Electronic Supplementary Material

Stratum corneum molecular mobility in the presence of natural moisturizers

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Table S1 ¹³C chemical shifts (ppm) of carbons in urea, glycerol, PCA, and UCA. The assignment is based on corresponding spectra from SDBS. (Web: http://sdbs.riodb.aist.go.jp, National Institute of Advanced Industrial Science and Technology). The measured spectra of pure UCA showed non-resolved clusters of CP peaks. Therefore, the chemical shifts for UCA is given here by the values from the database (SDBS).

	H_2N 1 NH_2	ОН H0ОН 2 1_2'	0 5 1 2 0 4 0 H 0 H 0 H 0 H	N 3 4 HN 1 5 0 0 0 0 0 0 0 0 0 0 0 0 0
Carbon no.	Urea	Glycerol	PCA	UCA
1	163.3	63.9	25.5	115.0
2		73.3	30.4	123.5
3			57.1	134.1
4			177.1	135.4
5			182.5	137.7
6				168.0



Fig. S1 Standard numbering of cholesterol carbons.



Fig. S2 Sorption isotherms of pure glycerol, urea, PCA, and UCA at 32 °C. Glycerol is a hygroscopic liquid that takes up water continuously upon increasing RH. Urea is a solid that starts to take up water around 72% RH, which corresponds to the vapor pressure over a saturated solution of urea, and the solution is then diluted when the RH increases further. The sorption isotherm for PCA is similar to the isotherm obtained for urea, but PCA starts to take up water at a higher RH of approx. 92%. The sorption isotherm for UCA is more complex as it shows signs of a non-equilibrium effect (a kink around ~ 4wt% and ~ 95% RH), which can be associated to amorphous recrystallization. To investigate the reproducibility of this non-equilibrium effect we performed triplicate measurements on UCA. Although some small differences are observed, the characteristic kink was reproduced, suggesting that the samples contained varying amount of amorphous material at the start of the experiment.



Fig. S3 Close-up PT ssNMR 13 C spectra (DP = grey, CP = blue, INEPT = red) of selected lipid resonances in SC samples with or without glycerol, urea, PCA, or UCA.



Fig. S4 Close-up PT ssNMR 13 C spectra (DP = grey, CP = blue, INEPT = red) of selected protein resonances in SC samples with or without glycerol, urea, PCA, or UCA.