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Insight into cholesterol transport in different lipid environments: a simulation study KLAS KARIS, URSULA PEREZ-SALAS, FATEMEH KHALILI-ARAGHI, Univ of Illinois - Chicago — With molecular dynamics simulations employing the MARTINI coarse grained force field, we investigate the difference in the dynamic behavior of cholesterol, linked to the absorption and desorption of cholesterol in two phospholipid environments consisting of either an uncharged, zwitterionic lipid (POPC) or the charged counterpart (POPS). The work is motivated by results from recent neutron scattering experiments measuring the transfer rate of inter-membrane cholesterol transfer, revealing that cholesterol intermembrane transport is significantly slower in lipid membranes composed of charged lipids, than in membranes composed of uncharged lipids. By systematically investigating dynamical and equilibrium parameters such as the free energy of desorption, lateral diffusion, tilt angle distribution, structural parameters and estimated absorption rates, we map the key differences in interaction of the two lipid species with cholesterol. Results point towards a shift in cholesterol absorption rates for POPS compared to POPC.

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