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Moving-window 2D correlation spectroscopy in studies of fluphenazine-DPPC dehydrated film as a function of temperature.

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The effect of incorporating fluphenazine (FPh) into the dipalmitoylphosphatidylcholine (DPPC) multibilayers was studied by means of two-dimensional correlation spectroscopy (2DCOS) applied to attenuated total reflection (ATR) infrared spectra. DPPC is used as a model membrane that mimics the organization of lipids in biological membranes and their interaction with FPh. ATR-IR spectra for both DPPC dry film alone and the film doped with FPh were recorded as a function of temperature to provide information about the interaction between FPh molecules and DPPC lipid. The chain-melting phase-transition temperature changes are strictly correlated with the conformational order of the lipid hydrocarbon chains. To gain deeper insight into the accompanying spectral changes, we employed moving-window 2D correlation spectroscopy. Subdividing all the measurements from 10 to 90 °C into 20° subsets enables a detailed identification of spectral features induced by embedding FPh into DPPC multilayers. Moving-window analysis of the power spectra for the $\nu_{asym,sym}CH_2$, δ_sCH_2, and δ_rCH_2 vibrations provides evidence that FPh is embedded in the region between the bilayers, penetrating their hydrophilic part, which destabilizes the interchain interaction. Above 60 °C the FPh–DPPC system reaches the liquid crystalline phase with the well-established location of FPh. A further temperature increase to 90 °C has little effect on the intrachain conformational order and the packing character of the FPh–DPPC system in the liquid crystalline phase. In addition, FPh hinders the formation of large domains. Comparison of the moving-window analysis done by using slice spectra for DPPC and FPh-doped DPPC dry film for $\nu_{asym,sym}CH_2$, νCO, and shows that the interaction between the DPPC and FPh molecules is accompanied by very distinct spectral changes located in a both lower and narrower temperature range than those observed in pure DPPC film.

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Dipalmitoylphosphatidylcholine (DPPC), Fluphenazine (FPh), Multilayers, Attenuated total reflection (ATR) infrared spectra, Two-dimensional correlation spectroscopy (2DCOS), Moving-window 2D correlation

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