Electronic Supplementary Material (ESI) for RSC Advances.

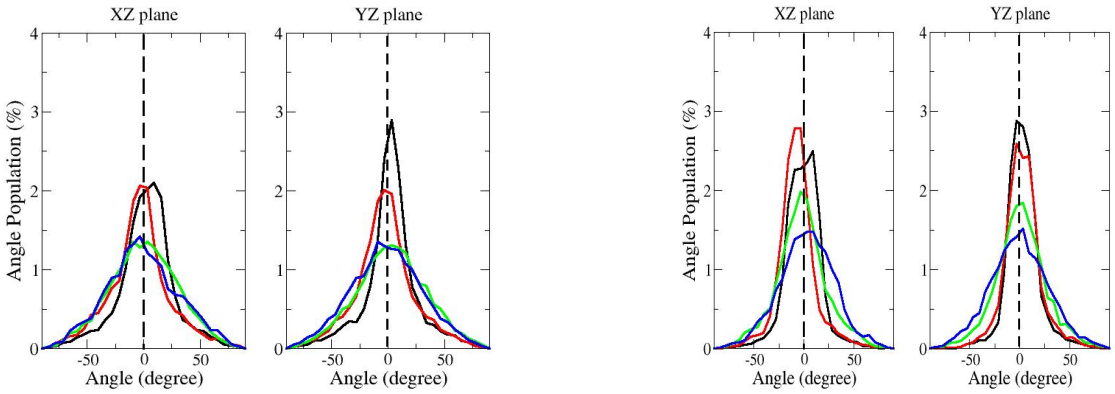

Fig. S1 Normalized angle distributions computed for the DPPC acyl chain C atoms during the atomistic MD simulations carried out for DPPC (left) and DPPC + Cer (right) systems at four temperatures: 20 ºC (in black), 30 ºC (in red), 37 ºC (in green) and 52 ºC (in blue). The XZ and YZ angles were measured with respect to the perpendicular of the node plane (see Figure 3). Ten snapshots extracted from each simulation (see Computational Details) were considered.

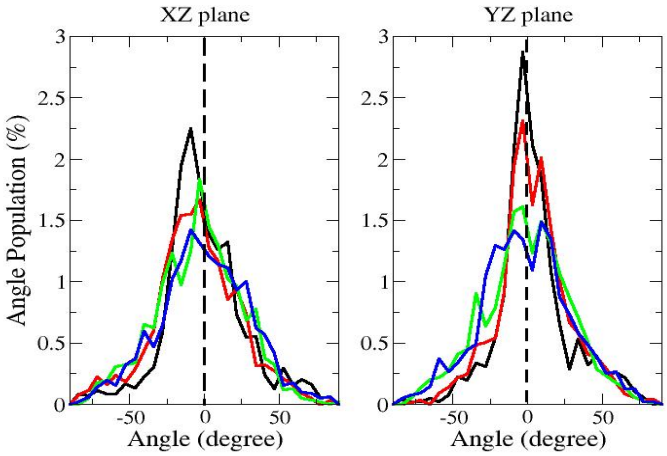

Fig. S2 Normalized angle distributions for the Cer acyl chain C atoms during atomistic MD simulations carried out for DPPC + Cer system at four temperatures: 20ºC (in black), 30ºC (in red), 37ºC (in green) and 52ºC (in blue). The XZ and YZ angles were measured with respect to the perpendicular of the node plane (see Figure 3). Ten snapshots extracted from each simulation (see Computational Details) were considered.

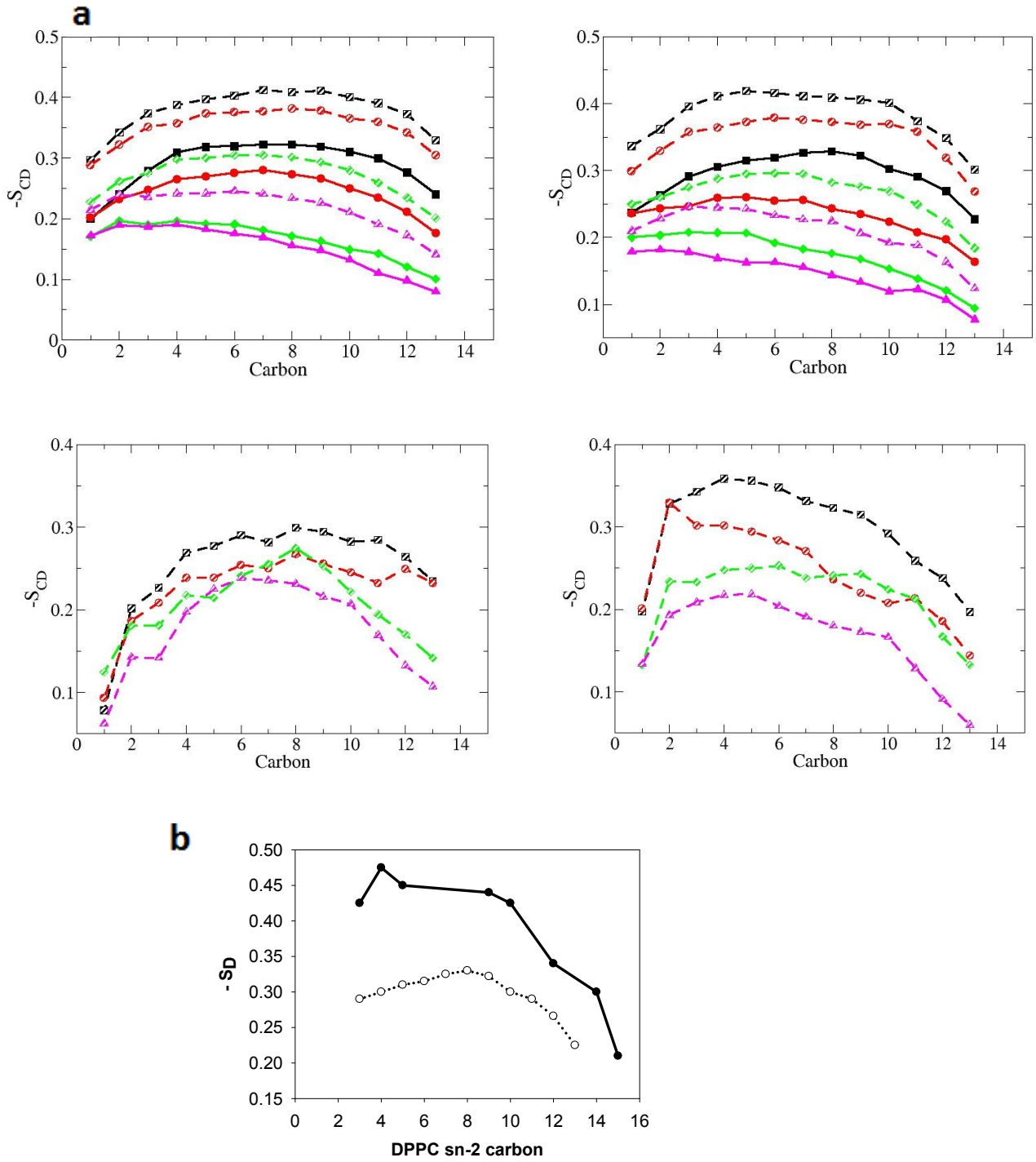

Fig. S3 a) S_{CD} order parameter profiles for sn-1 (left) and sn-2 (right) acyl chain C atoms (see definitions in Figure 3) of DPPC (above) and Cer (below, left: sphingoid chain, right: N-acyl chain) determined from the atomistic molecular dynamics carried out at four temperatures: 20 ºC (squares in black), 30 ºC (circles in red), 37 ºC (diamonds in green) and 52 ºC (triangles in magenta). Data shown in solid lines refer to DPPC, while data in dash lines refer to DPPC + Cer. The values were determined by calculating the average value over the 10 structures extracted from each simulation. b) Comparison between chain order parameters measured for sn-2 acyl chains of pure DPPC experimentally by ^{2}H-NMR (redrawn from Seelig and Seelig [52], solid black line) and our MD profile at 20 ºC (white circles, dotted lines).