

# Supplementary Information

## Thermodynamic and Kinetic Characterization of Transmembrane Helix Association<sup>†</sup>

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### 1 Supplementary Tables

System	Simulations No.	Lipids No.	Water No.	Box Size (nm)	Simulation Length ( $\mu$ s)
Long Unbiased	1	256	4000	12X6	320
Biased	36 windows	256	4000	12X6	6
Multiple Short Unbiased	100	94	863	5X5	1

**Supplementary Table 1** Overview of the coarse-grain simulations performed

<sup>†</sup> Electronic Supplementary Information (ESI) available. For review purposes, see attached file. For the final version see DOI: 10.1039/b000000x/

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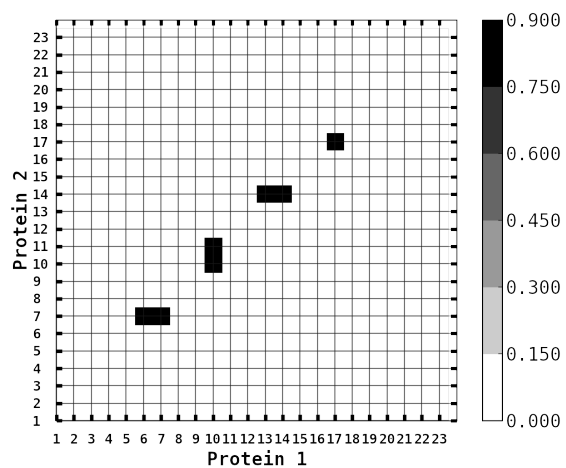
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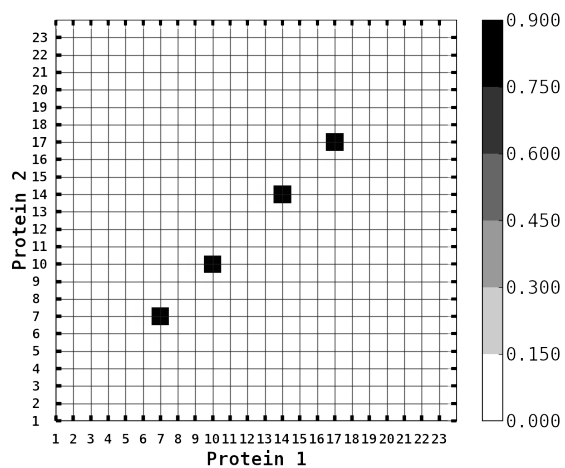
## 2 Supplementary Figures

**Supplementary Fig. 1** A contact map of the helix-helix interface for (a) 1-5  $\mu\text{s}$  (b) 300-320  $\mu\text{s}$  of the long unbiased simulation. A value of 1.0 correspond to a well preserved contact where as 0.0 correspond to no contacts. A cut-off of 0.8nm was used to calculate the contacts.

(a) 1-5  $\mu\text{s}$

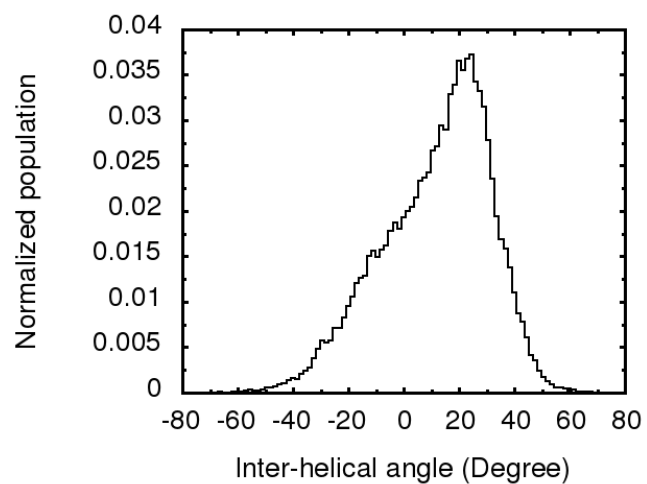


(b) 300-320  $\mu\text{s}$

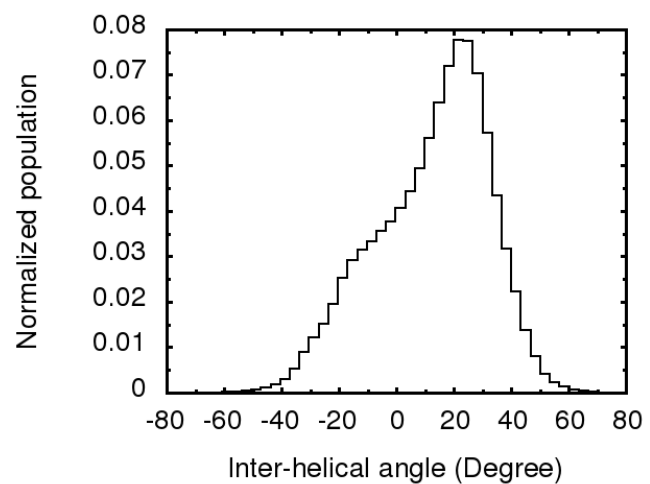


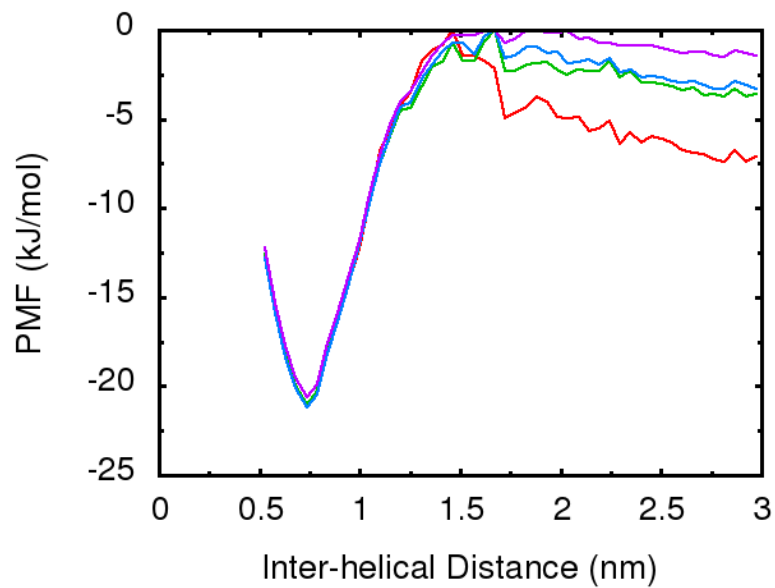
**Supplementary Fig. 2** The population distribution of the inter-helical angles sampled during (a) 1-5  $\mu$ s (b) 300-320  $\mu$ s of the long unbiased simulations.

(a) 1-5  $\mu$ s

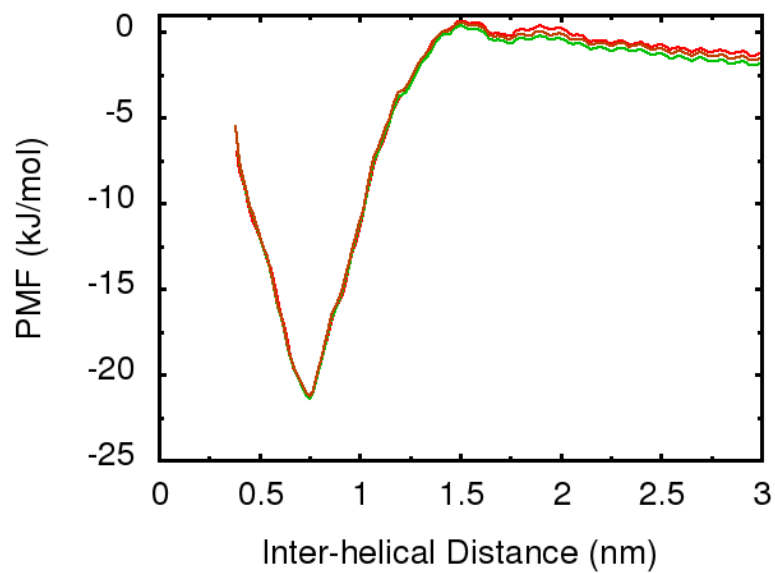


(b) 300-320  $\mu$ s

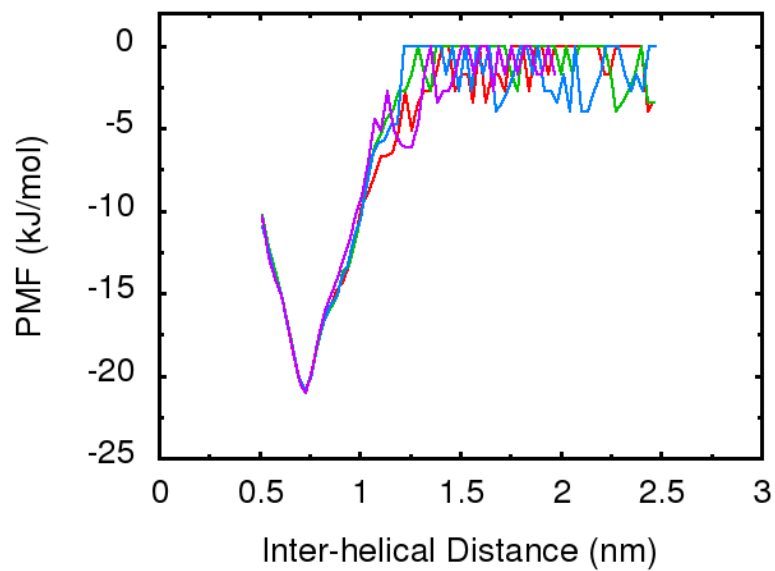




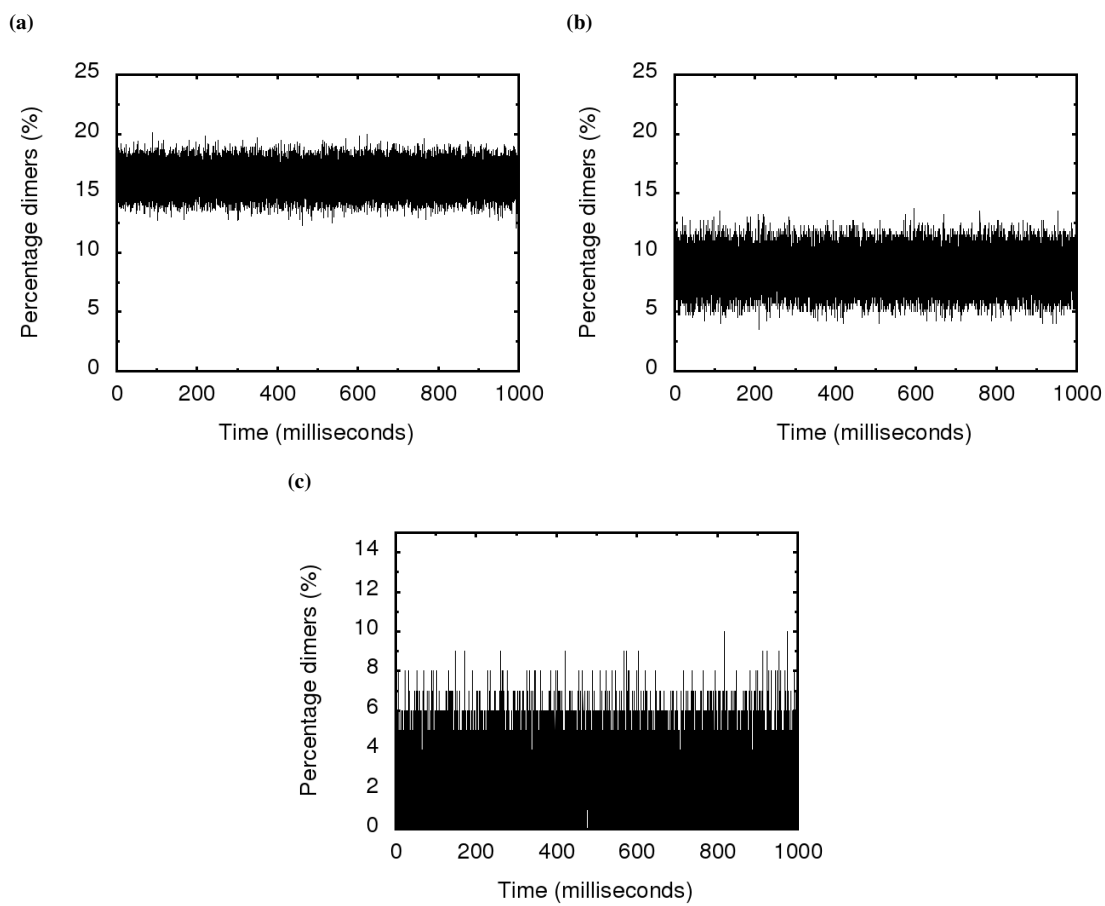
**Supplementary Fig. 3** The potential of mean force (PMF) of polyaniline transmembrane helices along the inter-helical distance calculated from long ms-timescale unbiased simulations. The profiles were calculated for 0-10  $\mu\text{s}$  (red), 0-50  $\mu\text{s}$  (green), 0-100  $\mu\text{s}$  (blue) and 0-320  $\mu\text{s}$  (magenta) time intervals.



**Supplementary Fig. 4** The PMF of polyalanine transmembrane helices along the inter-helical distance calculated from umbrella sampling biased simulations. The PMF were calculated at different time intervals: 0-1  $\mu$ s (red), 0-2  $\mu$ s (green), 0-3  $\mu$ s (blue), 0-4  $\mu$ s (magenta), 0-5  $\mu$ s (cyan) and 0-6  $\mu$ s (brown).



**Supplementary Fig. 5** The PMF of polyalanine transmembrane helices along the inter-helical distance calculated from the ensemble of biased simulations. The profiles were calculated for the time intervals: 600-700 ns (red), 700-800 ns green, 800-900 ns (blue), 900 ns-1  $\mu$ s (magenta).



**Supplementary Fig. 6** The time evolution of the percentage of the dimers formed in the meso-scale simulation at protein-lipid ratios (a)1:20, (b)1:50, and (c)1:200.