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Supporting Information : Investigation of the influence of surface defects on peptide adsorption onto carbon nanotubes

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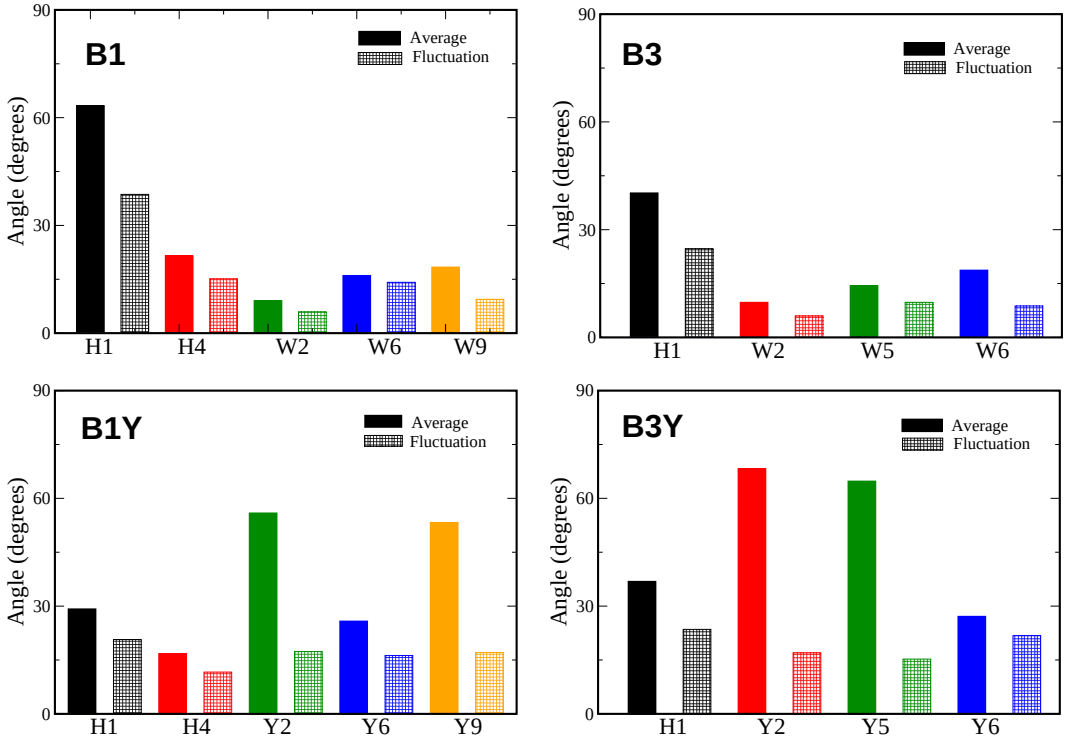

Figure S1: Average and fluctuation of ring tilt for the interface between each sequence and a pristine CNT. A tilt of zero indicates the ring is oriented flat on the surface.

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Table S1: Peptide end-to-end distances, *d* (Å), averaged over the lowest trajectory for each sequence (B1, B3, B1Y and B3Y) for each peptide-nanotube interface.

Pristine (no defects)				
Sequence		*d*		
B1		27.3		
B3		27.0		
B1Y		13.3		
B3Y		16.7		
‘Hydroxy’ defects				
Sequence	Distribution	*d*	Distribution	*d*
B1	Close	26.7	Distant	26.9
B3	Close	20.4	Distant	21.2
B1Y	Close	16.9	Distant	13.4
B3Y	Close	36.9	Distant	12.8
‘Carboxyl’ defects				
Sequence	Distribution	*d*	Distribution	*d*
B1	Close	27.0	Distant	27.0
B3	Close	21.2	Distant	20.5
B1Y	Close	16.8	Distant	14.2
B3Y	Close	17.7	Distant	24.5

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