

# Supporting information

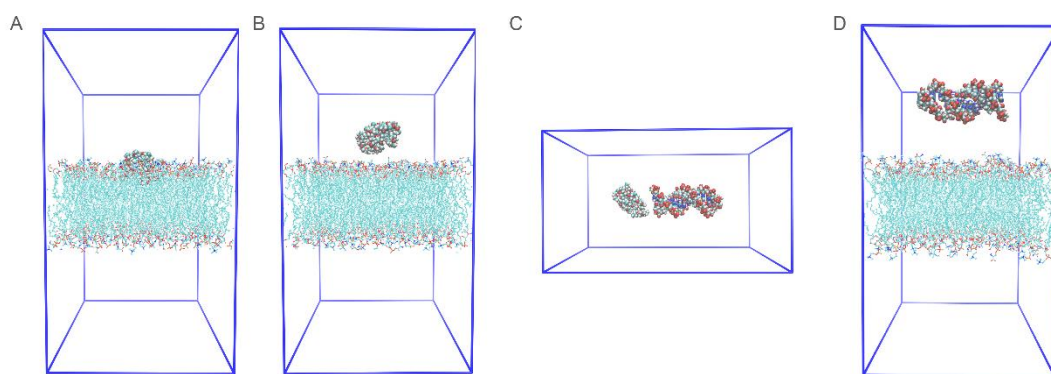
## The Interaction Mechanism of Intramuscular Gene Delivery Materials with Cell Membranes

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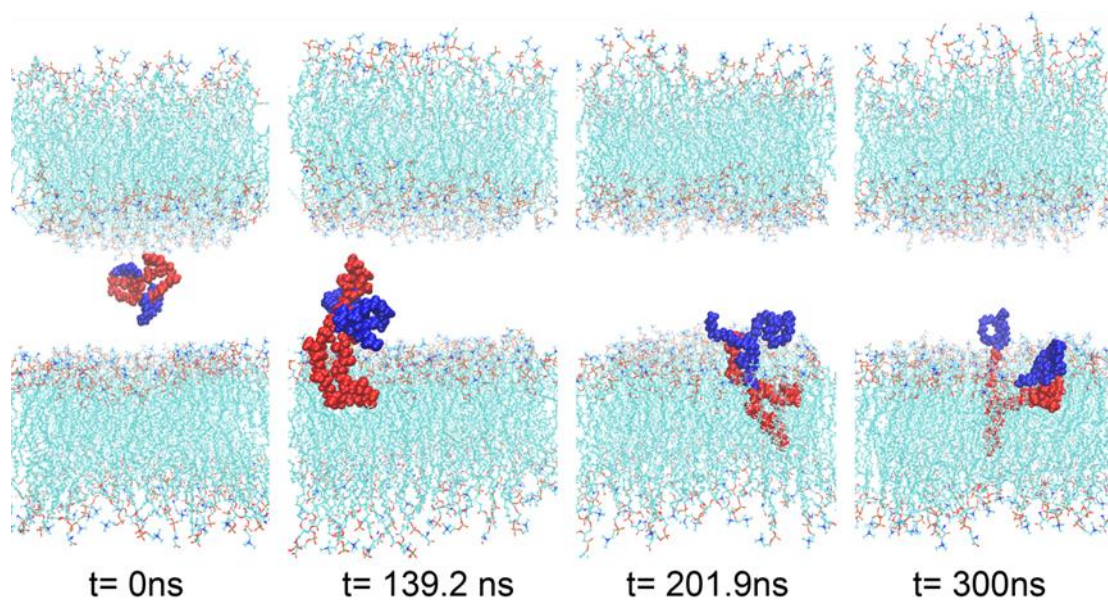
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**Table S1.** Details of the various systems simulated in this study.

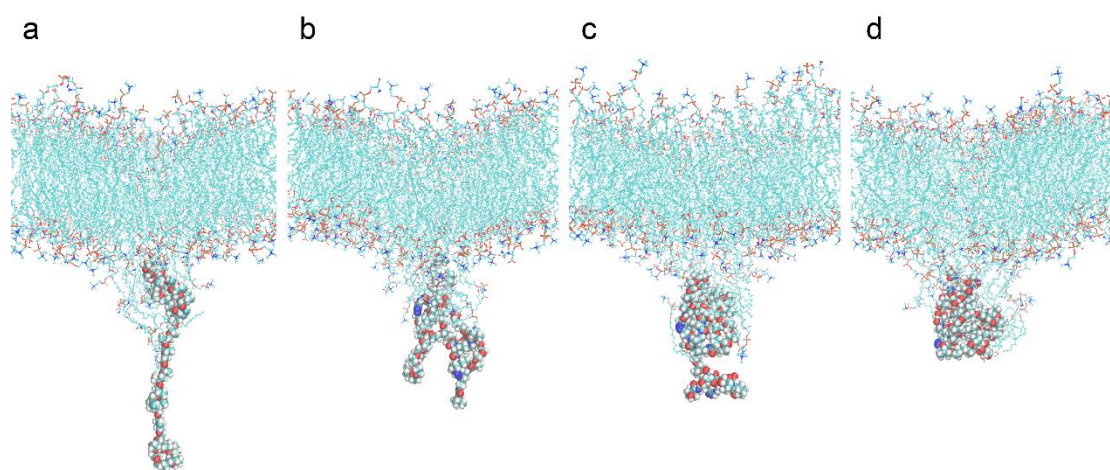
System label	Box size (nm <sup>3</sup> )	Water quantities	Description
A	9.0 × 9.0 × 16.0	29794	L64 & 240 Lipids
B	9.0 × 9.0 × 16.0	29794	LPL & 240 Lipids
C	9.0 × 9.0 × 16.0	29794	LPL & 240 Lipids (LPL in the Lipids membrane)
D	9.0 × 9.0 × 16.0	29794	rL <sub>2</sub> PL <sub>2</sub> & 240 Lipids
E	9.0 × 9.0 × 16.0	29794	rL <sub>3</sub> PL <sub>3</sub> & 240 Lipids
F	9.0 × 9.0 × 16.0	29764	PMF: L64 & 240 Lipids
G	9.0 × 9.0 × 16.0	29764	PMF: LPL & 240 Lipids
H	9.0 × 9.0 × 16.0	29764	PMF: rL <sub>2</sub> PL <sub>2</sub> & 240 Lipids
I	9.0 × 9.0 × 16.0	29764	PMF: rL <sub>3</sub> PL <sub>3</sub> & 240 Lipids
J	9.0 × 9.0 × 16.0	29764	PMF: rL <sub>3</sub> PL <sub>3</sub> -2 & 240 Lipids (Hydrophilic parts face down)
K	14.0 × 8.0 × 8.0	28958	L64 & DNA (No Lipids)
L	14.0 × 8.0 × 8.0	28958	LPL & DNA (No Lipids)
M	14.0 × 8.0 × 8.0	28958	rL <sub>2</sub> PL <sub>2</sub> & DNA (No Lipids)
N	14.0 × 8.0 × 8.0	28958	rL <sub>3</sub> PL <sub>3</sub> & DNA (No Lipids)
O	9.0 × 9.0 × 16.0	29766	PMF: DNA & 240 Lipids (None)
P	9.0 × 9.0 × 16.0	29766	PMF: DNA & 240 Lipids (L64)
Q	9.0 × 9.0 × 16.0	29766	PMF: DNA & 240 Lipids (DNA met the LPL)
R	9.0 × 9.0 × 16.0	29766	PMF: DNA & 240 Lipids (LPL)
S	8.5 × 8.5 × 18.9	25938	L64 & 240 Lipids (2 membranes)
T	7.1 × 7.1 × 7.8	6368	LPL & 160 Lipids
U	7.1 × 7.1 × 7.8	6368	rL <sub>2</sub> PL <sub>2</sub> & 160 Lipids



**Figure. S1.** Initial model of four-groups. (A)System A,B,D,E;(B)System F-J;(C) System K-N; (D) System O-R;



**Figure. S2.** The process of L64 entering the phospholipid membrane (the model of 2 membranes).



**Figure. S3** Final conformations of four molecules in PMF across phospholipid membranes: (a) L64; (b) LPL; (c) rL2PL2; (d) rL3PL3.