Buckling Under Pressure: Curvature Based Lipid Segregation and Stability Modulation in Cardiolipin Containing Bilayers

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SUPPORTING INFORMATION

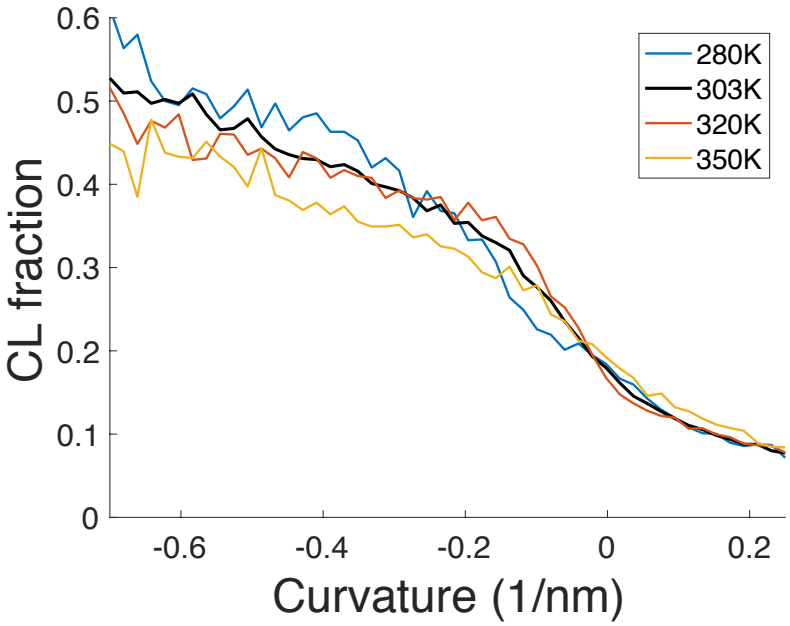

Figure S1. CL partitioning in PC/CL (4:1) system at γ=0.3 as a function of temperature. There is very little temperature dependence to the partitioning in this temperature range.

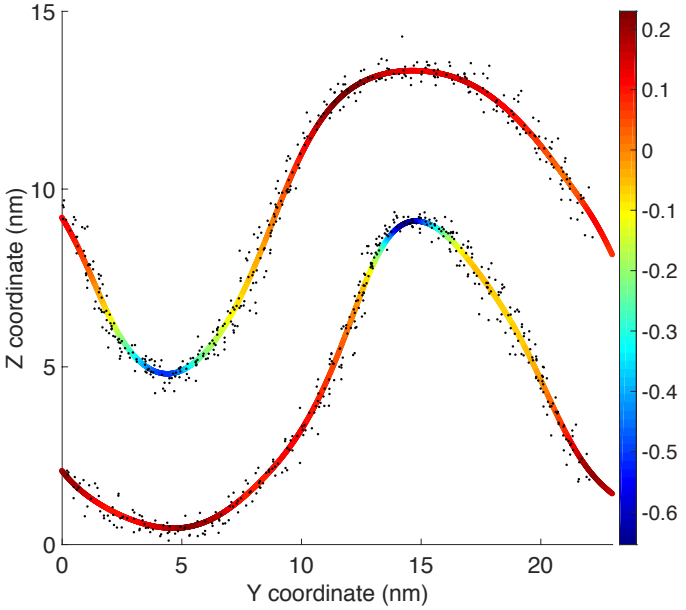

Figure S2. The spline fit (multicolored line) is overlaid with the phosphate head groups (black dots) used to generate the curve fit. The color-coding of the fit is the curvature (units of nm^{-1}), calculated from eq. 2 in main text. The phosphate positions are taken from a random snapshot of the IM^{-1} system at γ=0.3 compression.

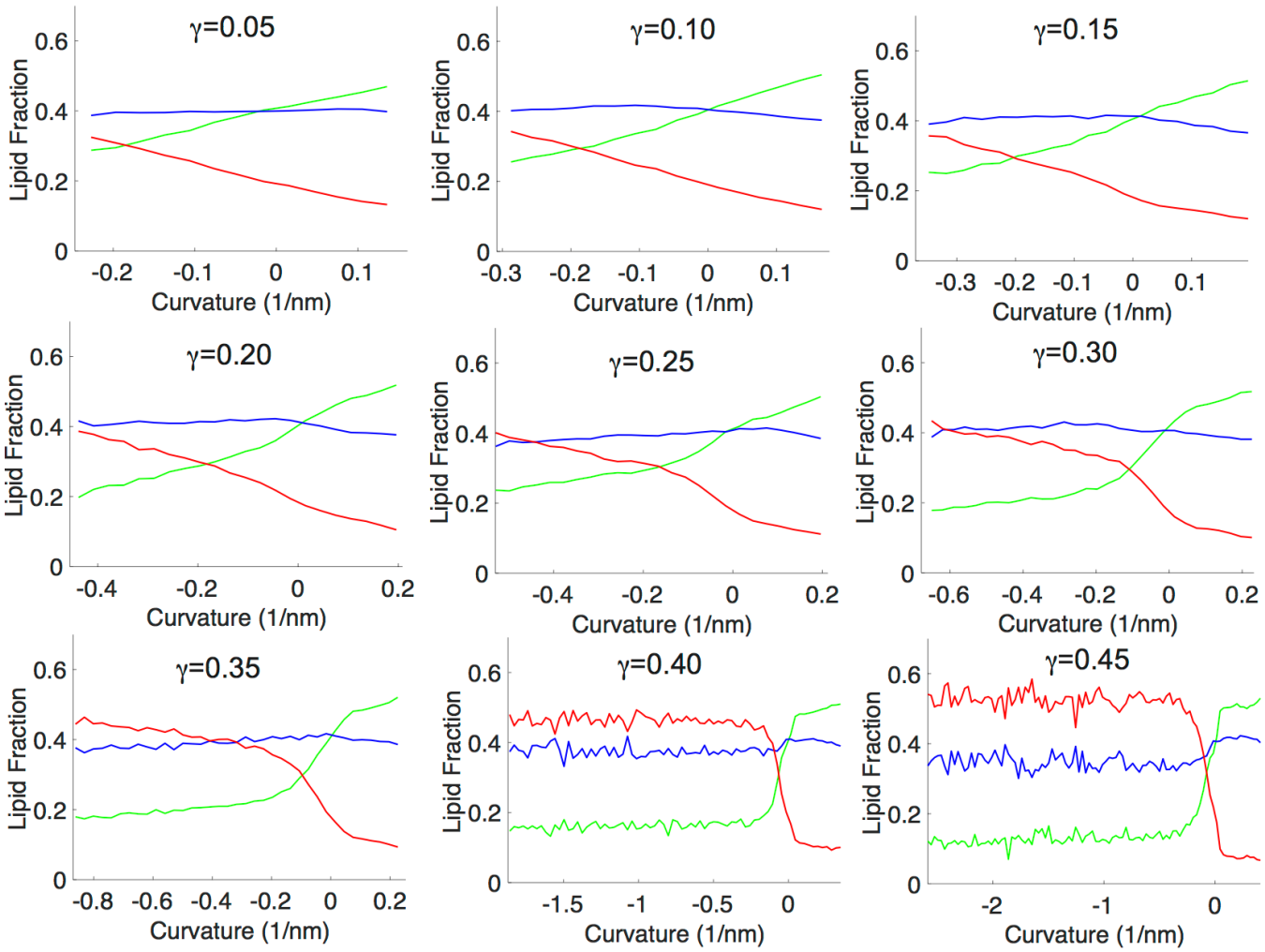

Figure S3. Lipid fractions a function of curvature for the IM^{-1} system, for γ=0.05-0.45. Line colors are the following: PC=green, PE=Blue, CL=Red. The *X*-axis range was fixed at curvatures encompassing 98% of head group curvature data points, discarding points at extreme positive and negative curvature due to poor sampling.

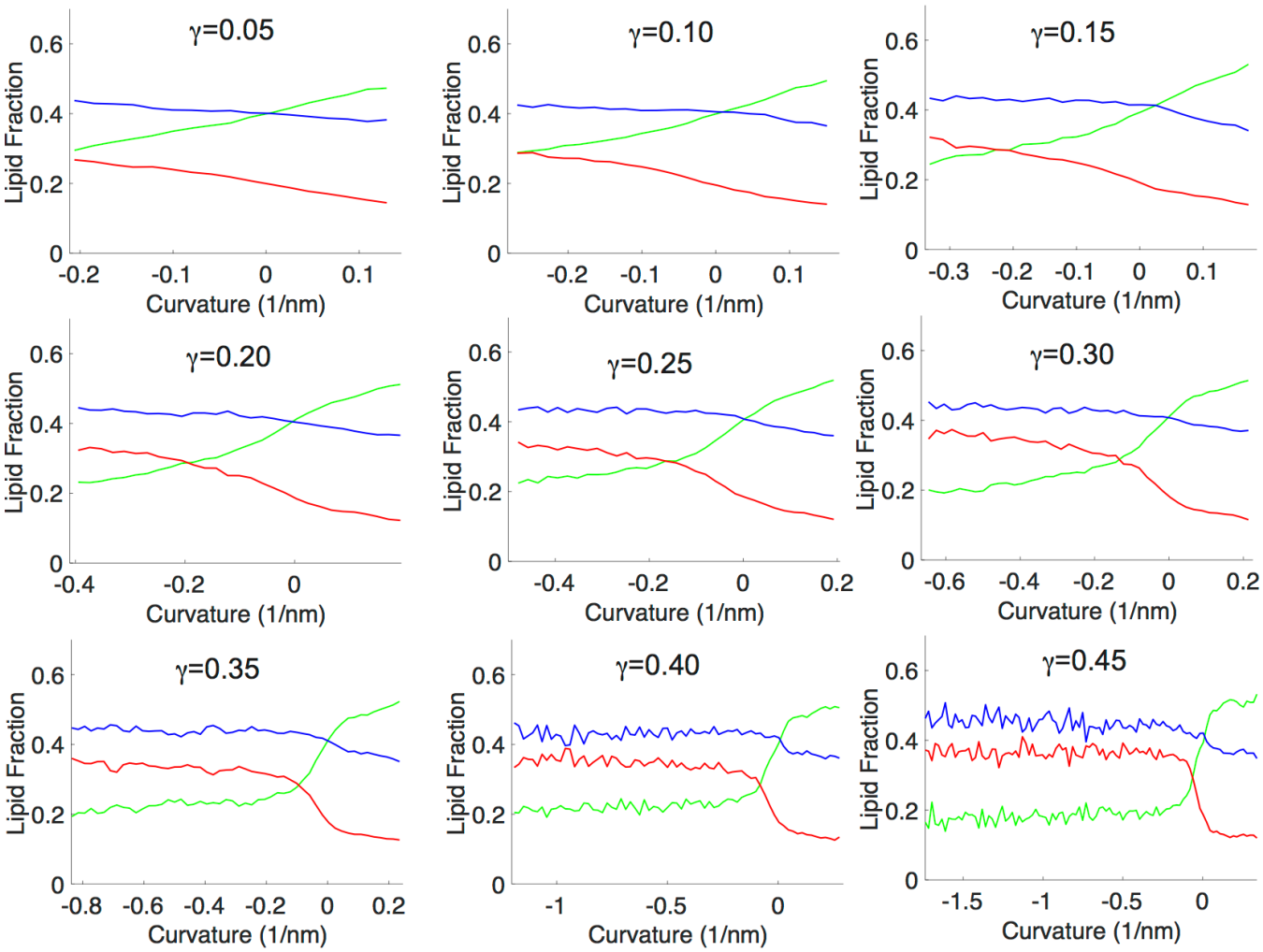

Figure S4. Lipid fractions a function of curvature for the IM^{-2} system, for γ=0.05-0.45. Line colors are the following: PC=green, PE=Blue, CL=Red. The *X*-axis range was fixed at curvatures encompassing 98% of head group curvature data points, discarding points at extreme positive and negative curvature due to poor sampling.

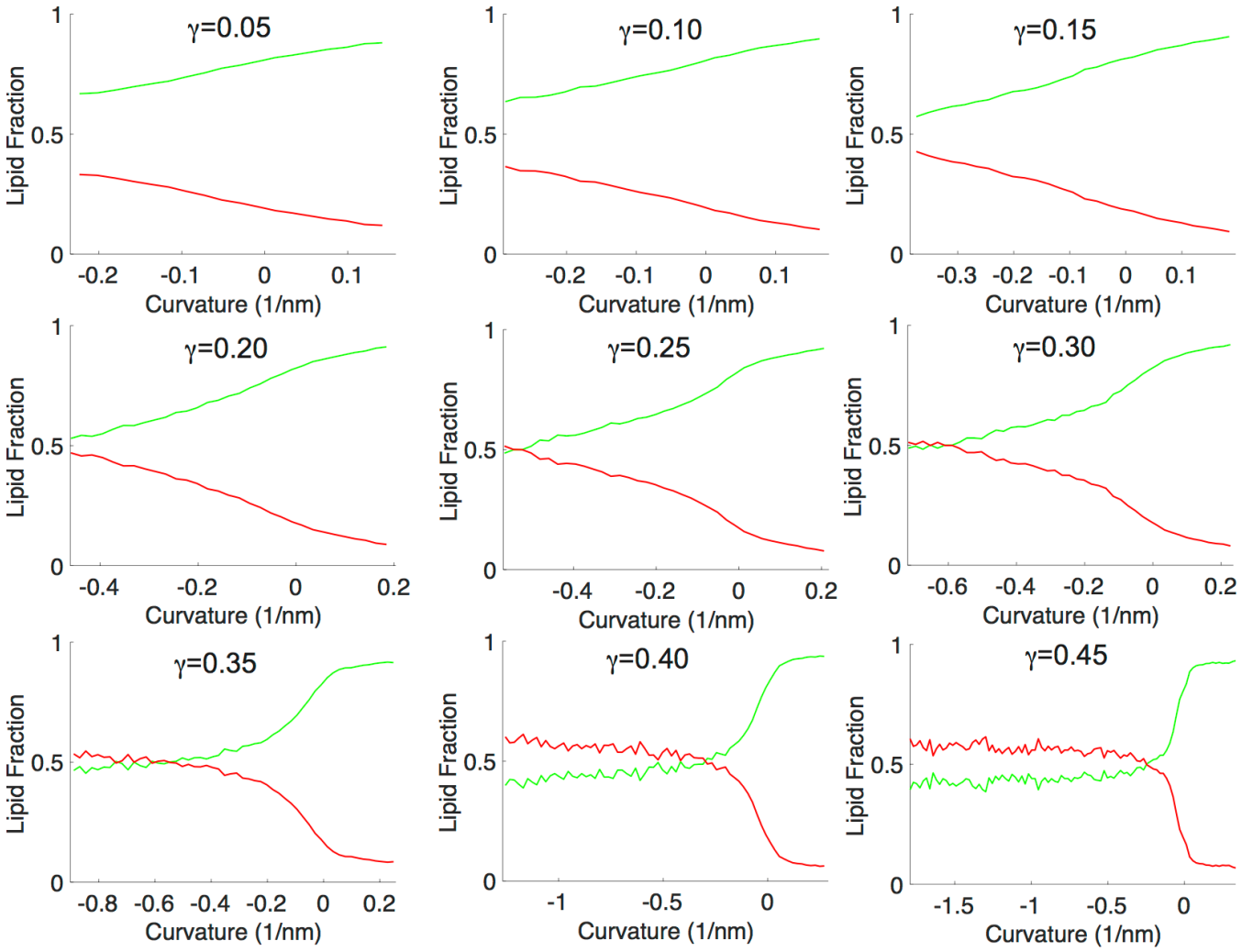

Figure S5. Lipid fractions a function of curvature for the PC/CL (4:1) system, for γ=0.05-0.45. Line colors are the following: PC=green, CL=Red. The *X*-axis s range was fixed at curvatures encompassing 98% of head group curvature data points, discarding points at extreme positive and negative curvature due to poor sampling.

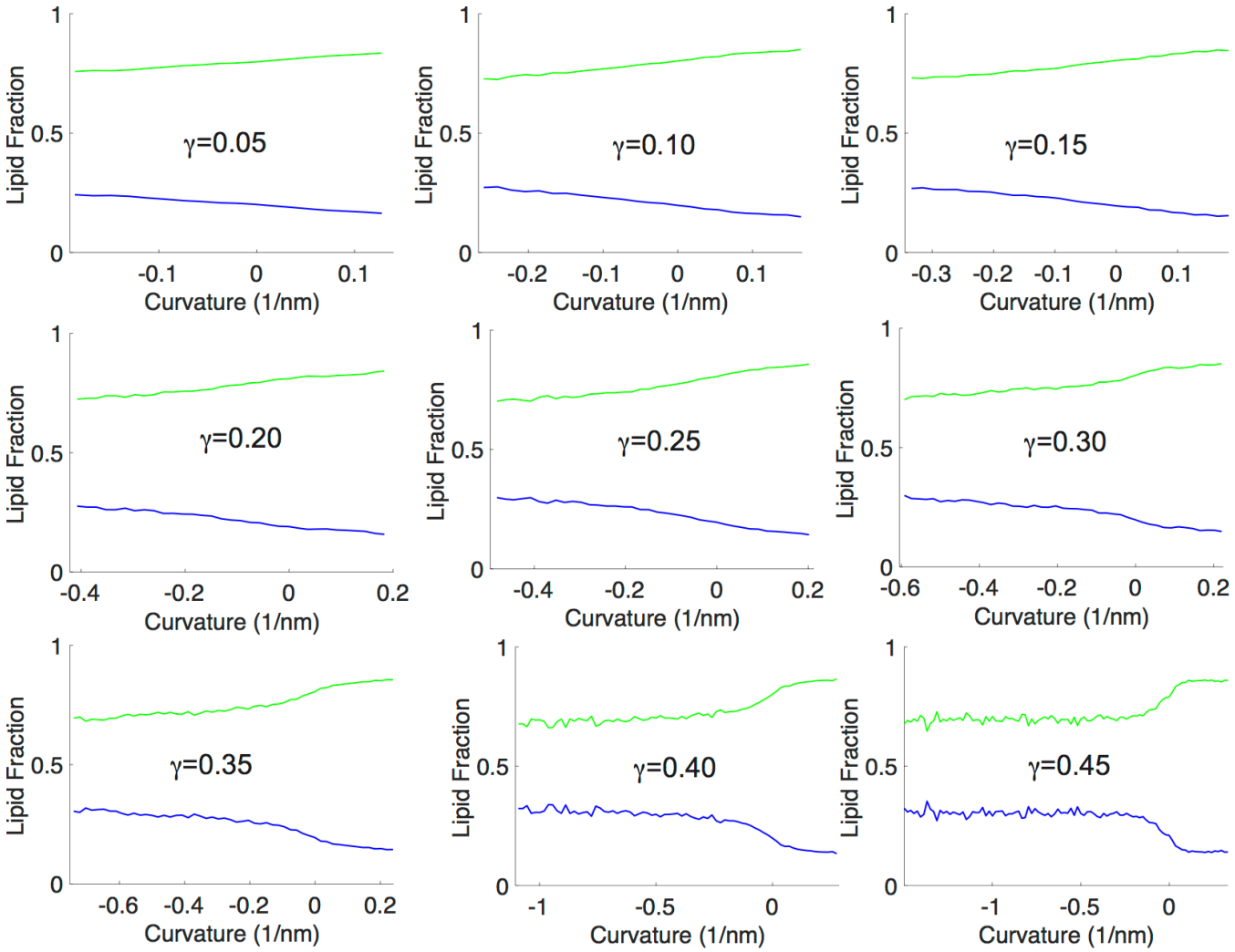

Figure S6. Lipid fractions a function of curvature for the PC/PE (4:1) system, for γ=0.05-0.45. Line colors are the following: PC=green, PE=Blue. The *X*-axis range was fixed at curvatures encompassing 98% of head group curvature data points, discarding points at extreme positive and negative curvature due to poor sampling.

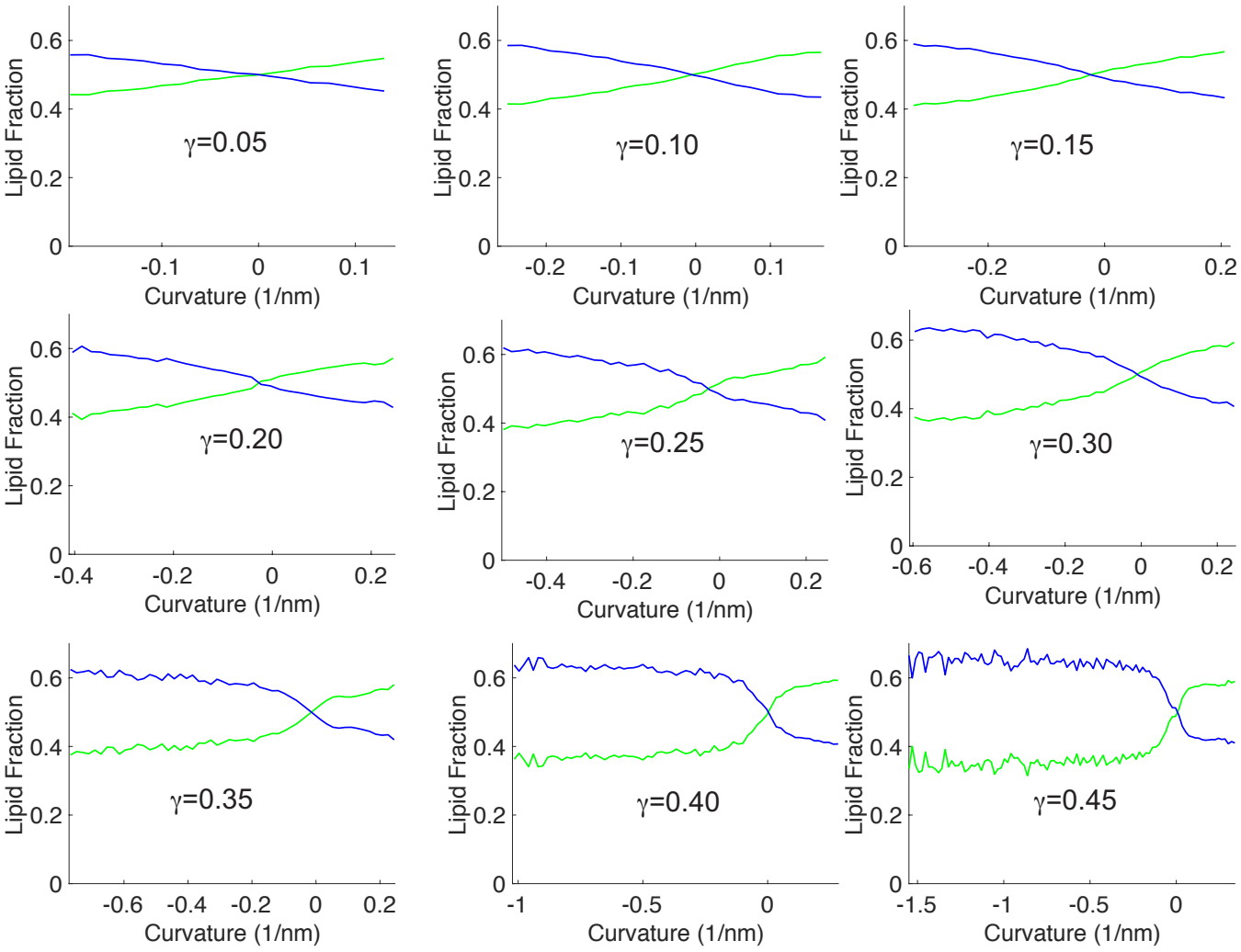

Figure S7. Lipid fractions a function of curvature for the PC/PE (1:1) system, for γ=0.05-0.45. Line colors are the following: PC=green, PE=Blue. The *X*-axis range was fixed at curvatures encompassing 98% of head group curvature data points, discarding points at extreme positive and negative curvature due to poor sampling.

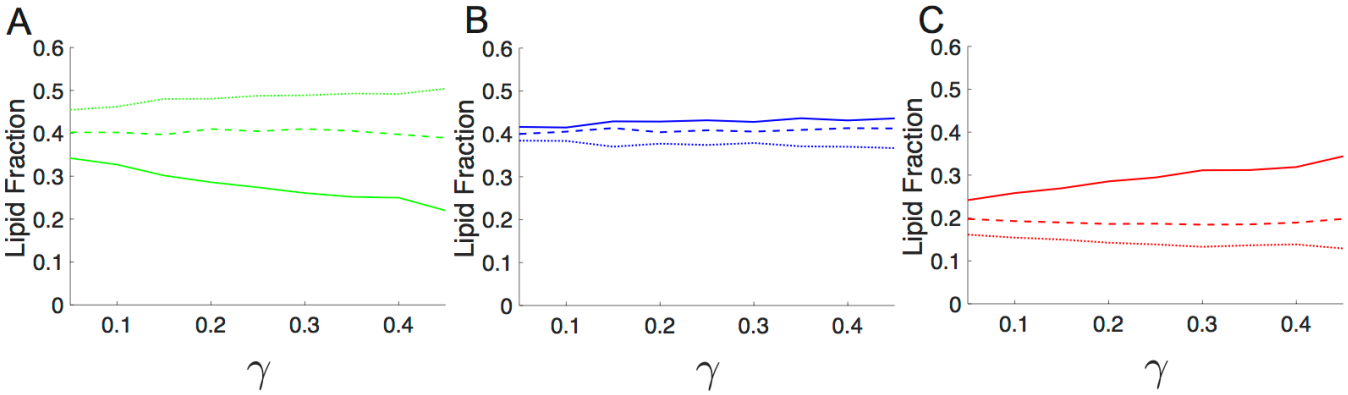

Figure S8. Lipid fractions as a function of compressional strain for the IM^{-2} system. The lipid fraction of PC (A), PE (B) and CL^{-2} (C) are shown. The solid lines represent the negative curvature region, the dashed lines represent the neutral curvature regions, and the dotted lines represent the positively curved regions. The curvature regions were defined as follows: negative: $C < -0.05$; neutral: $-0.05 \leq C \leq 0.05$; positive: $C > 0.05$, where curvature units are nm^{-1}.

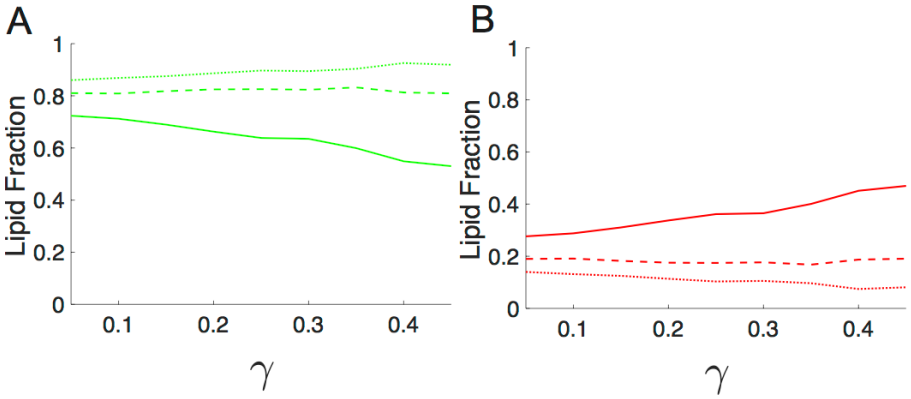

Figure S9. Lipid fractions as a function of compressional strain for the PC/CL (4:1) system. The lipid fraction of PC (A), and CL^{-1} (B) are shown. The solid lines represent the negative curvature regions, the dashed lines represent the neutral curvature regions, and the dotted lines represent the positively curved regions. The curvature regions were defined as follows: negative: $C < -0.05$; neutral: $-0.05 \leq C \leq 0.05$; positive: $C > 0.05$, where curvature units are nm^{-1}.

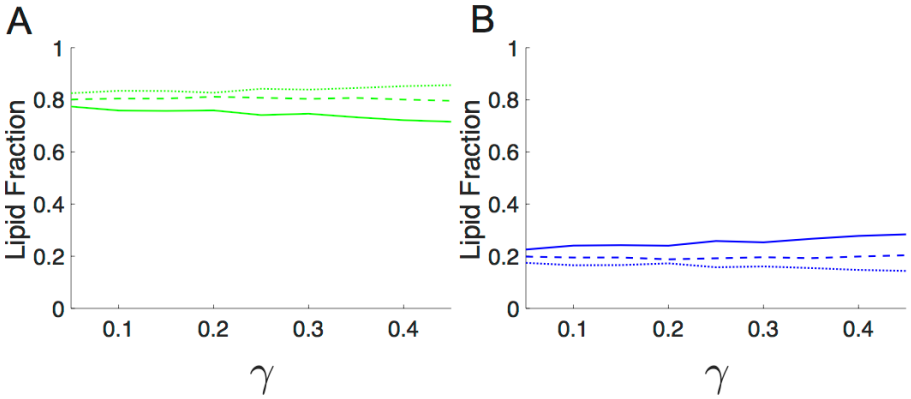

Figure S10. Lipid fractions as a function of compressional strain for the PC/PE (4:1) system. The lipid fraction of PC (A), and PE (B) are shown. The solid lines represent the negative curvature regions, the dashed lines represent the neutral curvature regions, and the dotted lines represent the positively curved regions. The curvature regions were defined as follows: negative: $C < -0.05$; neutral: $-0.05 \leq C \leq 0.05$; positive: $C > 0.05$, where curvature units are nm^{-1}.

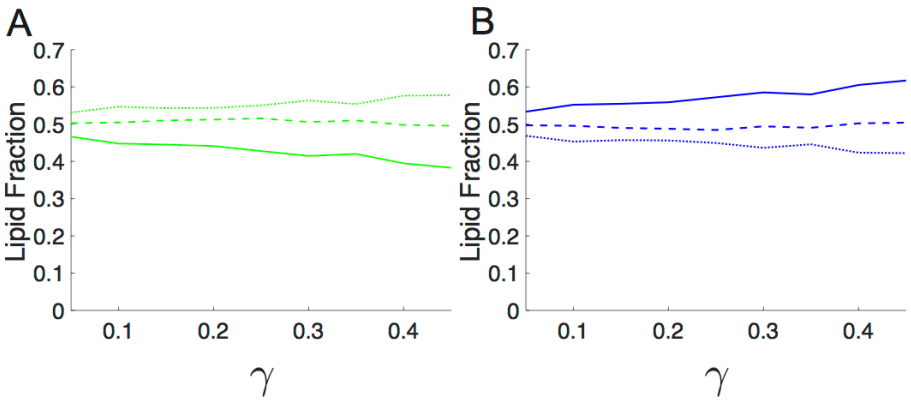

Figure S11. Lipid fractions as a function of compressional strain for the PC/PE (1:1) system. The lipid fraction of PC (A), and PE (B) are shown. The solid lines represent the negative curvature regions, the dashed lines represent the neutral curvature regions, and the dotted lines represent the positively curved regions. The curvature regions were defined as follows: negative: $C < -0.05$; neutral: $-0.05 \leq C \leq 0.05$; positive: $C > 0.05$, where curvature units are nm^{-1}.

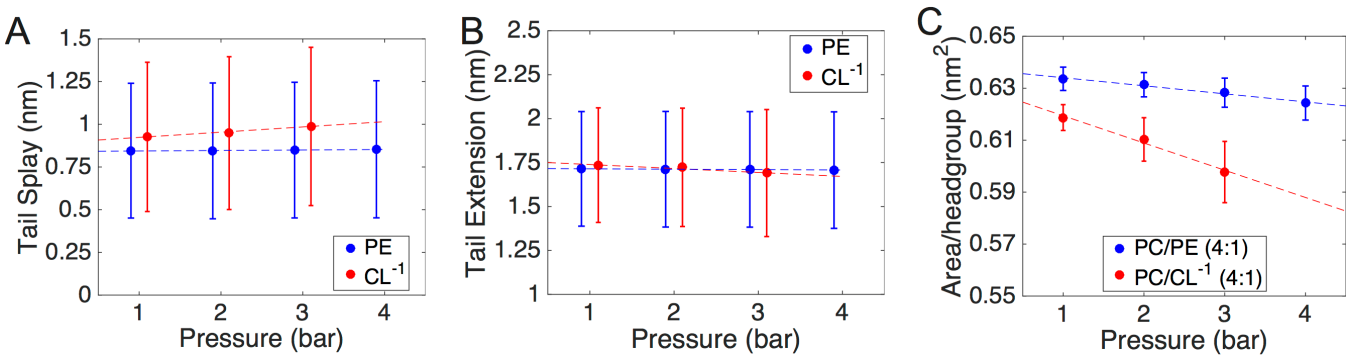

Figure S12. Molecular geometry of PE and CL in PC/PE (4:1) and PC/CL-1 (4:1) systems, respectively. A) The lateral splay of the lipids tails. B) The normal direction extension of the lipid tails. C) The area per lipid head group, each CL is considered as having two head groups. The pressure is the applied Y-dimension pressure.