

Monday, November 5th, 2018 – 12h15
Department of Physiology, Bugnon 7, 1005 Lausanne
Seminar room, 6th floor

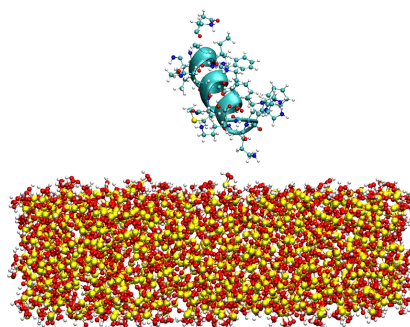
Molecular Modeling as virtual microscope to study the molecular mechanisms of delivery nanosystems : some examples

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In this talk, some examples will be presented showing how Molecular Modeling can act as virtual microscope to have insight on molecular mechanisms related to different class of delivery systems. So-called Critical Nanoscale Design Parameters (CNDP) that characterize the behavior of well-defined nanoscale building blocks allow, in principle, to control the final behavior of a given molecule. However, CNDPs are somewhat entangled, and they do not take into account explicitly the influence of the external environment as thought as the presence of polar solvent molecules, salt ions and eventually other charged molecules. In this context, we will present some modeling studies performed to explore the efficiency of dendrimeric structures as gene delivery systems and Cell Penetrating Peptides as candidates for magnetic nanoparticles functionalization, in order to enhance their adsorption stability and efficiency

References

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