# **Supporting Information**

# Non-covalent Pyrene-PEG Coatings of Carbon Nanotubes Achieve *In Vitro* Biocompatibility

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## **Molecular Dynamics Results**

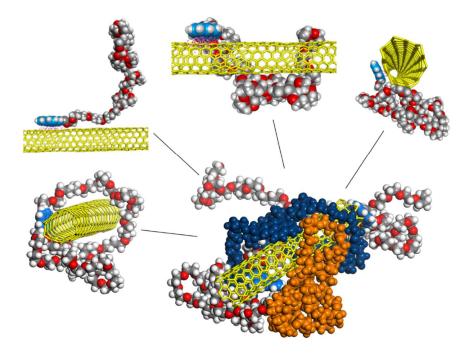


Figure S1. Dynamics of PEG chains on SWNTs and coating of the SWNT by four PEG<sub>2000</sub>

chains in different conformations (from M<sub>4</sub>)

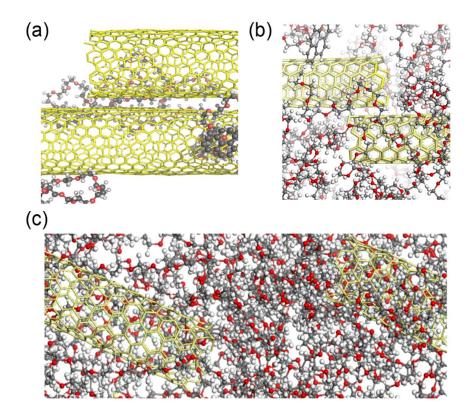


Figure S2. (a) π-π interactions between SWNTs (yellow) from neighboring box in simulation
(a) M<sub>2</sub> and (b) M<sub>3</sub>. (c) SWNTs from neighboring simulation boxes do not interact in simulation M<sub>6</sub>. Water molecules are not shown for clarity.

## **SWNT Synthesis**

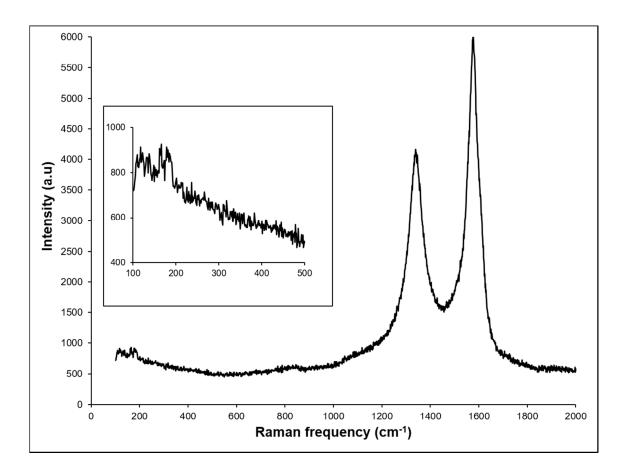


Figure S3. Raman spectra of SWNTs synthesized at 800 °C

Thermogravimetric analysis of SWNTs coated with Pyr-PEG<sub>5000</sub>

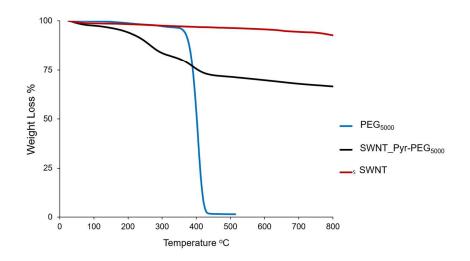
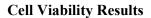
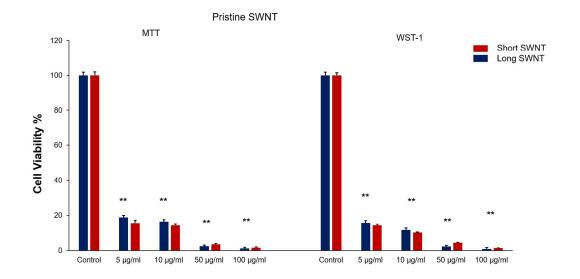
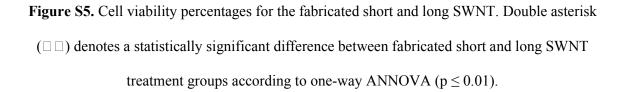


Figure S4. Thermogravimetric results of PEG<sub>5000</sub>, short SWNT and short SWNT coated with

Pyr-PEG<sub>5000</sub>







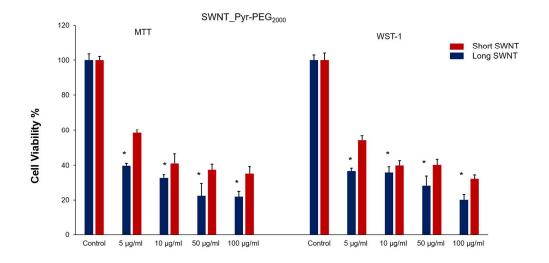


Figure S6. Cell viability percentages for the fabricated short and long SWNT. The asterisk ( $\Box$ ) denotes a statistically significant difference between long SWNT and short SWNT coated with Pyr-PEG<sub>2000</sub> treatment groups according to Student's t-test (p  $\leq$  0.05).

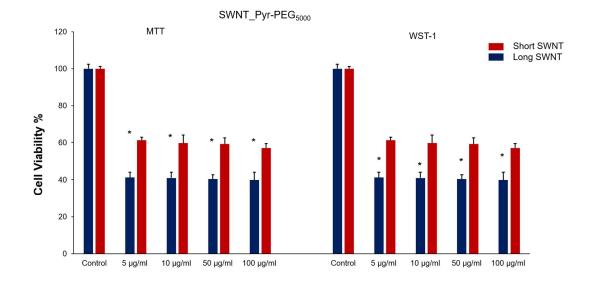


Figure S7. Cell viability percentages for the fabricated short and long SWNT. The asterisk ( $\Box$ ) denotes a statistically significant difference between long SWNT and short SWNT coated with Pyr-PEG<sub>5000</sub> treatment groups according to Student's t-test (p  $\leq$  0.05).