Electronic Supplementary Information for

"Edge Effects Control Helical Wrapping of Carbon Nanotubes by Polysaccharides"

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Table S1. Detail of systems for molecular dynamics simulation.

Simulation	Number of atoms	Box dimensions	Time (ns)
MP	14280	~4.0 × 4.0 × 9.8 nm^3	217
EP	13659	~3.0 × 3.0 × 14.4 nm^3	120
MO	45306	~6.0 × 8.0 × 9.8 nm^3	209
EO	40749 (left-handed)	~6.0 × 8.0 × 8.8 nm^3	200
	40752 (right-handed)	~6.0 × 8.0 × 8.8 nm^3	210

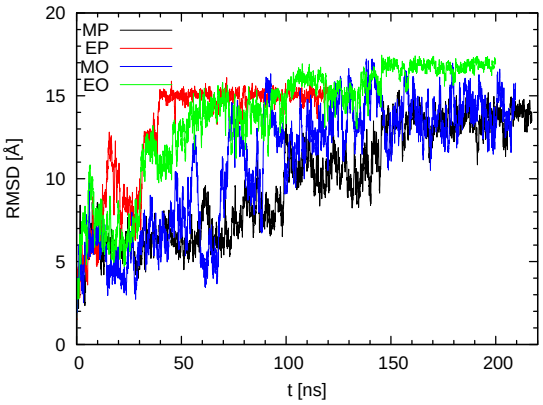

Figure S1. Distance root-mean-square deviation over the heavy atoms of the AMYL chain with respect to the initial structure as a function of time.

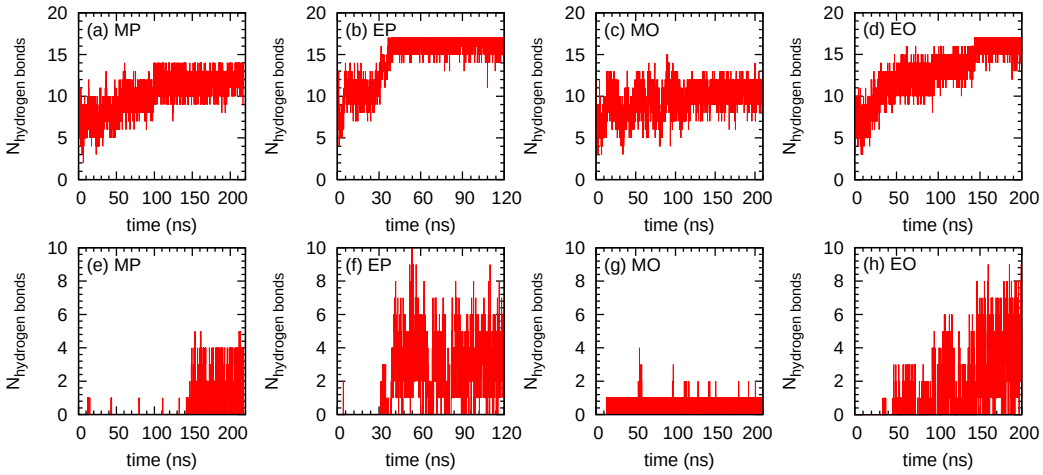

Figure S2. Time evolution of number of hydrogen bonds for the system of (a) MP, (b) EP, (c) MO, and (d) EO. The top panels represent the inter-residue hydrogen bonds (O2-O3) and the top panels represent the inter-turn hydrogen bonds (O2/O3-O6), respectively. The hydrogen-bond criterion here is the angle O-H···O > 135º and the distance O···O < 3.5 Å.

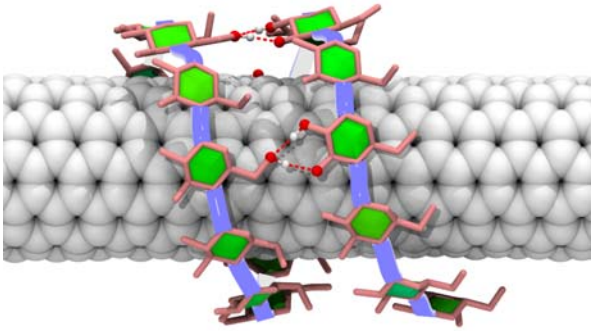

Figure S3. Final structure of the self-assembly of the inherent right-handed AMYL chain on the tubular surface.