Electronic Supplementary Material (ESI) for Soft Matter

Cholesterol affects C_{60} translocation across lipid bilayers

Dandan Sun, Xubo Lin and Ning Gu[*]

State Key Laboratory of Bioelectronics and Jiangsu key Laboratory for Biomaterials and Devices, School of Biological Science & Medical Engineering, Southeast University, Nanjing, 210096, People's Republic of China

Calculation of C_{60} permeability

In order to characterize the dynamic of C_{60} penetration into the bilayer, we calculate the permeability coefficient P of C_{60}. Marrink and Berendsen[1-2] have applied molecular dynamic simulations to estimate lipid membrane permeability coefficients long ago. Here, the same method is used to infer the permeability coefficient P of C_{60}. The C_{60} is constrained at chosen depths in the membrane and aqueous layer and the constraint forces are calculated. The free energy of C_{60} transferring from water into various depths z of the membrane, i.e., $\Delta G(z)$, is accessible as the potential of the mean force

$$\Delta G(z) = -\int_{5.0}^{z} < F(z) >_t dz \tag{1}$$

The force correlation method can be applied to compute the diffusion constant $D(z)$:

$$D(z) = \frac{(RT)^2}{\int_0^{\infty} < \Delta F(z,t) \Delta F(z,0) > dt} \tag{2}$$

where R is the universal gas constant, T is the absolute temperature and

$$\Delta F(z,t) = F(z,t) - < F(z) >_t \tag{3}$$

is the deviation of the instantaneous force $F(z, t)$ from mean force $<F(z)>_t$ at z. According to the solubility diffusion model, the permeability coefficient P can be

defined as

$$\frac{1}{P} = \int_0^{5.0} \frac{\exp(\Delta G(z)/RT)}{D(z)} dz \tag{4}$$

Diffusion coefficient $D(z)$ profiles are plotted in Figure S1.

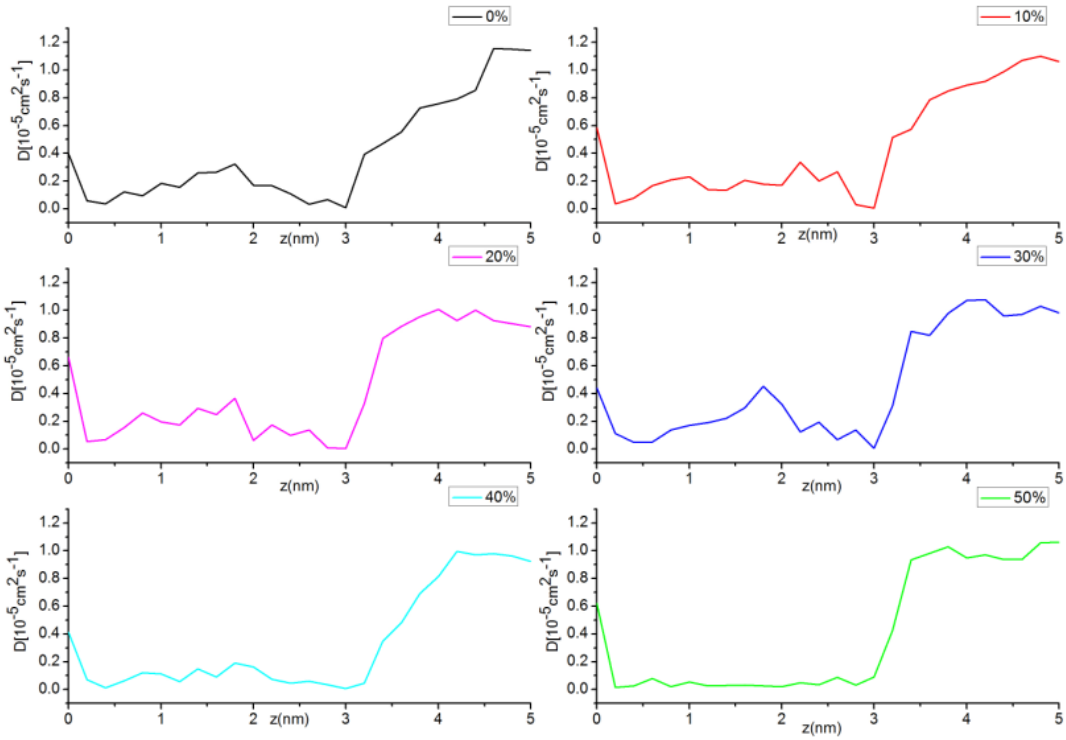

Figure S1 Diffusion coefficients of C_{60} as a function of position relative to the bilayer center-of-mass. The colors of the curves represent the DPPC/CHOL bilayers at the cholesterol concentration of 0 mol % (black), 10 mol % (red), 20 mol % (Magenta), 30 mol % (blue), 40 mol % (cyan), and 50 mol %(green).

References

1 S. J. Marrink and H. J. C. Berendsen, *J. Phys. Chem.*, 1994, **98**, 4155-4168.

2 S. J. Marrink and H. J. C. Berendsen, *J. Phys. Chem.*, 1996, **100**,16729-16738.