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Supplementary Information

The chains order of binary unsaturated lipid bilayers modulated by aromatic residues containing peptides: an ATR-FTIR spectroscopy study

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Polarised ATR-FTIR data analysis

The electric fields of incident light for the ATR experiment were computed using the following formulae[1].

$$E_x = \frac{2\cos\vartheta\sqrt{\sin^2\vartheta - n_{21}^2}}{\sqrt{(1 - n_{21}^2)[(1 + n_{21}^2)\sin^2\vartheta - n_{21}^2]}}$$

$$E_y = \frac{2\cos\vartheta}{\sqrt{(1 - n_{21}^2)}}$$

$$E_z = \frac{2\sin\vartheta\cos\vartheta}{\sqrt{(1 - n_{21}^2)[(1 + n_{21}^2)\sin^2\vartheta - n_{21}^2]}}$$

where ϑ is the angle of a light beam to the prism normal at the point of reflection and $n_{21} = n_2/n_1$ (n_1 is the refractive index of ZnSe, and n_2 is the refractive index of the membrane sample). In our experiments, ϑ was equal to 45°. When n_1 was taken to be 2.4 and n_2 was taken to be 1.5,[2] E_x, E_y and E_z were 1.09, 1.81 and 2.32, respectively.

The R^{ATR} is the ratio between the absorption of light polarised parallel and perpendicular to the surface of the internal reflection element and is defined by the following formula. The electric field components together with the R^{ATR} are used to calculate the orientation order parameter f.

$$R^{ATR} = \frac{A_{\parallel}}{A_{\perp}} = \frac{E_x^2}{E_y^2} + \frac{\frac{E_z^2}{E_y^2}(f\cos^2\alpha + \frac{1-f}{3})}{\frac{f\sin^2\alpha}{2} + \frac{1-f}{3}}$$

where R^{ATR} is the dichroic ratio, $A_{\parallel}$ is the parallel polarised incident light, $A_{\perp}$ is the perpendicularly polarised incident light and α is the angle between the transition moment of the ν_{as} (CH_2) (~2920 cm^{-1}) and the helix axis. Lipid order parameters were computed from the symmetric (~2850 cm^{-1}) and asymmetric (~2920 cm^{-1}) stretching mode of the lipid with α set as 90°[2]. The value of f is known; therefore, the average angle of lipid chains relative to the membrane normal γ can be calculated as follows:

$$f = \frac{3\cos^2\gamma - 1}{2}$$

Orientation Analysis from Polarised ATR-FTIR data

The order parameter (S) of helical peptide was computed using the following formulae[3-7].

$$S = \frac{\left[(E_x^2 - R^{ATR} E_y^2 + E_z^2) \Big/ (E_x^2 - R^{ATR} E_y^2 - 2E_z^2) \right]}{\left[(3\cos^2 a - 1) / 2 \right]}$$

where E_x, E_y and E_z were the integrated absorption coefficients. If the film refractive index was independent of the wavelength, E_x, E_y and E_z were 1.398, 1.516 and 1.625[3], respectively, the above equation can be written as below:

$$S = \frac{\left[(R^{ATR} - 2) / (R^{ATR} + 1.45) \right]}{\left[(3\cos^2 a - 1) / 2 \right]}$$

where α was the angle between the principal transition moment and the molecular director. For the amide I mode, α was 39°[4]. The tilt angle β from the normal can be calculated as follows:

$$S = (3\cos^2 \beta - 1) / 2$$

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