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Computational discovery of bioactive compounds binding to hepatic HMGCR

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The hypocholesterolemic effect of tomato juice has been investigated in an intervention study with rats, along with the possible inhibition effect of bioactive tomato compounds binding to the HMGCR enzyme. Two experimental groups (n=8 Sprague-Dawley rats) were fed ad libitum for five weeks, with water or tomato juice provided to the control and intervention groups, respectively. Total, LDL and HDL cholesterol, and total triglycerides were analysed in plasma, and the lycopene content and the expression and activity of the enzyme HMGCR were determined in liver samples. A computational molecular modelling was carried out to determine the interactions between HMGCR and lycopene, chlorogenic acid and naringenin. Total, LDL and HDL cholesterol were significantly lower in the intervention group after the intake of tomato juice. In addition, a significant reduction in HMGCR activity was observed, although this was not accompanied by changes in gene expression. The molecular modelling showed that components of tomato can bind to the active site of the enzyme and compete with the ligand HMGCoA. Lycopene, from tomato juice, accumulates in the liver and can inhibit the activity of the rate-limiting enzyme of cholesterol biosynthesis, HMGCR.

Biography

Horacio Perez-Sanchez graduated in Theoretical and Computational Chemistry from the University of Murcia (Spain) in 1999, where he also obtained his PhD degree in 2006. He has carried out research in several European Institutions such as the Institute of Structural Biology, where he successfully developed and applied computational methodologies for the prediction and interpretation of macromolecular behaviour in solution, and at the Karlsruhe Institute of Technology (Karlsruhe, Germany), where he developed new methodologies for drug discovery and implemented them in Supercomputers. Currently he is full-time researcher and Principal Investigator of the "Bioinformatics and High Performance Computing" research group at the Catholic University of Murcia (Spain). He has co-authored more than 50 international conference contributions and journal papers, book chapters and European patents. He has served as a reviewer for several conferences/journals/book editorials. His primary research interests are in the areas of Bioinformatics, mainly Drug Discovery.

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