

Supporting Information:
Dynamics of aqueous suspension of short Hyaluronic acid chains
near DPPC bilayer

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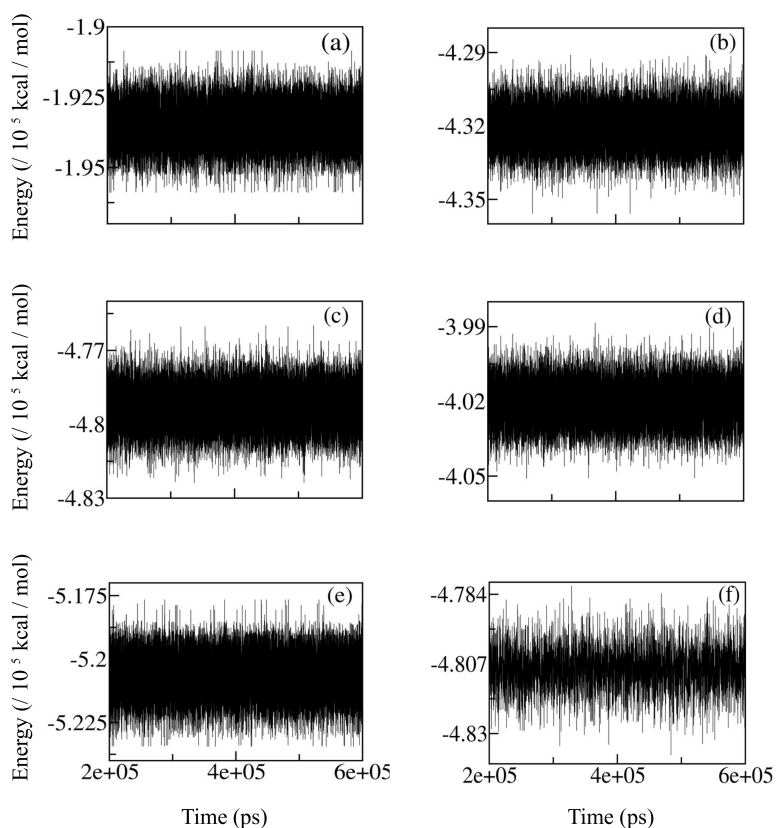


Figure S1: Total energy of the system at equilibrium for (a) $n_{\text{HA}5}=0$, (b) $n_{\text{HA}5}=10$, (c) $n_{\text{HA}5}=30$, (d) $n_{\text{HA}5}=50$, (e) $N=1$ and (f) $N=10$.

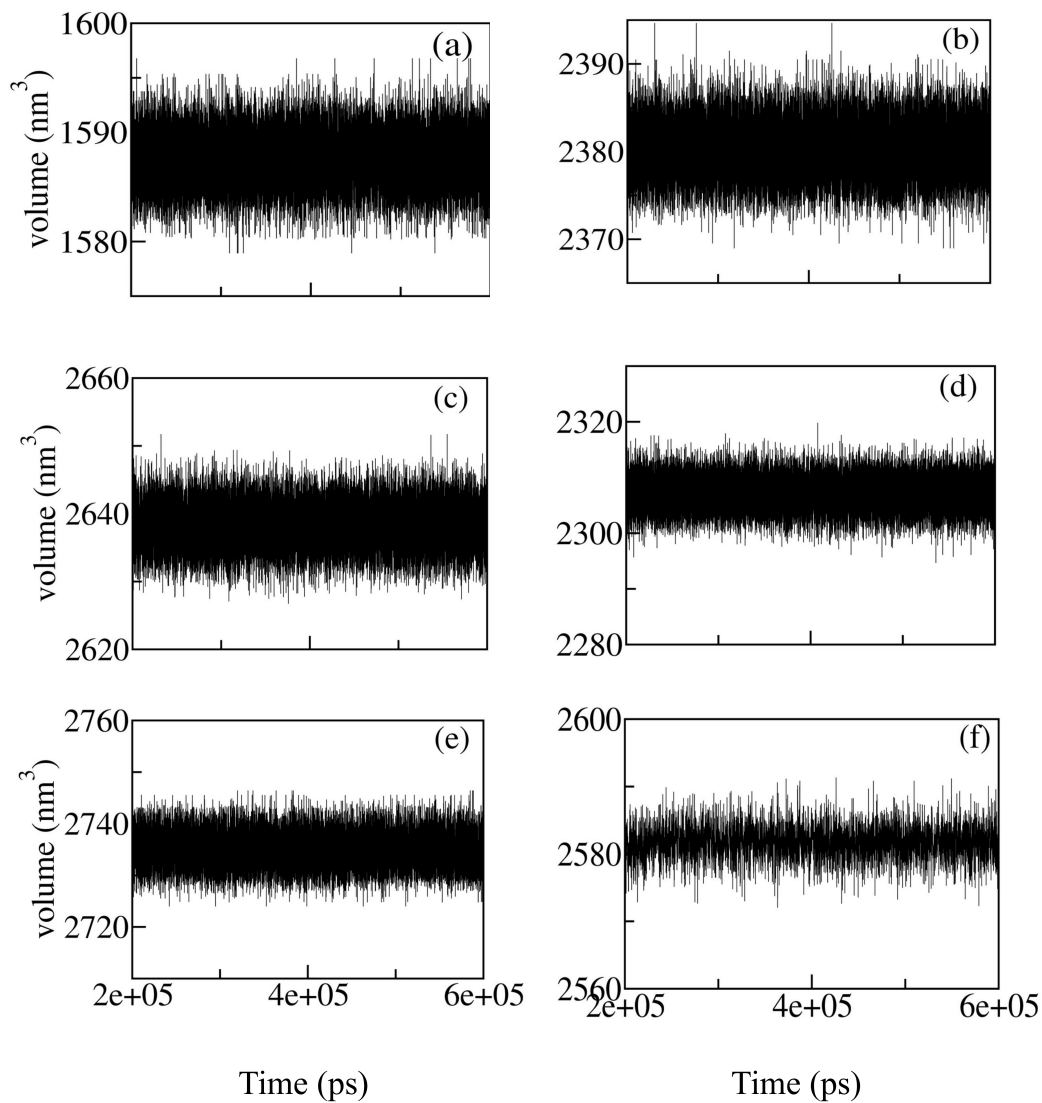


Figure S2: Volume of the simulation box at equilibrium for (a) $n_{\text{HA5}}=0$, (b) $n_{\text{HA5}}=10$, (c) $n_{\text{HA5}}=30$, (d) $n_{\text{HA5}}=50$, (e) $N=1$ and (f) $N=10$.

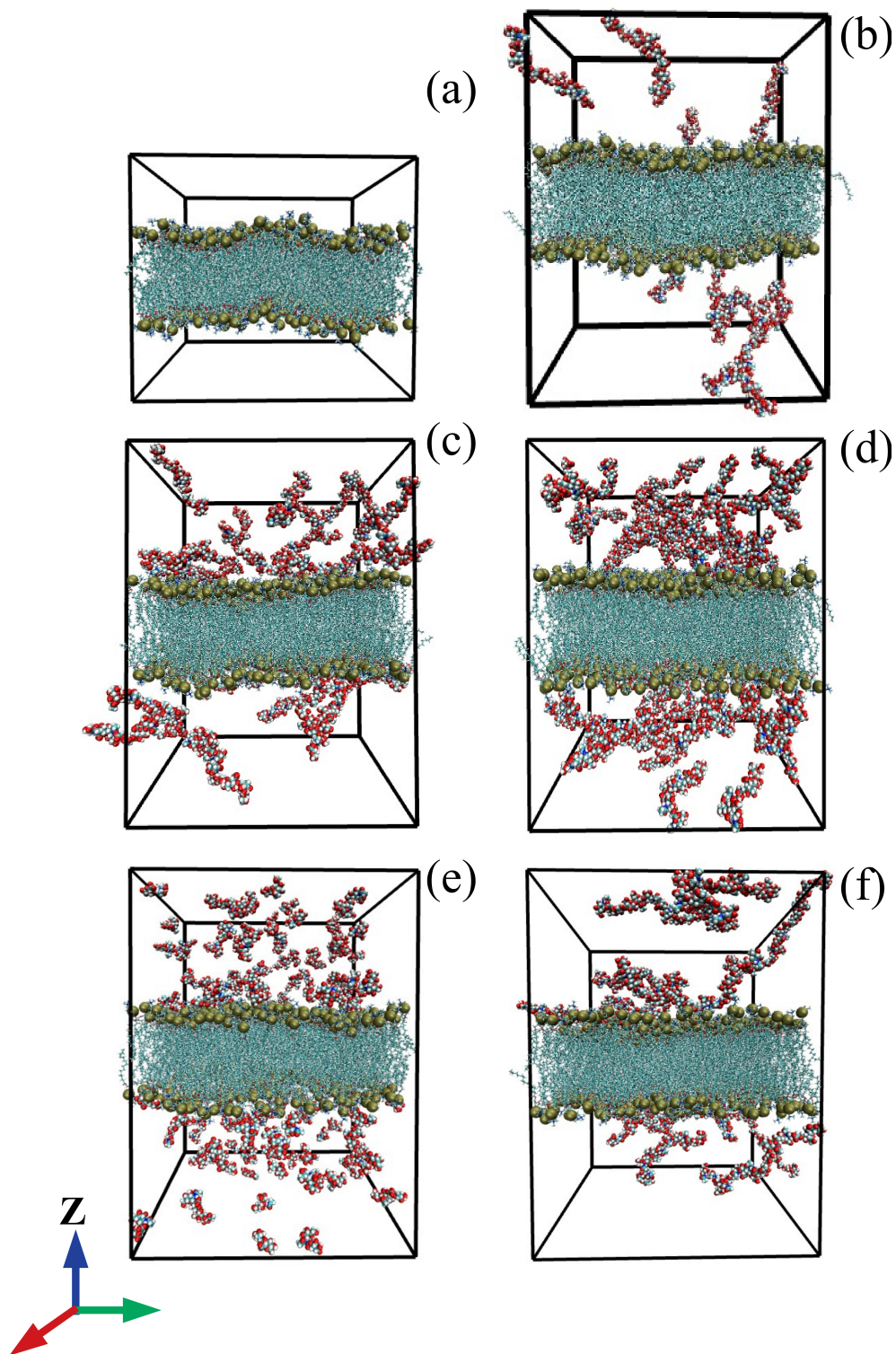


Figure S3: Typical equilibrium snapshot of (a) $n_{HA5}=0$, (b) $n_{HA5}=10$, (c) $n_{HA5}=30$, (d) $n_{HA5}=50$, (e) $N=1$ and (f) $N=10$. Hyaluronic acids (HA) and lipid bilayer are shown in vdw and bonds representation respectively with the following color codes: *Cyan* for Carbons, *red* for Oxygens, and *blue* for Nitrogens. The normal of the lipid bilayer is along z axis. Water molecules are not shown.

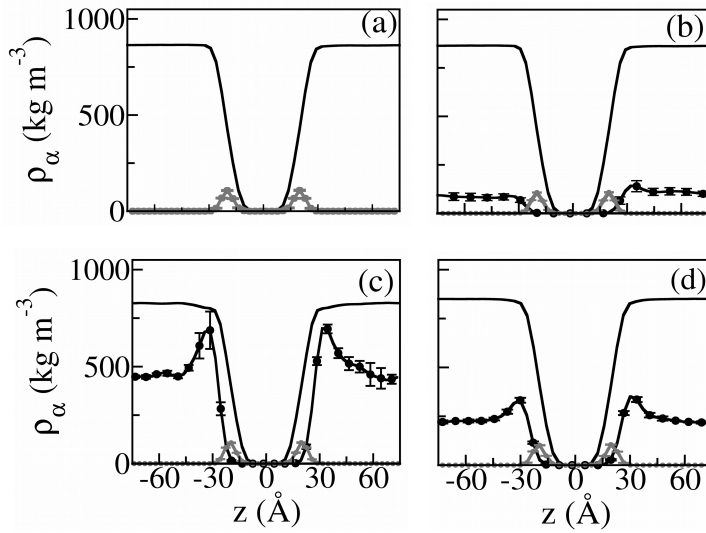


Figure S4: (a) Density profiles of Phosphorus atoms ($\rho_P(z)$, *grey solid line*), HA ($\rho_H(z)$, *dotted black line*), and water ($\rho_W(z)$, *solid black line*) along the bilayer normal for $n_{HA5}=0$, (b) $n_{HA5}=10$, (c) $n_{HA5}=50$ and (d) $N=1$. Origin is set at the bilayer center. $\rho_H(z)$ is amplified by a factor of 5.

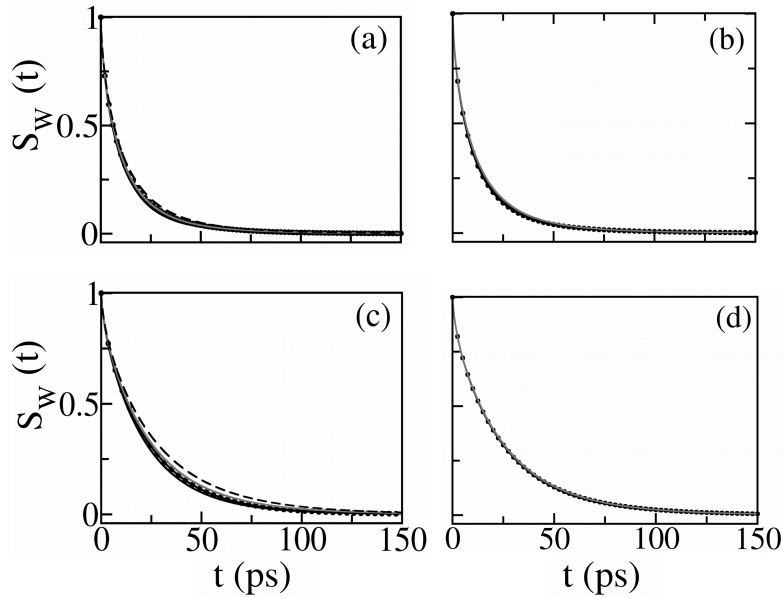


Figure S5: (a) Survival probability of water $S_W(t)$ in region A for different HA concentrations: $n_{HA5}=0$ (*solid black line*), $n_{HA5}=10$ (*dotted black line*), $n_{HA5}=30$ (*solid gray line*), $n_{HA5}=50$ (*dashed black line*) and (b) for varying HA chain size: $N=1$ (*solid black line*), $N=1$ (*dotted black line*), $N=10$ (*solid gray line*). (c) $S_W(t)$ in region B for different n_{HA5} and (d) for different N . The same line type as (a)-(b) is used.

Table S1: Mean residence time of water in region A (τ_W^A) and in region B (τ_W^B), obtained from $S_W(t)$ in respective regions (Figure S5). $\tau_W^{A,0}$ and $\tau_W^{B,0}$ are shown.

system	τ_W^A (ps)	τ_W^B (ps)
$n_{\text{HA}5}=0$	10.86 ($\tau_W^{A,0}$)	20.07 ($\tau_W^{B,0}$)
$n_{\text{HA}5}=10$	11.86	21.24
$n_{\text{HA}5}=30$	11.83	22.90
$n_{\text{HA}5}=50$	13.40	25.27
N=1	12.37	22.32
N=5	11.83	22.90
N=10	12.79	23.08

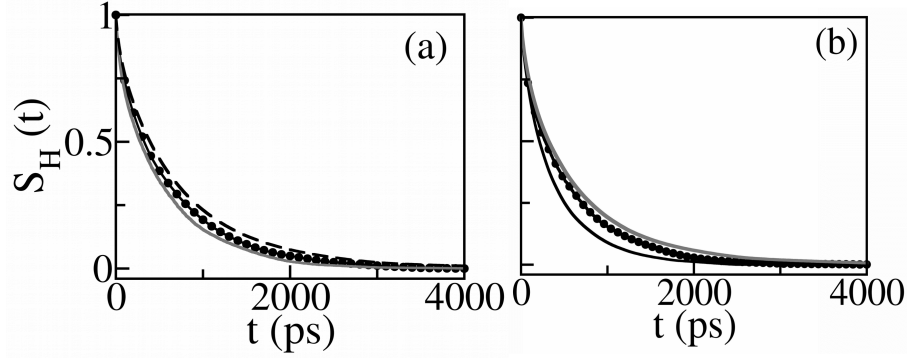


Figure S6: Survival probability of HA monomers $S_H(t)$ in region B for (a) $n_{\text{HA}5}=10$ (dotted black line), $n_{\text{HA}5}=30$ (solid gray line), $n_{\text{HA}5}=50$ (dashed black line), and (b) N=1 (solid black line), N=5 (dotted black line), N=10 (solid gray line).

Table S2: Mean residence time of HA monomers (τ_H) in region B, computed from $S_H(t)$ (Figure S6). τ_H^1 is indicated.

system	τ_H (ps)
$n_{\text{HA}5}=0$	-
$n_{\text{HA}5}=10$	568.84
$n_{\text{HA}5}=30$	494.87
$n_{\text{HA}5}=50$	677.04
N=1	372.48 (τ_H^1)
N=5	494.87
N=10	588.65

Table S3: Translational diffusion exponents (β_W) of $\langle r_W^2 \rangle$ in region A

system	β_W
$n_{\text{HA}5}=0$	0.75
$n_{\text{HA}5}=10$	0.73
$n_{\text{HA}5}=30$	0.73
$n_{\text{HA}5}=50$	0.72
N=1	0.73
N=5	0.73
N=10	0.73

Table S4: Rotational diffusion exponents (γ_W) of $\langle \phi_W^2 \rangle$ in region A

system	γ_W
$n_{\text{HA5}}=0$	0.73
$n_{\text{HA5}}=10$	0.72
$n_{\text{HA5}}=30$	0.74
$n_{\text{HA5}}=50$	0.72
N=1	0.73
N=5	0.73
N=10	0.75

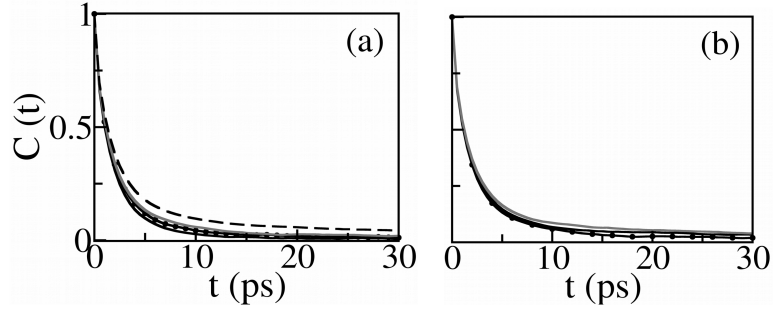


Figure S7: Rotational autocorrelation function of the water molecules ($C(t)$) in region B for different HA concentrations: $n_{\text{HA5}}=0$ (*solid black line*), 10 (*dotted black line*), 30 (*solid gray line*) and 50 (*dashed black line*) (b) $\langle r_W^2 \rangle$ in region B for varying HA chain sizes: N=1 (*solid black line*), N=5 (*dotted black line*) and N=10 (*solid gray line*)

Table S5: First rank rotational autocorrelation time of water molecules, t_1^W in region B (computed from $C(t)$ in SI Figure S7) and the product of t_1^W and rotational diffusion, D_R^W

system	t_1^W (ps)	$t_1^W \cdot D_R^W$
$n_{\text{HA5}}=0$	1.84	0.51
$n_{\text{HA5}}=10$	2.13	0.55
$n_{\text{HA5}}=30$	2.21	0.56
$n_{\text{HA5}}=50$	2.53	0.59
N=1	2.13	0.53
N=5	2.21	0.56
N=10	2.53	0.60

Table S6: translational diffusion exponents (β_H) of HA monomers in region B.

system	β_H
$n_{\text{HA5}}=0$	-
$n_{\text{HA5}}=10$	0.80
$n_{\text{HA5}}=30$	0.80
$n_{\text{HA5}}=50$	0.79
N=1	0.88
N=5	0.80
N=10	0.79

Table S7: First rank rotational autocorrelation time t_1^H for interfacial HA monomers

system	t_1^H (ns)
$n_{\text{HA}5}=0$	-
$n_{\text{HA}5}=10$	6.1
$n_{\text{HA}5}=30$	6.8
$n_{\text{HA}5}=50$	7.7
$N=1$	0.2
$N=5$	6.8
$N=10$	24.6

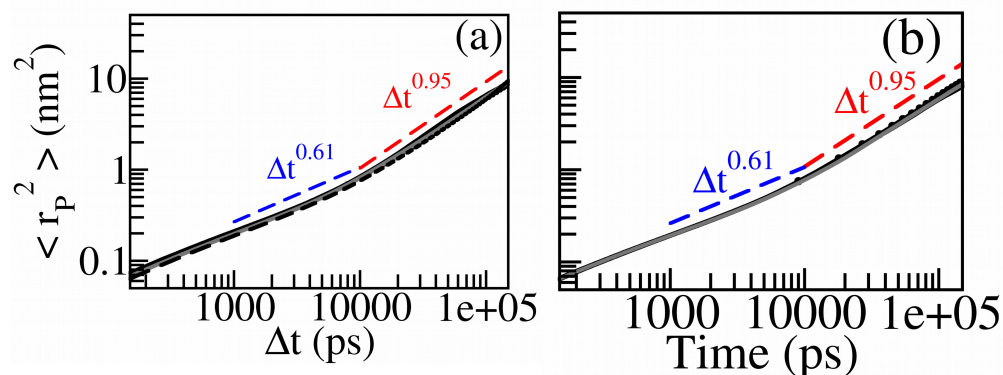


Figure S8: (a) Translational mean squared displacements of the Phosphorus atoms ($\langle r_P^2 \rangle$) in the lateral plane of the bilayer for varying HA concentrations: $n_{\text{HA}5} = 0$ (solid black line), 10 (dotted black line), 30 (gray solid line), 50 (dashed black line) and (b) for different HA chain sizes: $N=1$ (solid black line), $N=5$ (dotted black line) and $N=10$ (solid gray line)

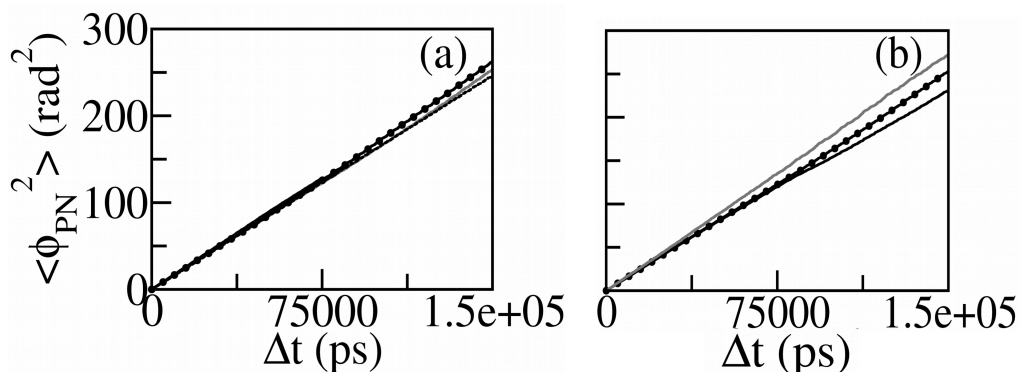


Figure S9: (a) Rotational mean squared displacements of the lipid PN vectors ($\langle \phi_{PN}^2 \rangle$) for $n_{\text{HA}5} = 0$ (solid black line), 10 (dotted black line), 30 (gray solid line), 50 (dashed black line) and (b) for $N=1$ (solid black line), $N=5$ (dotted black line) and $N=10$ (solid gray line)