

**Supplementary Information for: "Chemistry
specificity of DNA-polycation complex salt
response: A simulation study of DNA, polylysine
and polyethyleneimine"**

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Summary of simulated systems

Table 1: The summary of systems simulated in this work, along with the number of protonated (N^+) and non-protonated (N) nitrogens, and the number of ions in each simulation

System	Nitrogens		NaCl							
	N^+	N	counter		0.27 M		0.52 M		1.04 M	
			Na	Cl	Na	Cl	Na	Cl	Na	Cl
2PEI25-DNA	10	30	22	10	162	150	312	300	624	612
2PEI50-DNA	20	20	22	20	162	160	312	310	624	622
2PLL-DNA	40	0	22	40	162	180	312	330	642	642
4PEI50-DNA	40	40	22	40	137	155	-	-	-	-
5PEI25-DNA	25	75	22	25	152	155	-	-	-	-

System	Nitrogens		CaCl ₂									
	N^+	N	0.13 M		0.27 M		0.39 M		0.52 M		1.04 M	
			Ca	Cl	Ca	Cl	Ca	Cl	Ca	Cl	Ca	Cl
2PEI25-DNA	10	30	81	150	162	312	234	456	312	612	624	1263
2PEI50-DNA	20	20	81	160	162	322	622	234	466	312	-	-
2PLL-DNA	40	0	81	180	162	342	324	486	312	642	-	-

Time development of minimum distance between polycation chains and DNA

The minimum distance between the polycations and DNA at the different salt concentrations are shown in 1 for PLL, 2 for PEI25, and 3 for PEI50. The data is shown to complement the average distances presented in the main article Figure 4. Data here shows the excess salt induced momentary fluctuations and precise time of detachments not visible in the averaged data.

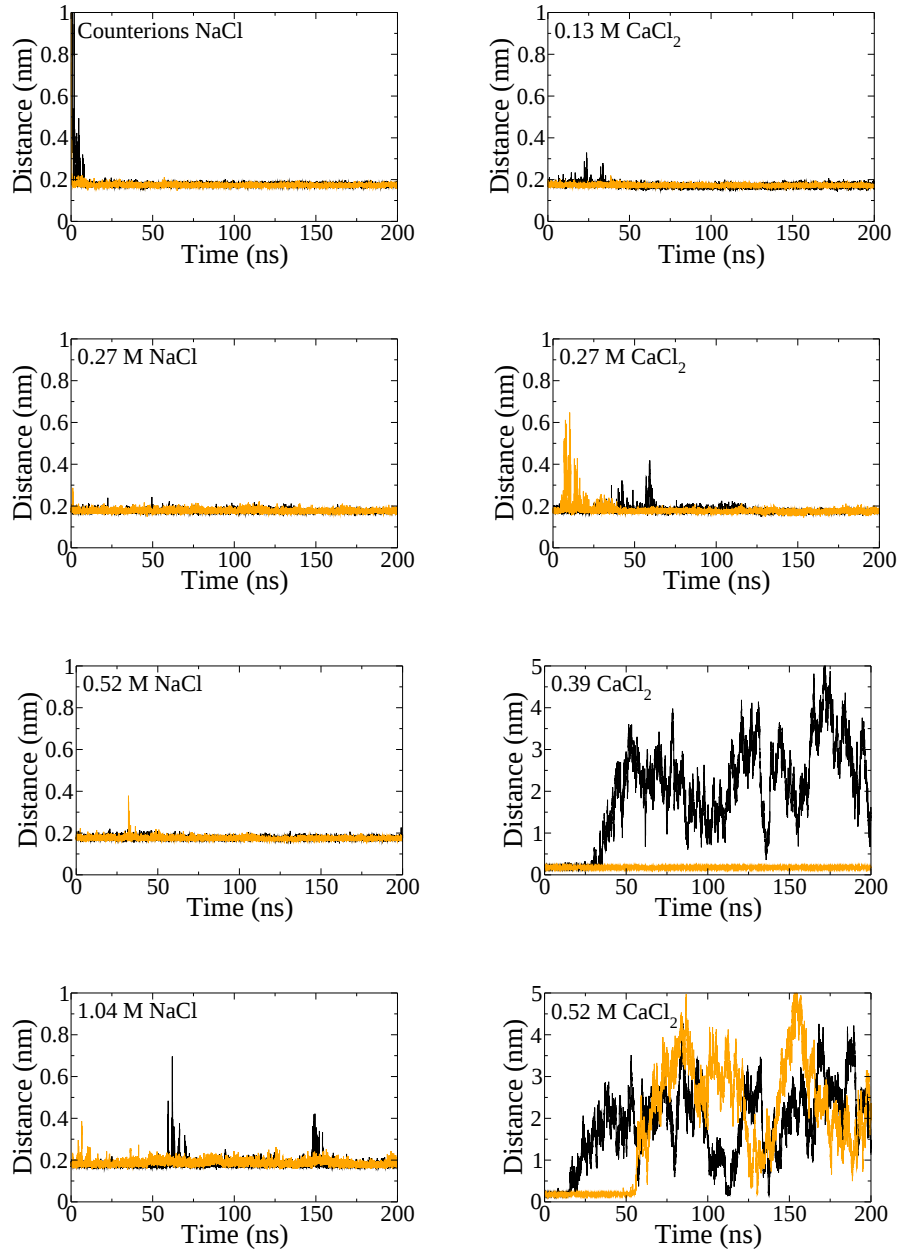


Figure 1: Time development of minimum distance between DNA and PLL in varying excess salt concentrations. Different colors denote the two separate PLL strands. The distance is measured as the closest distance between DNA and PLL.

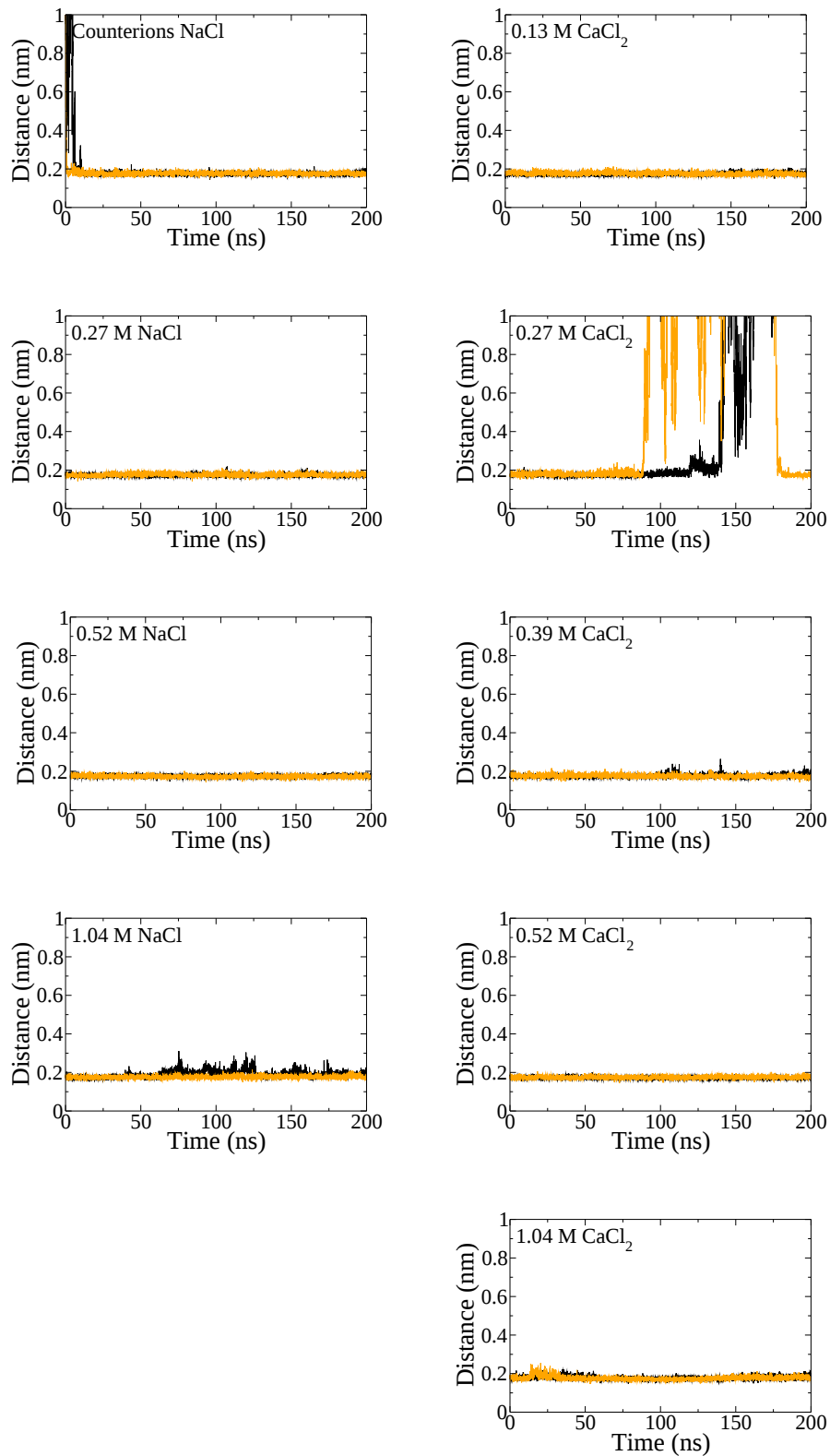


Figure 2: Time development of minimum distance between DNA and PEI25 in varying excess salt concentrations. Different colors denote the two separate PEI25 strands. The distance is measured as the closest distance between DNA and PEI25.

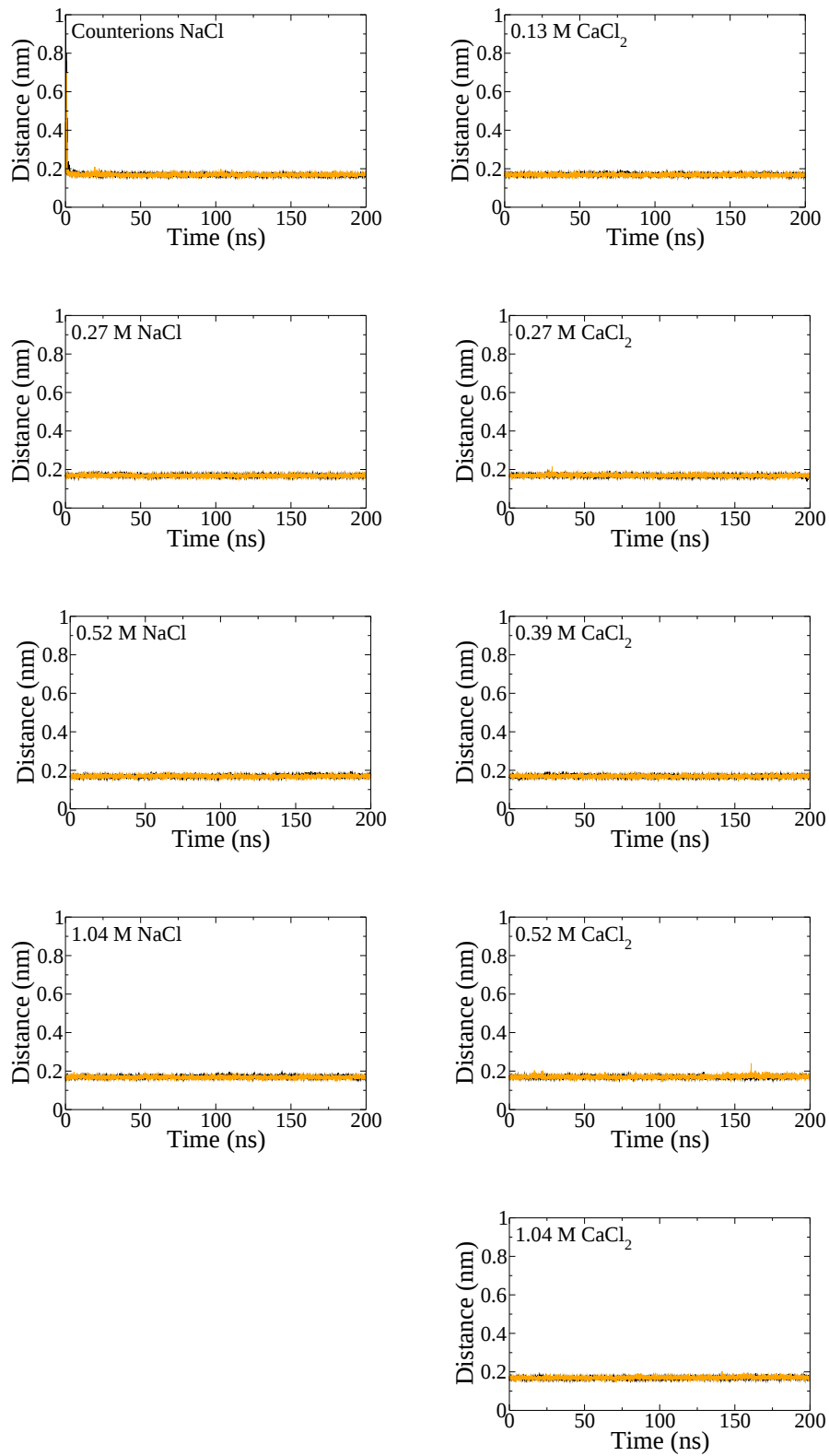


Figure 3: Time development of minimum distance between DNA and PEI50 in varying excess salt concentrations. Different colors denote the two separate PEI50 strands. The distance is measured as the closest distance between DNA and PEI50.

Open complex conformation for 25% protonated PEI in 1.04 M NaCl

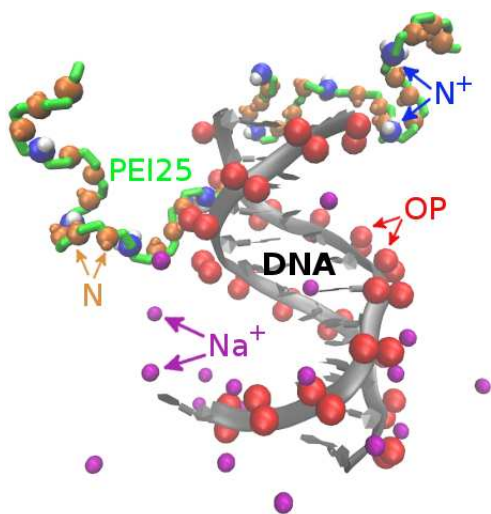


Figure 4: Representative simulation snapshot of open complex conformation detected with 2PEI25-DNA complex in 1.04 M NaCl. The figure shows the effect of high excess of NaCl in loosening the complex structure.