9-6-2012

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Key Players in Reverse Cholesterol Transport: The Plasma Enzyme LCAT

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Abstract

Lecithin cholesterol acyltransferase (LCAT) is a plasma enzyme that remodels nascent high density lipoprotein (HDL) into a mature form called spherical HDL. The impeding of this critical step in reverse cholesterol transport (RCT, the transport of cholesterol from periphery cells to liver), leads to atherosclerosis. Our goal is to use computational chemistry and molecular modeling tools to build molecular models for LCAT and its complex with nascent HDL. The molecular models are constructed from low resolution structures of LCAT and LCAT-HDL complex obtained by small angle neutron scattering (SANS) with contrast variation. Ultimately, we combine various experimental data (SANS data, hydrogen-deuterium exchange tandem mass spectrometry, other biochemical data) with computational techniques (bioinformatics, molecular modeling, SANS modeling, protein-protein docking, molecular dynamics simulation) to produce a molecular model for LCAT and its complex with nascent HDL. The model will be used in the future to map the amino acid residues from LCAT and the protein component of nascent HDL (apoA1) involved in mutual interaction, and to identify LCAT residues interacting with the lipid phase of nascent HDL.