Electronic Supplementary Information

Thermodynamic and structural study of DMPC-alkanol system

Mária Klacsová[a*], Attila Bóta[b], Peter Westh[c], Sérgio de Souza Funari[d], Daniela Uhríková[a] and Pavol Balgavý[a]

[a.] *Department of Physical Chemistry of Drugs, Faculty of Pharmacy, Comenius University in Bratislava, Odbojárov 10, 832 32 Bratislava, Slovakia. E-mail: klacsova@fpharm.uniba.sk*
[b.] *Biological Nanochemistry Research Group, Research Centre for Natural Sciences, Magyar tudósok blv.2, 1117 Budapest, Hungary.*
[c.] *Department of Biotechnology and Biomedicine, Technical University of Denmark, Søltofts Plads, Building 224, 2800 Kongens Lyngby, Denmark.*
[d.] *HASYLAB at DESY, Notkestrasse 85, 22607 Hamburg, Germany*

Figure S1 Temperature dependence of the heat capacity C_p of the DMPC-C10OH (left) and DMPC-C12OH system (right) at different CnOH:DMPC molar ratios, obtained upon cooling. The insets represent 10 times enlarged areas of the pre-transition peak.

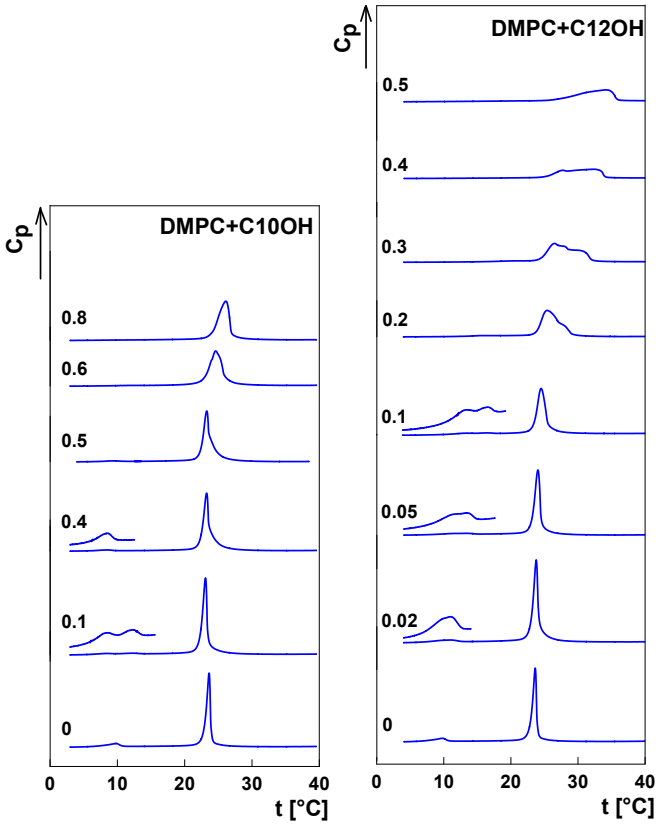


Figure S2 Temperature dependence of the heat capacity C_p of the DMPC-CnOH systems with n = 8 – 18 at n_{CnOH}:n_{DMPC} = 0.2 mol/mol obtained on heating. For systems containing C14OH, C16OH and C18OH, respectively, the dependences were enlarged two times for better resolution.

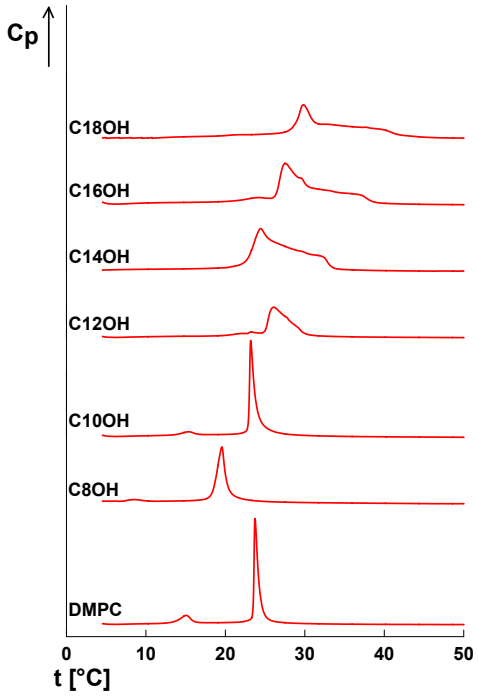


Figure S3 Example of DSC heat capacity curve simulation for DMPC-C12OH sample at n_{C12OH}:n_{DMPC} = 0.3 mol/mol by five Pearson functions (depicted without background correction).

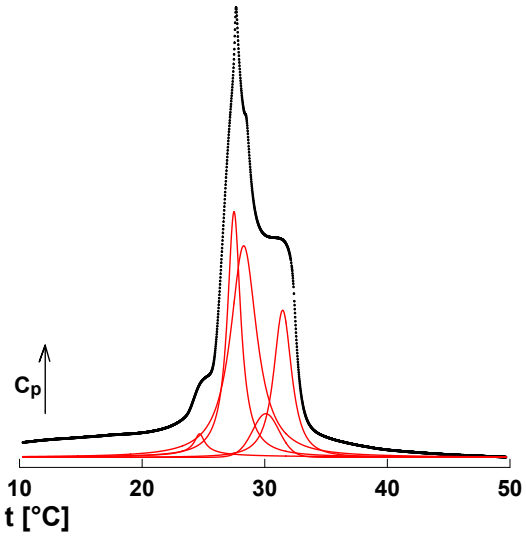


Figure S4 SAXD patterns obtained for the DMPC-C12OH system at n_{C12OH}:n_{DMPC} = 0, 0.1, 0.2, 0.4 mol/mol (panel A, B, C, D, respectively) in the temperature range 10-50°C. Signal loss seen at s □ 0.308 nm^{-1} is an electronic artefact of the SAXD detector. (This artefact was deleted in Figure 2 for the representative diffractograms.)

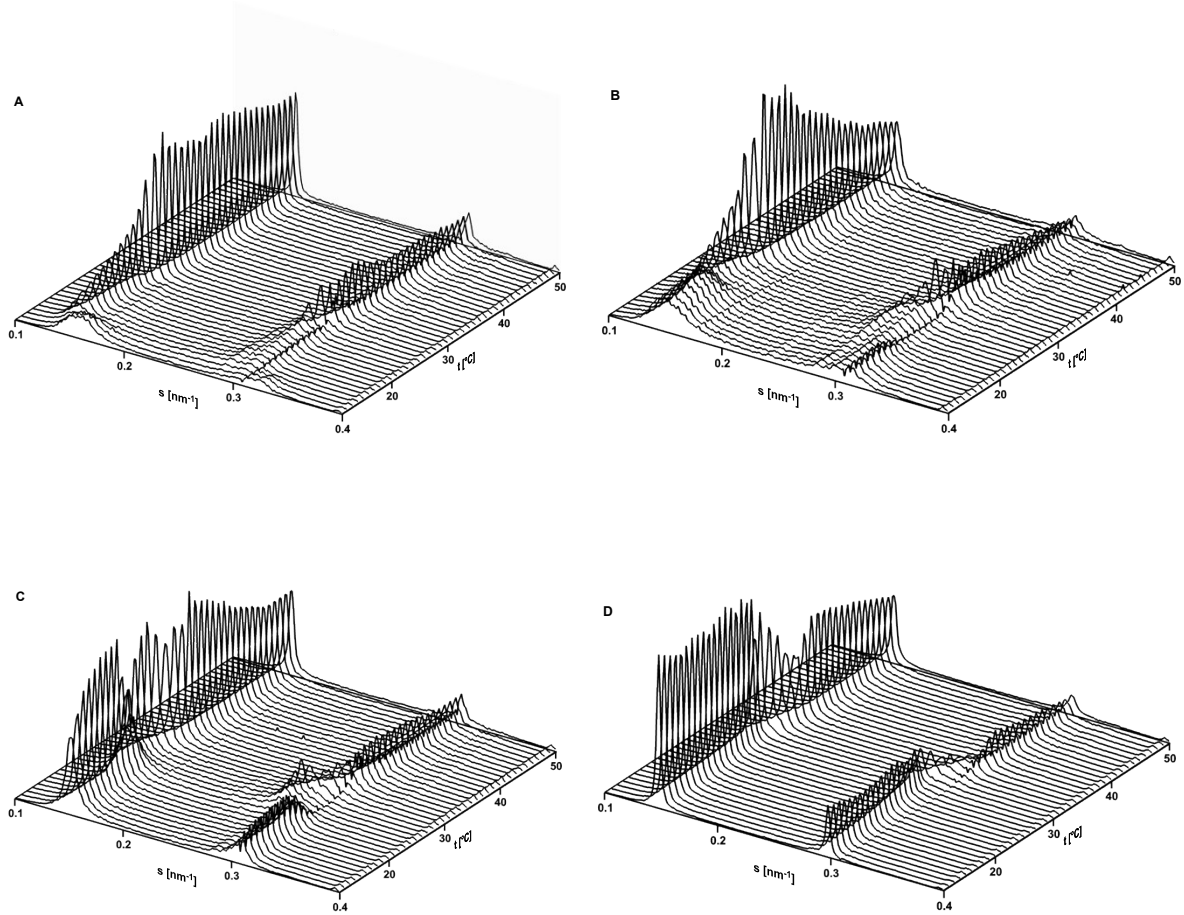
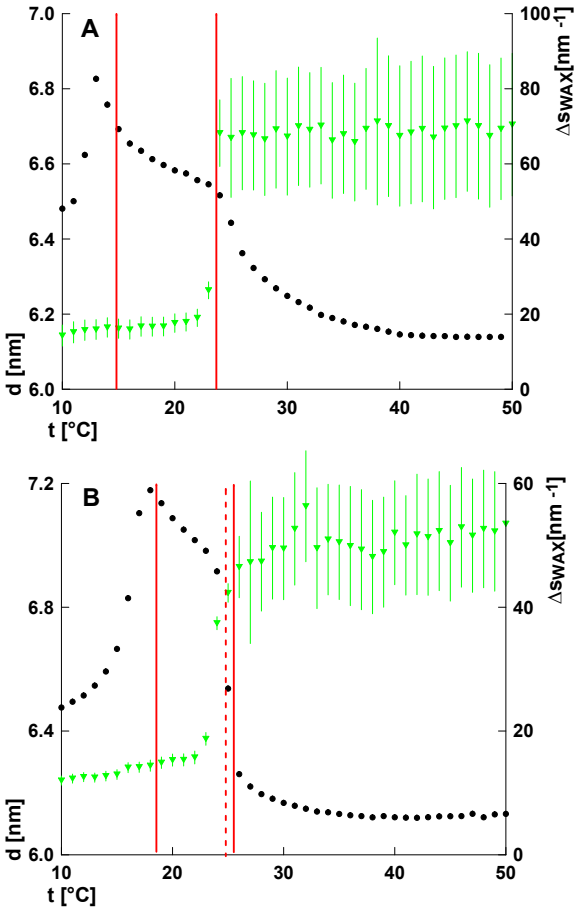


Figure S5 Temperature dependence of the repeat distance d (black symbols) and the half-width of the WAX reflection Δs_{WAX} (green symbols) for the DMPC-C12OH system at n_{C12OH}:n_{DMPC} = 0, 0.1, 0.2, 0.4 mol/mol (panel A, B, C, D, respectively). Red vertical lines denote the transition temperatures determined from DSC heating scan: pre-transition and end of the main-transition (solid lines) and onset of the main-transition (dashed lines).



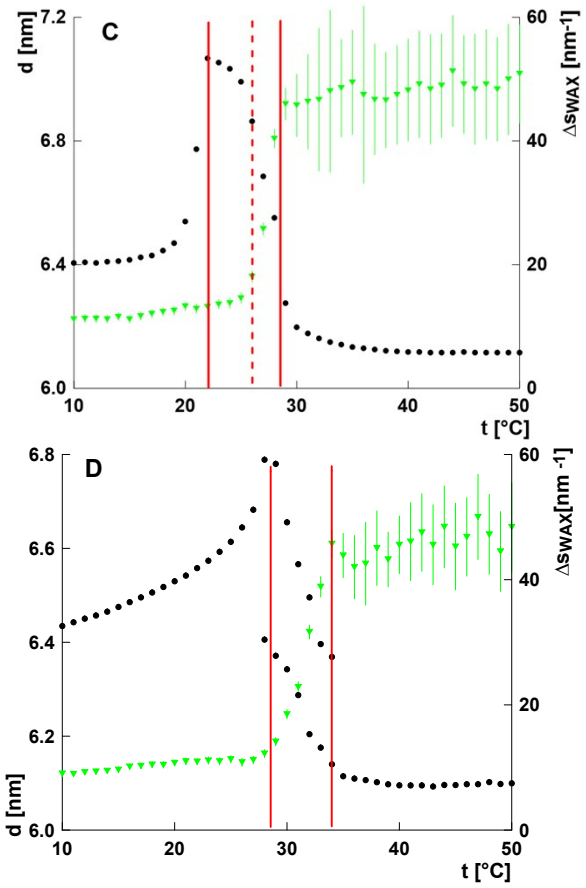

C
d [nm]
7.2
6.8
6.4
6.0
10
20
30
40
50
t [°C]
60
40
20
0
ΔsWAX [nm-1]
D
d [nm]
6.8
6.6
6.4
6.2
6.0
10
20
30
40
50
t [°C]
60
40
20
0
ΔsWAX[nm -1]

Figure S6 Predicted pseudo-binary phase diagram of the DMPC-C12OH system. Dots represent transition temperatures obtained by DSC and SAXD/WAXD, solid lines are just guiding to the eyes. Dashed lines represent approximation of the data points.