Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Analysis of the orientation of cholesterol in high-density lipoprotein nanodiscs using solid-state NMR

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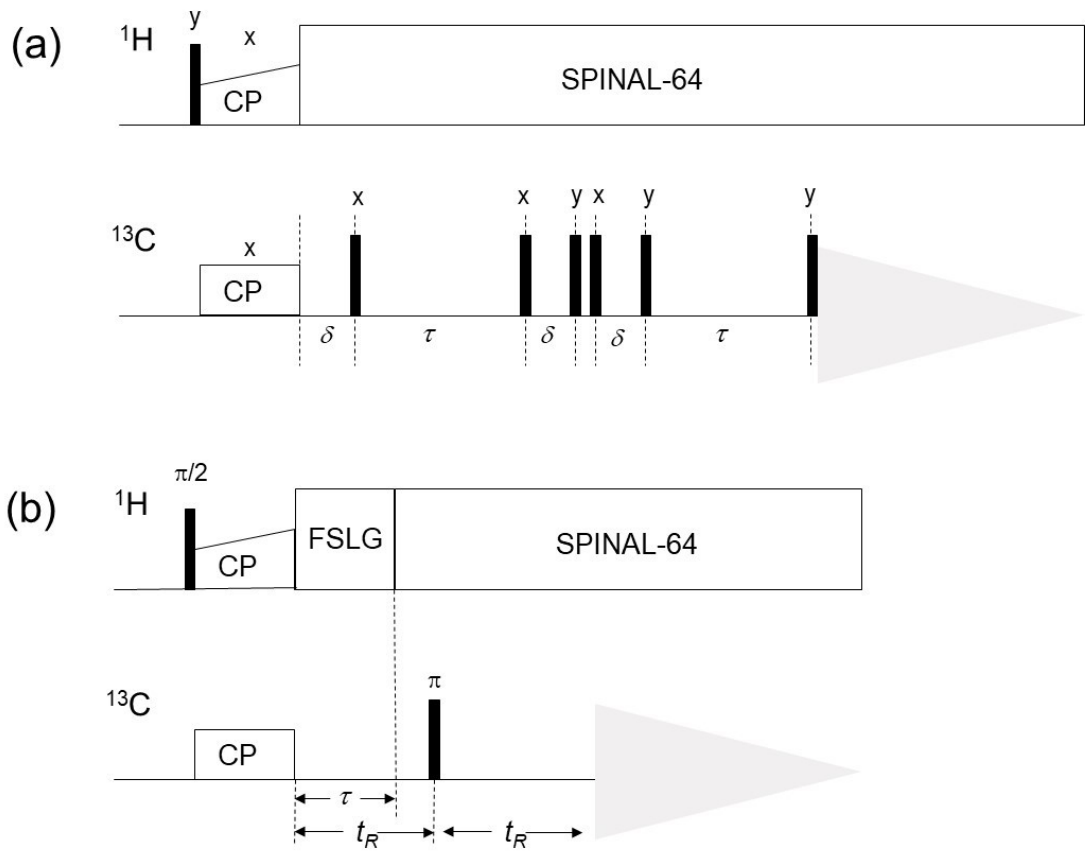

Figure S1. (a) NMR pulse scheme for the selective measurement of ^{13}C-^{13}C zero quantum build-up rates. The transmitter frequency is set to half way between the resonance frequencies of the two nuclear spins of interest. After cross-polarisation, a delay δ equal to the frequency difference of the two spins, S_1 and S_2, followed by a $\pi/2$ pulse stores S_1 and S_2 along the +z and -z axes. The delay τ allows for mechanical excitation of zero quantum coherence at rotational resonance. The next $\pi/2 - \delta - \pi/2$ sequence converts zero quantum into double quantum coherence and then a further $\pi/2 - \delta - \pi/2$ sequence converts the double quantum coherence back to zero quantum coherence. After a second delay τ, a final $\pi/2$ readout pulse is applied. With appropriate phase cycling, only the magnetisation that has passed through the double quantum filter is observed. Peaks in the spectrum are 180° out of phase with respect to each other. (b) The DIPSHIFT pulse sequence.

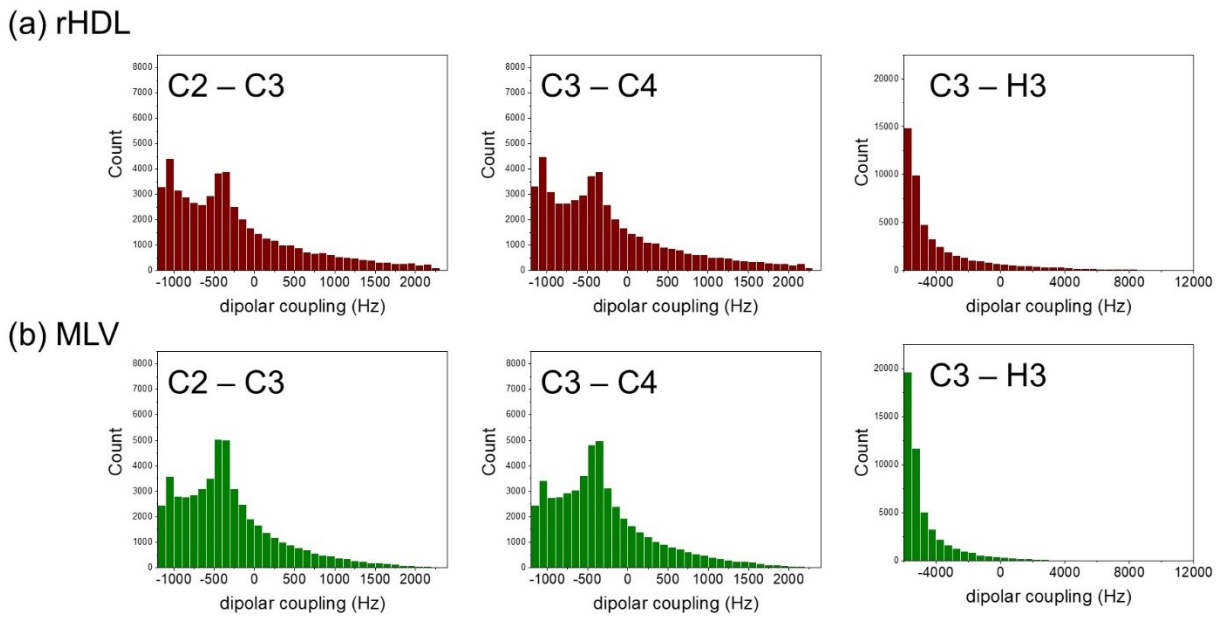

Figure S2. Dipolar couplings calculated from 50,000 cholesterol orientations generated using the Gaussian distribution procedure described in Figure 4 of the main text. The values of the three parameters, α_{MR}, β_{MR} and σ_{RN} used to calculate the distributions are given in Tables 2 and 3 of the main text.