Supplementary Material (ESI) for Soft Matter
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**Supplementary Data**

# Effect of functionalization on the self-assembling propensity of β-sheet forming peptides

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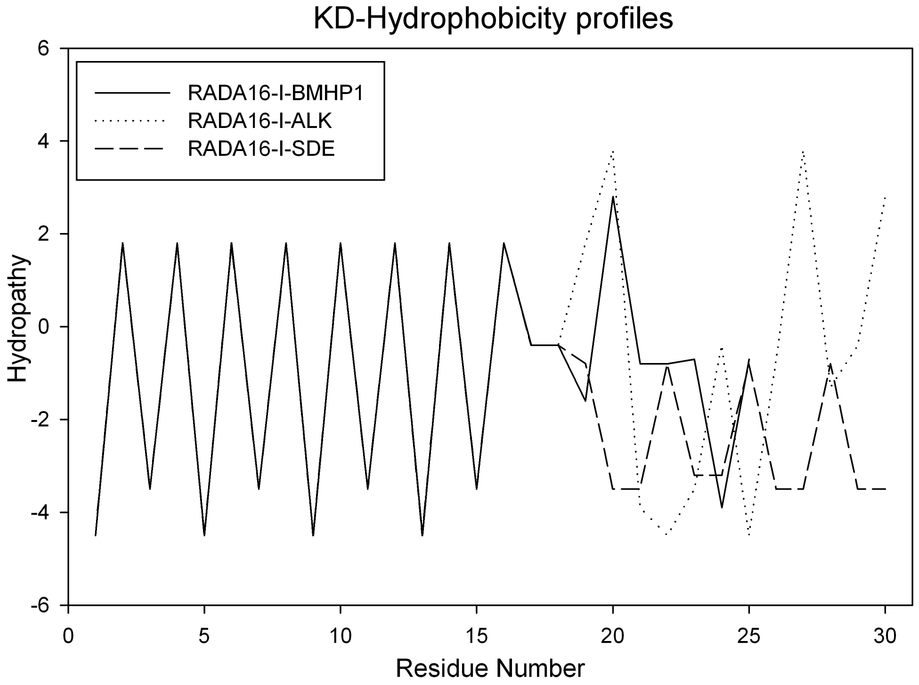
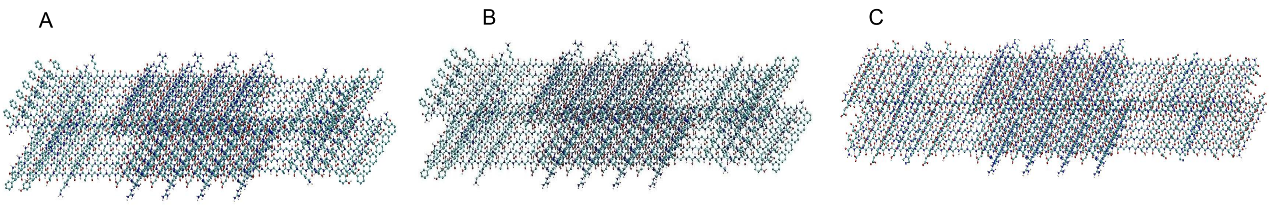
## Section 1

Hydrophobicity profiles calculated via the Kyte-Doolittle scale (J. Kyte and R.F. Doolittle, *J. Mol. Biol.* 1982, **157**,105-132). According to this scale positive values stand for hydrophobic residues while negative values stand for the hydrophilic residues. Hydrophobicity profiles are similar to those obtained with the White and Smith scale.



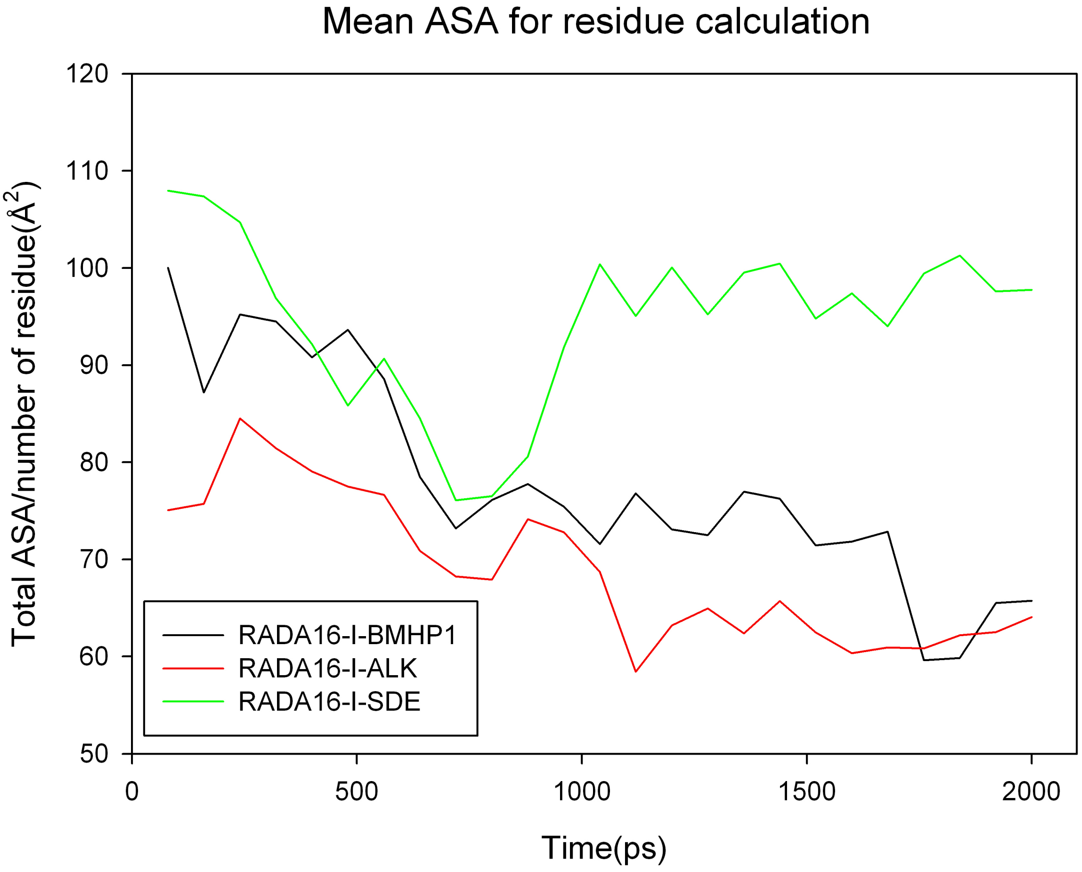
## Section 2

Initial FP arrangement in each MD. The image shows the starting cross-β of each peptide in the CPK mode of visualization. A) RADA16-I-BMHP1, B) RADA16-I-ALK, C) RADA16-SDE



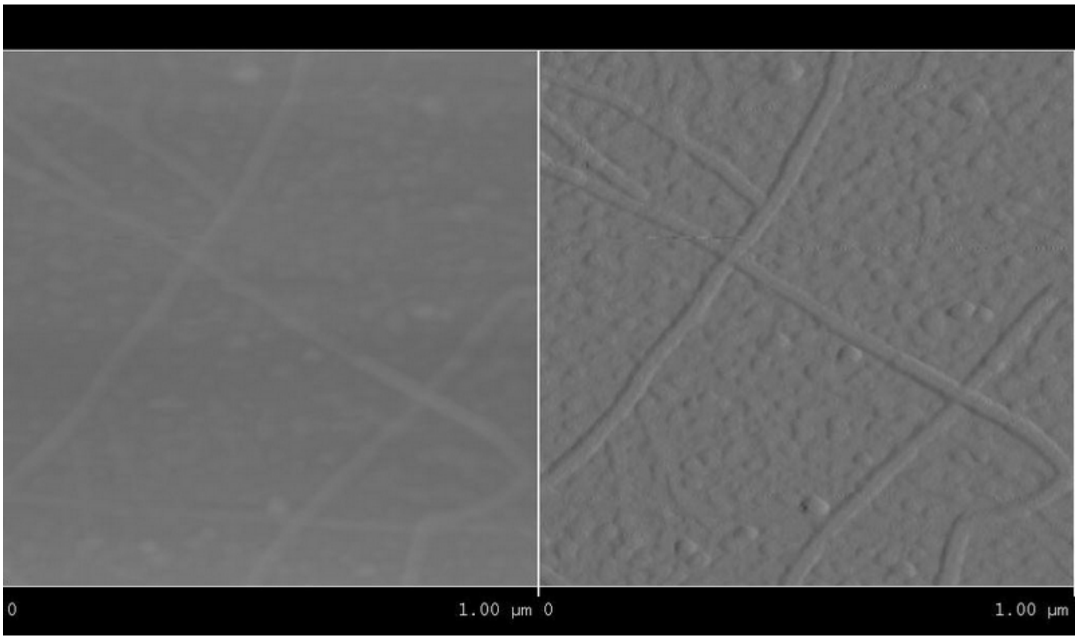
## Section 3

Total ASA value normalized over residue number for each peptide. Time step is 80ps.



## Section 4

RADA16-I-ALK solution in MilliQ was used to a peptide final concentration of 1% w/v. 5µl peptide solution was placed on mica surface and after 1 minute of adsorption the sample was washed with MilliQ water and dried under a stream of nitrogen.
All images were processed using Digital Instrument (Nanoscope 5.31r1) software.

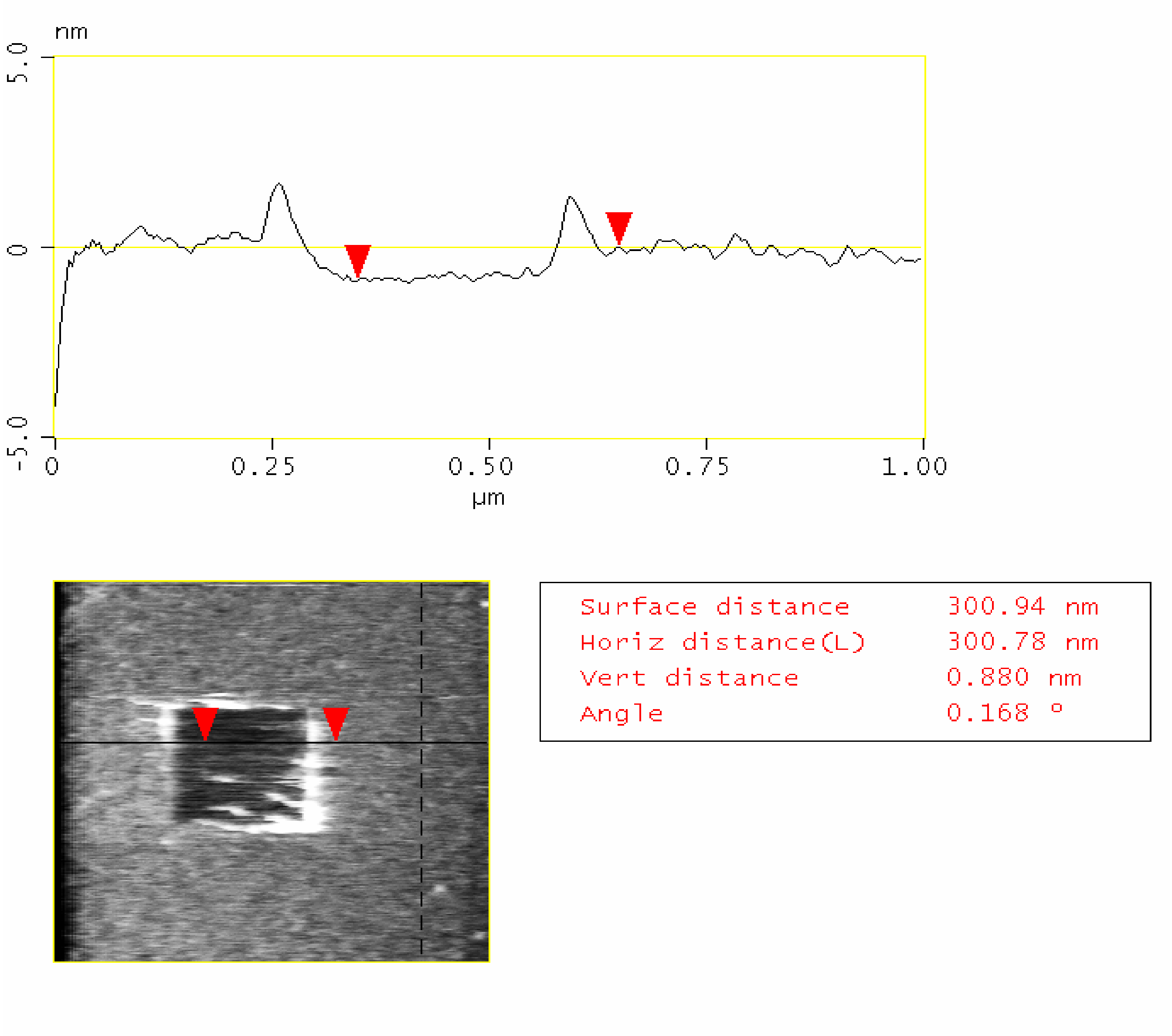


<u>Section 5</u>

RADA16-I-SDE solution was diluted to a final concentration of 0.01% w/v. 5µl peptide solution was placed on mica surface and after 1 minute of adsorption the sample was washed with MilliQ water and dried carefully under a stream of nitrogen.

All the images were obtained in air in contact mode with a nominal spring constant of 0.16 N/m.

All the images were processed using Digital Instrument (Nanoscope 5.31r1) software.



| | |
|---|---|
| Surface distance | 300.94 nm |
| Horiz distance(L) | 300.78 nm |
| Vert distance | 0.880 nm |
| Angle | 0.168 ° |