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S E M I N A I R E

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**« A multiscale approach for rationalizing molecule diffusion
through nano-pores »**

In this talk I'll summarize the effort of our group to combine numerical simulations and electrophysiology with a multi-scale approach for quantifying the passive transport of small molecules through membrane proteins.

Starting from some general bacterial pores used as model systems we identified the way in which molecules are selectively transferred in and out from bacteria. The two structural features controlling transport are (i) the hourglass shape of the pore, and (ii) a segregation of charges in the central region. The former property avoids the uncontrolled flux of molecules, creating an unselective barrier for penetration. The latter on the other hand can be very specific: by creating a transversal electric field, it allows molecules with a particular dipole moment to have high flux. This mechanism, an entropic general barrier compensated by specific electrostatic properties, has the advantage to avoid saturation. Further these structural features can be easily transferred in designing synthetic nanopores for selecting/sensing specific molecules.

Jeudi 12 mai à 14h00
Salle de conférence