Supporting Information

Effect of Monovalent Salt Concentration and Peptide Secondary Structure in Peptide-Micelle binding

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Table S1. Size of MD simulation models.

	P^{c}*	P^{c}_SDS (NaCl= 0.0% w/v)	P^{c}_SDS (NaCl= 0.5% w/v)	P^{c}_SDS (NaCl= 1.0% w/v)	P^{h}*	P^{h}_SDS (NaCl= 0.0% w/v)	P^{h}_SDS (NaCl= 0.5% w/v)	P^{h}_SDS (NaCl= 1.0% w/v)
Total no of atoms	98307	268911	268062	267241	98295	268833	268038	266918
Water molecules	32667	88675	88300	87933	32663	88649	88292	87925
Na^{+}	-	60	198	338	-	60	198	338
Cl^{-}	7	7	145	285	7	7	145	285

	SDS (NaCl= 0.0% w/v)	SDS (NaCl= 0.5% w/v)	SDS (NaCl= 1.0% w/v)	DPC (NaCl= 0.0% w/v)
Total no of atoms	269046	268494	267934	270642
Water molecules	88822	88546	88266	88994
Na^{+}	60	198	338	-
Cl^{-}	-	138	278	-

Table S2. Number of independent replicas (varying the initial velocities) considered for each simulation model and the post-equilibrated production MD run-length. Multiple relative orientation has been considered for studying LL-14:micelle binding (Setup A, Setup B, Setup C: see Figure S1). Total MD run-lenth= 14.2 μs.

Salt (NaCl)	**Free in Water** Replica (Run-length)				**LL-14: Micelle interaction** Replica (Run-length)			
	P^c	P^h	SDS	DPC		P^c:SDS	P^h:SDS	P^c:DPC
0.0%	Rep1 (200ns) Rep2 (500ns) Rep3 (1μs)	Rep1 (200ns) Rep2 (500ns) Rep3 (1μs)	Rep1 (20 ns)	Rep1 (20ns)	Setup A	Rep1 (50ns) Rep2 (50ns) Rep3 (50 ns)	Rep1 (50ns) Rep2 (50ns) Rep3 (50 ns)	Rep1 (1μs)
					Setup B	Rep1 (50ns) Rep2 (50ns)	Rep1 (50ns) Rep2 (50ns)	
					Setup C	Set1(d_{com} = 5.8 nm) Rep1 (6 μs) Rep2 (50ns) Rep3 (50ns) Rep4 (50ns) Rep5 (50ns) Set2 (d_{com} = 5.1 nm) Rep1 (50ns) Rep2 (10ns) Rep3 (10ns) Set 3 (d_{com} = 8.6 nm) Rep1 (50ns)	Set1(d_{com} = 5.8 nm) Rep1(50ns) Rep2 (50ns) Rep3 (50ns) Rep4 (50ns) Rep5 (50ns) Set2 (d_{com} = 5.1 nm) Rep1 (50ns) Rep2 (10ns) Rep3 (10ns) Set 3 (d_{com} = 8.6 nm) Rep1 (50ns)	
0.5%			20 ns		Setup A	Rep1 (50ns) Rep2 (50ns) Rep3(50 ns)	Rep1 (50ns) Rep2 (50ns) Rep3(50 ns)	
					Setup B	Rep1 (50ns) Rep2 (50ns)	Rep1 (50ns) Rep2 (50ns)	

					Setup C	Set1(d_{com} = 5.8 nm) Rep1 (50ns) Rep2 (50ns) Rep3 (50ns) Rep4 (50ns) Rep5 (50ns) Set2 (d_{com} = 5.1 nm) Rep1 (50ns) Rep2 (10ns) Rep3 (10ns) Set2 (d_{com}= 8.6 nm) Rep1 (50ns)	Set1(d_{com} = 5.8 nm) Rep1 (50ns) Rep2 (50ns) Rep3 (50ns) Rep4 (50ns) Rep5 (50ns) Set2 (d_{com} = 5.1 nm) Rep1 (50ns) Rep2 (10ns) Rep3 (10ns) Set2 (d_{com} = 8.6 nm) Rep1 (50ns)	
1.0%			20 ns		Setup A	Rep1 (50ns) Rep2 (50ns) Rep3(50 ns)	Rep1 (50ns) Rep2 (50ns) Rep3(50 ns)	
					Setup B	Rep1 (50ns) Rep2 (50ns)	Rep1 (50ns) Rep2 (50ns)	
					Setup C	Set1(d_{com} = 5.8 nm) Rep1 (50ns) Rep2 (50ns) Rep3 (50ns) Rep4 (50ns) Rep5 (50ns) Set2 (d_{com} = 5.1 nm) Rep1 (50ns) Rep2 (10ns) Rep3 (10ns) Set3 (d_{com} = 8.6 nm) Rep1 (50ns)	Set1(d_{com} = 5.8 nm) Rep1 (50ns) Rep2 (50ns) Rep3 (50ns) Rep4 (50ns) Rep5 (50ns) Set2 (d_{com} = 5.1 nm) Rep1 (50ns) Rep2 (10ns) Rep3 (10ns) Set3 (d_{com} = 8.6 nm) Rep1 (50ns)	

Table S3. Micelle eccentricity (averaged from the last 20 ns of the first 50 ns trajectory) independent of salt concentration.

System (Salt concentration)	**Eccentricity**	**I_{min}/I_{max}**
SDS:P^c (NaCl = 0.0% w/v)	0.15 ± 0.06	1.34 ± 0.15
SDS:P^c (NaCl = 0.5% w/v)	0.17 ± 0.05	1.38 ± 0.18
SDS:P^c (NaCl = 1.0% w/v)	0.16 ± 0.06	1.39 ± 0.18
SDS:P^h (NaCl = 0.0% w/v)	0.22 ± 0.08	1.53 ± 0.21
SDS:P^h (NaCl = 0.5% w/v)	0.21 ± 0.08	1.52 ± 0.22
SDS:P^h (NaCl = 1.0% w/v)	0.22 ± 0.07	1.52 ± 0.20

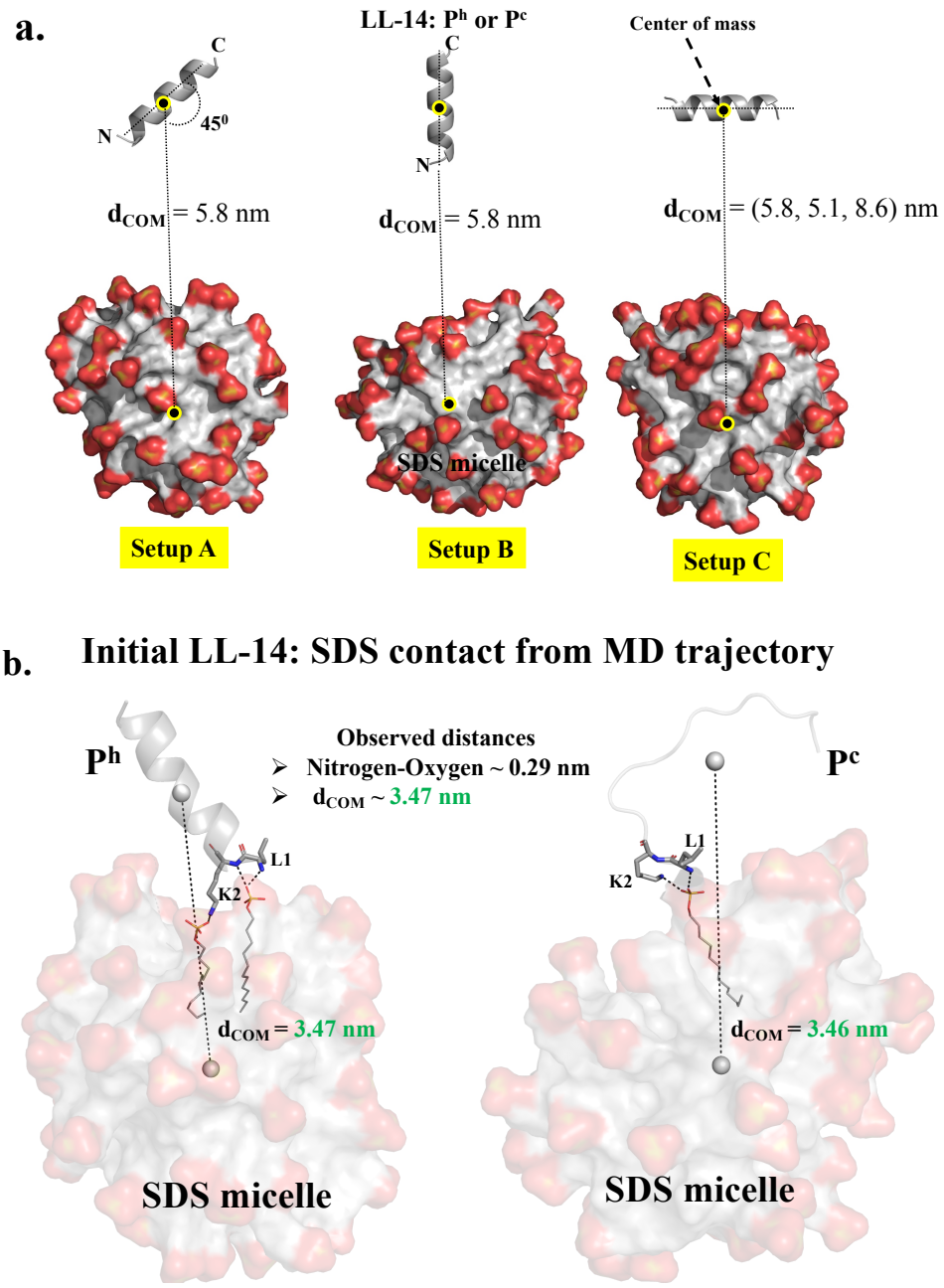

Fig. S1. (a) Relative position of LL-14 and SDS micelle considered as initial model for MD simulations. (b) Representative snapshot from MD simulation highlighting the initial contact between LL-14 and SDS micelle. Center of mass represented by grey sphere.

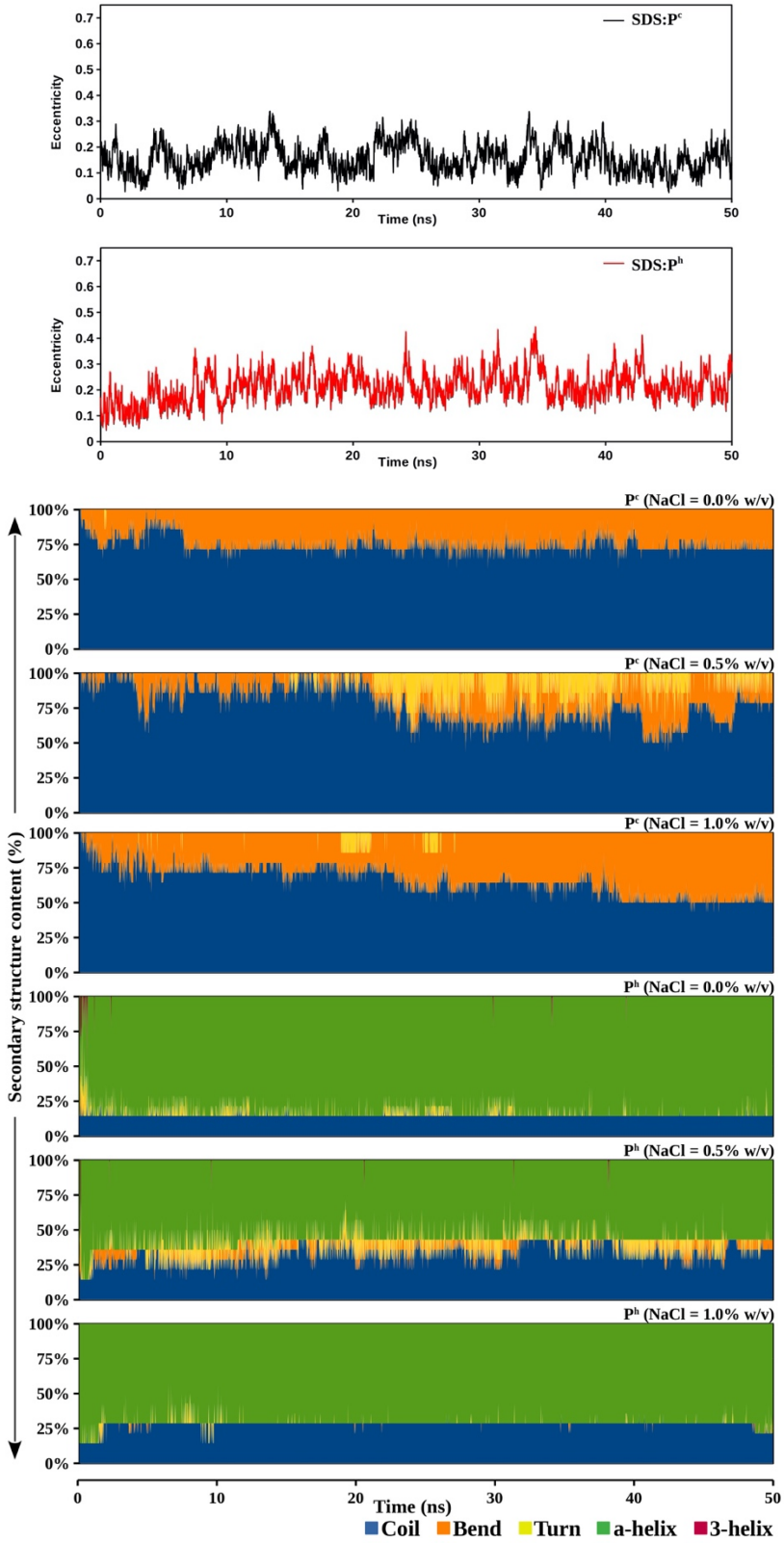

Fig. S2. Eccentricity vs Time plot (NaCl =0.0%). Secondary structural content of the peptide (P^c or P^h) estimated from the MD trajectory in presence of SDS micelle at various salt concentrations.

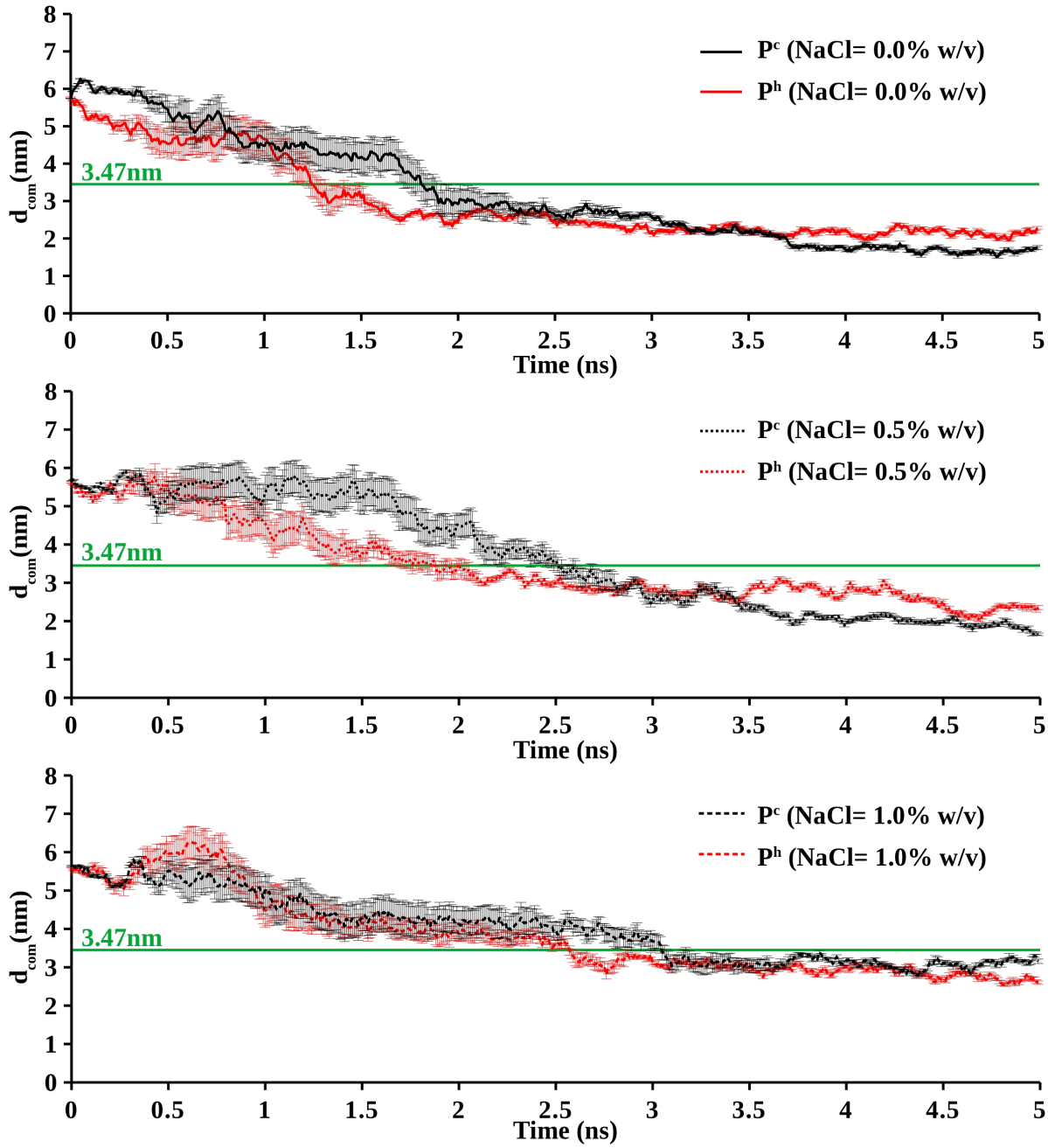

Fig. S3. Lines in the Figure 3 of the main-text has been divided into three groups (based on salt-concentrations). 5 independent replicas (obtained from Setup C of Fig. S1a, d_{COM} = 5.8 nm) were considered to calculated the temporal average for each simulation models. Error are reported as s.e.m from 5 replicas and shown as vertical bars. The same trend has been confirmed starting with various other setups (Fig. S1a).

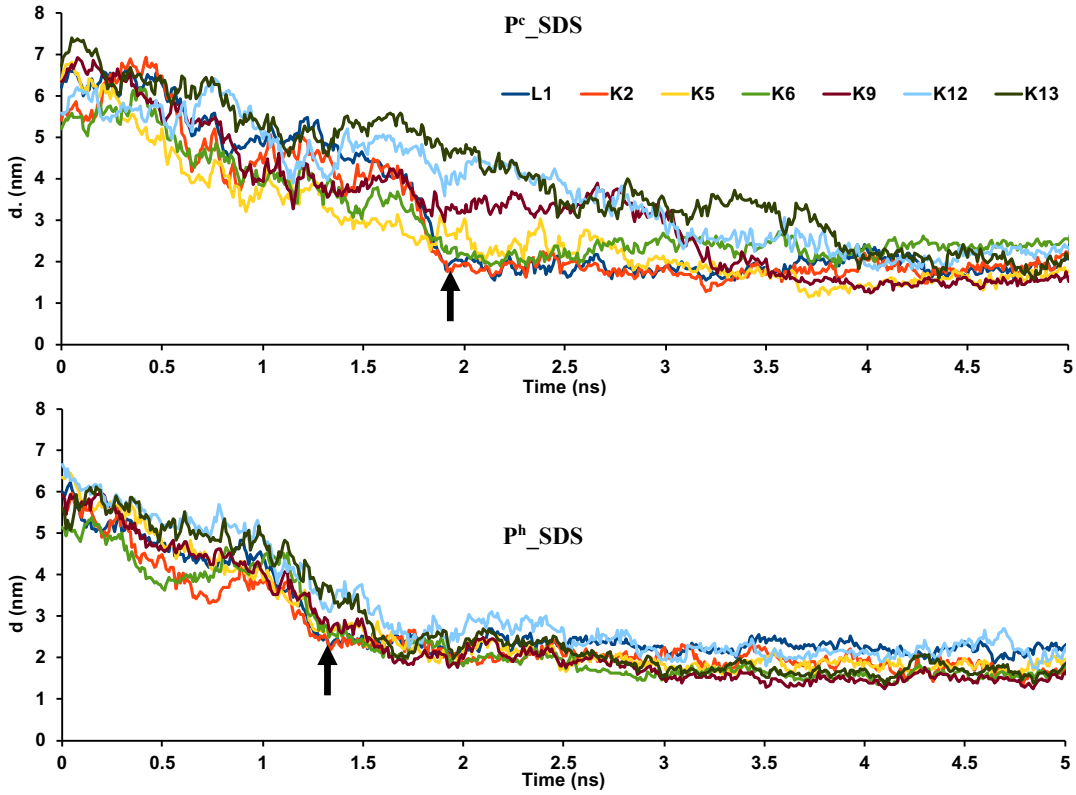

Fig. S4. "d" is the distance between positively charged nitrogen of the LL-14 residues and the centre of mass of SDS micelle. Distance plot (d vs. time) is shown along the MD trajectories (0% NaCl). Different colours represent different $-NH_3^+$ containing residues. N-terminal (L1, blue) and side-chain of K2 (red) forms the initial contact (represented as vertical arrow) with the micelle surface. The trend is same for simulations in presence of salt (not shown).

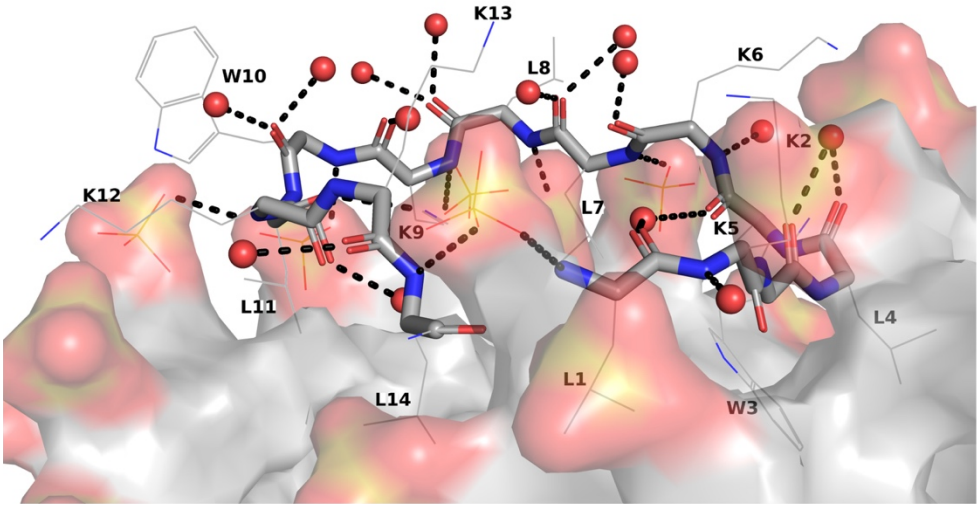

Fig. S5. Peptide backbone of P^c satisfied its hydrogen bonding requirement by forming H-bond with water molecules or sulphates of the SDS micelle or both. Snapshot after 50ns of MD. Peptide in sticks, water in red sphere, SDS (surface representation, lines represent sulphate).

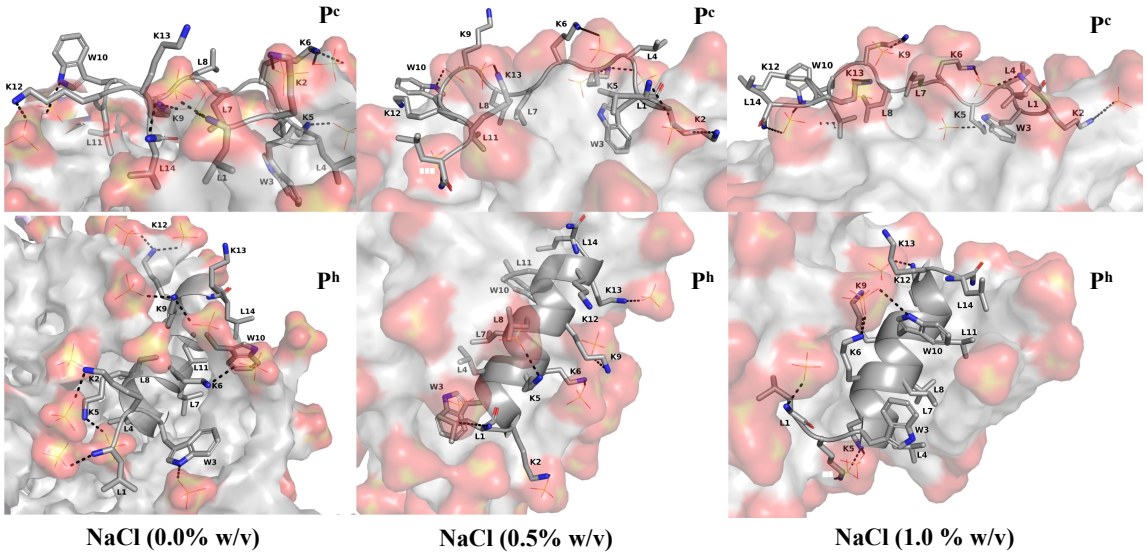

Fig. S6. Final structure of the peptide: micelle complex after 50 ns of MD simulations from three different NaCl-concentrations: 0.0% (given also in the main-text), 0.5% , and 1.0% w/v.

Description of Movie files

Mov1_Pc_in_Water.mpg :
1 μs MD trajectory starting with free P^c conformation of LL-14 in water. 1000 equally spaced frames (1 ns apart) from the MD trajectory was used for the movie.

Mov2_Ph_in_water.mpg :
1 μs MD trajectory starting with free P^h conformation of LL-14 in water. 1000 equally spaced frames (1 ns apart) from the MD trajectory was used for the movie.

Mov3_Pc_DPC.mpg :
1 μs MD trajectory starting with LL-14 (P^c) in presence of DPC micelle in water. 200 equally spaced frames (5 ns apart) from the MD trajectory was used for the movie.

Mov4_Pc_SDS.mpg:
6 μs MD trajectory starting with LL-14 (P^c) in presence of SDS micelle in water. 600 equally spaced frames (10 ns apart) from the MD trajectory was used for the movie.