Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Table S1. Structures by group using the clustering tool of Gromacs and % of structures collected in the first five groups.

Non-phosphorylated peptide							
Group	Free	N1	N2	N3	N4	N5	N6
1	300	558	396	412	465	1853	1227
2	208	283	235	312	274	130	546
3	161	234	197	294	190	16	83
4	135	94	135	116	154	1	60
5	111	87	128	111	145	1	43
% Structures	45.7	62.7	54.5	62.2	61.3	99.9	97.8
Phosphorylated peptide							
	Free	P1	P2	P3	P4	P5	
1	344	878	332	341	865	591	
2	324	394	294	196	719	233	
3	292	188	189	174	177	185	
4	118	109	142	147	66	159	
5	114	72	99	142	61	112	
% Structures	59.5	82.0	52.7	50.0	94.3	64.0	

Note S1

The geometry optimizations of the aluminum complexes with the phosphorylated derivative displayed some proton transfer from water molecules to the closer carboxyl group; in the P1 went to E2, in P2 went to E4, in P3 double proton transfer to PO_4, and in P4 and P5 none proton transfer.