



Investigation of the polarization dependent attenuated total reflection infrared spectra of ordered lipids assisted by principal component analysis.

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The information about molecular architecture of oriented lipid multibilayers stacks is frequently extracted from linearly polarized infrared spectra. Usually, the measurements are limited only to the parallel and perpendicular direction of the vector of the electric field relative to the plane of incidence. The absorbance differences are measured by linear dichroism, defined as the change in absorbance that occurs when the electric vector of the radiation beam is rotated by 90°. On a basis of the dichroism value, the so-called infrared order parameter that depends on the orientation of the transition dipole moment vector with respect to the surface normal can be determined. In the studies reported here, the measurements have been carried out at angles of the electric field changing with the step of 5° in a range between the parallel and perpendicular direction. The polarization-dependent spectra were pretreated by a procedure to eliminate from the total absorbance the component shaped solely by the specific dependence of the ATR absorbance on the effective penetration depth. The principal component analysis (PCA) done for the standard normal variate (SNV) pretreated spectra has shown that the obtained model based on one component is able to describe spectral variability with a reproducibility better than 95%. Lack of any other phenomenon that modulates the analysed spectral variations is undeniable proof that the raw data were well "cleaned" from the unwanted effect. The loading value for a given variable strictly correlates with orientation of the transition dipole moment vector for the corresponding mode with respect to the surface normal. PCA results obtained for the polarization-dependent spectra of the dry lipid film measured as function of temperature give information about the contribution of different parts of the DPPC molecule in the melting of the lipid film within the gel phase.

Słowa kluczowe

Attenuated total reflection (ATR) infrared spectra, Polarized radiation, Dipalmitoylphosphatidylcholine (DPPC), Principal component analysis, Standard normal variate (SNV), Orientational analysis, Molecular ordering

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