Supporting Information

Mixed Carboxyl and Hydrophobic Dendrimer Surface Inhibits Amyloid-β Fibrillation? New Insight from Generation Number Effect

Ziyuan Wang, Xiaoyan Dong, Yan Sun*

Department of Biochemical Engineering and Key Laboratory of Systems Bioengineering of the Ministry of Education, School of Chemical Engineering and Technology, Tianjin University, Tianjin 300354, China
Table S1. Molecular mass and terminal group number of the PAMAM dendrimer (Gn, n=3-6), reaction conditions for the synthesis of the four phenyl-derivatized dendrimers (Gn-P, n=3-6), and the final DS values obtained from the reactions.

<table>
<thead>
<tr>
<th></th>
<th>G3</th>
<th>G4</th>
<th>G5</th>
<th>G6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Terminal group number (-)</td>
<td>32</td>
<td>64</td>
<td>128</td>
<td>256</td>
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<tr>
<td>Molecular mass (Da)</td>
<td>10109</td>
<td>20615</td>
<td>41626</td>
<td>83648</td>
</tr>
<tr>
<td>EDC concentration (mg/mL)</td>
<td>3.7</td>
<td>2.4</td>
<td>2.8</td>
<td>7.3</td>
</tr>
<tr>
<td>PEA concentration (v/v%)</td>
<td>2.4</td>
<td>1.6</td>
<td>2.3</td>
<td>4.8</td>
</tr>
<tr>
<td>DS of Gn-P (%)</td>
<td>28.8</td>
<td>28.2</td>
<td>30.5</td>
<td>28.8</td>
</tr>
</tbody>
</table>
Figure S1. Structures of PAMAM dendrimers of different generations (G0 to G4).
Figure S2. UV absorption spectra of the PAMAM dendrimers, their phenyl derivatives and phenethylamine (PEA).
Figure S3. The calibration curve for PEA determined by UV absorption at 260 nm.
Figure S4. ThT fluorescence intensities of G6 solutions at different concentrations.
Figure S5. Surface models of Aβ42 in aqueous solution. Positive and negative potentials are represented in blue and red, respectively. Hydrophobic areas are in silver. Neutral regions are in orange. Analysis of the surface models was performed by the visual molecular dynamics (VMD) software (http://www.ks.uiuc.edu/Research/vmd/).
Figure S6. ITC isotherms for the titration of (A) G3, (B) G3-P, (C) G4, and (D) G4-P (250 μM each) to Aβ42 (25 μM) at 37 °C.
Figure S7. ITC isotherms for the titration of (A) G5, (B) G5-P, (C) G6, and (D) G6-P (250 μM each) to Aβ_{42} (25 μM) at 37 °C.
Figure S8. Aggregation kinetics of Aβ_{42} (25 μM) incubated with and without an equimolar dendrimer. The final (maximum) ThT fluorescence of Aβ_{42} aggregates without a dendrimer was defined as 100%.
Reference: