CHEMPHYSCHEM

Supporting Information

Lipid Internal Dynamics Probed in Nanodiscs

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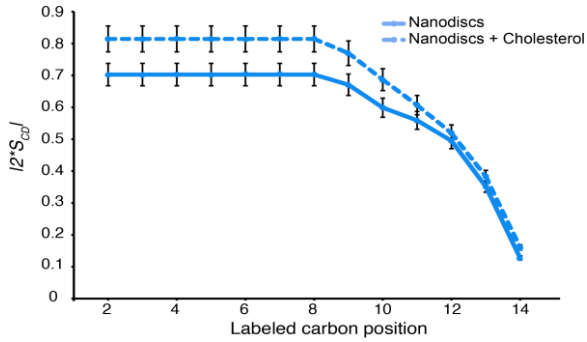
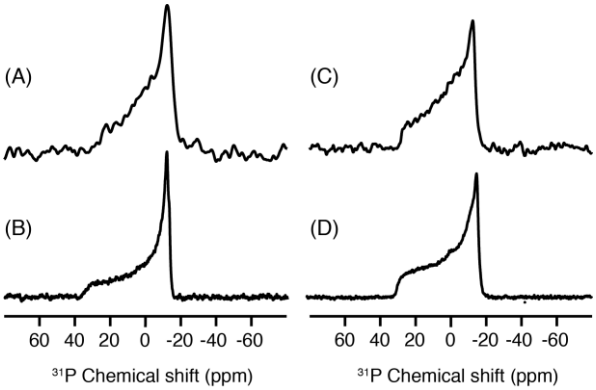
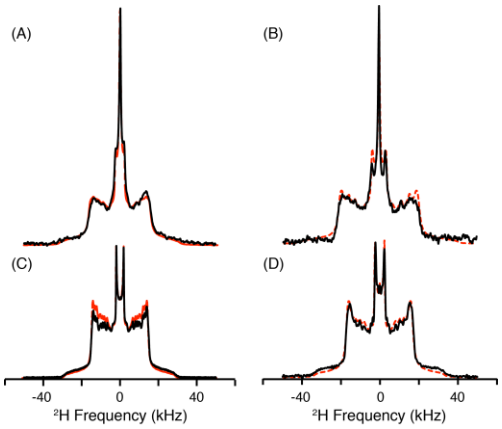
SI figures



S1. C-^{2}H order parameter as a function of labeled carbon position**.** Lipid ordering was determined at 289K in nanodiscs (blue) and supplemented with cholesterol (dotted blue). De-Pake-ing and simulation of ^{2}H ssNMR spectra were applied to measure individual quadrupolar splittings for DMPC-d_{54} and determine accurately order parameters. Error bars due to calculation procedures are estimated to be ca. 10%.



S2. ^{31}P solid-state NMR spectra of pure DMPC in nanodiscs (A), pure liposomes (B), DMPC nanodiscs with cholesterol (C) and DMPC liposomes supplemented in cholesterol (D). Spectra show the chemical shift anisotropy from the phospholipid head group due to the angular dependence of the phosphorus nucleus according to the magnetic field.



S3. Experimental (black lines) and simulated (red, dotted) deuterium NMR spectra for DMPC-d_{54} (A) in nanodiscs (a) and liposomes (b) and for DMPC-d_{54} / cholesterol (B) in nanodiscs (a) and in liposomes (b). Spectral simulations were realized using an in-house software and NMRdePaker program to determine individual experimental quadrupolar splittings.