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Dynamics of apolipoprotein B-100 assessed by elastic incoherent neutron scattering

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Protein dynamics is pivotal to fulfill protein function. Apolipoprotein B-100 is a giant monomeric protein with a fascinating dynamical history: it mediates the conversion from very low density lipoprotein (VLDL, ~50 nm) to low density lipoprotein (LDL, 22 nm). As a key-player in the cholesterol transport system, the protein is intimately linked to the development of atherosclerosis and cardiovascular diseases.

We here employed elastic incoherent neutron scattering (EINS) experiments to assess the local motions in isolated apo B-100 and compare it to those in VLDL and LDL complexes. All samples were lyophilized and hydrated with D₂O to finally obtain approximately one single hydration layer around the protein. EINS scans were carried out from 20 to 315 K at the backscattering spectrometer IN13 (energy resolution of 8 μ eV) at the Institut Laue Langevin (ILL), Grenoble, France. The mean-square displacements (MSD) as a measure of flexibility and the mean environmental force constant $\langle k \rangle$ to quantify structural resilience were calculated.

Our results suggest that apo B-100 with an MSD of 1.5 \AA^2 at 310 K is a highly flexible protein. Apo B-100's force constant $\langle k \rangle$ is comparable to that of VLDL, whereas their values substantially differentiate from LDL. LDL shows a much higher molecular resilience and thus can be considered much more rigid than VLDL and apo B-100.

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