Cholesterol affects C<sub>60</sub> translocation across lipid bilayers

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**Calculation of C<sub>60</sub> permeability**

In order to characterize the dynamic of C<sub>60</sub> penetration into the bilayer, we calculate the permeability coefficient \( P \) of C<sub>60</sub>. Marrink and Berendsen<sup>1-2</sup> 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<sub>60</sub>. The C<sub>60</sub> is constrained at chosen depths in the membrane and aqueous layer and the constraint forces are calculated. The free energy of C<sub>60</sub> transferring from water into various depths \( z \) of the membrane, i.e., \( \Delta G(z) \), is accessible as the potential of the mean force

\[
\Delta G(z) = - \int_{z_0}^{z} < F(z) >, dz
\]

(1)

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

\[
D(z) = \frac{(RT)^2}{\int_{0}^{\infty} < \Delta F(z,t) \Delta F(z,0) > dt}
\]

(2)

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

\[
\Delta F(z,t) = F(z,t) - < F(z) >
\]

(3)

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

\[ \frac{1}{P} \int_{0}^{5.0} \exp(\Delta G(z) / RT) \frac{d\Delta}{D(z)} \, dz \]  

(4)

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

Figure S1 Diffusion coefficients of \( \text{C}_{60} \) 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
