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Aggregation of chlorophylls on plant thylakoid membranes using coarse-grained simulations

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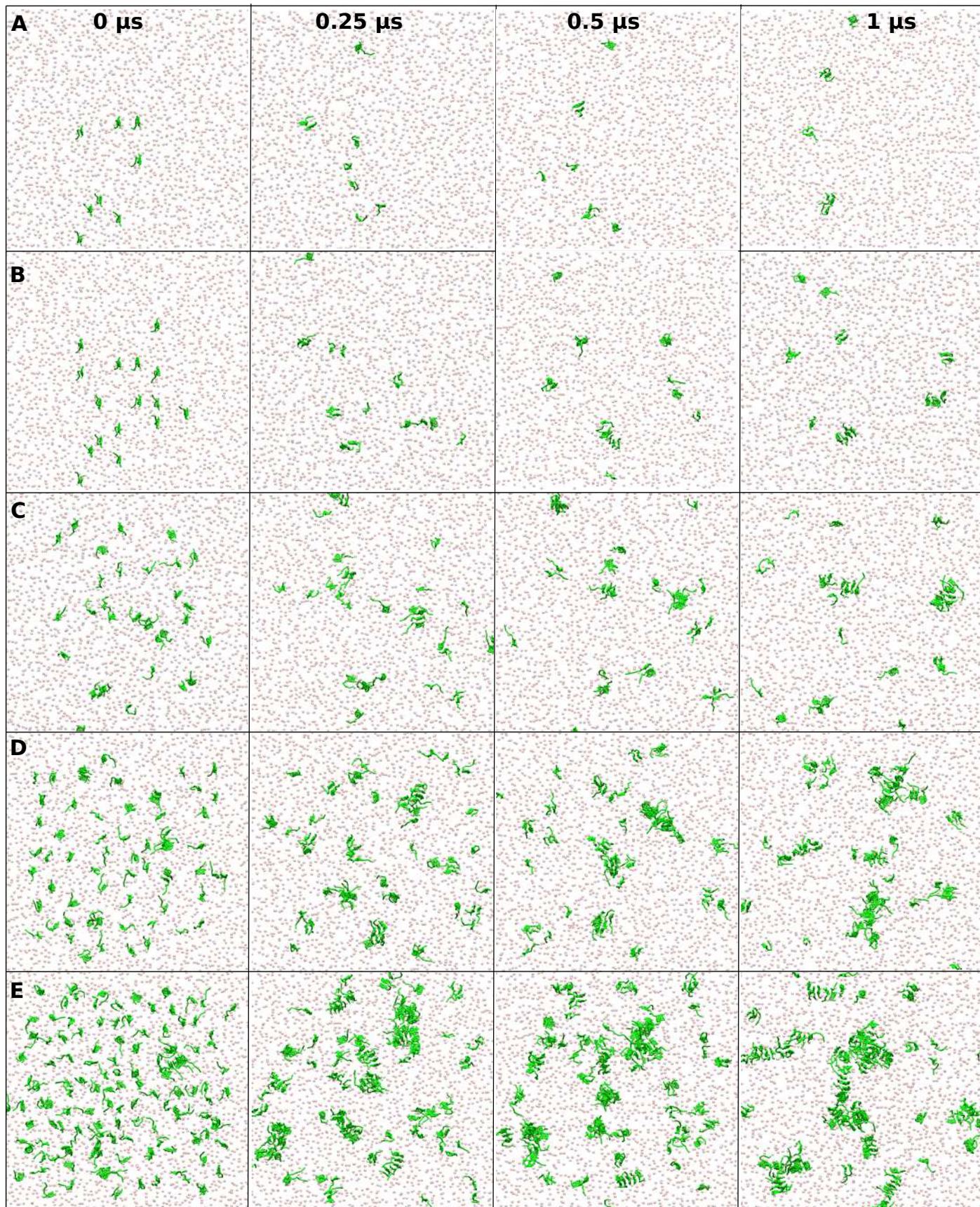


Fig. S1 Top view of the bilayer heads in presence of CLA to represent the time evolution of the aggregation of CLA molecules at $0\mu s$, $0.25\mu s$, $0.5\mu s$ and $1\mu s$ for (A) 8 (B) 16 (C) 32 (D) 64 (E) 128 CLA. Color code: green: CLA, pink: lipid heads. Other components are not shown for the sake of clarity.

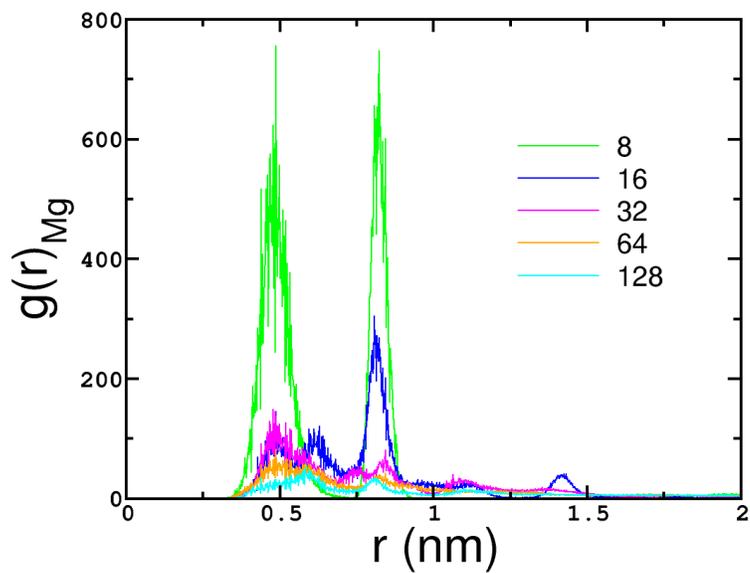


Fig. S2 Radial distribution function of central Mg atom (P5N) of CLA.

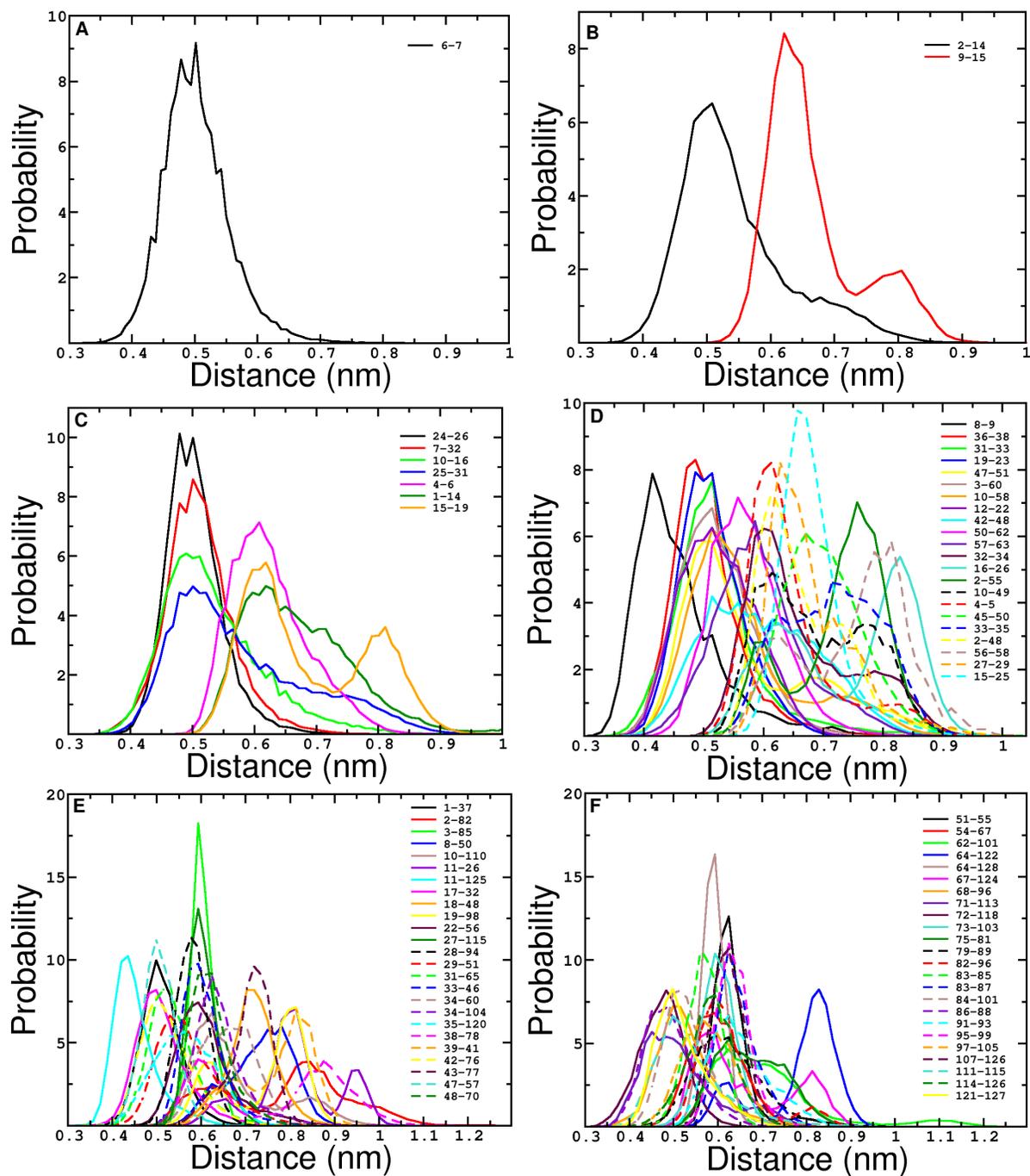


Fig. S3 Distance distribution of all possible dimer pairs for (A) 8 [1], (B) 16 [2], (C) 32 [7], (D) 64 [22], and (E),(F) 128 CLA [49]. The number in "[]" represents the total number of dimers in respective bilayers. Since the total number of dimers for the bilayer with 128 CLA is 49 and very high, dimers are shown into two figures (E) and (F) due to the sake of clarity. The legends in the figure refer to the residue ID of the CLA dimers.

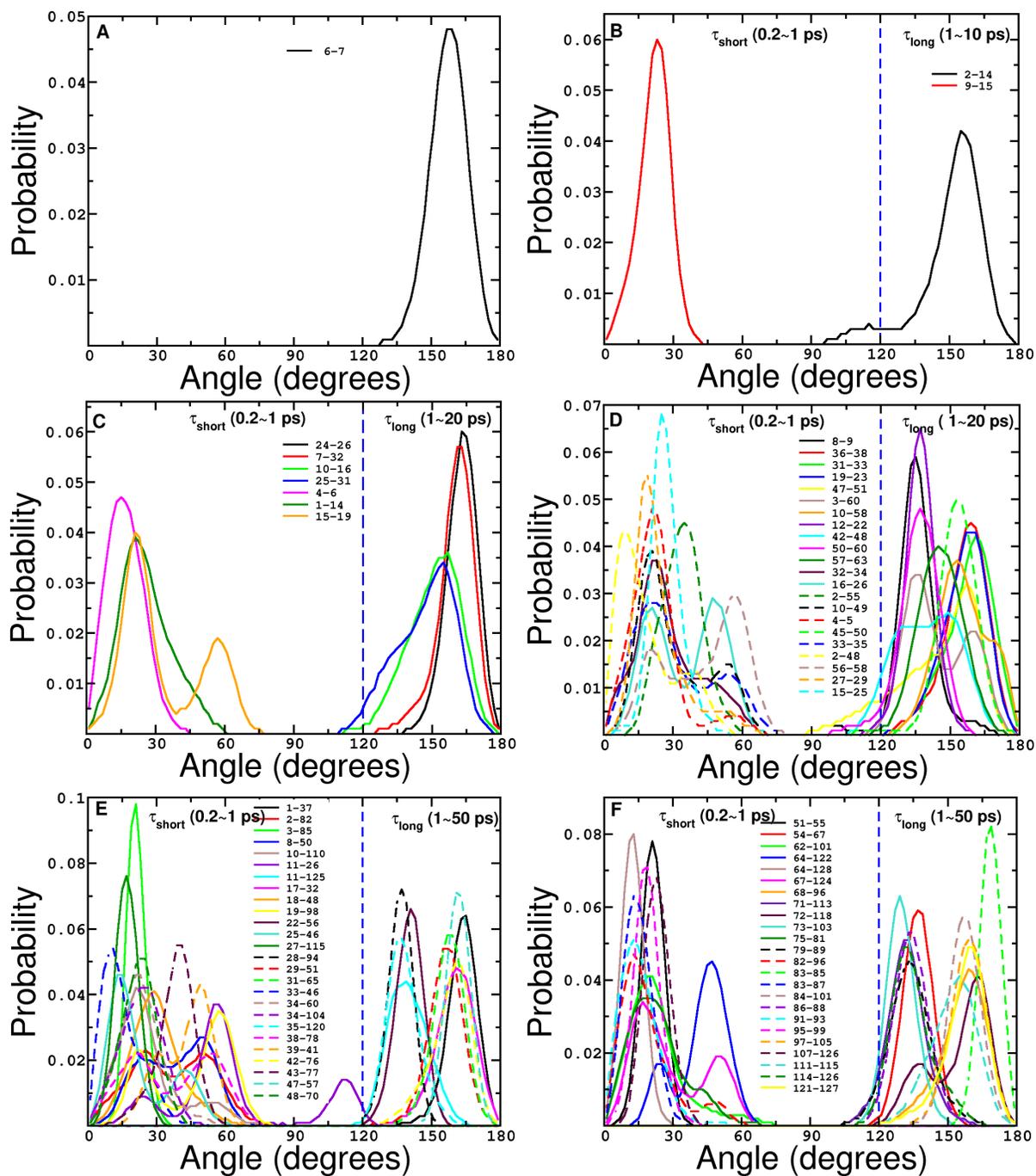


Fig. S4 Angle distribution of all possible dimer pairs for (A) 8, (B) 16, (C) 32, (D) 64, and (E),(F) 128 CLA

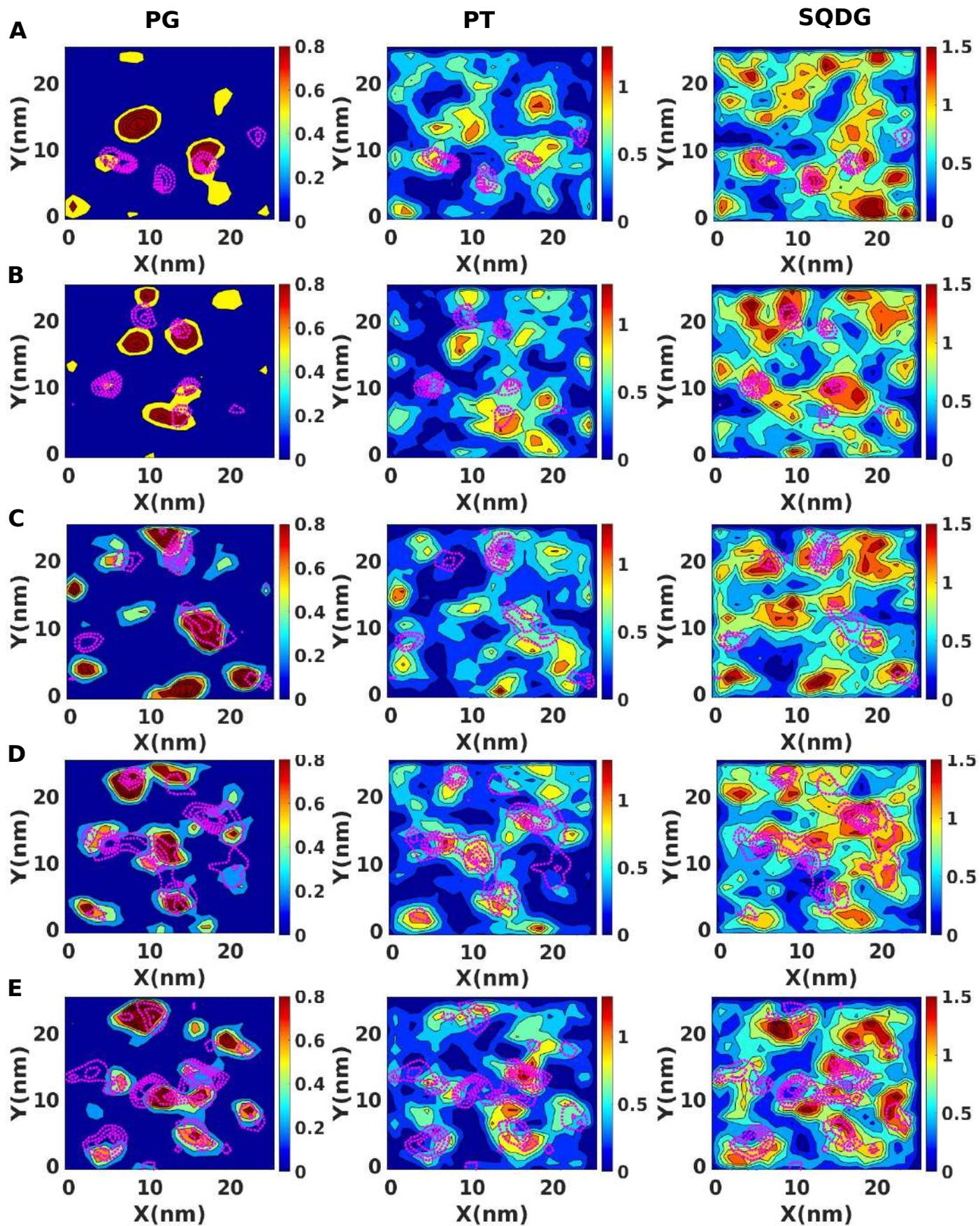


Fig. S5 The density of PG, PT, and SQDG lipids around CLA for (A) 8, (B) 16, (C) 32, (D) 64, and (E) 128 CLA lipid bilayer. The density of CLA represents in a magenta contour line.

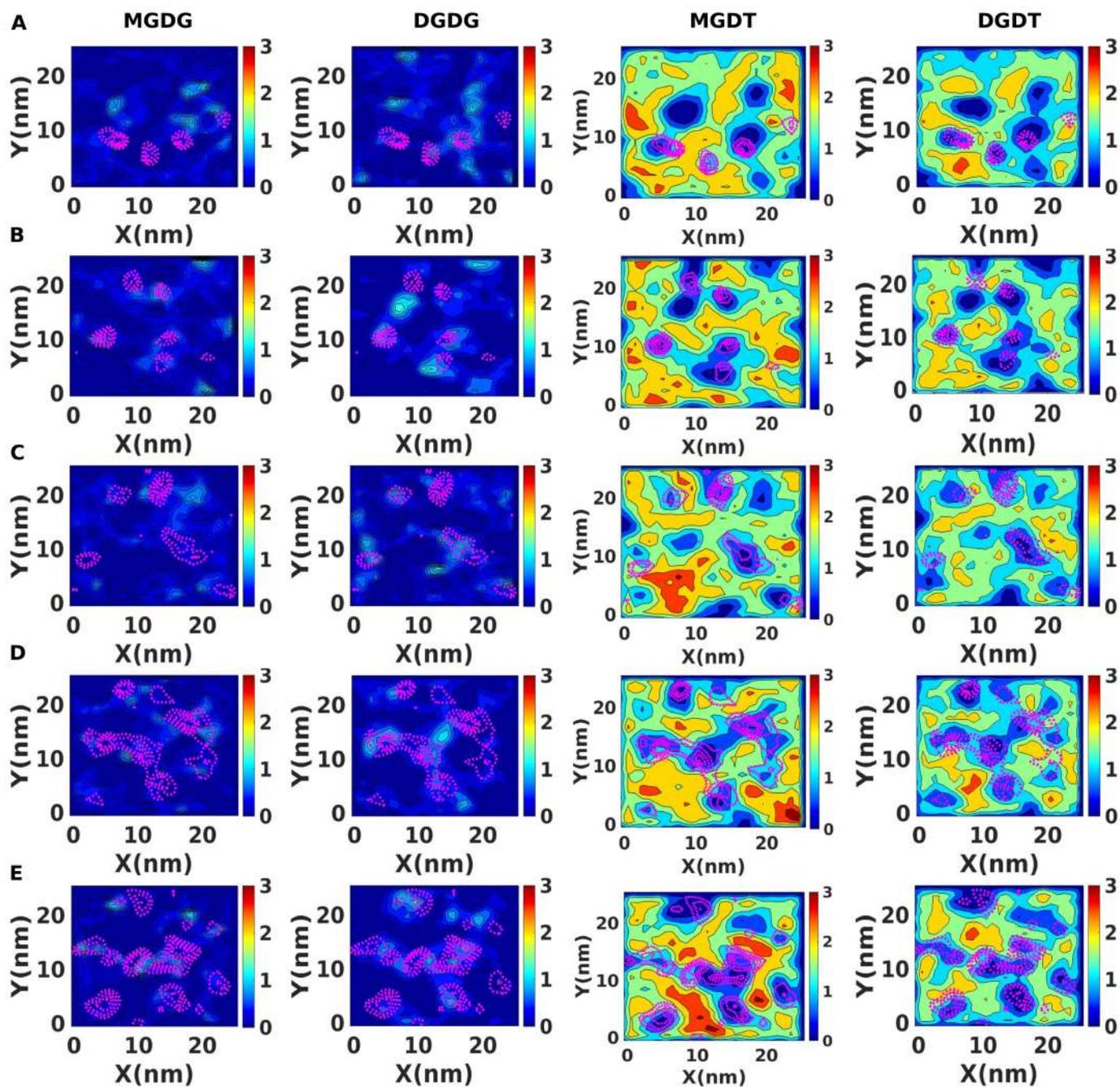


Fig. S6 The density of MGDG, DGDG, MGD, and DGD lipids for (A) 8, (B) 16, (C) 32, (D) 64, and (E) 128 CLA lipid bilayer. The density of CLA represents in a magenta contour line.

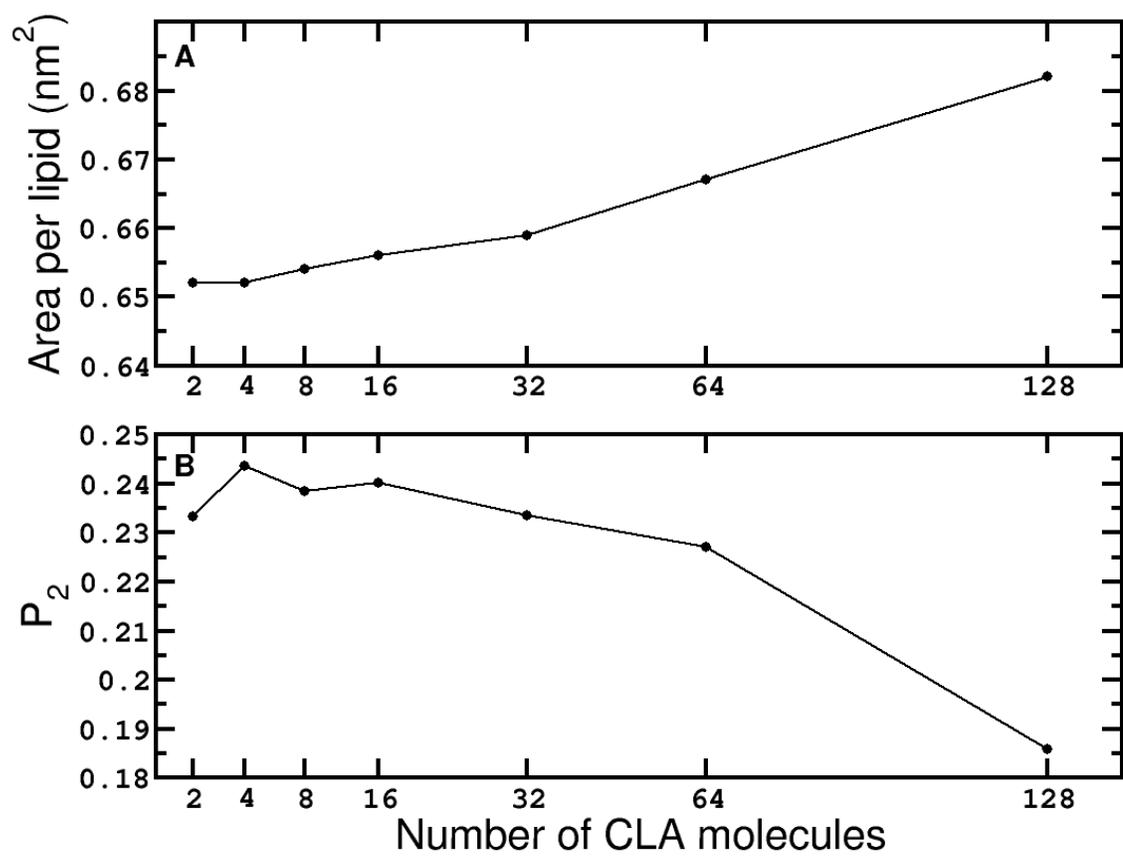


Fig. S7 (A) Area per lipid and (B) order parameter vs number of CLA molecules.

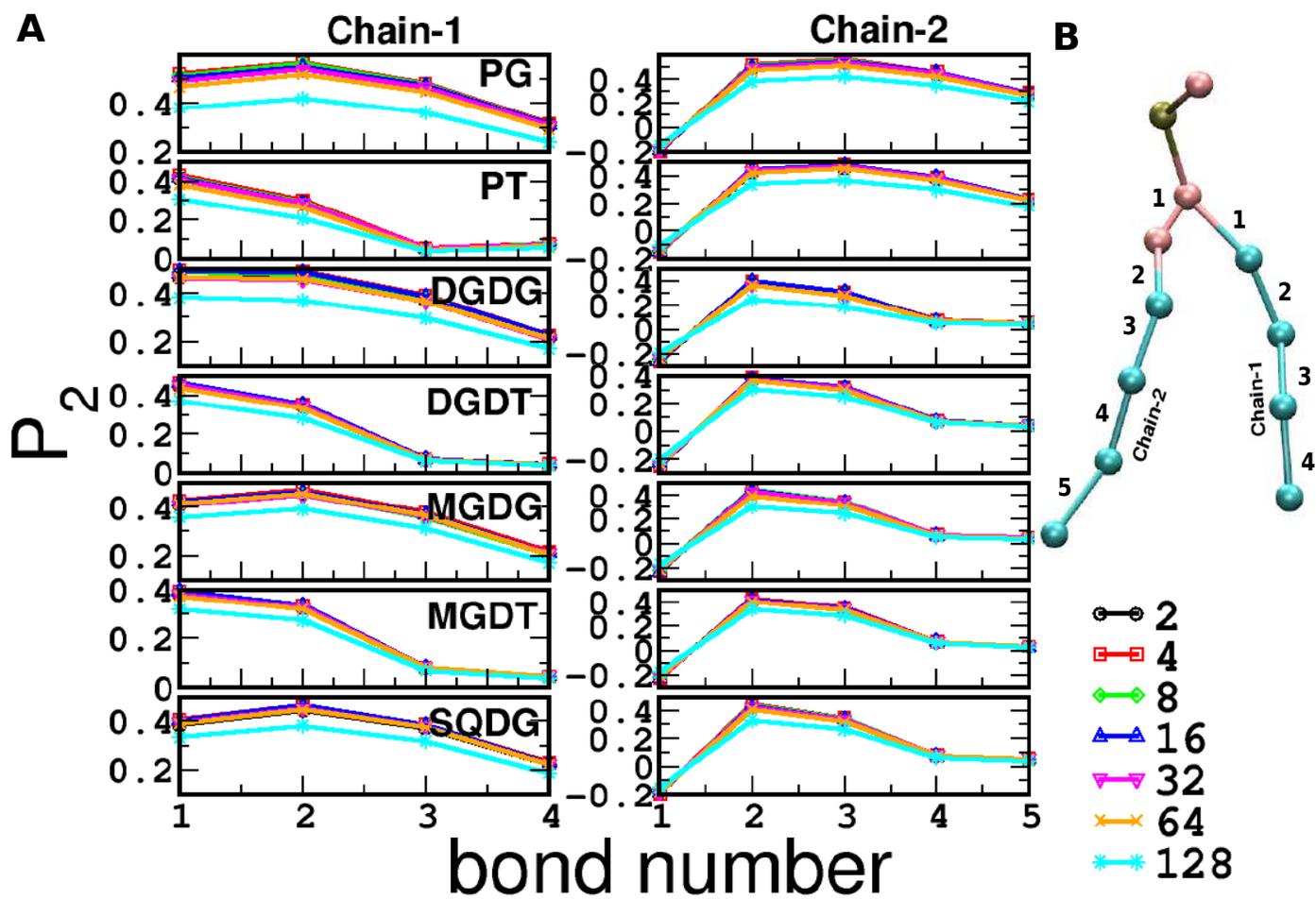


Fig. S8 (A) P_2 order parameter of two chains of all lipids of the plant thylakoid bilayer (B) Representation of a PG lipid with corresponding bond and chain numbers.

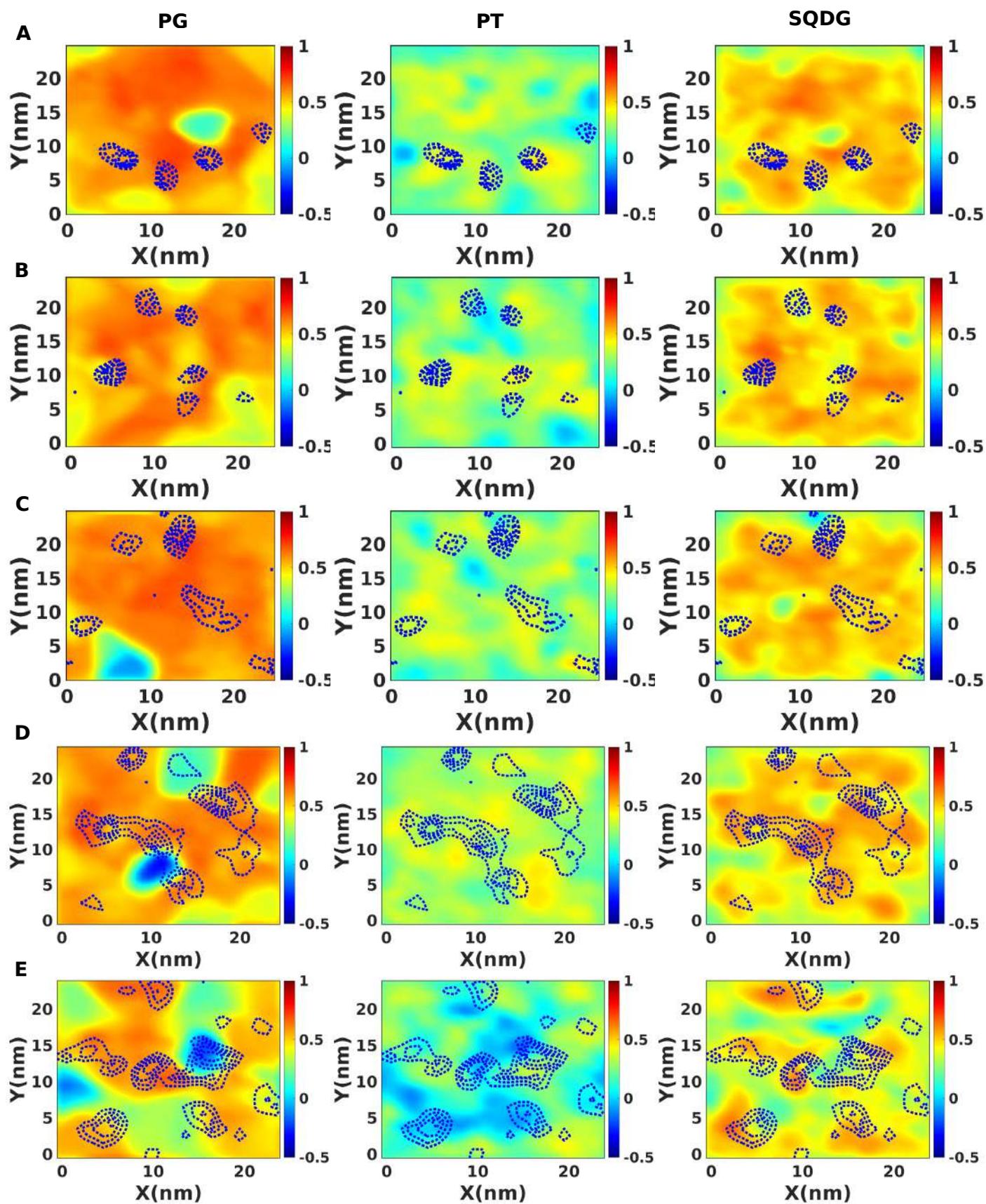


Fig. S9 The orientational order parameter of PG, PT, and SQDG lipids for (A) 8, (B) 16, (C) 32, (D) 64, and (E) 128 CLA lipid bilayer. Blue contour lines represent the density of CLA.