Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Molecular dynamics simulations to elucidate translocation and permeation of active from lipid nanoparticle to skin: complemented by experiments

Krishna M. Gupta*, Surajit Das, Pui Shan Chow

Institute of Chemical & Engineering Sciences, A*STAR (Agency for Science, Technology and Research), 1 Pesek Road, Jurong Island, Singapore 627833

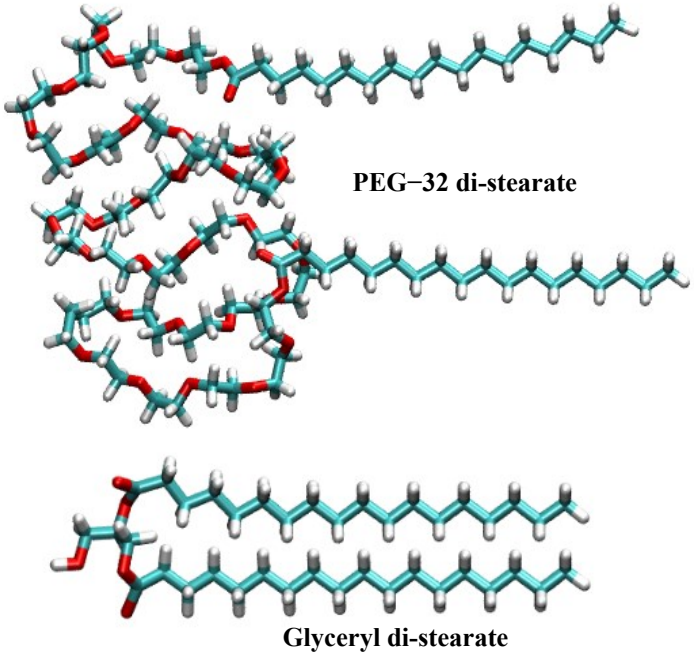


Fig. S1. Three-dimensional (3D) molecular structure of Gelucire® 50/13 which is a mixture of polyethylene glycol−32 (PEG-32) di-stearate and glyceryl di-stearate (close to supplier's information). Color code: O, red; C, cyan; H, white.

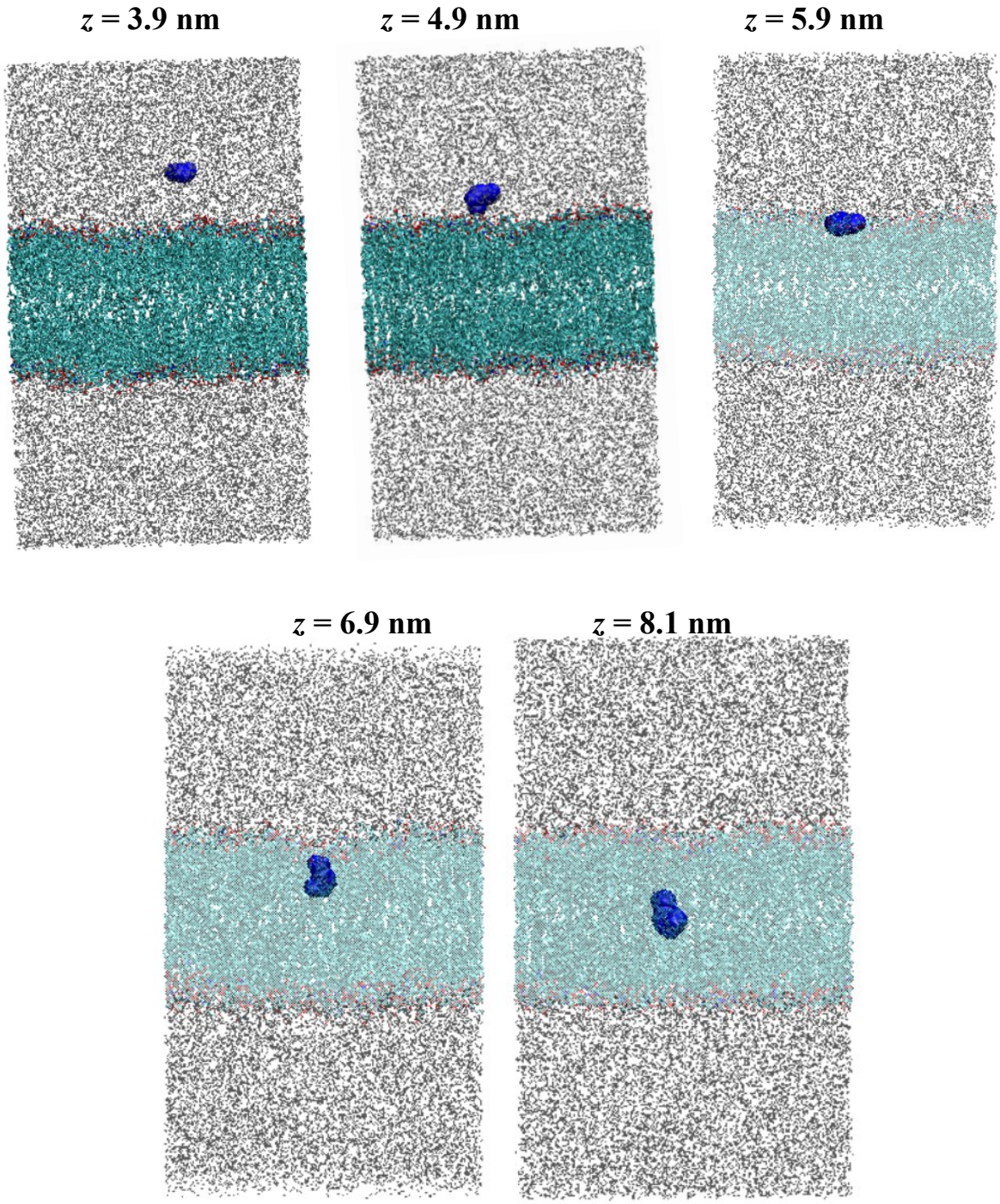
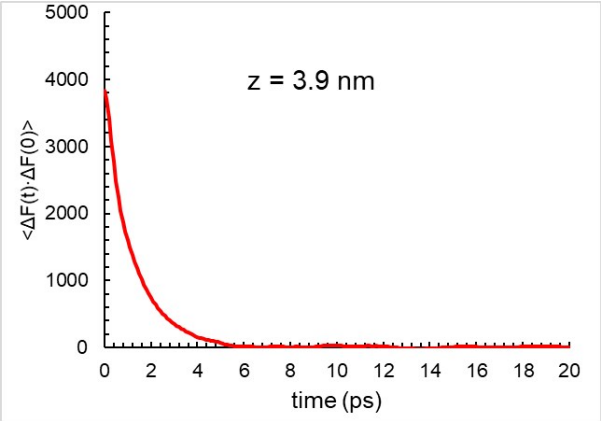
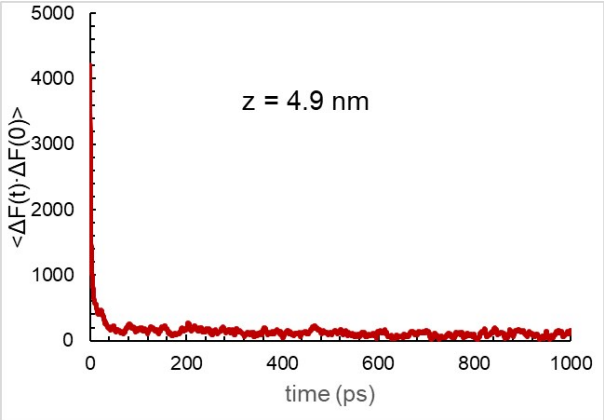
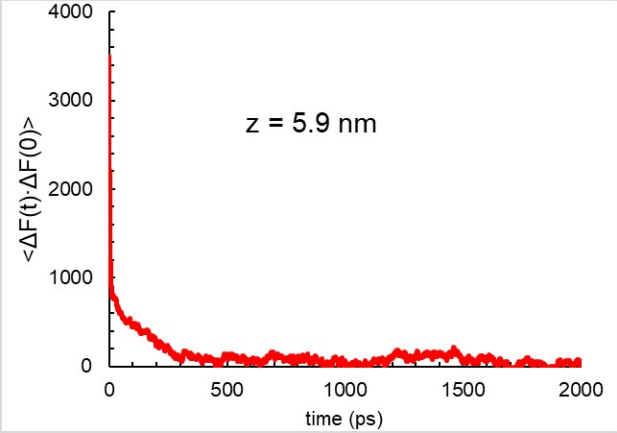
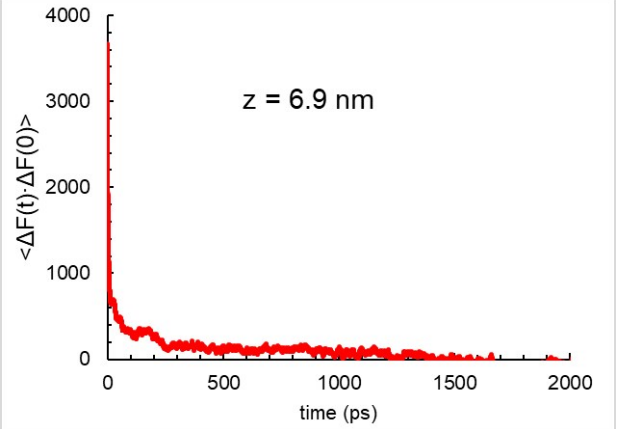


Fig. S2. Initial simulation snapshots for umbrella sampling simulations at few *z* locations of FA. For clear visualization, the skin bilayer is made transparent when FA molecule enters into skin.


z = 3.9 nm
<ΔF(t)·ΔF(0)>
time (ps)
0
1000
2000
3000
4000
5000
0
2
4
6
8
10
12
14
16
18
20


z = 4.9 nm
<ΔF(t)·ΔF(0)>
time (ps)
0
1000
2000
3000
4000
5000
0
200
400
600
800
1000


z = 5.9 nm
<ΔF(t)·ΔF(0)>
time (ps)
0
1000
2000
3000
4000
0
500
1000
1500
2000


z = 6.9 nm
<ΔF(t)·ΔF(0)>
time (ps)
0
1000
2000
3000
4000
0
500
1000
1500
2000

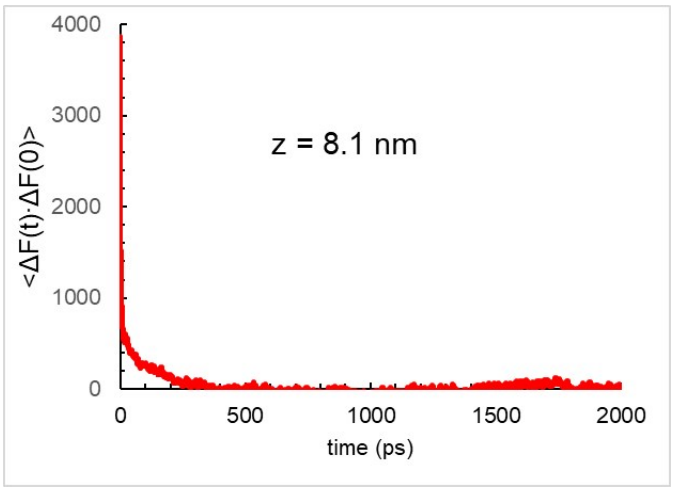
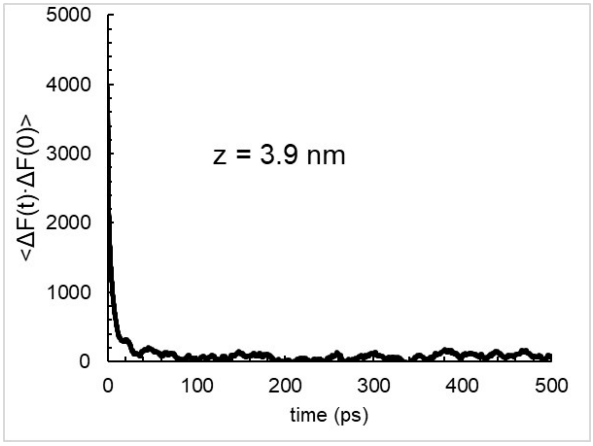
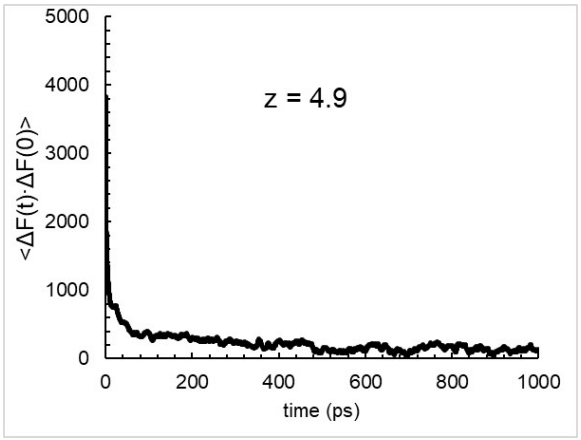
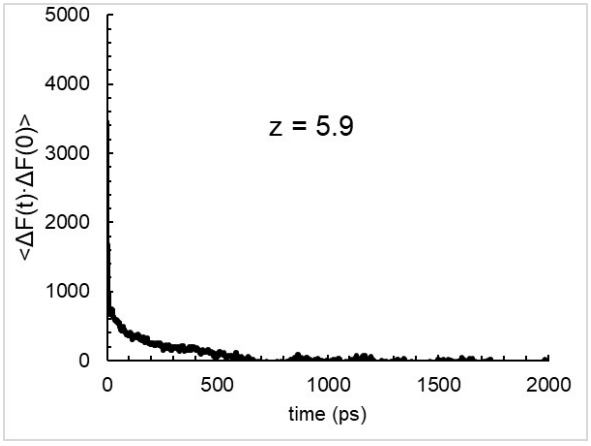
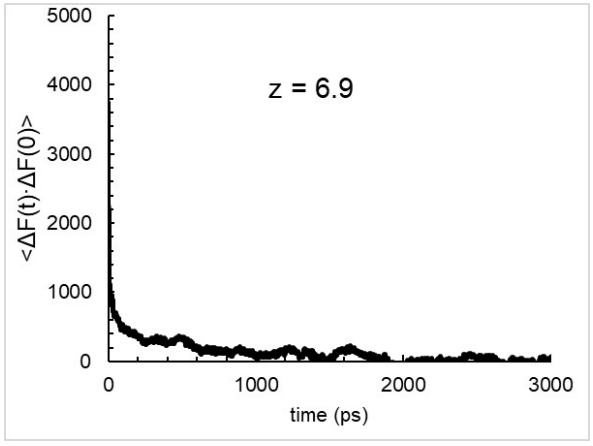


Fig. S3: Autocorrelation functions of ΔF using 20 ns simulation trajectories at z locations corresponding to Fig. S2 without NP.









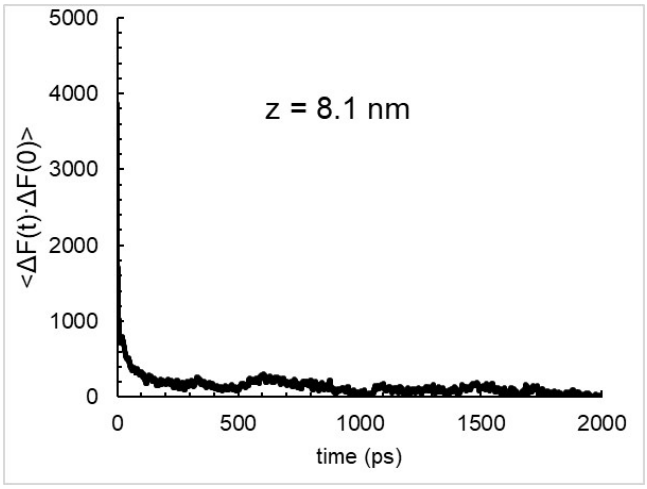


Fig. S4: Autocorrelation functions of ΔF using 20 ns simulation trajectories at z locations corresponding to Fig. S2 in the presence of NP.

Table S1: Composition of nanoparticle dispersion.

Ingredients	% (w/w)
Gelucire® 50/13	10.0
Ferulic acid	0.5
Water	89.5

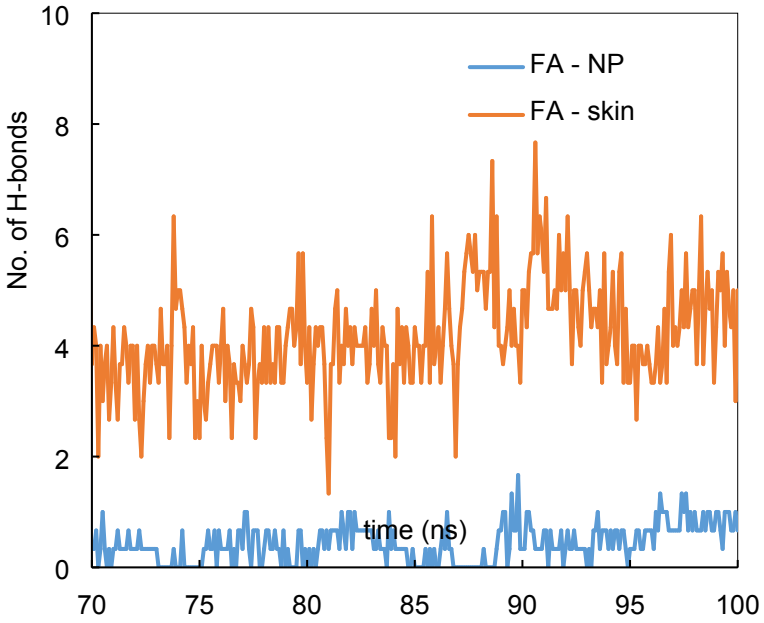


Fig. S5. Hydrogen-bonds between FA and NP as well as FA and skin.

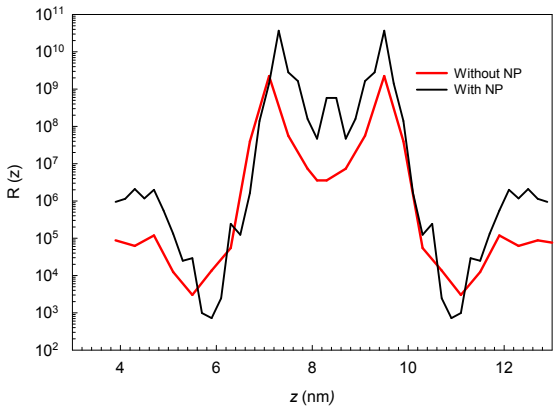


Fig. S6. Resistance of permeation $R(z)$ of FA along the skin bilayer normal with and without NP.