

**Supporting Information:**

**Effect of Ionic Strength on Ibuprofenate**

**Adsorption on a Lipid Bilayer of**

**Dipalmitoylphosphatidylcholine from**

**Molecular Dynamics Simulations**

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# 1 Ibuprofenate Topology

**Table S1:** Ibuprofenate structure, atom number (nr), type of atoms and charge parameters for each atom in the molecule.

Structure	nr	Type of atoms	Charge
	1	OM	-0.779
	2	CPos	0.716
	3	OM	-0.779
	4	CH1	-0.038
	5	CH3	-0.030
	6	CAro	0.057
	7	CAro	-0.168
	8	HCR	0.123
	9	CAro	-0.224
	10	HCR	0.134
	11	CAro	0.102
	12	CAro	-0.224
	13	HCR	0.134
	14	CAro	-0.168
	15	HCR	0.123
	16	CH2	-0.003
	17	CH1	0.082
	18	CH3	-0.030
	19	CH3	-0.028

# 2 Time evolution of the area per lipid

Figure S1 shows the time evolution of the area per lipid when the IBU is at the minimum energy for the  $\zeta_1^{0.0}$ ,  $\zeta_1^{0.13}$ , and  $\zeta_1^{1.0}$  systems. It is clearly appreciated that the area per lipid is stabilized along the simulated trajectory in the  $\zeta_1^{0.0}$ ,  $\zeta_1^{0.13}$ , and  $\zeta_1^{1.0}$  systems.

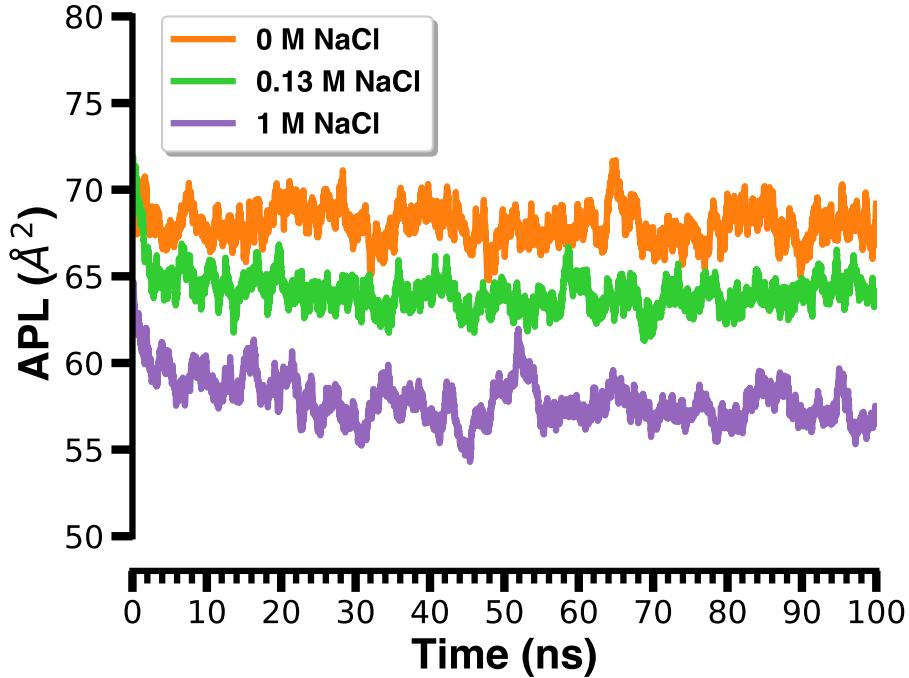


Figure S1: Time evolution of the area per lipid for the  $\zeta_1^{0.0}$ ,  $\zeta_1^{0.13}$ , and  $\zeta_1^{1.0}$  systems throughout the 100 ns of productive simulation when the IBU is at the minimum of free energy.

### 3 Convergence of the free energy profile

The 100 ns MD-US trajectory was divided into five independent 20 ns blocks. In order to show that the US simulations were long enough for the simulated time. Figure S2 shows the convergence of the free energy profiles for the  $\zeta_1^{0.0}$ ,  $\zeta_1^{0.13}$ , and  $\zeta_1^{1.0}$  systems.

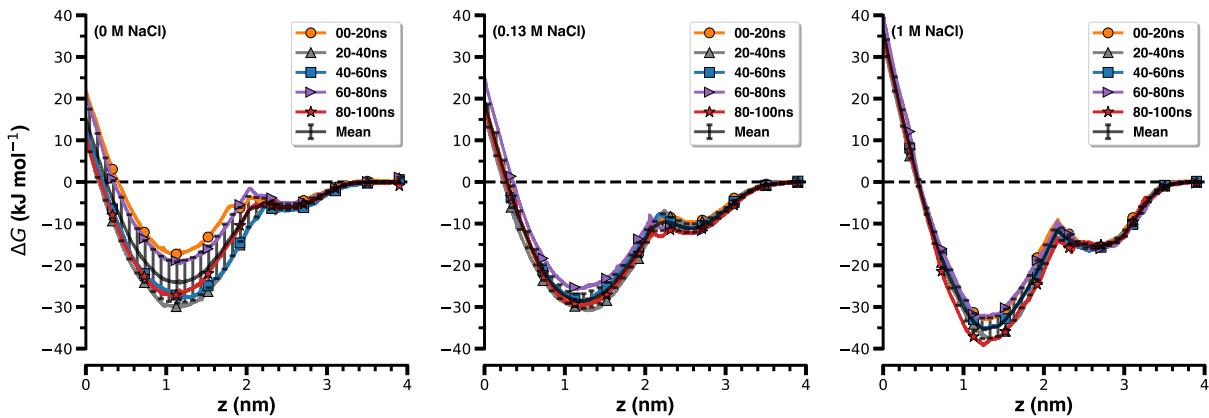


Figure S2: Free energy profile for systems:  $\zeta_1^{0.0}$ ,  $\zeta_1^{0.13}$ , and  $\zeta_1^{1.0}$  at different NaCl concentrations