

Supporting Information

Structure and Interaction in 2D Organized Assemblies of Cationic Lipids with Tryptophan: An Experimental and Computational Investigation

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Table S1. Critical packing parameters (CPP) calculated from experimental (a_0) and DFT study (l_c and V values).

Lipids	a_0	l_c	V	CPP
DPPC	58.87±0.29	21.2765	569.028	0.454±0.002
EPC	44.39±0.16	23.8415	703.019	0.664±0.002
EPCU	79.59±0.28	20.0435	814.643	0.510±0.001

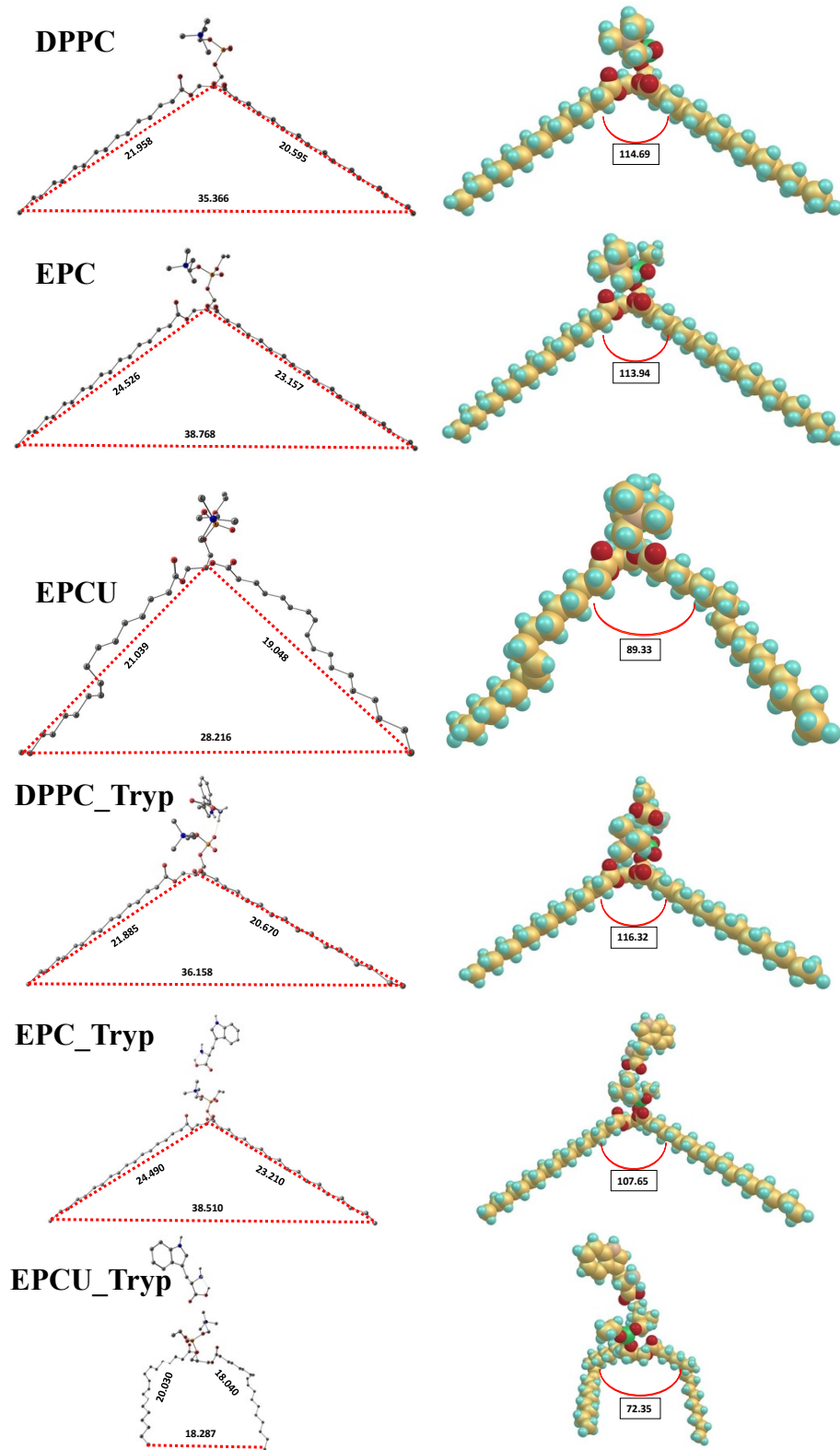


Figure S1(a). The optimized geometries (alkyl chain lengths and angles) of DPPC, EPC and EPCU lipids in the absence and presence of tryptophan.

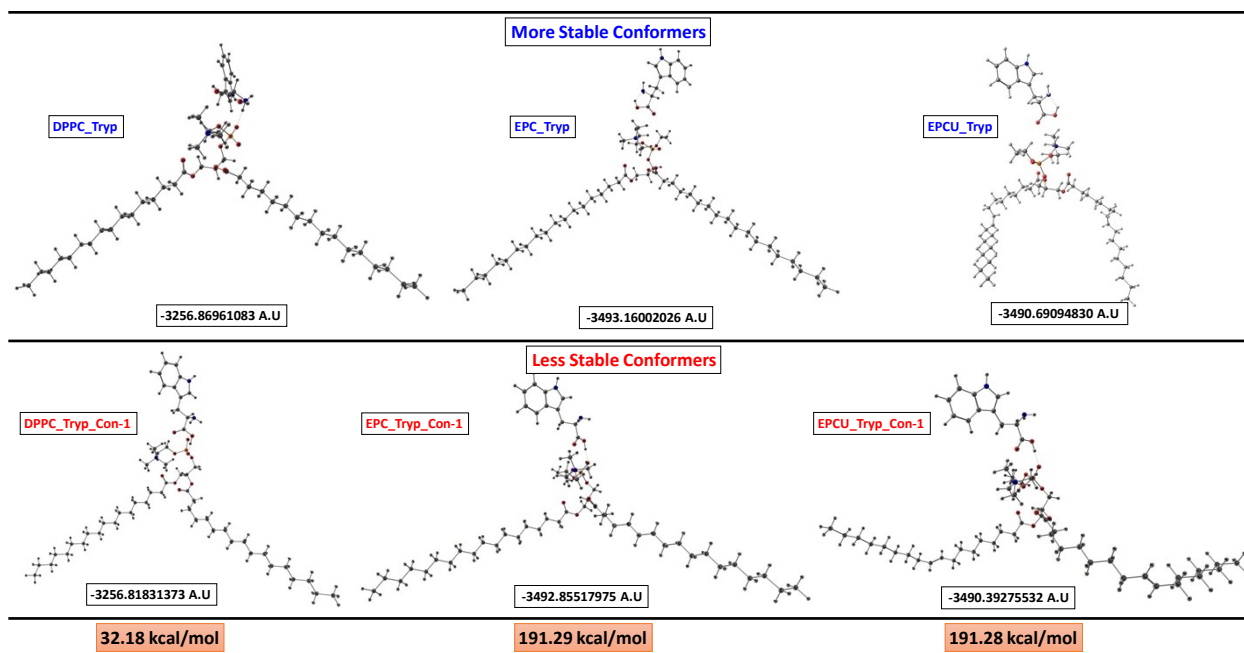


Figure S1(b). The conformational analysis for optimized geometries (alkyl chain lengths and angles) of DPPC, EPC and EPCU lipids in the presence of tryptophan.

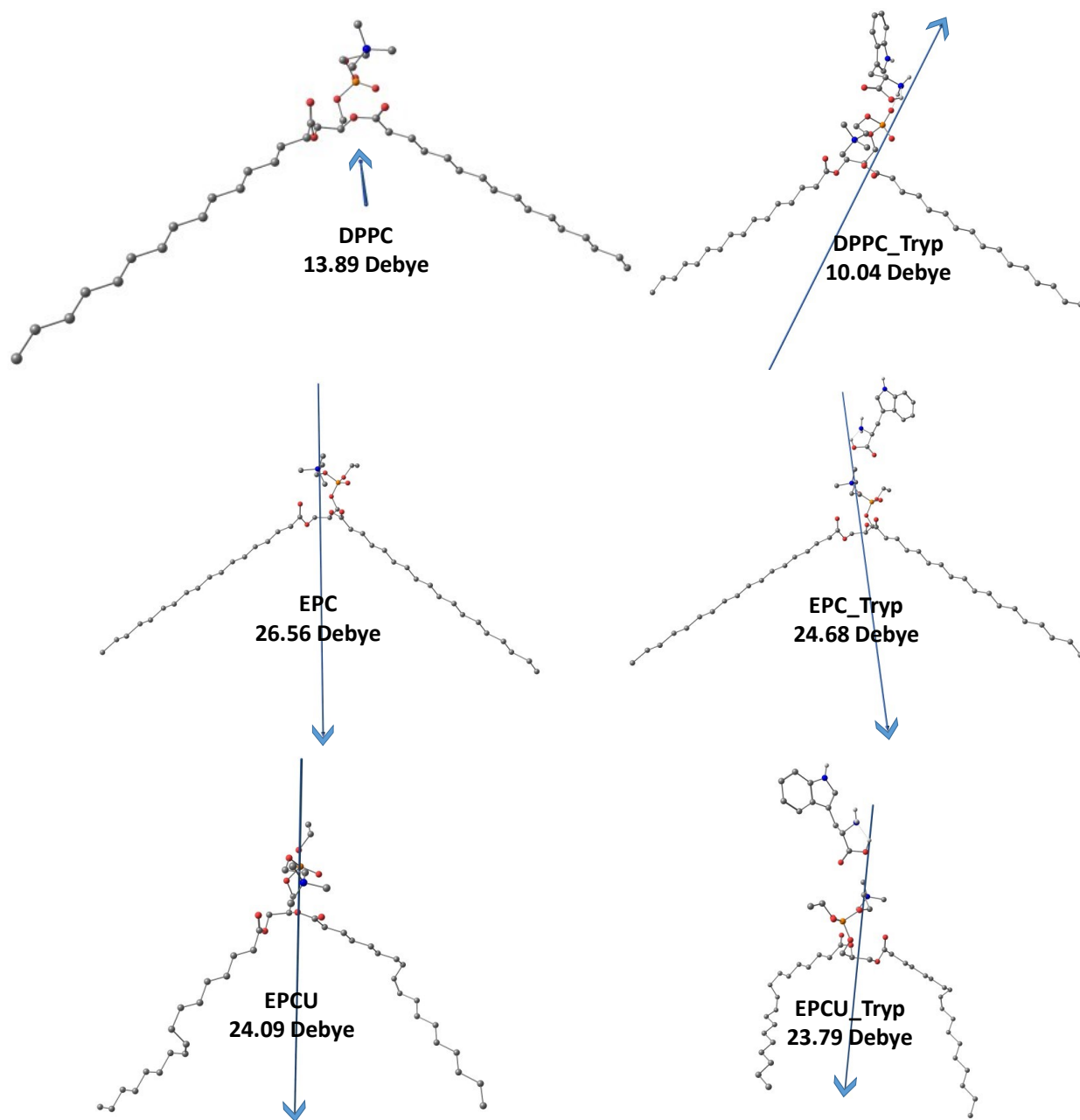


Figure S2. The dipole moment values and their directionality for all the three lipid molecules in presence and absence of tryptophan.

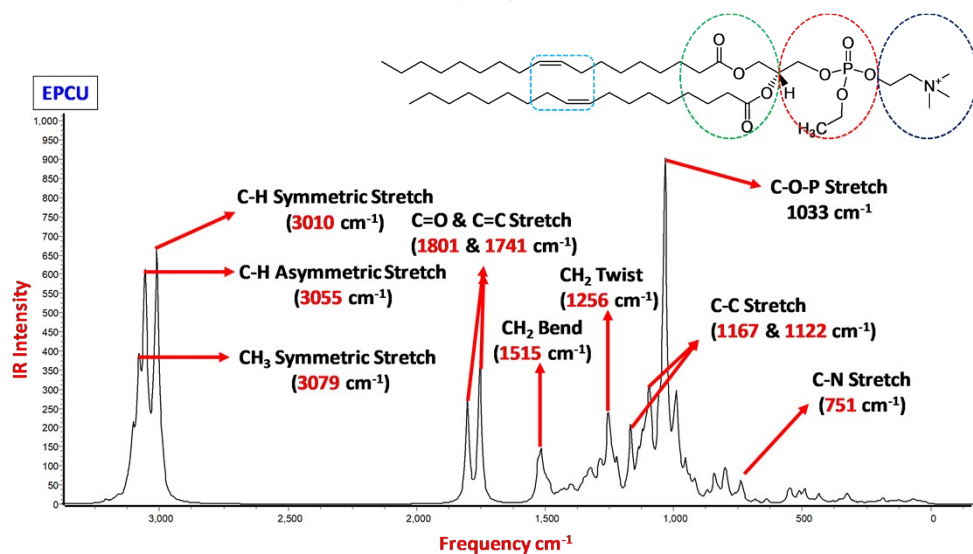
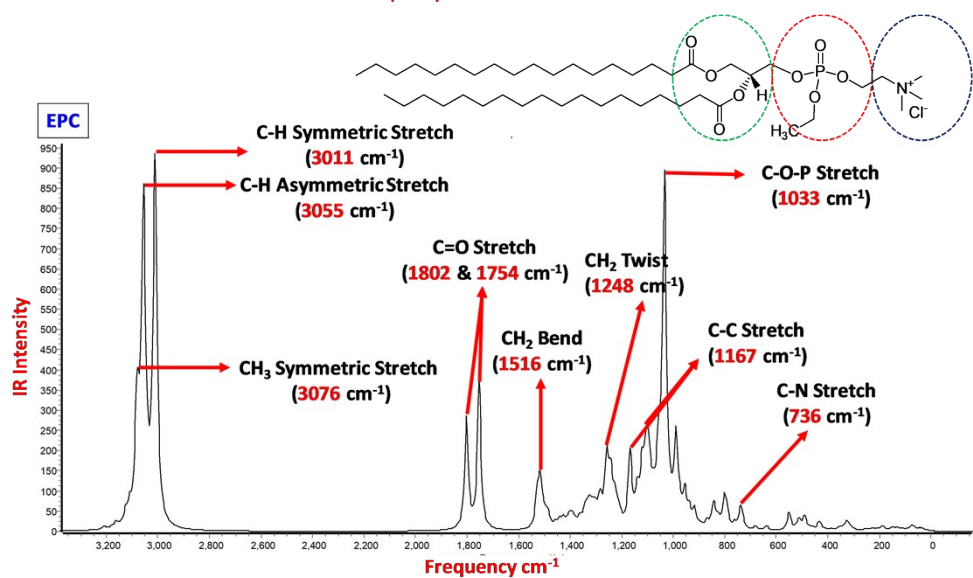
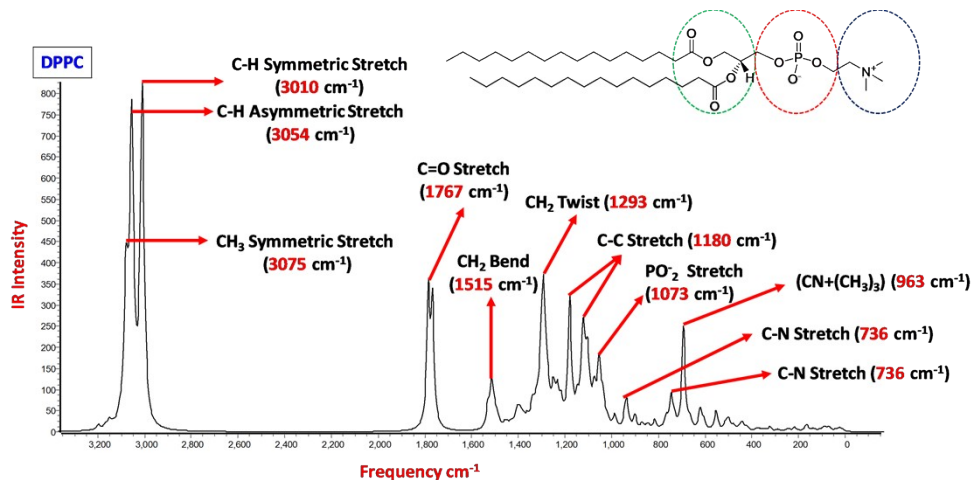


Figure S3. Calculated IR spectra and peak assignments for pristine DPPC, EPC and EPCU lipids.

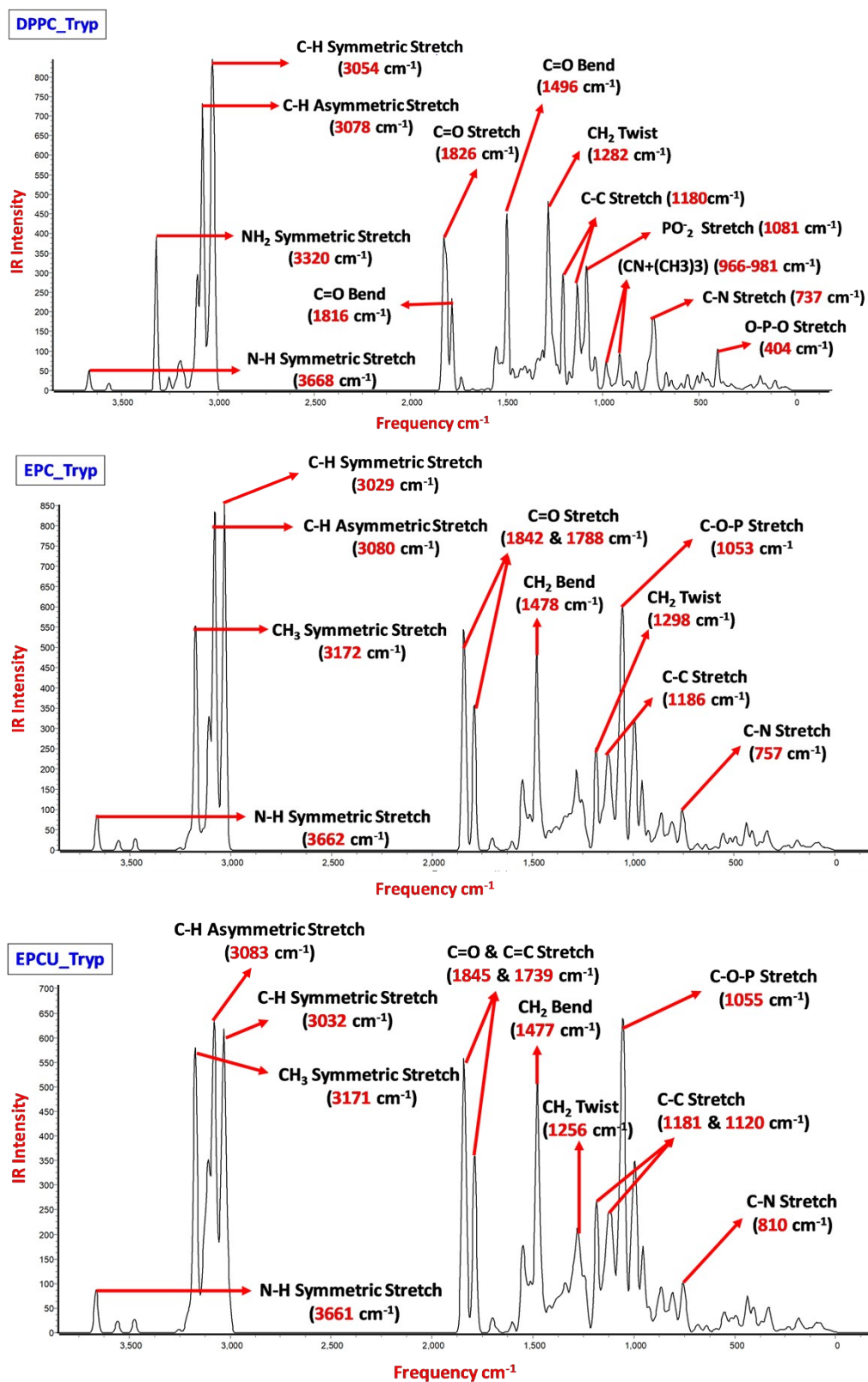


Figure S4. Calculated IR spectra and peak assignments for DPPC, EPC and EPCU lipids in interaction with Tryptophan.

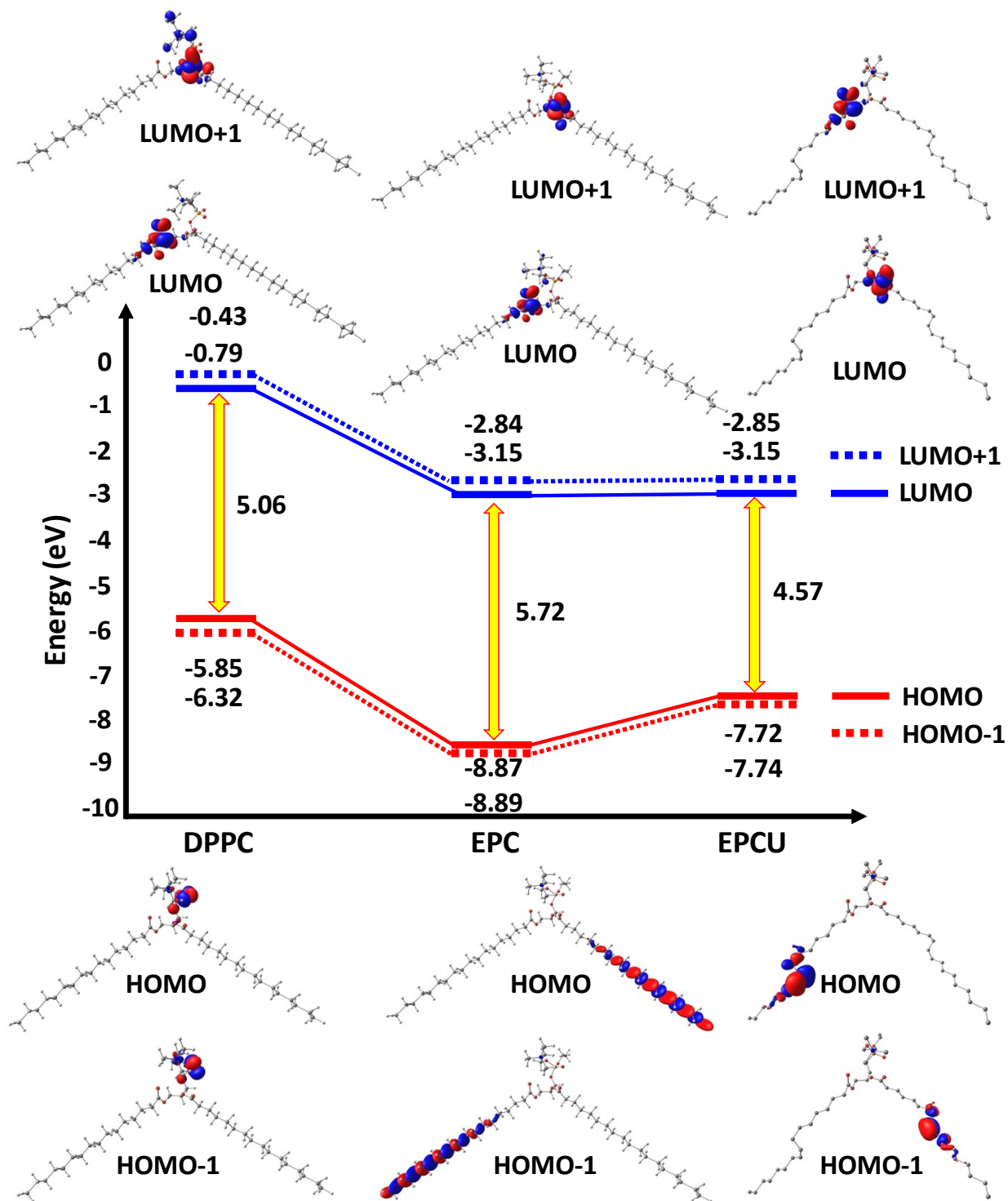


Figure S5. The frontier molecular orbitals (FMO) of pristine DPPC, EPC and EPCU lipids and their electronic band gaps.

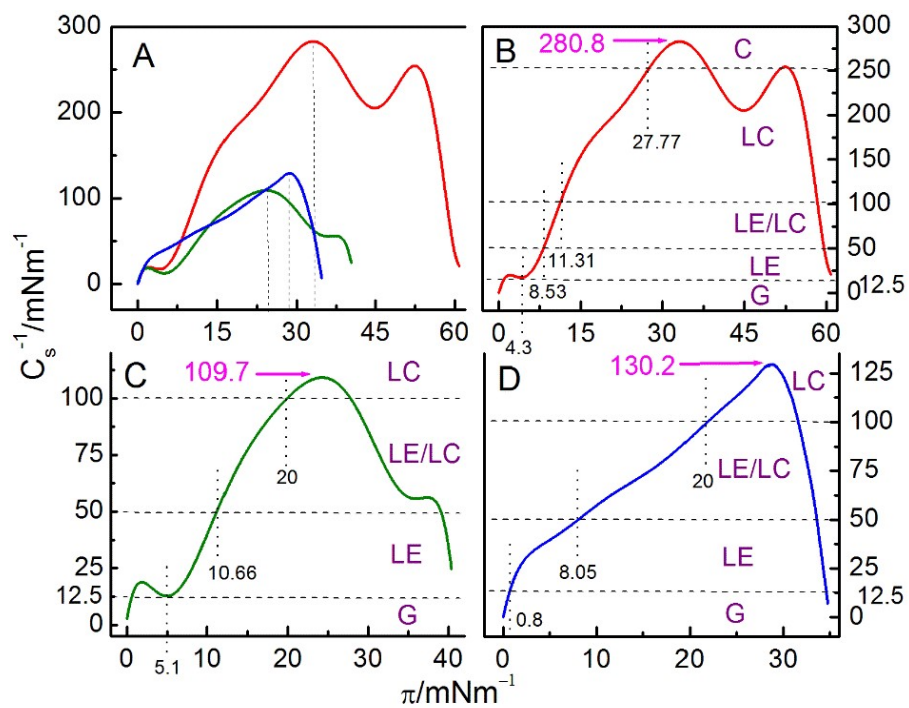


Figure S6. Compressibility coefficient (C_s^{-1}) vs. surface pressure (π) curves of pure lipids for different phases at 25 °C. Red, DPPC; green, EPC and blue, EPCU.

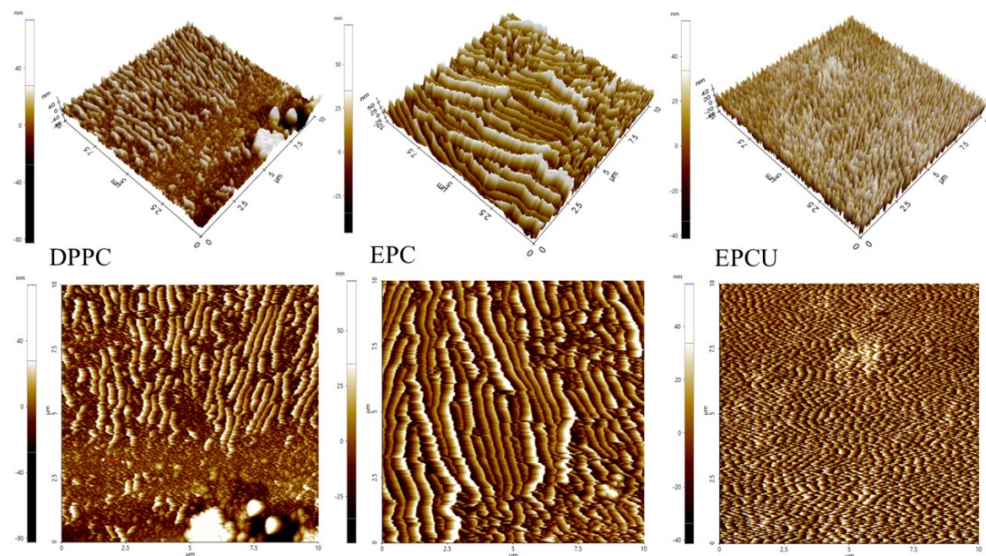
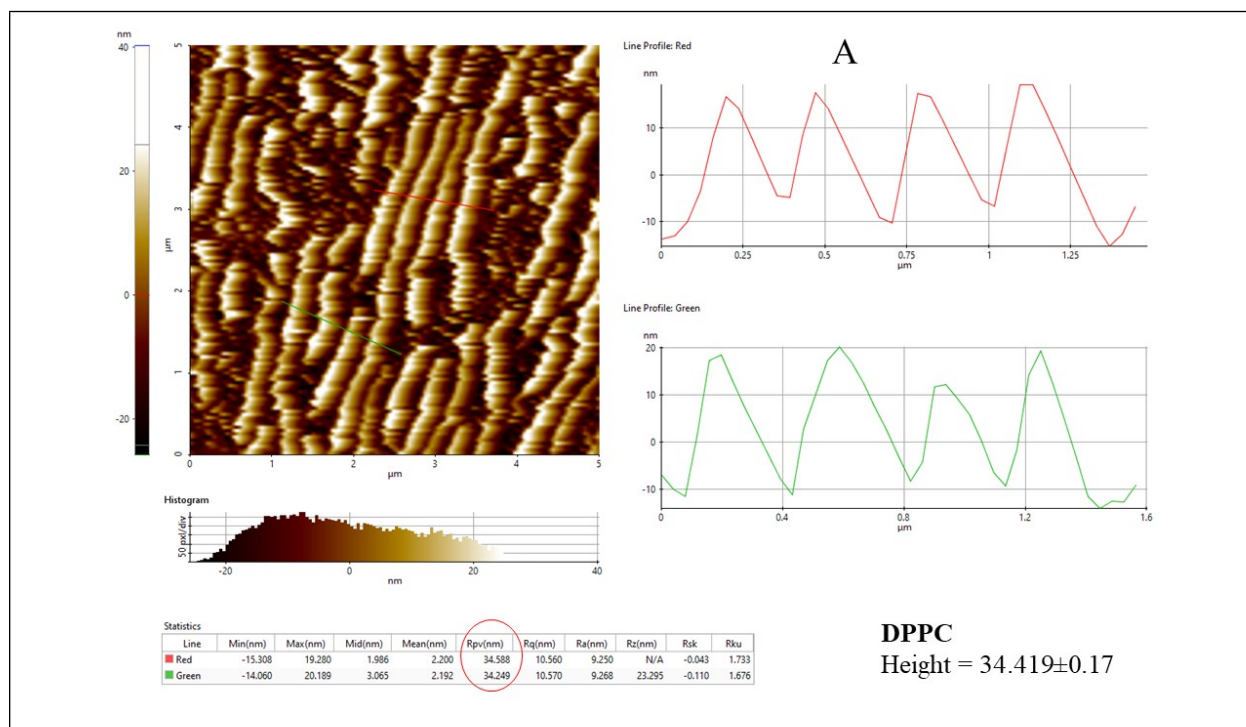


Figure S7. Condensed phase lipid lattices of different lipids (3D and 2D images). Dimension 10 x 10 μm^2 .



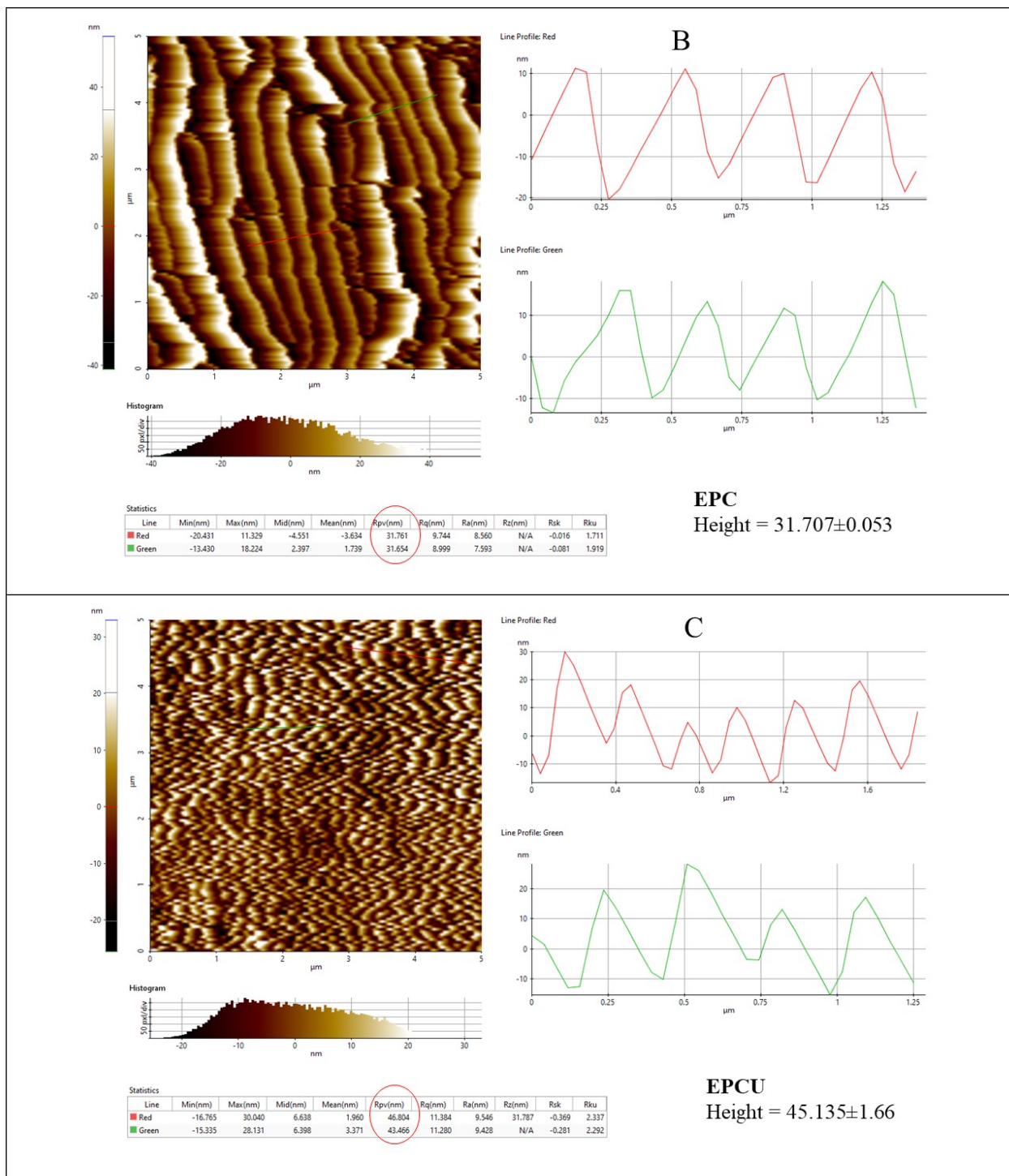


Figure S8. Average height measurements by statistical analysis of condensed phase lipid lattices in different locations of different lipids. Panel A, DPPC; Panel B, EPC and Panel C, EPCU. Dimension $5 \times 5 \mu\text{m}^2$.

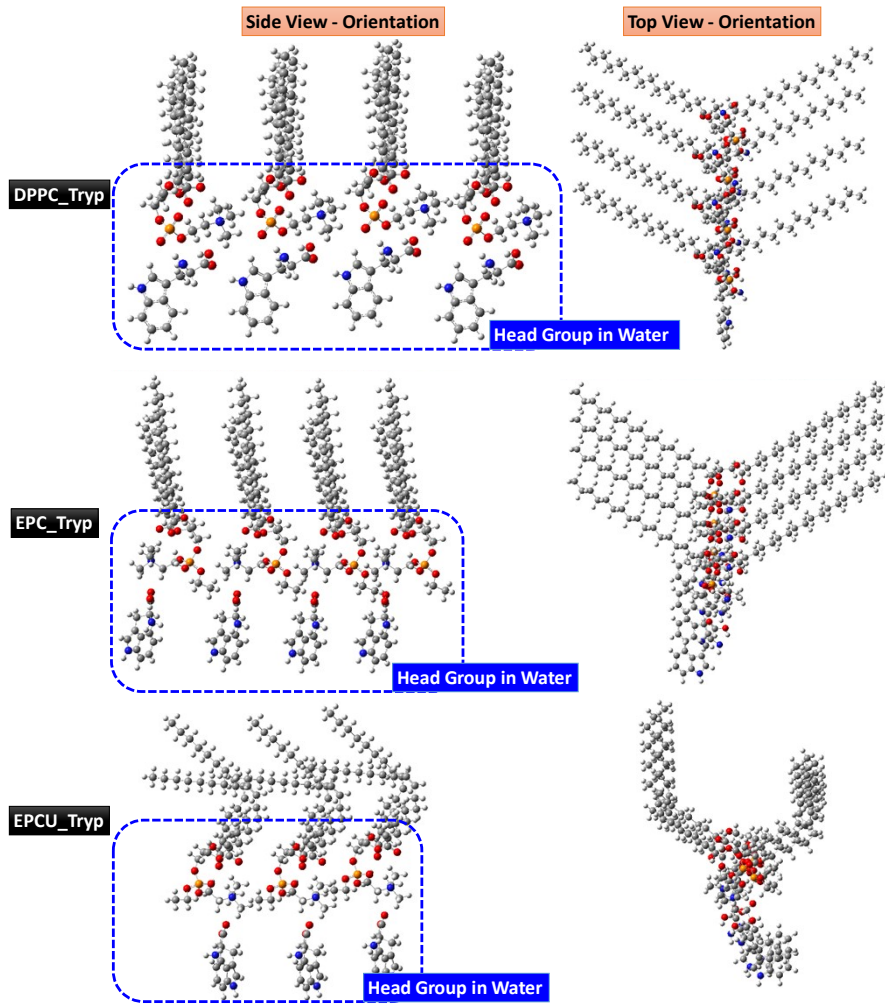


Figure S9. Probable side view and top view orientations during formation of the lipid monolayers over the tryptophan sub-phase.

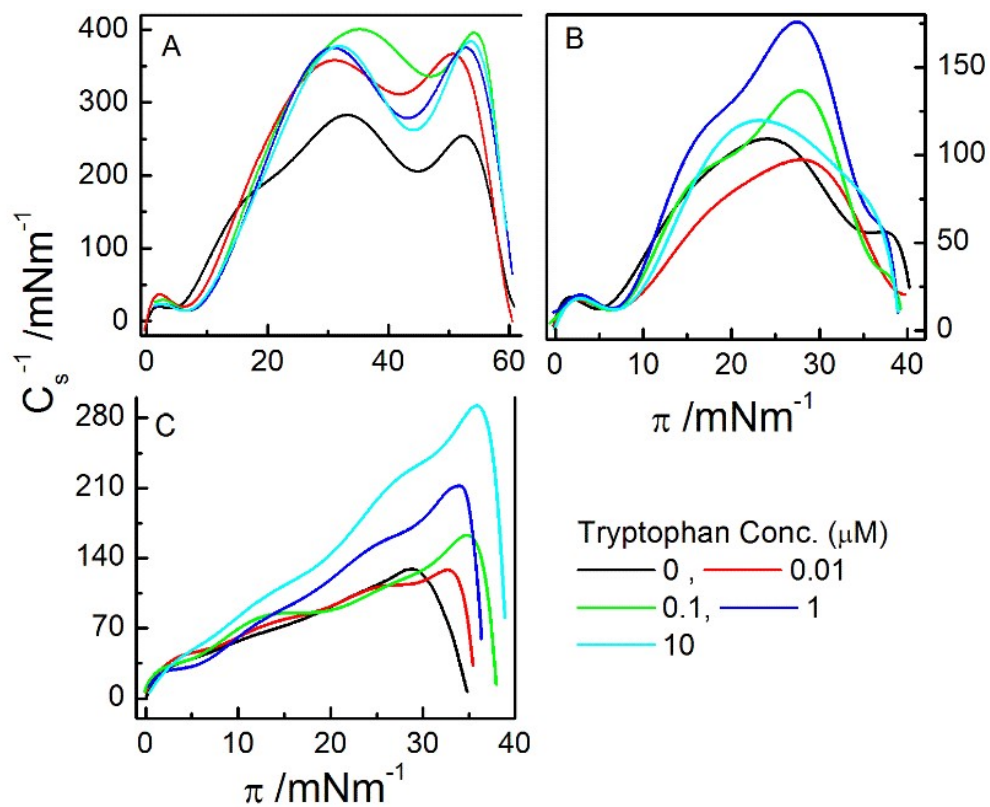


Figure S10. The compressibility coefficient -surface pressure curves of DPPC (panel A), EPC (panel B) and EPCU (panel C) lipids in presence and absence of tryptophan. Lipid concentration: 1 mM.

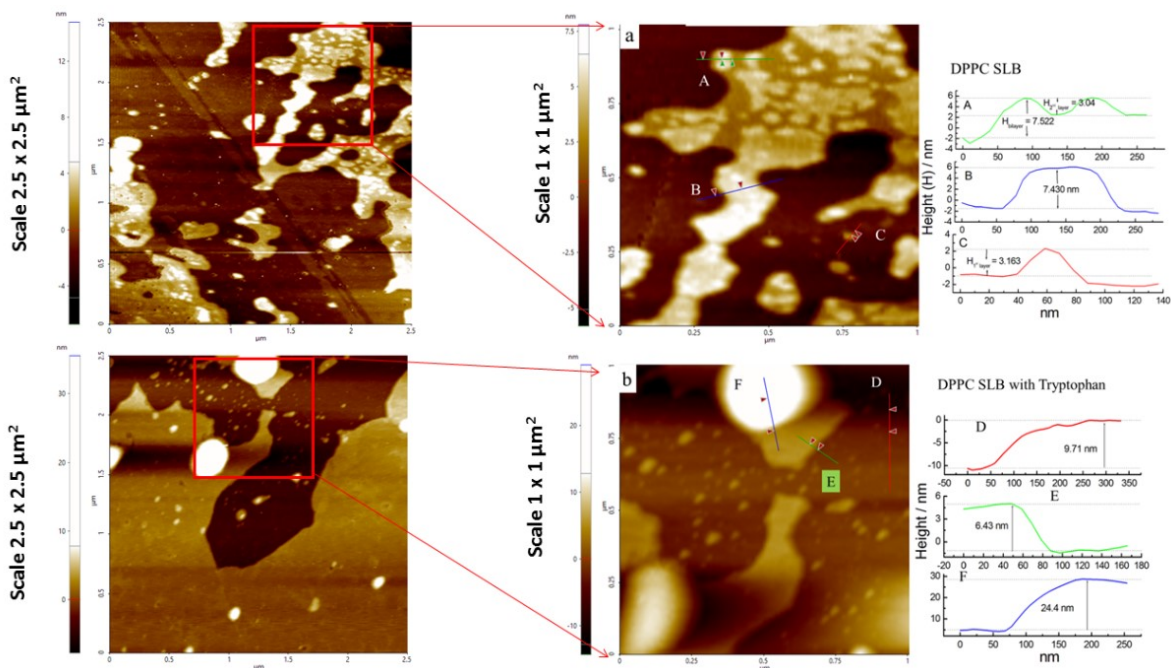


Figure S11. Supported lipid bilayers (SLB) of DPPC lipid in absence (panel a) and presence (panel b) of tryptophan on mica substrate transferred at 20 mN/m. The insets for panels described different heterogeneous phases and SLBs with varying heights. Red and Green lines are height analysis of two different regions of the same sample. Blue line is the sum of two layers. Average values with standard deviations are written in the main manuscript.

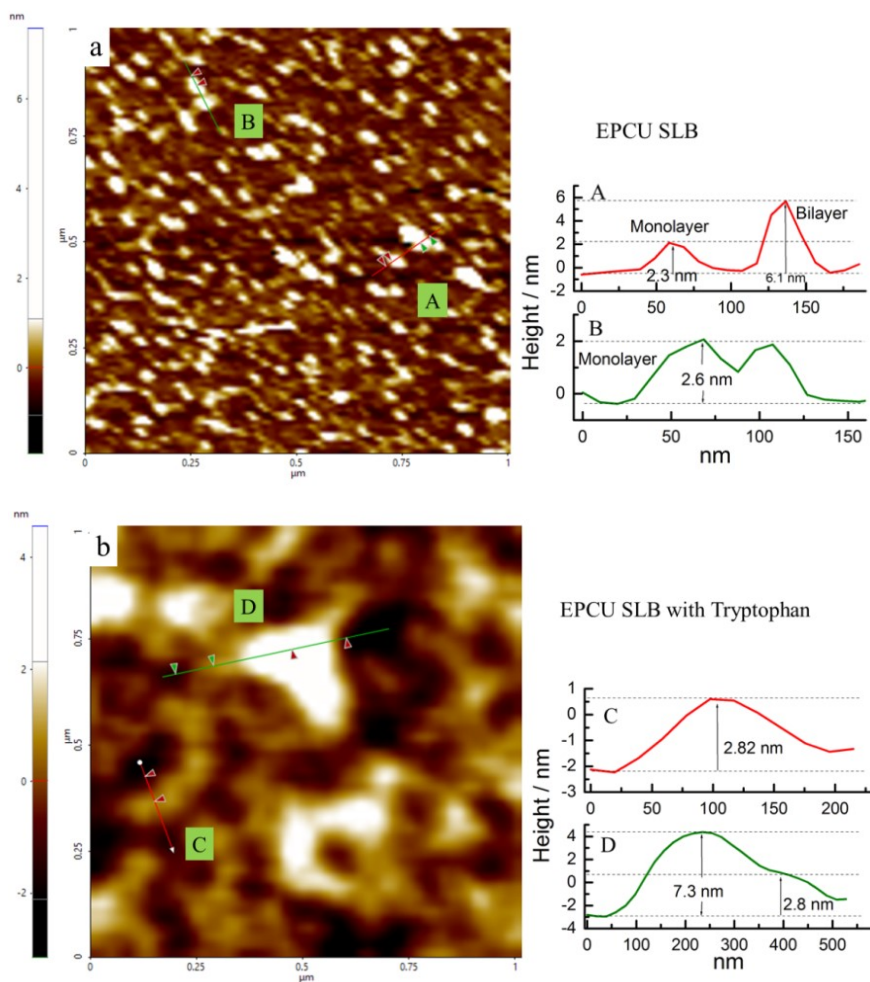


Figure S12. Supported lipid bilayers (SLB) of EPCU lipid in absence (panel a) and presence (panel b) of tryptophan on mica substrate, transferred at 20 mN/m. The insets for panels describe different heterogeneous phases and SLBs with varying heights. Red and Green lines are height analyses of two different regions of the same sample. Average values with standard deviations are written in the main manuscript.