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The use of epitopes against schistossomiasis: The role of molecular modelling

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The schistossomiasis is an important parasitic disease that affects more than 200 million people around the world in 76 countries. The primary weapon used against Schistossoma mansoni is chemotherapy, but reinfections and occurrence of drug resistant parasites was related. Thus, thevaccines using the epitopes existing in the parasitic tegument could be effective against this disease. The main event where the epitopes can be used against schistossomiasis is its interaction with theMHC class II complex (MHC-II). Then, the complex formed by MCH/epitope would interactwith the TCR (T cell receptor) triggering one immunization cascade. These interactions arefundamental to development of any kind of vaccine based on the epitopes and the understandinghow it occurs is mandatory for this process. The contribution of the bioinformatics and molecular modeling (MM) can be helpful in the sense to improve the knowledge about the interaction ofthe epitopes with MHC complex because the molecular modelling tools can provide information about binding energy, unbinding process, orbital energies and electrostatic interaction amongothers. In addition, the use of molecular modelling results can decrease the amount ofexperimental work providing some insights about what kind of epitopes use and why use them. Keeping this in mind, this speak attempt to show what have been done in the study of interactionbetween epitopes and MCH-II involving bioinformatics, molecular docking, molecular dynamicsand quantum chemical calculations. Besides, some experimental results will be compared withtheoretical ones.

Biography

Moacyr Comar Junior has completed his PhD at the age of 31 years from University of São Paulo. At the end of PhD he went to Amazonas to work in the Theoretical Chemistry Lab at theFederal University of Amazonas. In 2009 he went to Federal University of São João del Rei tothe Molecular Modeling Lab. He has published articles about different subjects in reputedjournals and has been serving as reviewer member of some journals of biotechnology.

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