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ESI

Elucidating the mechanism of interaction between peptides and inorganic surfaces

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Peptide sequences

The protected peptide sequences that were used for tip functionalization were

1. Fmoc-Gln(Trt)-Pro-Ala-Ser(tBu)-Ser(tBu)-Arg(pbf)-Tyr(tBu)-COOH
2. Fmoc-Ala-Pro-Ala-Ser(tBu)-Ser-(tBu)Arg(pbf)-Tyr(tBu)-COOH
3. Fmoc-Gln(Trt)-Ala-Ala-Ser(tBu)-Ser(tBu)-Arg(pbf)-Tyr(tBu)-COOH
4. Fmoc-Gln(Trt)-Pro-Ala-Ala-Ser(tBu)-Arg(pbf)-Tyr(tBu)-COOH
5. Fmoc-Gln(Trt)-Pro-Ala-Ser(tBu)-Ala-Arg(pbf)-Tyr(tBu)-COOH
6. Fmoc-Gln(Trt)-Pro-Ala-Ser(tBu)-Ser(tBu)-Ala-Tyr(tBu)-COOH
7. Fmoc-Gln(Trt)-Pro-Ala-Ser(tBu)-Ser(tBu)-Arg(pbf)-Ala-COOH

Detailed version of Fig. 2 (this figure contains the number of measurements and MPF for each experiment).

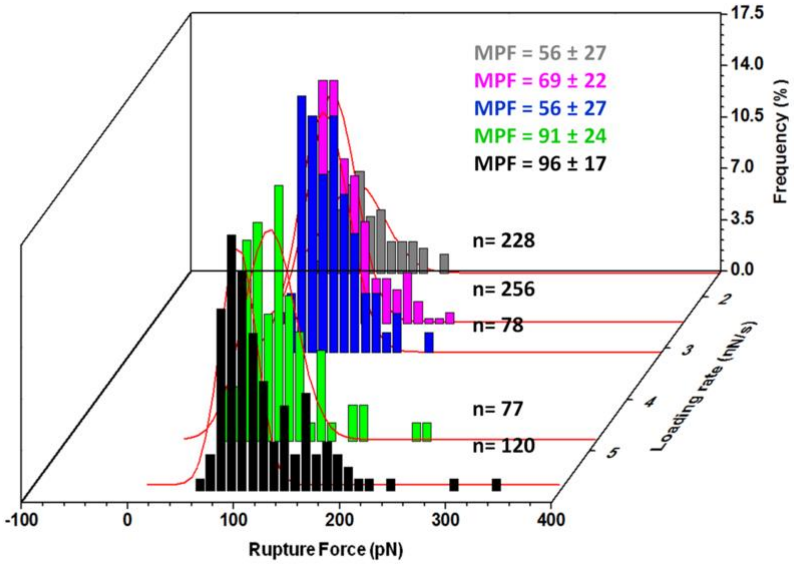

Fig 2. Waterfall representation of a pull-off force histogram for the Q4 interaction between peptide 1 and mica at different apparent loading rates (1.54 nN, 2.52 nN, 3.08 nN, 4.82 nN and 5.80 nN) at 298 K in TDW. The red lines represent the Gaussian fit for each histogram. n is the number of curves used for generating a histogram.

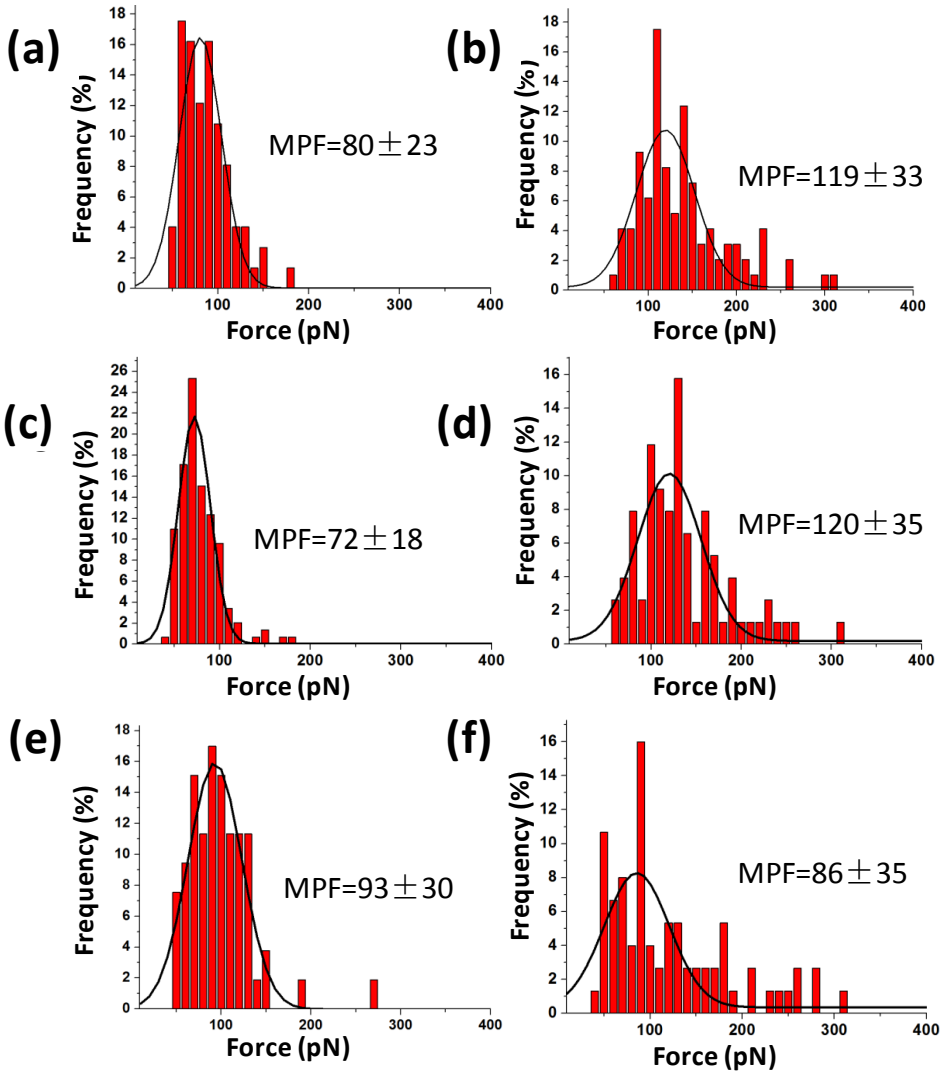

Fig. S1 Force histogram with Gaussian fit (black curve) for the different peptides and mica at different apparent loading rate at 298K. (a) peptide **1** at 3.1±0.6nN/s (n=78) (b) peptide **2** at 3.8±0.9nN/snN/s (n=107) (c) peptide **4** at 3.2± 0.7nN/s (n=140) (d) peptide **5** at 3.3±0.8 nN/s (n=122) (e) peptide **6** at 2.9±0.7 nN/s (n= 112) and (f) peptide **7** at 3.5±1.1nN/s (n=71). n is the number of curve used for preparing histogram.

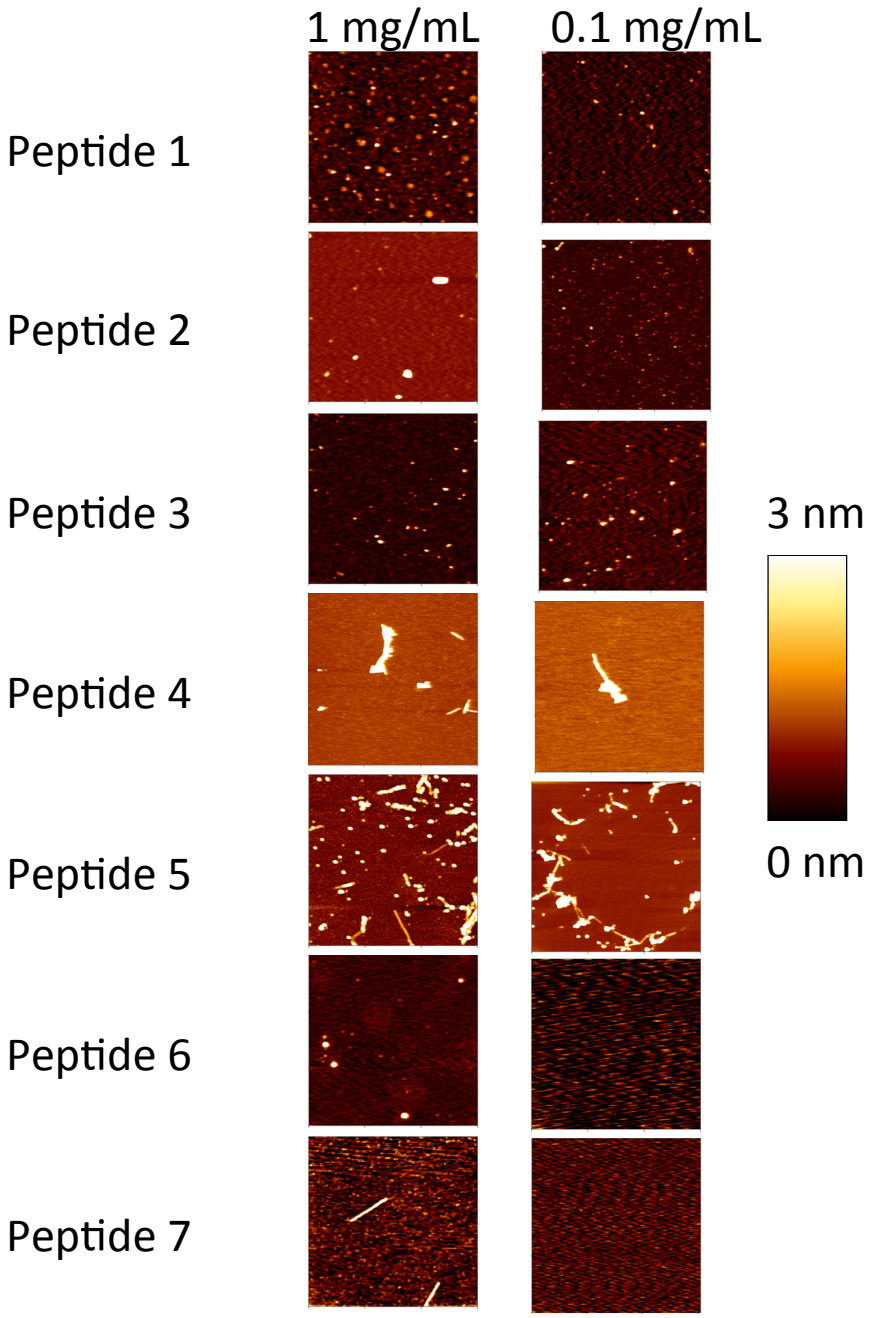

Fig. S2 AFM topography analysis of peptides **1-7** at different concentrations after one hour of incubation. The size scan of all images is 3x3 μm.

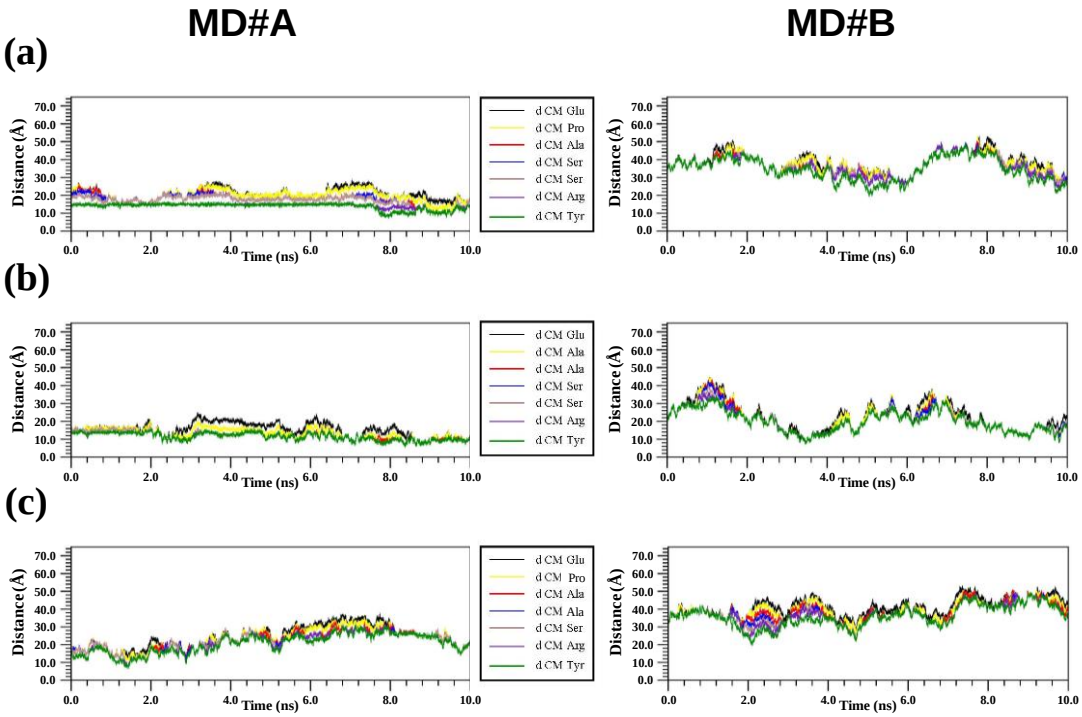

Fig. S3 Temporal evolution of the distance between the center of masses of each residue and the mica surface, calculated using the normal vector, for MD#A and MD#B simulations with #= (a) **1**; (b) **2** and (c) **3**.

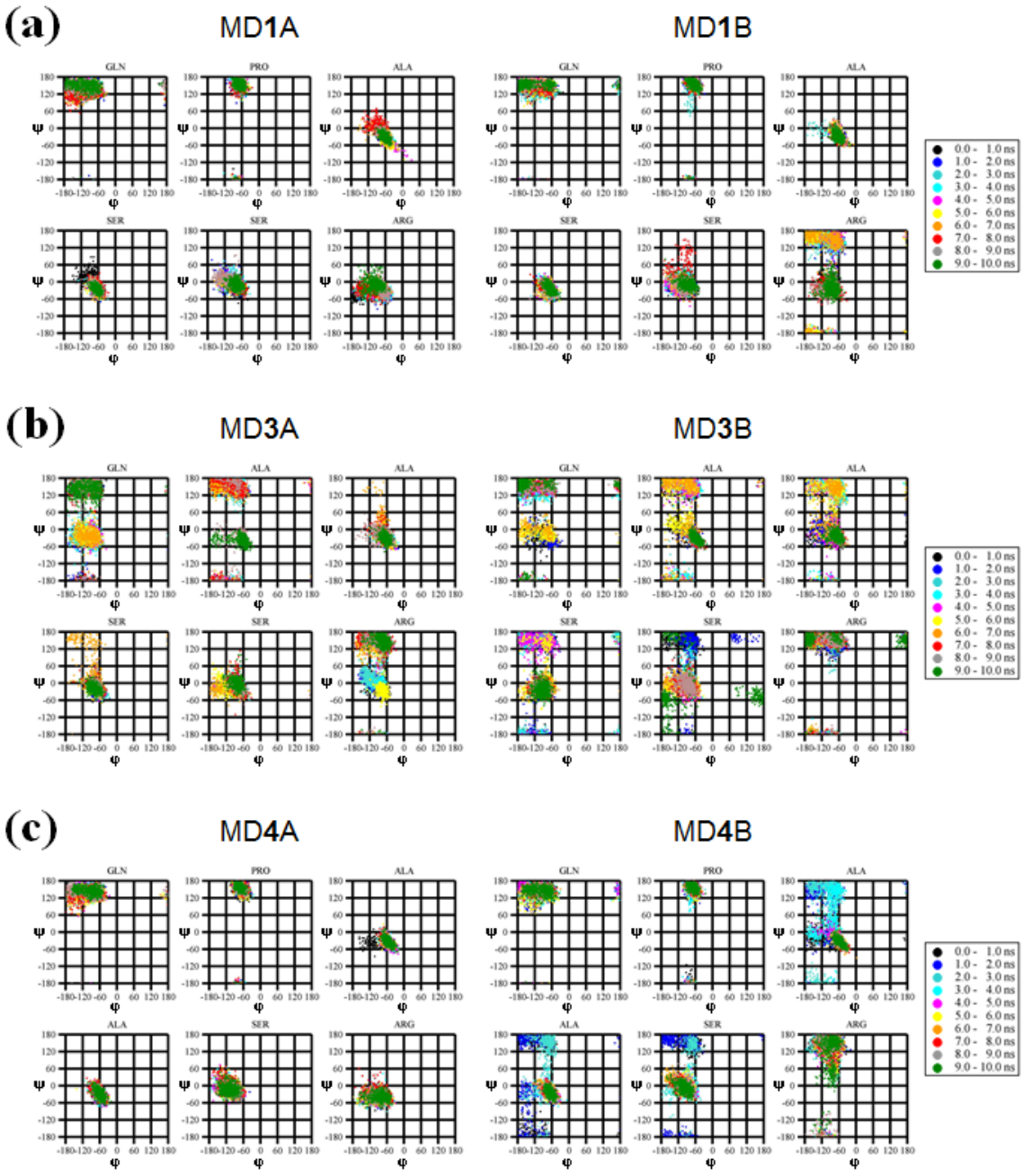

Fig. S4 Time dependent accumulated Ramachandran plots for (a) **1**, (b) **3** and (c) **4** depicted using snapshots recorded form from MD#A and MD#B simulations Each different color represents a time period of 1 ns.

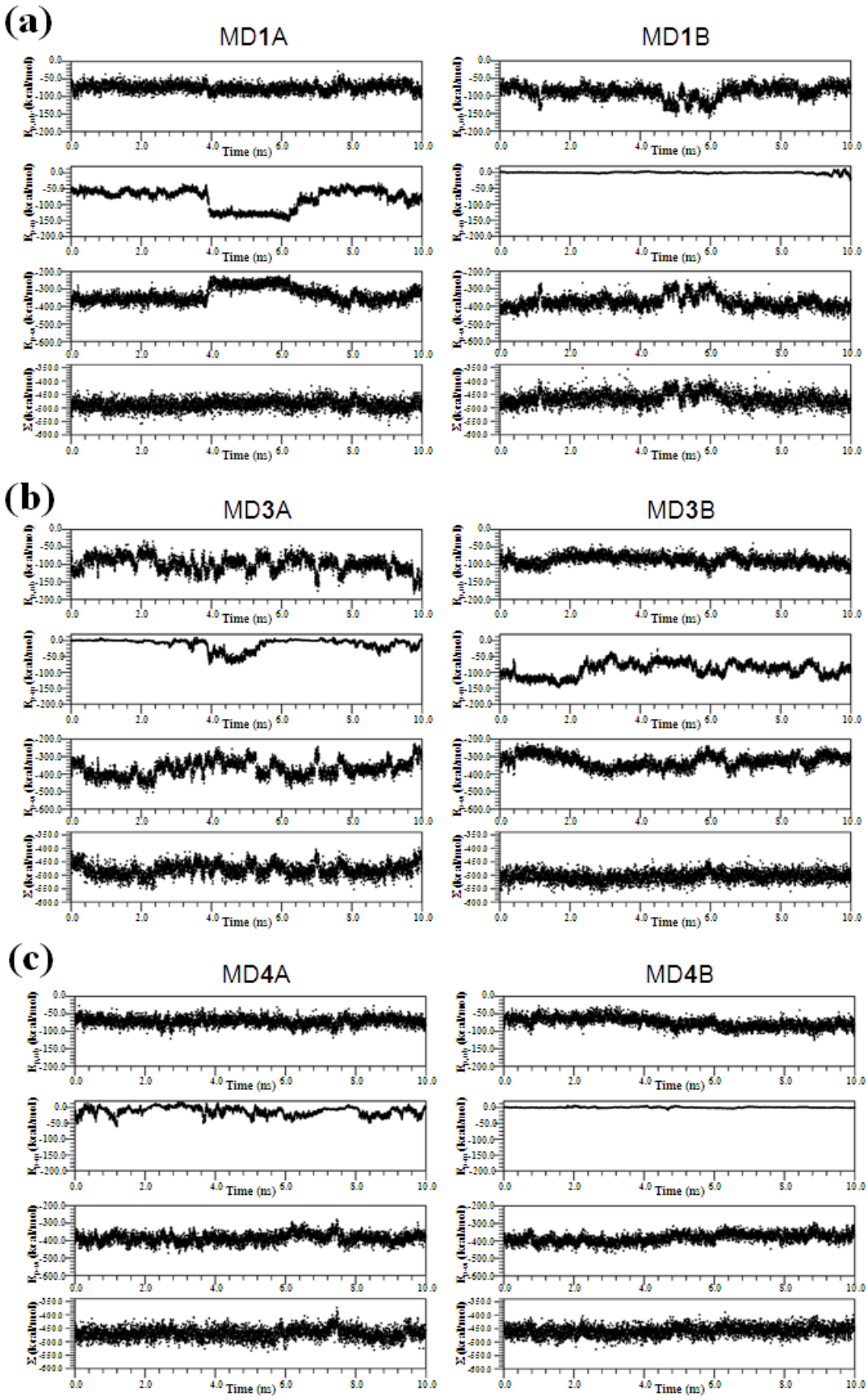

Fig. S5 Temporal evolution of $E_{p.nb}$, E_{p-m}, E_{p-w} and Σ (which is the sum of the three previous contributions) for MD#A and MD#B: (a) **1**; (b) **2** and (c) **3**.

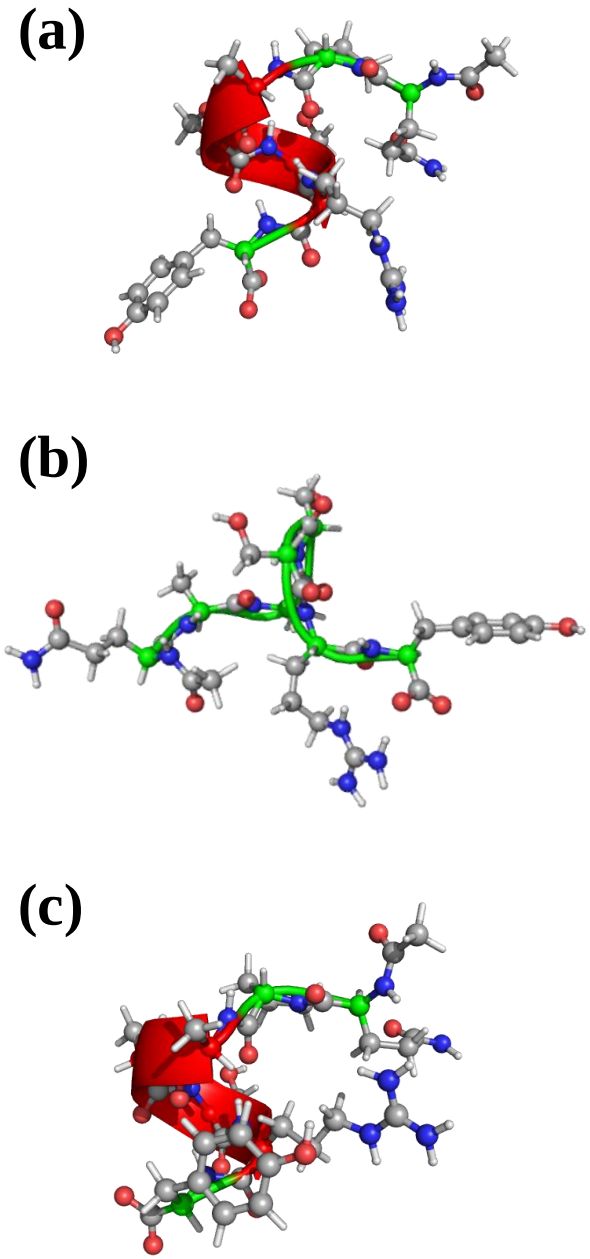

Fig. S6 Representative snapshots of peptides (a) **1**, (b) **3** and (c) **4** extracted from MD#**A** simulations.

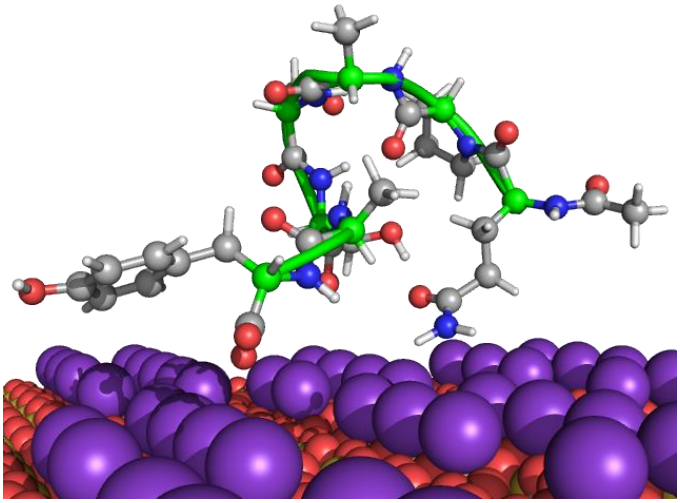

Fig. S7 Representative snapshot of peptides **6** adsorbed onto mica extracted from preliminary MD simulations performed according to the explanation given in the text.

Table S1. Results of the clustering analysis for MD#A and MD#B simulations, where # corresponds to peptides **1**, **3** and **4**.

	MD1A	**MD1B**	**MD3A**	**MD3B**	**MD4A**	**MD4B**
Total number of unique minima	361	695	758	1554	315	565
Number of minima with hydrogen bonds or salt bridges ($N_{hb/sb}$)[a]	353	672	706	1267	311	416
Number of interactions per minimum included in $N_{hb/sb}$	3.04	2.40	2.29	2.46	2.89	2.50
Number of clusters found in the $N_{hb/sb}$ minima	455	209	342	536	225	253
Number of clusters with more than 10 unique minima	11	13	17	11	9	13
Percentage of main chain – main chain hydrogen bonds (%)	53.92	87.63	79.88	53.46	80.69	60.41
Percentage of main chain – side chain hydrogen bonds (%)	42.30	8.59	14.06	43.41	14.18	36.99
Percentage of side chain – side chain hydrogen bonds (%)	3.80	3.81	6.07	3.14	2.16	2.62

[a] Salt bridges between the side chain of Arg and the COO^- groups of the C-terminal have not been found in any studied system.