

Table S1: Time-dependent distribution of protonation and deprotonation states of Aspartate and Glutamate residues.

Time Interval (ns)	Asp Protonated (%)	Asp Deprotonated (%)	Glu Protonated (%)	Glu Deprotonated (%)
1-10	70	30	80	20
10-20	65	35	75	25
20-30	60	40	70	30
30-40	55	45	65	35
40-50	50	50	60	40
50-60	45	55	55	45
60-70	40	60	50	50
70-80	35	65	45	55
80-90	30	70	40	60
90-100	75	25	65	35