Supporting Information

for

Unusual Behavior of Bipolar Molecule, 25-Hydroxycholesterol, at the Air/Water Interface – Langmuir Monolayer Approach Complemented with Theoretical Calculations

Anita Wnętrzak[a], Anna Chachaj-Brekiesz[a], Jan Kobierski[b],
Katarzyna Karwowska[c], Aneta D. Petelska[c], Patrycja Dynarowicz-Latka[a]

[a] Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland

[b] Department of Pharmaceutical Biophysics, Faculty of Pharmacy, Jagiellonian University Medical College, Medyczna 9, 30-688 Kraków, Poland

[c] Faculty of Chemistry, University of Bialystok, Ciolkowskiego 1K, 15-425 Bialystok, Poland

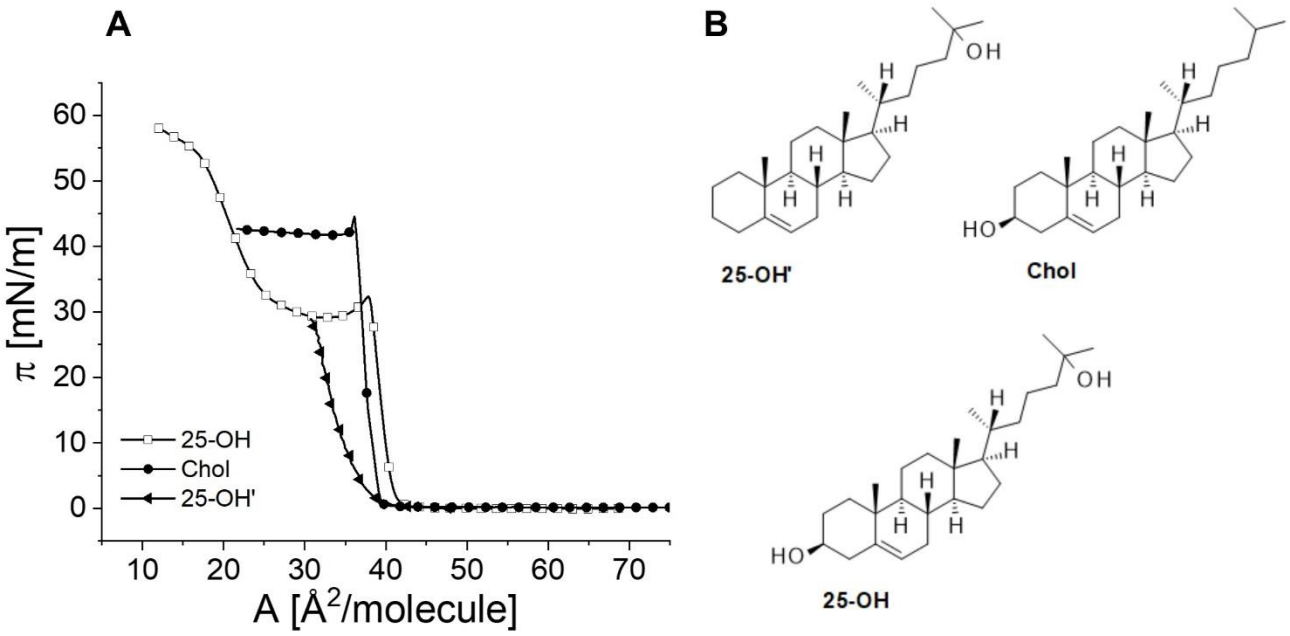


Figure S1. Surface pressure-area isotherms (A) and molecular formulas (B) of 25-OH and its homologs. The isotherm for 25-OH' was reconstructed with Origin program, based on the published data [V. Janout, S. Turkyilmaz, M. Wang, Y. Wang, Y. Manaka, S.L. Regen, An upside down view of cholesterol's condensing effect: does surface occupancy play a role? *Langmuir* **2010**, 26, 5316-5318].

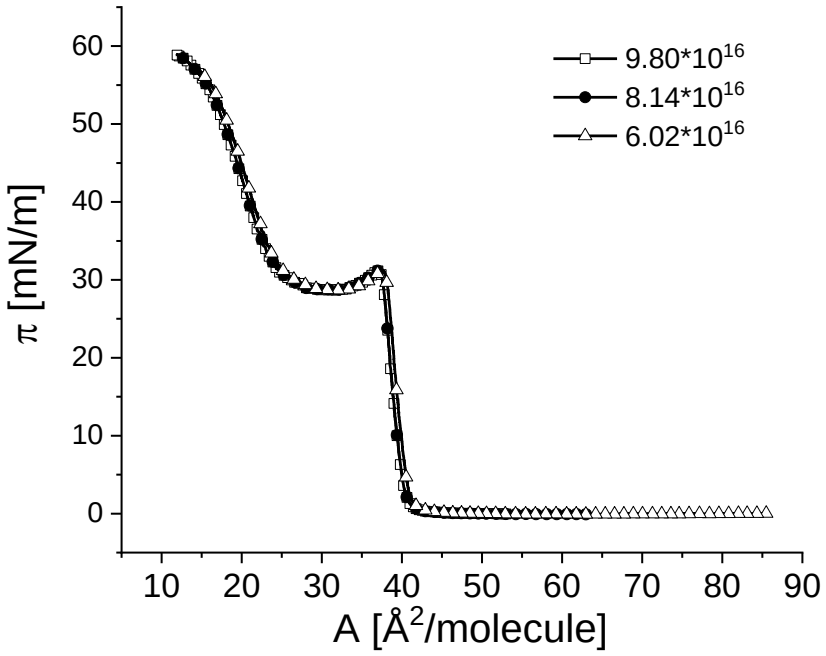


Figure S2. Influence of the number of molecules on surface pressure-area isotherms of 25-OH (recorded at 20 °C).

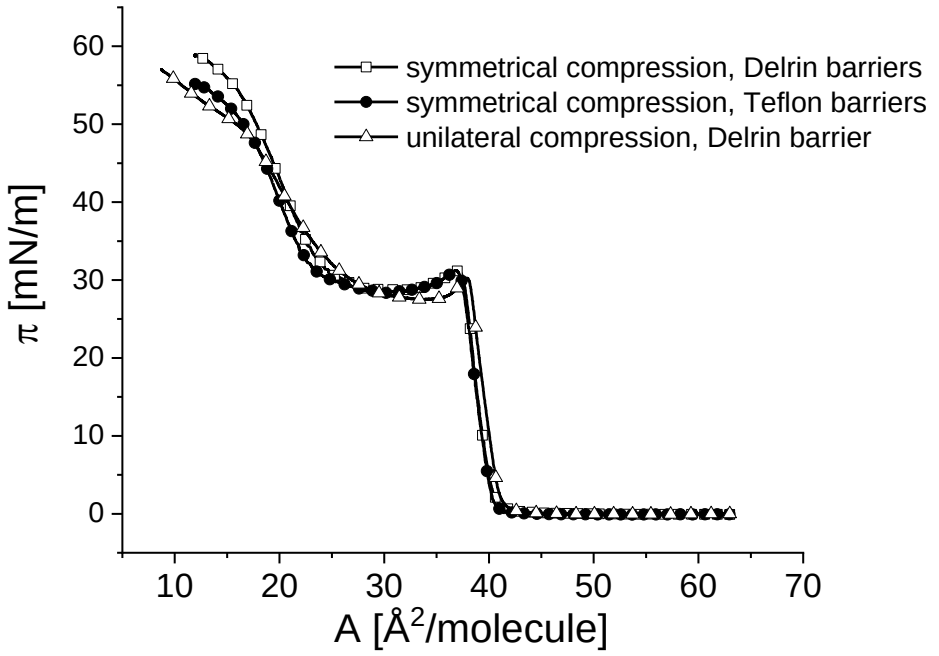


Figure S3. Influence of the type of compression (unilateral *vs* symmetrical) and barrier material (Delrin *vs* Teflon) on surface pressure-area isotherms of 25-OH (recorded at 20 °C).

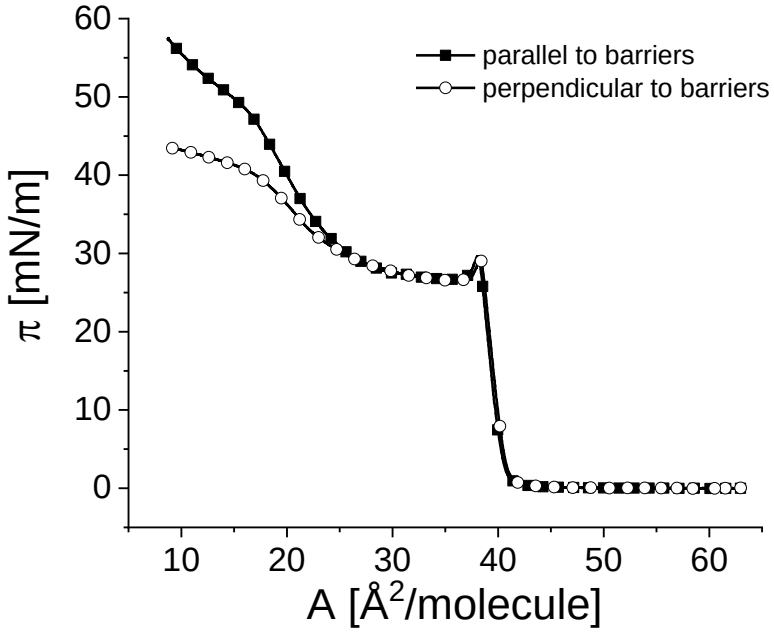


Figure S4. Influence of the orientation of Wilhelmy plate in respect to barriers position on surface pressure-area isotherms of 25-OH (recorded at 20 °C).

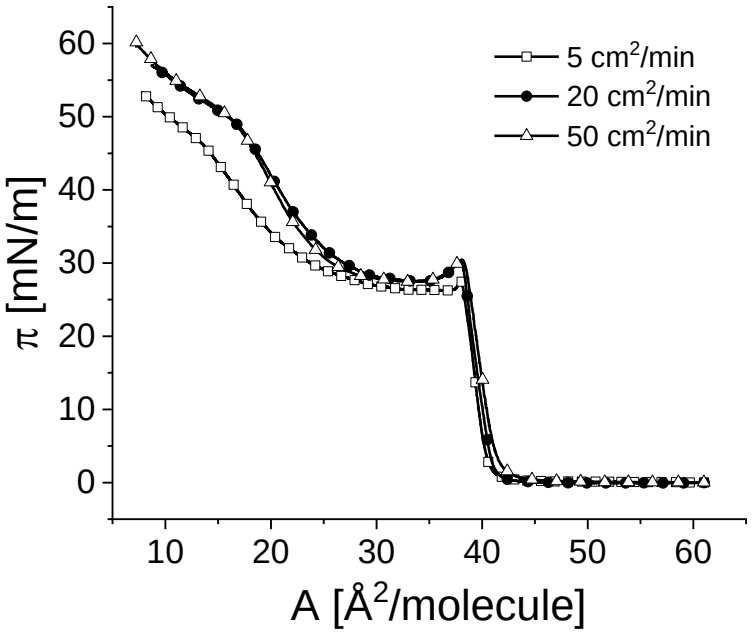


Figure S5. Influence of compression speed on surface pressure-area isotherms of 25-OH (recorded at 20 °C).

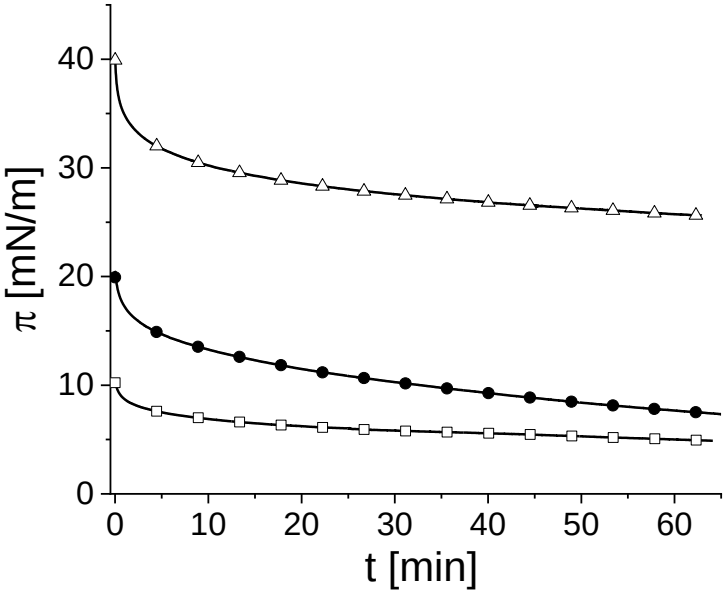
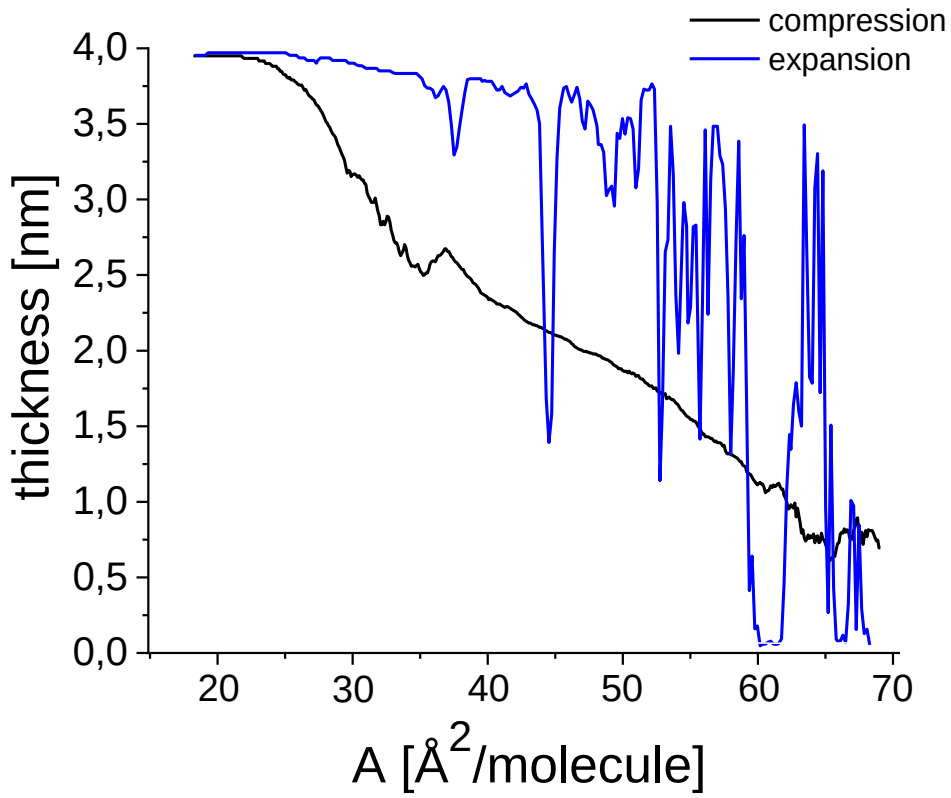
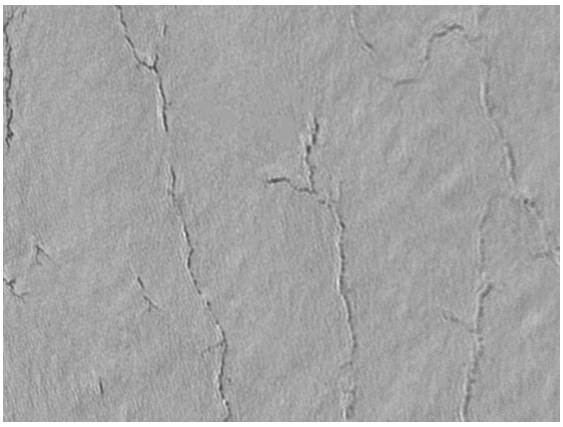


Figure S6. Stability of Langmuir monolayers from 25-OH (recorded at 20 °C).

A)



B)



C)

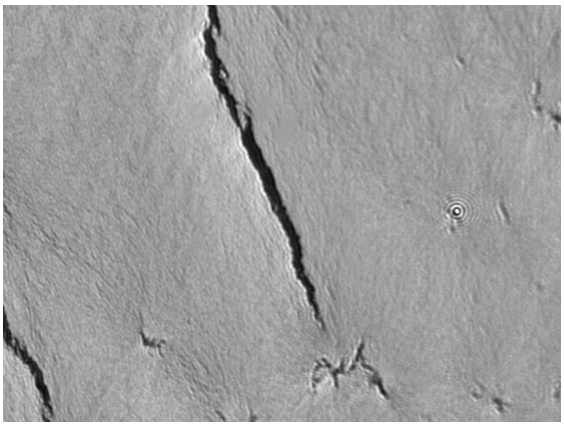


Figure S7. Thickness versus area per molecule plot registered during compression-expansion cycle for 25-OH monolayer spread on water at 20 °C (A). BAM textures of 25-OH films registered during expansion at different area per molecule values: 35 Å/molecule (B) and 50 Å/molecule (C).

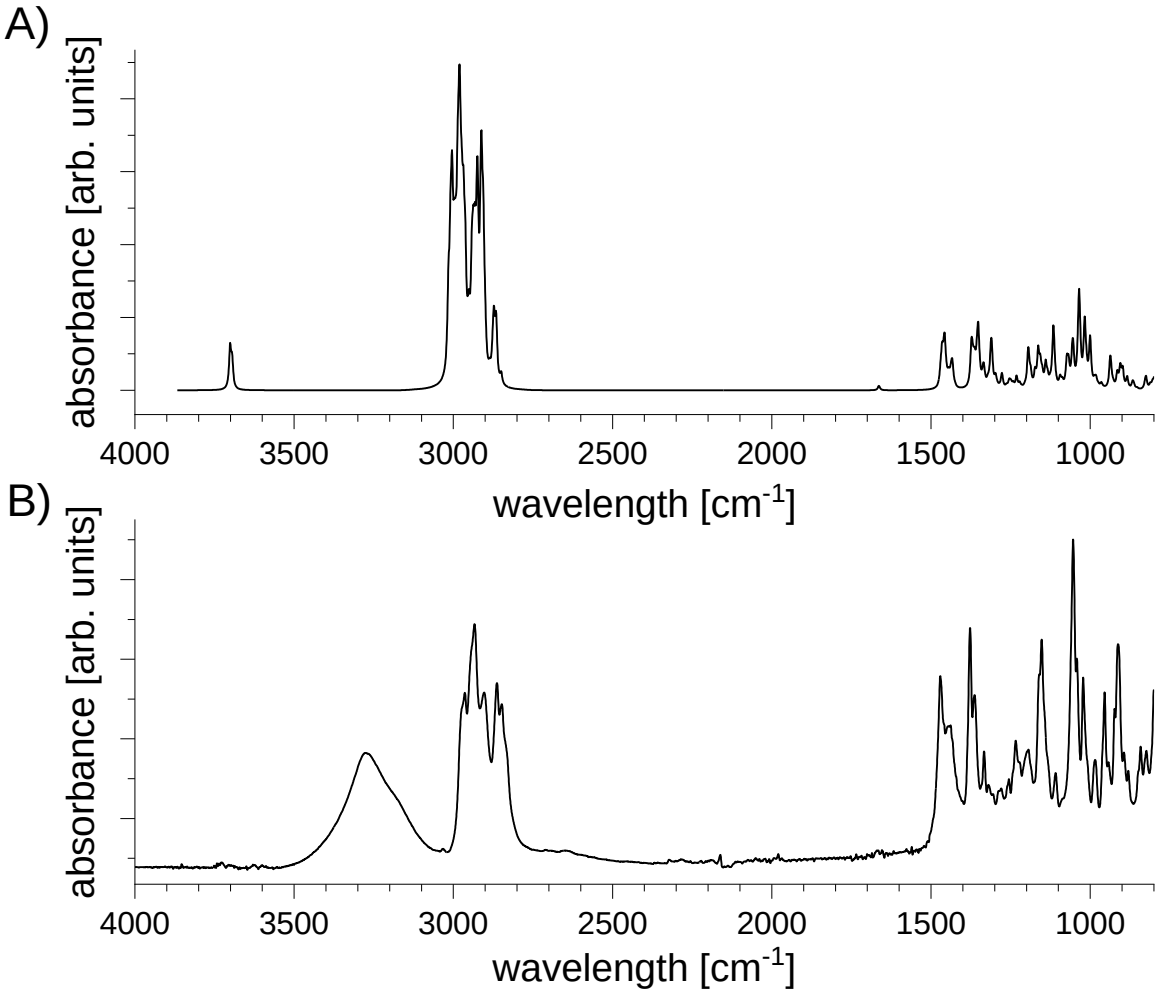


Figure S8. Comparison of IR spectra of 25-OH: calculated (A) and experimental ATR-FTIR (B).

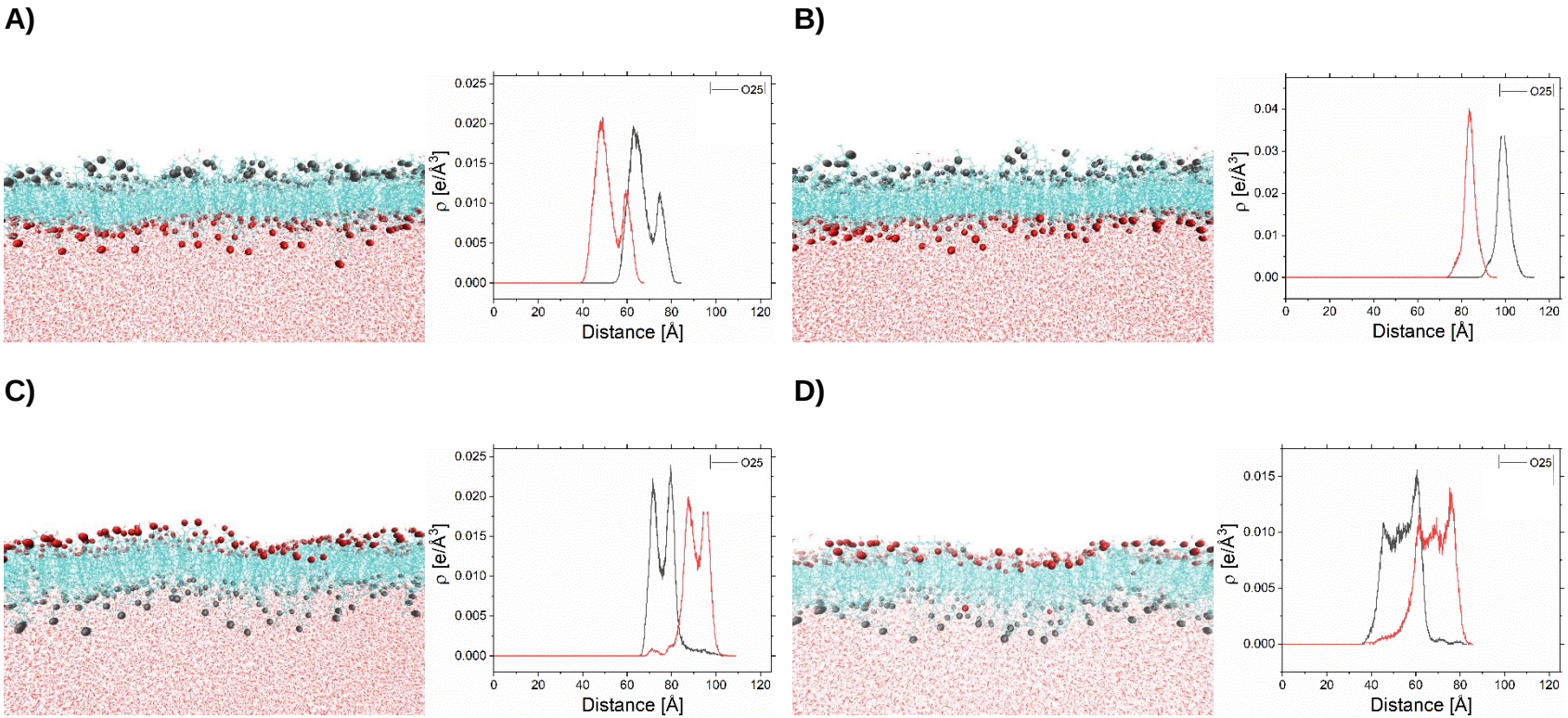


Figure S9. Models of monolayers and electron densities obtained after 110 ns production of molecular dynamics for systems with different mutual orientations: anchored with hydroxyl group at C(3) with surface pressure equal to 15 mN/m (A) or 35 mN/m (B) and anchored with hydroxyl group at C(25) with surface pressure equal to 15 mN/m (C) or 35 mN/m (D). Red balls and lines represent oxygen atom attached to C(3), dark grey represent oxygen atom attached to C(25).