Adsorption, Folding and Packing of an Amphiphilic Peptide at the Air/Water Interface

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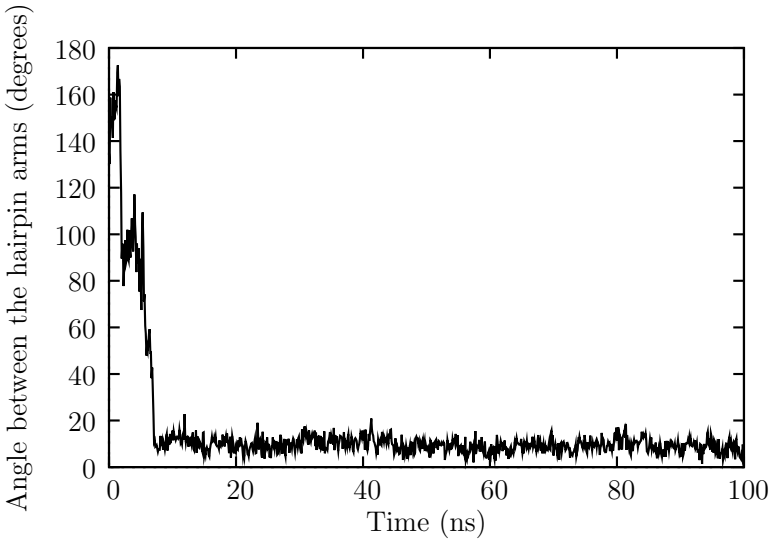
SI 1

Trajectory for the adsorption and folding of the peptide at the air/water interface. At the beginning of the movie, the interface system is shown from the side. The interface is shown as a transparent plane separating the bulk water (bottom) and air (top) phases. The hydrophobic and hydrophilic side chains are shown in licorice mode as blue and purple, respectively. The backbone of the peptide is shown in cartoon view, so that one can observe the evolution of the secondary structure as the peptide adsorbs to the interface. In the final part the system is shown looking down at the interface from vacuum side. The stability of the β-hairpin structure and local fluctuations can be seen in the movie.

Please watch the movie "adsorption.avi", which is available as part of the supporting information.

SI 2

The β-hairpin structure formed by the amphiphilic peptide molecule at the interface was preserved for the rest of the simulation. We used the angle between the arms for quantifying the alignment, where the time-line data for the angle is shown below. As seen from the figure, despite the changing β-sheet content in DSSP result, the arms of the β-hairpin remained well aligned.

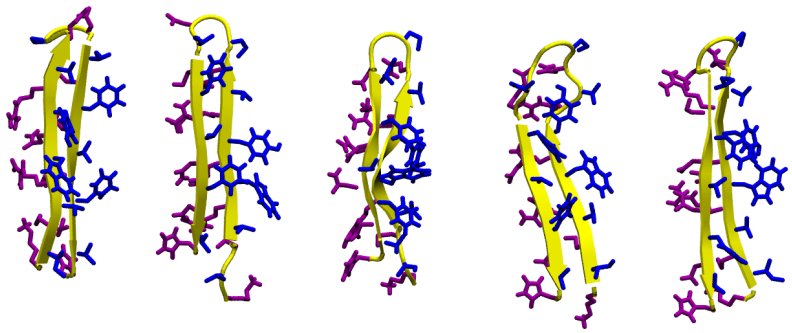


SI 3

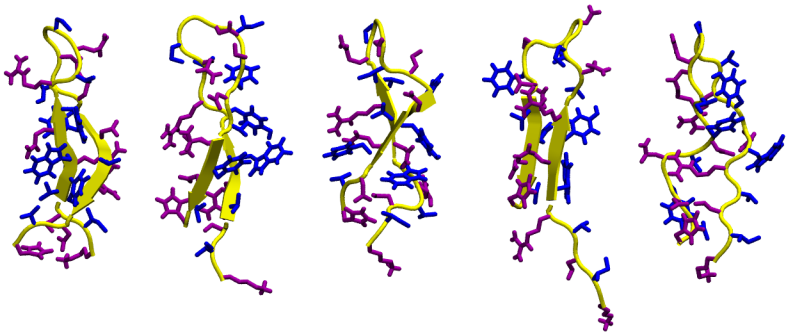
In order to test the dependence of the results presented in the paper we have performed 4 additional simulations with different initial conditions for both interface and bulk systems. Representative snapshots from all 5 of these simulations are given below for interface (a) and bulk (b) systems. As explained in the text the presence of the interface significantly reduces the conformational space of the molecule, such that except for small variations in the side chain orientations the structures look almost identical.

On the other hand in bulk, since the hydrophobic and hydrophilic side chains can not be partitioned completely, the peptide has more conformational flexibility.

a)

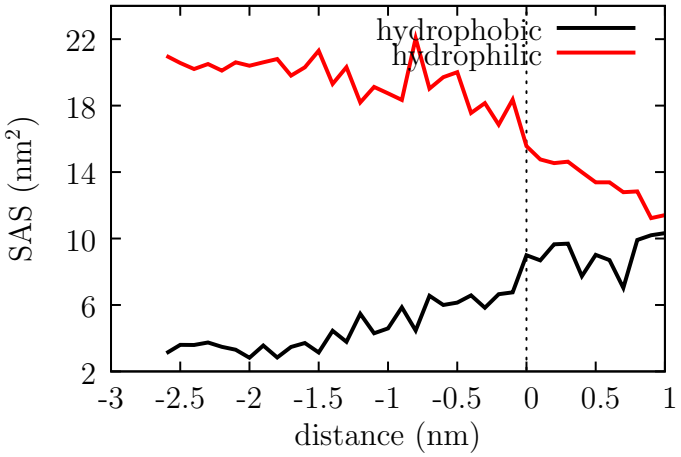


b)



SI 4

Surface area of hydrophobic groups accessible by air (black), and surface area of hydrophilic groups of the peptide accessible by water (red) as a function of the distance from the air/water interface. Due to the discrete nature of the side chains SAS values and the internal energy of the molecule display a zigzag pattern.



SI 5

The amphiphilic nature of the peptide provides such a large driving force that if the molecule is placed at the interface with its hydrophilic side facing the vacuum, the peptide quickly re-orients. Secondary structure time-line data obtained from the DSSP program (top) shows that β-hairpin structure of the molecule is destroyed during re-orientation and restored back when the hydrophilic face is in contact with water. Time-line data for the number of intra-peptide H-bonds confirm restoration of the secondary structure. The water accessible hydrophobic surface area (bottom) also demonstrate the re-orientation of the molecule.