



Asian Journal of Scientific Research

ISSN 1992-1454

science
alert
<http://www.scialert.net>

ANSI*net*
an open access publisher
<http://ansinet.com>

Computational Modeling Helps in Determining Individual Cholesterol-Related Information

Computational modeling increases our knowledge of lipoprotein properties that cannot be measured using experimental methods. Lipoproteins are particles that transport cholesterol in our bloodstream. According to the doctoral dissertation of Master of Science in Technology Linda Kumpula (Aalto University School of Science), the differences in the composition, size and number of lipoprotein particles transporting cholesterol in individuals can be computationally modeled using experimental data. The lipids transported by the particles have been established earlier, but it has not been possible to determine the content of one particle.

Modeling can be used to calculate the size of one lipoprotein particle when the number and volume of the lipids and proteins are known. The cholesterol-transporting particles of different individuals are slightly different in size. The size difference depends on issues such as how many cholesterol molecules there are in one lipoprotein particle. The risk of getting a cardiovascular disease varies depending on the size, number and possibly also the lipid composition of, for instance, LDL particles -- lipoproteins containing so-called bad cholesterol. If there is a significant number of LDL particles and they are small, the risk of cardiovascular disease may be greater since the small particles can enter the arterial walls more easily than larger ones.

A lot of research has been carried out on the structure and properties of lipoproteins, but the details of their structure are still fairly unknown. Computational modeling can be used to examine whether lipids are located in the core or on the

surface of lipoprotein particles. This study has disproved earlier hypotheses on the location of lipid molecules. The lipids that are more commonly found in the core can also be located on the surface of a particle.

"This study shows that there are differences between individuals when it comes to the particles that transport cholesterol. In the future, the significance of these differences from the point of view of preventing cardiovascular diseases would be an interesting area to explore," Linda Kumpula comments on her dissertation.

An important aspect of this study is its usefulness when applying new, experimental methods, such as NMR spectroscopy for example, to the study of lipoproteins and possible clinical use in the future.

Story Source: The above story is reprinted from materials provided by Aalto University.