Electronic Supplementary Material (ESI) for Soft Matter.

ELECTRONIC SUPPLEMENTARY INFORMATION

How to control interactions of cellulose-based biomaterials with skin: the role of acidity in the contact area

Andrey A. Gurtovenko*[,1] and Mikko Karttunen[2,3,4,1]

[1] *Institute of Macromolecular Compounds, Russian Academy of Sciences, Bolshoi Prospect V.O. 31, St.Petersburg, 199004 Russia;*

[2] *Department of Chemistry, the University of Western Ontario,1151 Richmond Street, London, Ontario, Canada N6A 3K7;*

[3] *Department of Applied Mathematics, the University of Western Ontario, 1151 Richmond Street, London, Ontario, Canada N6A 5B7;*

[4] *The Centre for Advanced Materials and Biomaterials Research, the University of Western Ontario, 1151 Richmond Street, London, Ontario, Canada N6A 5K7.*

E-mail: a.gurtovenko@gmail.com

Web: biosimu.org

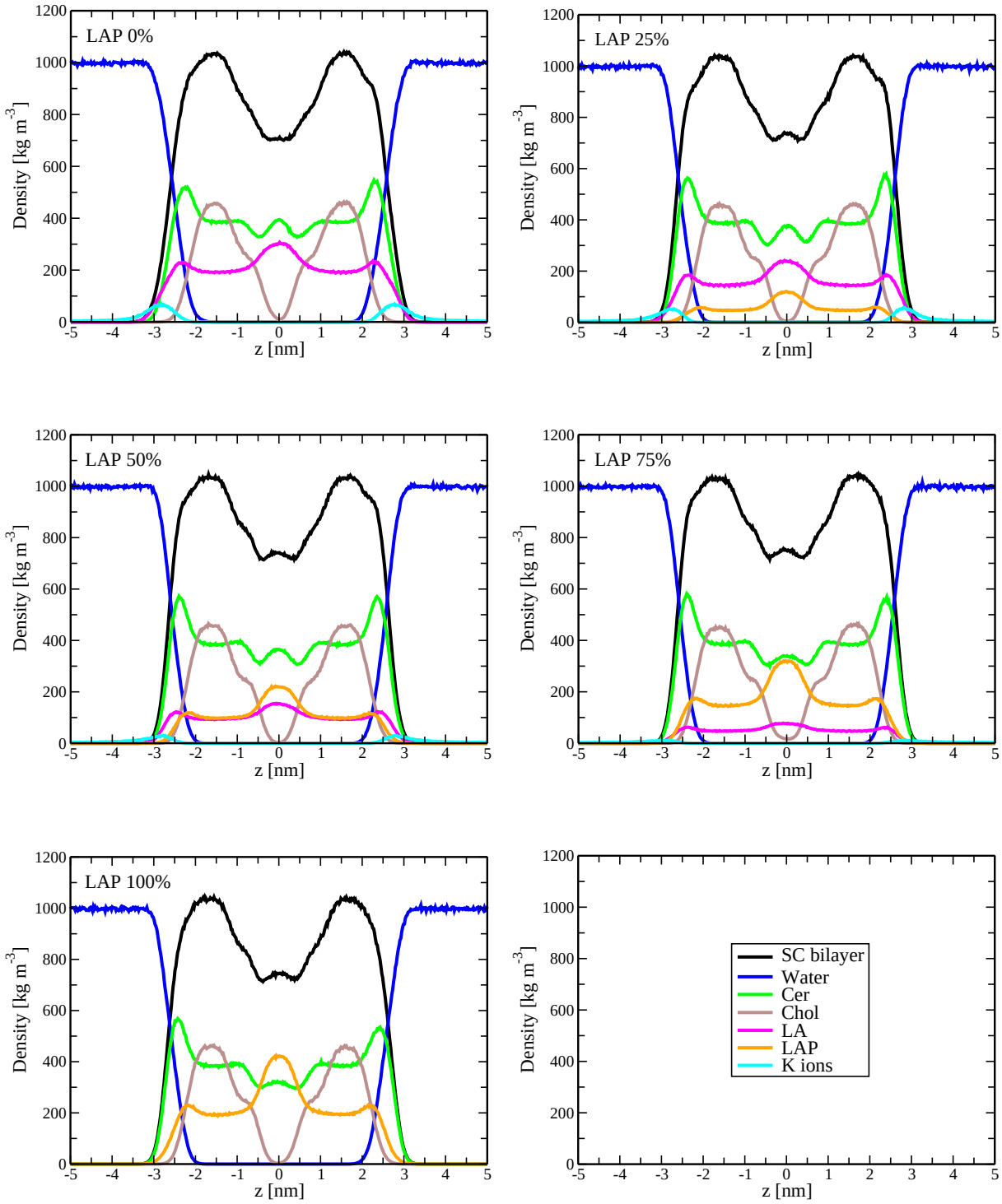

FIG. S1: Mass density profiles for components of a SC lipid bilayer, water, and K counterions as a function of the distance from the SC bilayer center (z = 0). Shown are results for the SC bilayers with LAP content of 0 %, 25 %, 50 %, 75 %, and 100 %.

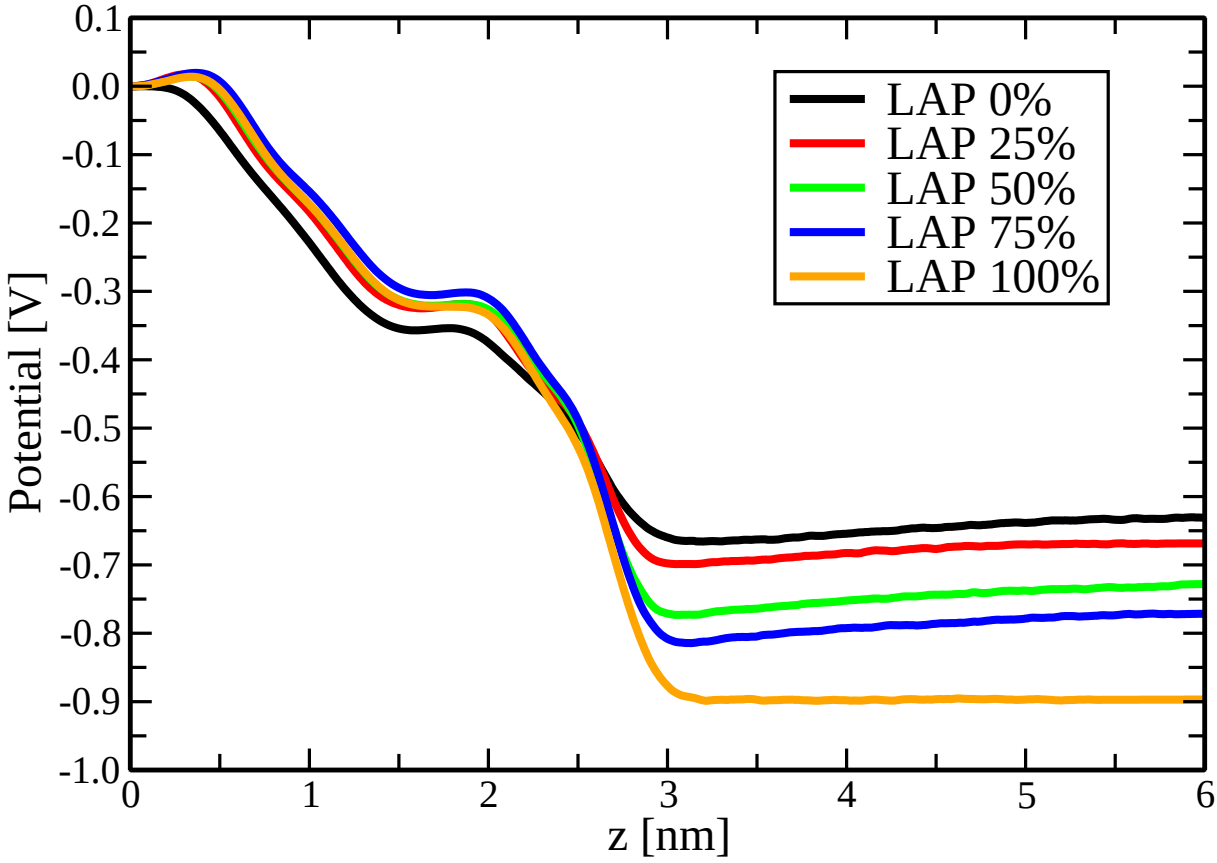

FIG. S2: Electrostatic potential of SC lipid bilayers as a function of the distance from the SC bilayer center (z = 0).

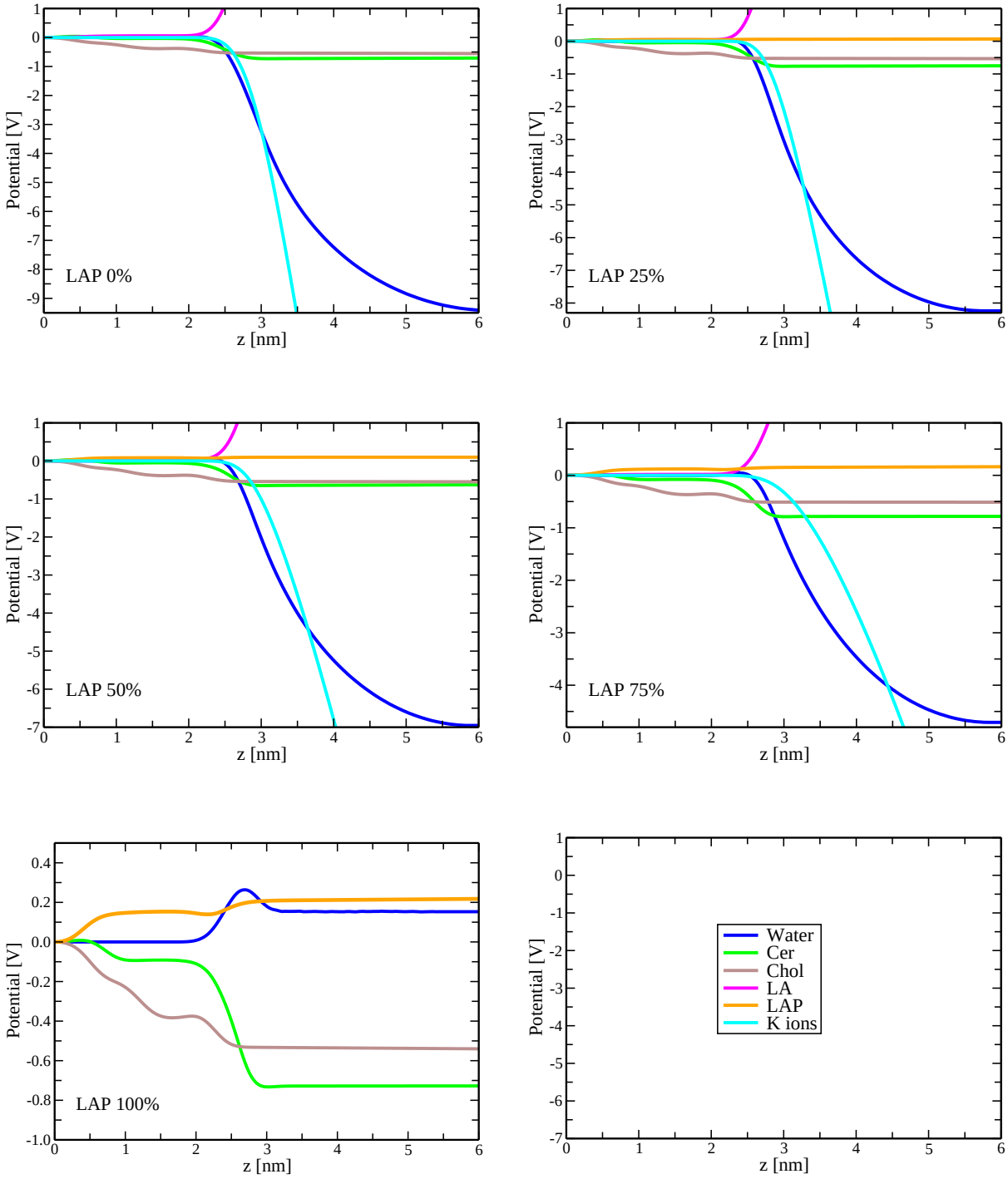

FIG. S3: Contributions of components of a SC lipid bilayer, water, and K counterions to the electrostatic potential as a function of the distance from the SC bilayer center (z = 0). Shown are results for the SC bilayers with LAP content of 0 %, 25 %, 50 %, 75 %, and 100 %.

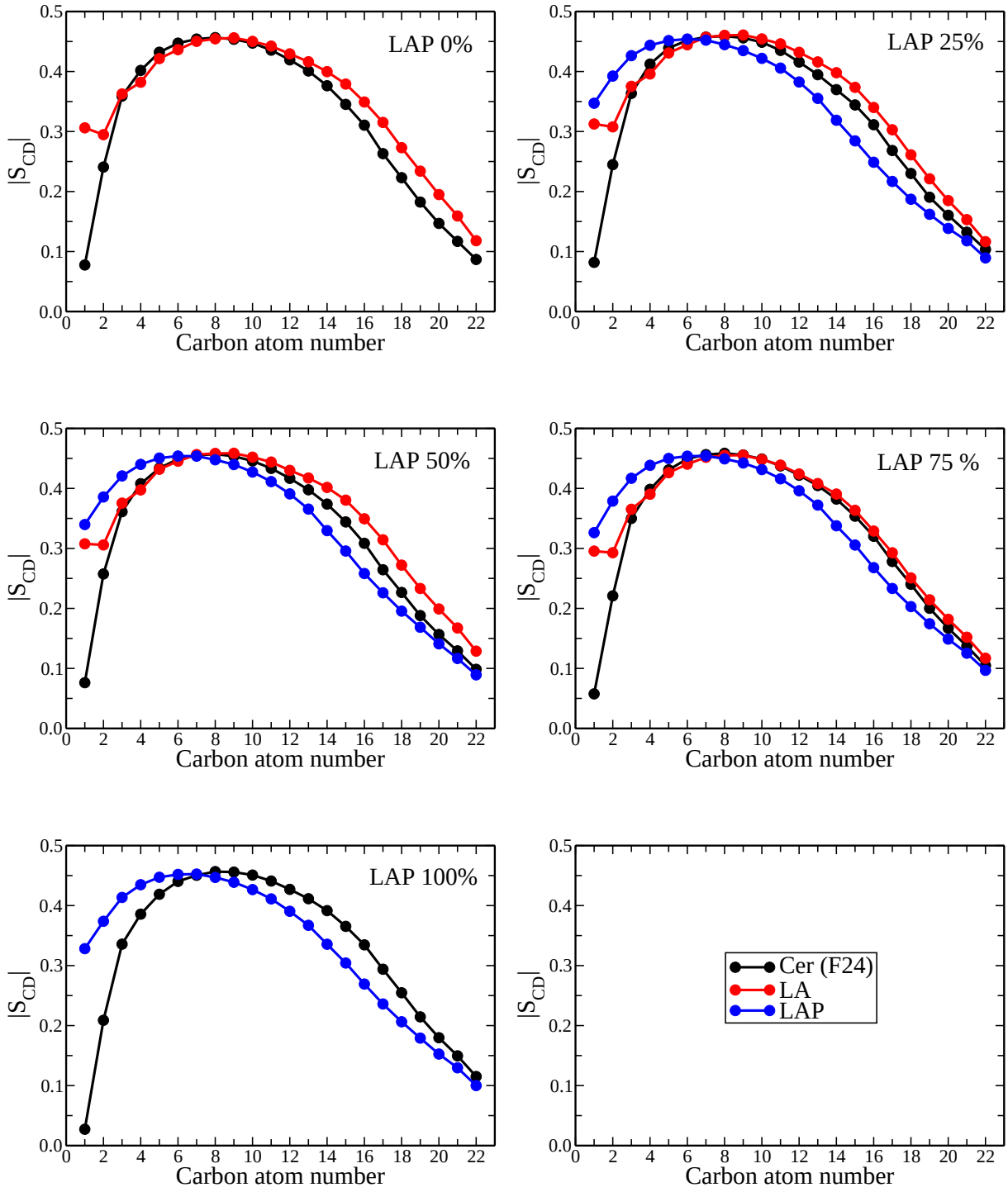

FIG. S4: Deuterium order parameter $|S_{CD}| = |(1/2)(3\langle\cos^2\theta\rangle - 1)|$ for the fatty acid chain (F24) of ceramide and for the fatty acid chains of LA and LAP (θ is the angle between the C-H vector in the hydrocarbon chain and the SC bilayer normal).

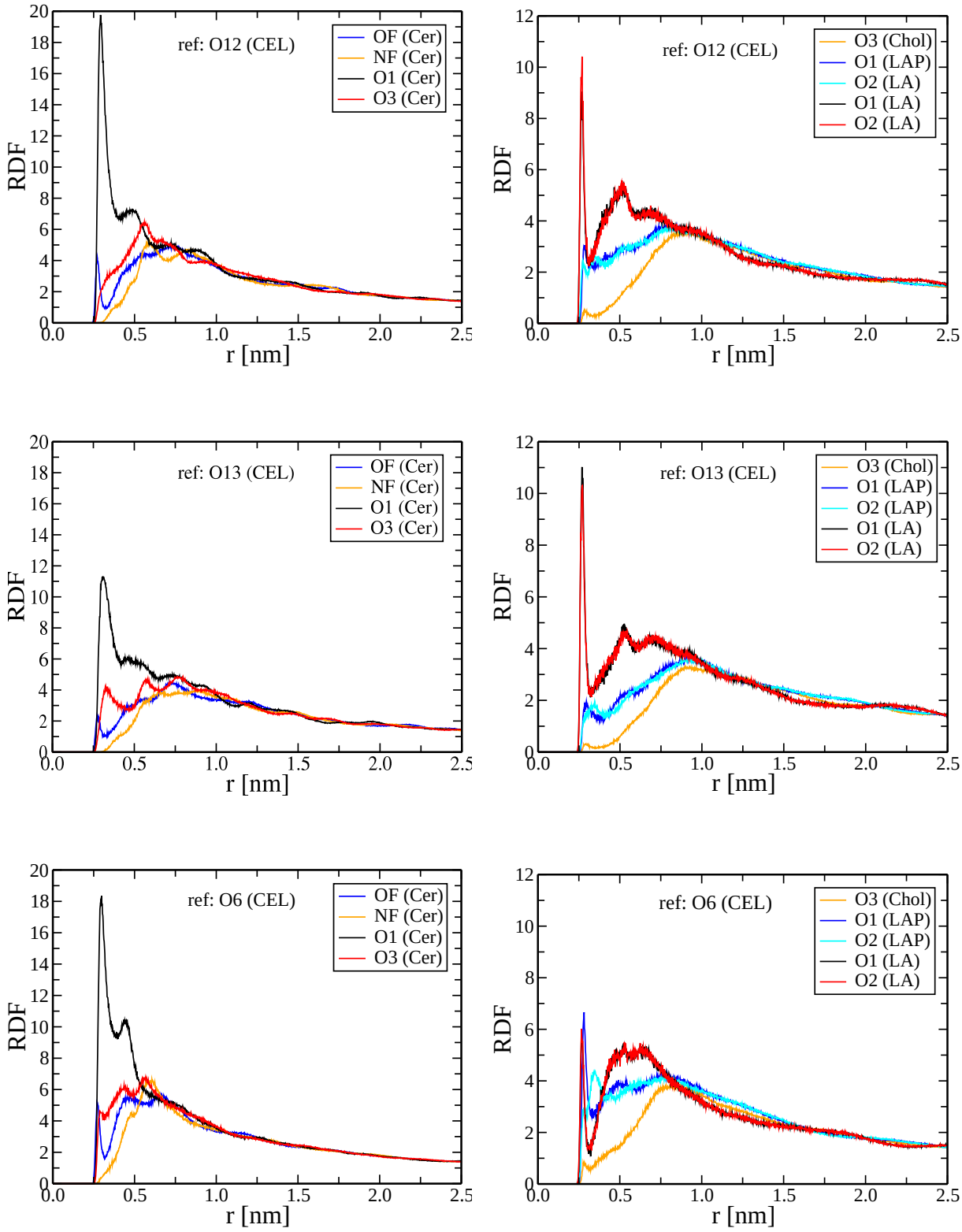

FIG. S5: Radial distribution functions (RDFs) of cellulose's oxygen atoms (O12, O13, and O6) and principal atoms of ceramides (left) and of fatty acids and cholesterol (right). Shown are results for the CEL-SC-P75 system.

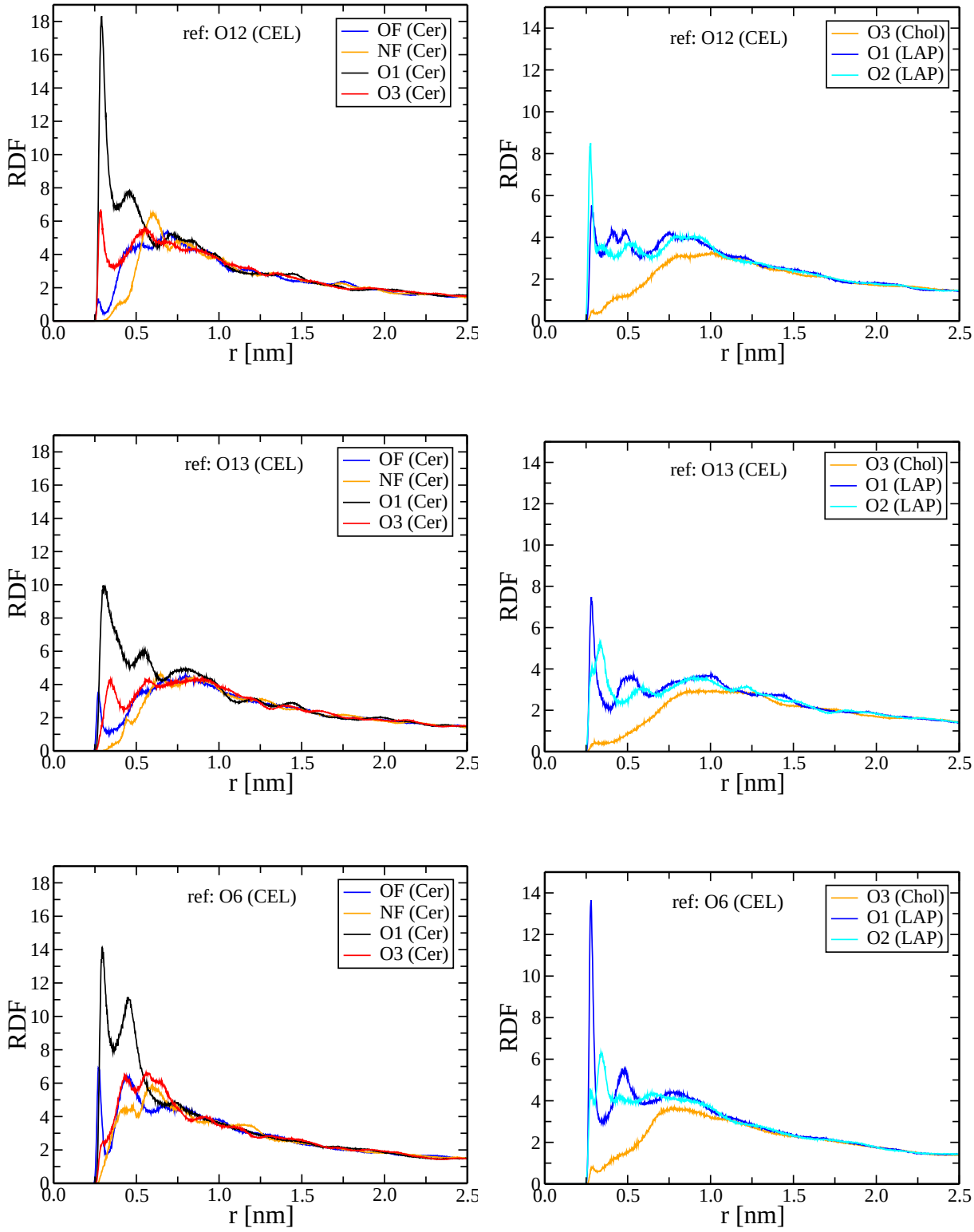

FIG. S6: Radial distribution functions (RDFs) of cellulose's oxygen atoms (O12, O13, and O6) and principal atoms of ceramides (left) and of fatty acids and cholesterol (right). Shown are results for the CEL-SC-P100 system.