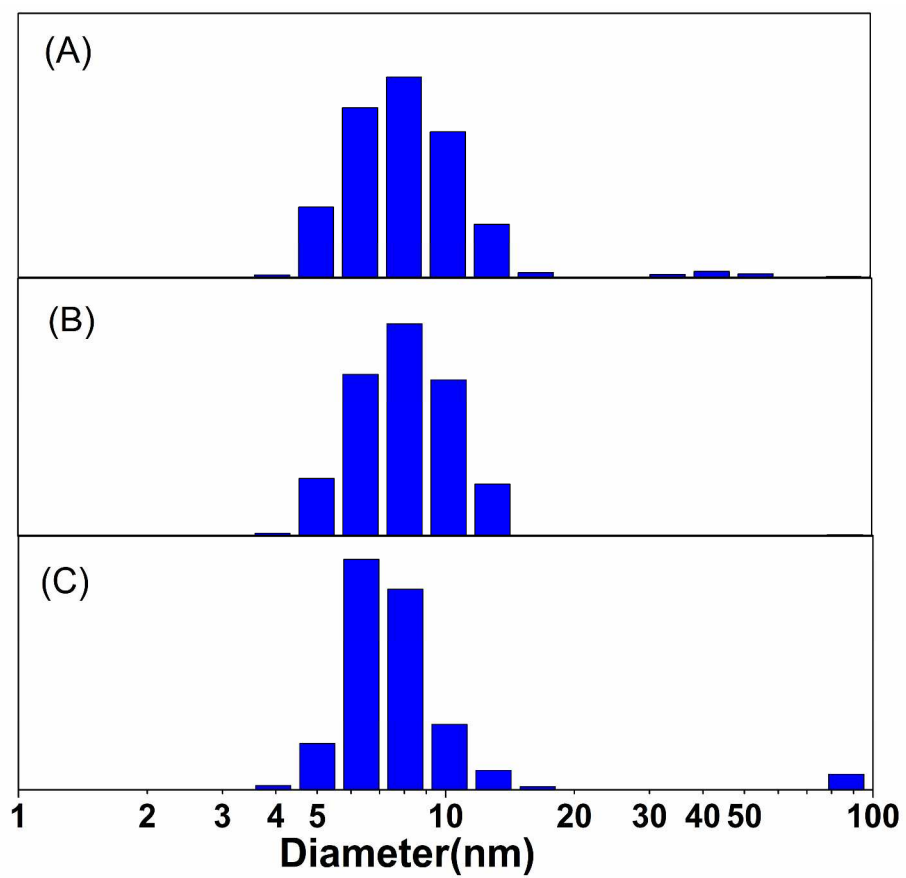
**Figure S4.** Water Contact Angle Measurement.



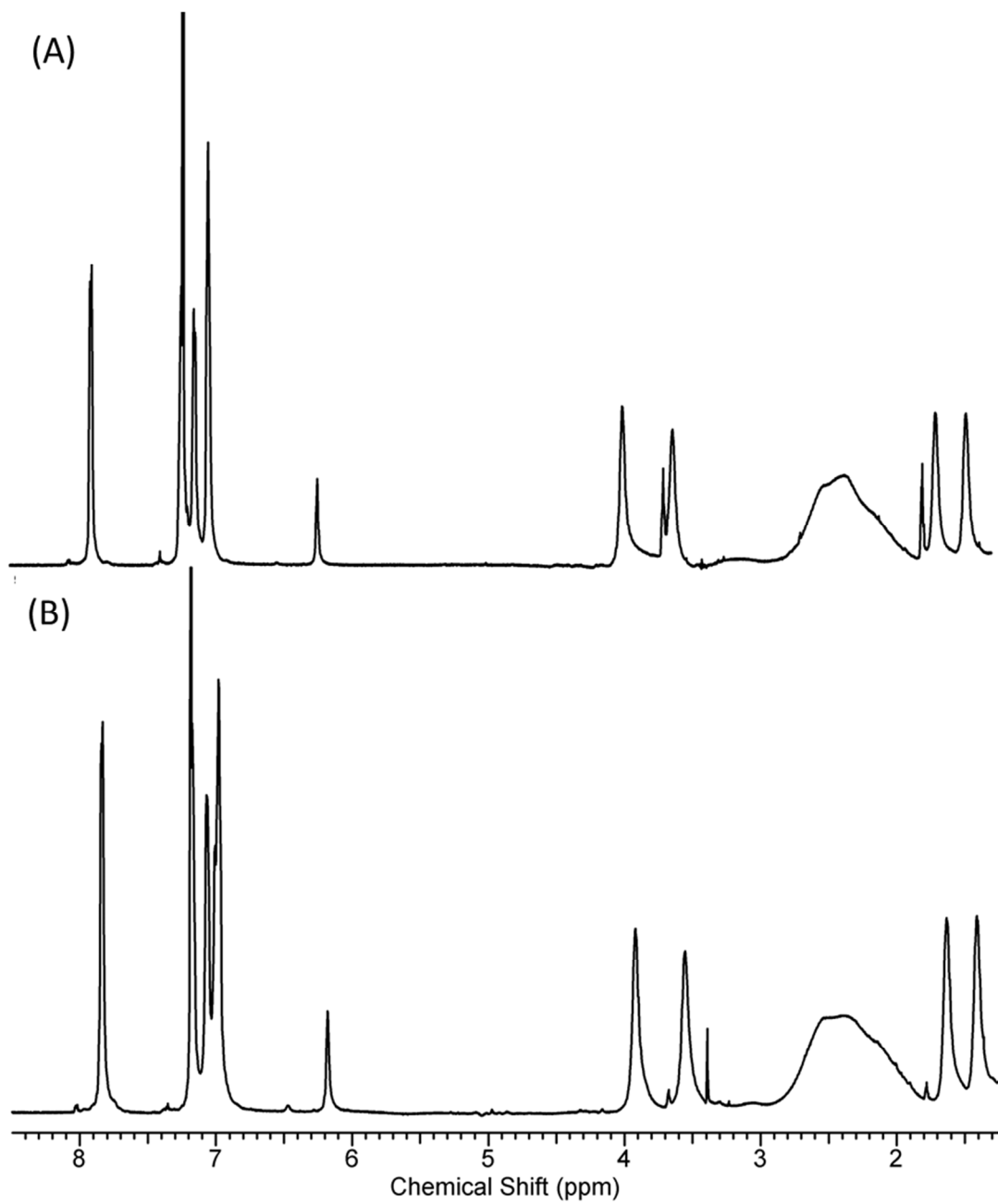
**Figure S5.** Comparative  $^1\text{H}$  NMR spectra of (A) PEI, G1-COOH and nanocomplex PEI-G1; (B) PEI, G2-COOH, and nanocomplex PEI-G2.



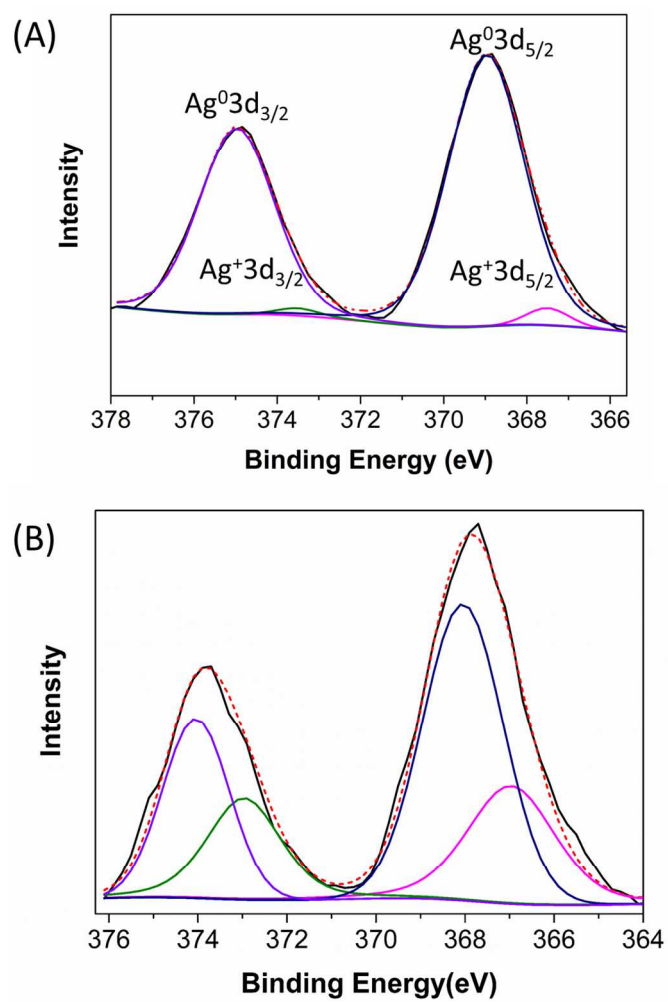
**Figure S6.** Comparative  $^1\text{H}$  NMR spectra of the nanocomplex PEI-G1: (A) fresh prepared and (B) two weeks after preparation.



**Figure S7.** Comparative DLS analysis of the nanocomplex PEI-G1: (A) fresh prepared, (B) one week after preparation and (C) two weeks after preparation.

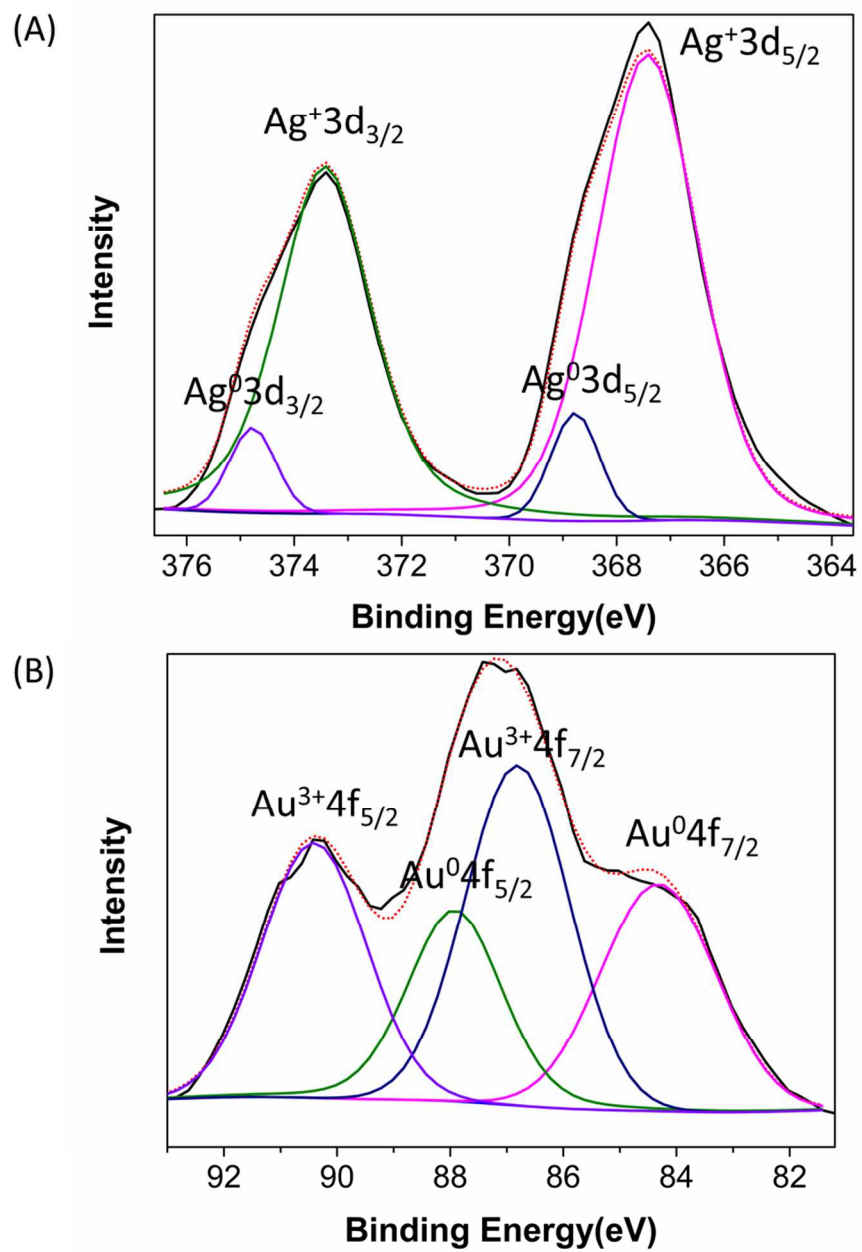


**Figure S8.** Comparative  $^1\text{H}$  NMR spectra of nanocomplex PEI-G1: (A) before mixing with water and (B) after mixing with water.



**Figure S9.** XPS spectra of (A) PEI-G0+1.0 AgNO<sub>3</sub>, and (B) PEI-G2+1.0 AgNO<sub>3</sub>.





**Figure S10.** XPS spectra of (A) PEI-PA+1.0 AgNO<sub>3</sub> and (B) PEI-PA+0.4 AuCl<sub>3</sub>.