

Molecular modeling: a numerical zoom to help fighting diseases

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<http://lcrbw.pharmacie.univ-paris5.fr/spip.php?article193&lang=fr>

Abstract

The essential challenge posed by human health requires the understanding of the cell's machinery at a molecular level. The interplay between proteins, DNA and RNA is key for the cell to perform its functions and contribute to the organism wellbeing. In the presence of diseases such as cancer, HIV, Hepatitis, Alzheimer, these interactions are perturbed and the cell either dies or starts acting against the organism's interest. The role of drugs is then to restore the correct function through the chemical interaction with the biomolecules and repair the cell's machinery. To understand these processes many experimental techniques are put in action but a microscopic view unveiling the detailed mechanisms of a virus or of a cancerous cell is still missing. This is however a necessary step to develop efficient and selective drugs. Molecular modelling, which is the science of studying molecular structure and function through model building and computation, allows to complement experiments and to propose models looking at each atom of the system and following its behaviour under different conditions. It constitutes therefore a "numerical zoom" for a detailed understanding of the molecular mechanism leading to a disease and pointing in the direction of its possible cure. In this presentation, I will describe some of the major health challenges of our times and give an outlook on how modelling contributed to our understanding of the diseases.