



**Figure 5.6. Time evolution of lipid positions and their orientations.** Top: Time evolution of positions of the centers of mass (CM) of headgroups for four representative flip-flopped lipids of a DMPC bilayer system in an aqueous solution with NaCl. The  $z = 0$  corresponds to the membrane center; solid black lines show the average positions of lipid headgroups in the two opposite leaflets, extracted from the intact membrane before pore formation. Bottom: Time evolution of the tail-to-head orientation for the same four flip-flopped lipids. The tail-to-head orientation is characterized as the angle between the bilayer normal and the vector directed from the CM of acyl chains to the CM of headgroups. Solid black lines again show typical values for the angle for lipids in the opposite leaflets. Adapted with permission from [34]. Copyright © 2007, American Chemical Society.