Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Microsecond Molecular Dynamics Studies of Cholesterol-Mediated Myelin Sheath Degeneration in Early Alzheimer's Disease

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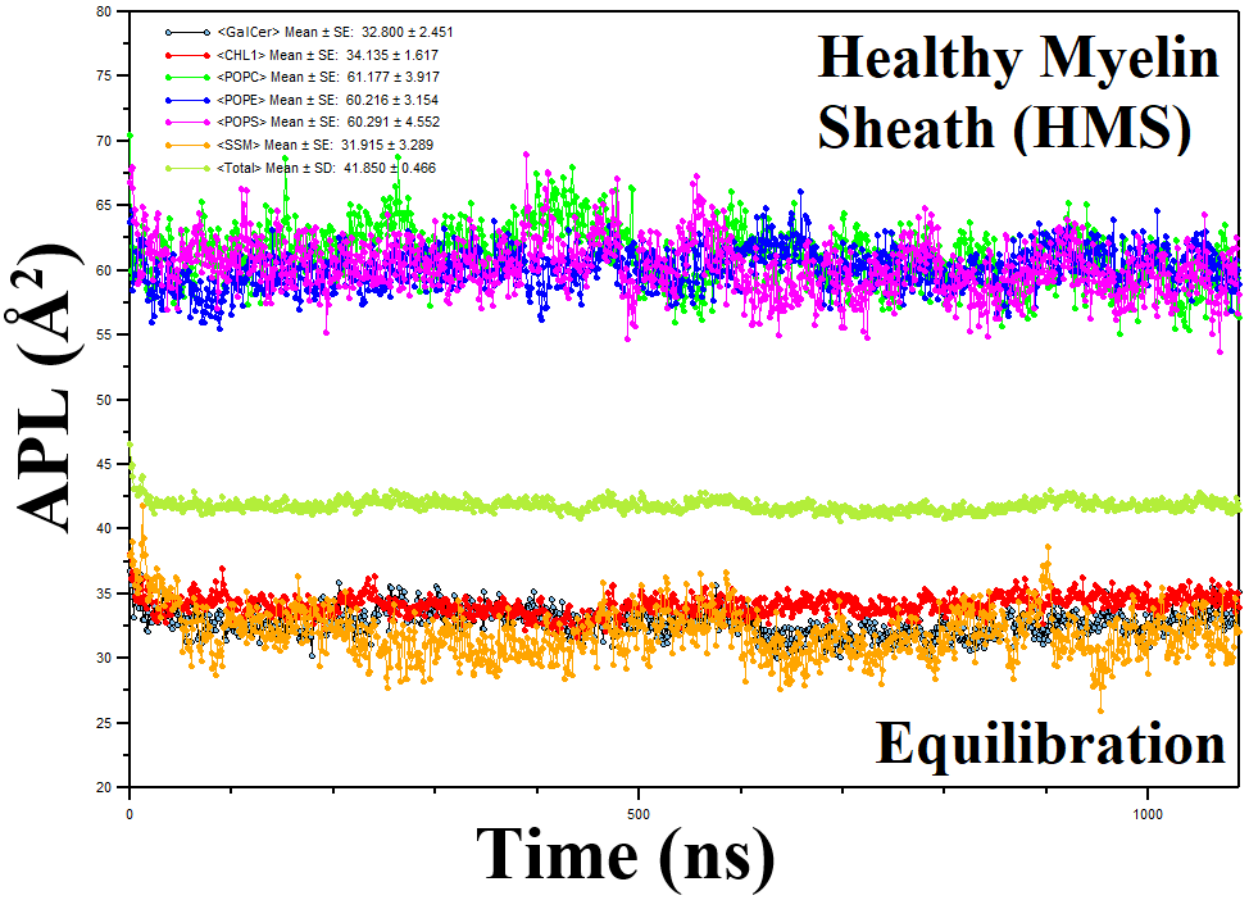

Figure S1: *Area per lipid (APL) as a function of equilibration time for healthy myelin sheath membrane (HMS) bilayer system. The component APL ($Å^2$) of specific lipid of AP bilayer i.e GalCer, CHL, POPC, POPE, POPS and SSM, is also shown.*

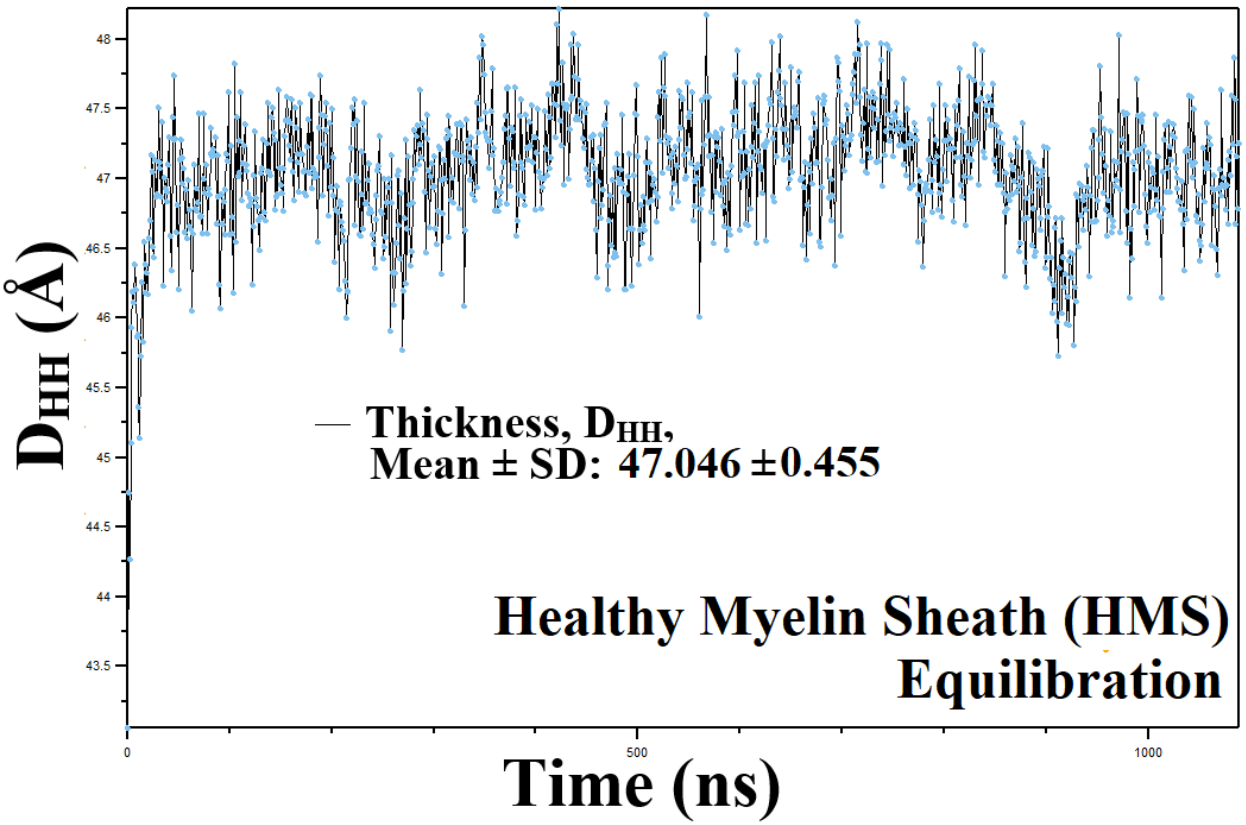

Figure S2: *Bilayer thickness (D_{HH}) as a function of equilibration time for healthy myelin sheath membrane (HMS) bilayer system.*

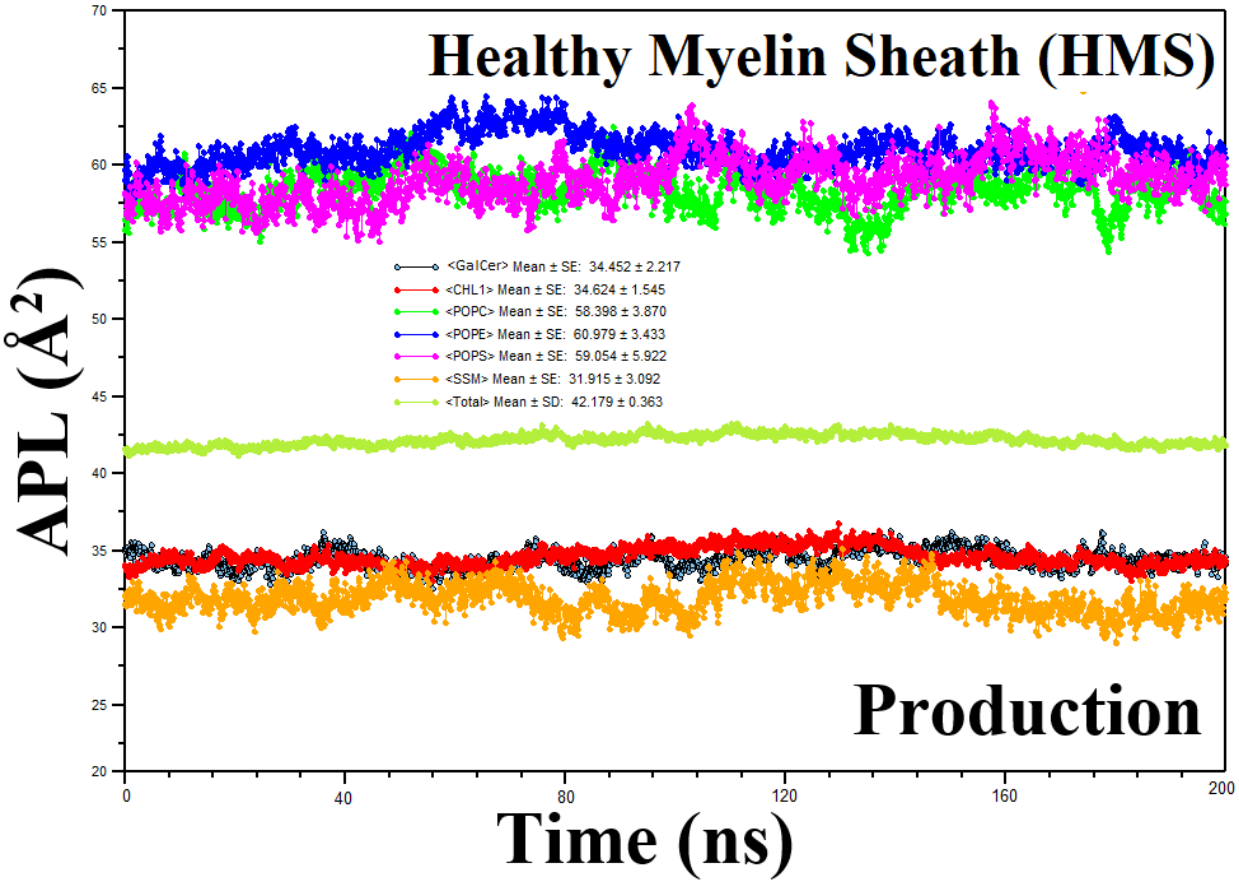

Figure S3: *Area per lipid (APL) as a function of time for healthy myelin sheath membrane (HMS) bilayer system at production stage (after equilibration). The component APL ($Å^2$) of specific lipid of AP bilayer i.e GalCer, CHL, POPC, POPE, POPS and SSM, is also shown.*

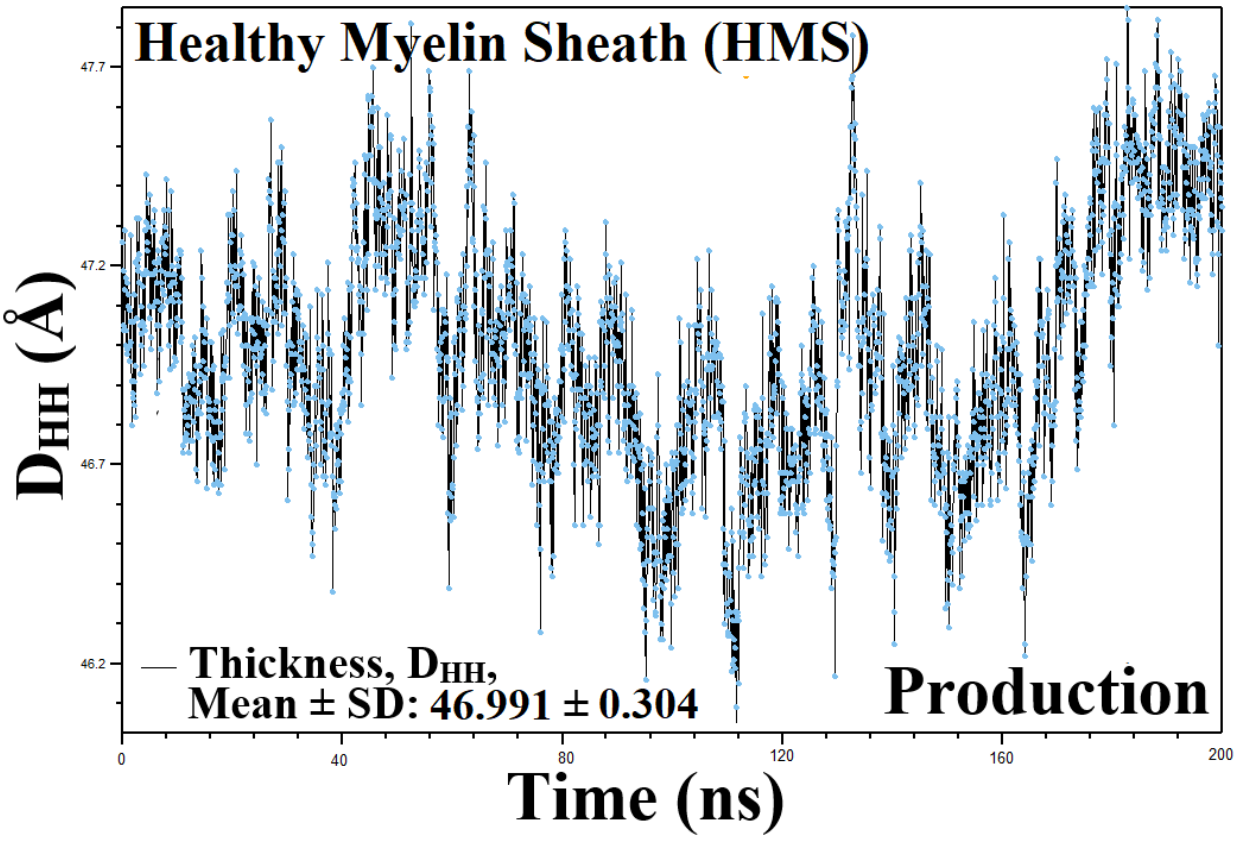

Figure S4: *Bilayer thickness (D_{HH}) as a function of time for healthy myelin sheath membrane (HMS) bilayer system at production stage (after equilibration).*

Table S1: The average P-N angle for POPC, POPE, POPS, SSM lipids and average cholesterol tilt angle (C13-C10) of reference membrane systems at 310 K. The standard deviation in the results over the 0.2 μS simulation trajectory is also given.

S. No.	Bilayer	χ_{CHL}	P-N angle (deg)				C13-C10 angle (deg)
			POPC	POPE	POPS	SSM	Cholesterol
1	PC	0	67.953+1.92	--	--	--	--
2	PC:PE	0	62.951+2.57	82.084+2.66	--	--	--
3	PC:PE:CHL	0.34	64.206+3.21	79.068+3.34	--	--	14.349+0.96
4	PC:PE:CHL:SSM	0.25	64.467+3.58	81.687+3.54	--	67.541+3.37	13.427+1.12
5	PC:PE:CHL:GalCer	0.25	63.320+3.72	77.892+3.79	--	--	11.967+0.92

Table S2: The average fraction of contacts and mass overlap, interdigitation within lipid bilayers systems of reference membrane systems at 310 K. The standard deviation in the results over the 0.2 μS simulation trajectory is also given.

S.No.	Bilayer	χ_{CHL}	Interdigitation of bilayer leaflets i.e. width of overlapping regions Wρ (nm)	Fraction of mass overlap (Iρ)	Fraction of contacts (Ic)
1	PC	0	0.520+0.050	0.288+0.019	0.053+0.004
2	PC:PE	0	0.468+0.049	0.252+0.020	0.047+0.004
3	PC:PE:CHL	0.34	0.323+0.044	0.164+0.019	0.033+0.003
4	PC:PE:CHL:SSM	0.25	0.314+0.049	0.153+0.016	0.031+0.003
5	PC:PE:CHL:GalCer	0.25	0.288+0.045	0.153+0.018	0.026+0.003

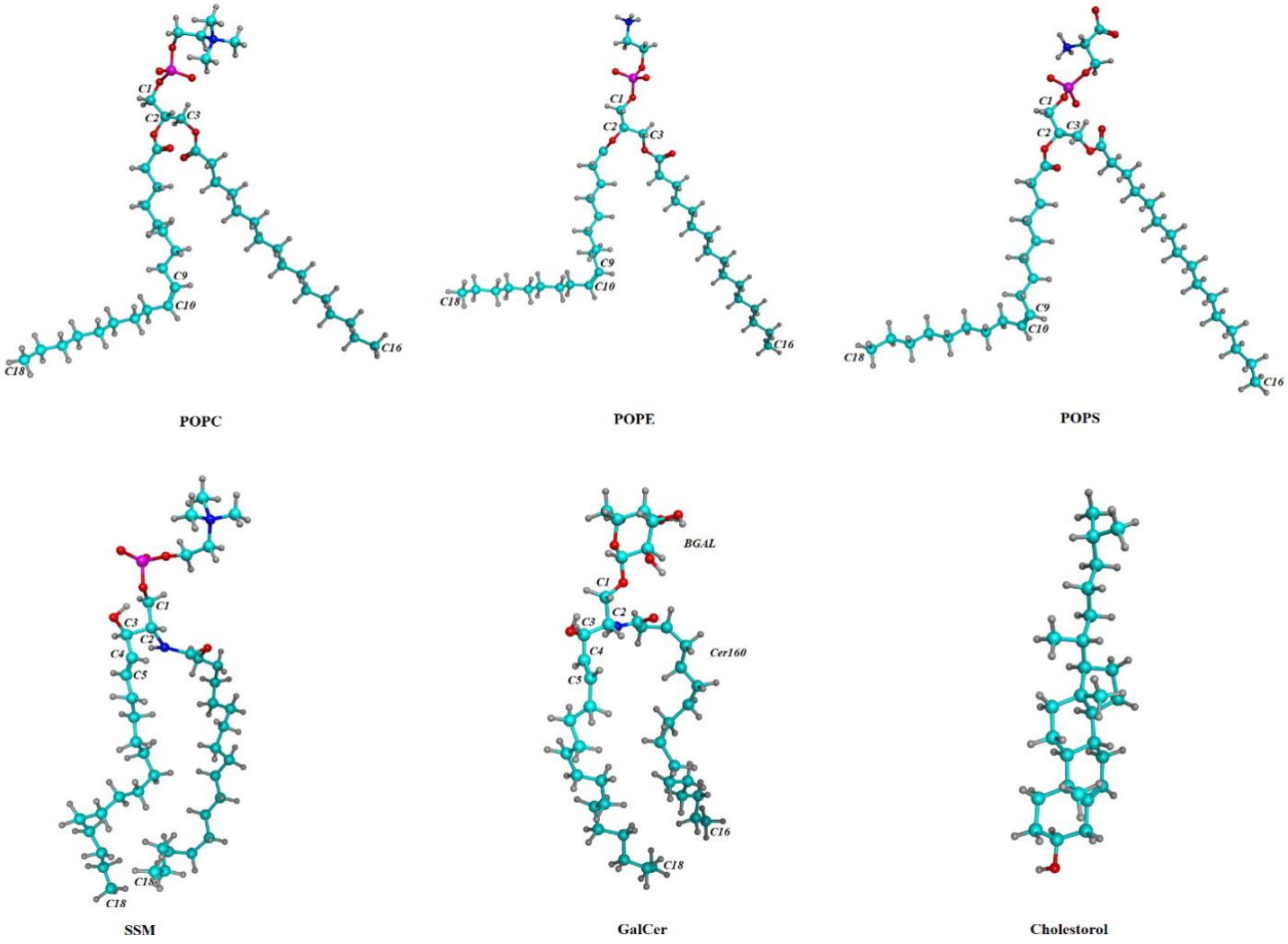

Figure S5*: Structure of various lipids and cholesterol molecules used in bilayer systems.*