Master « Sciences, Technologie, Santé »
Mention « In Silico Drug Design »
Second Year

OFFER AN INTERNSHIP
Academic Year 2014 – 2015

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Specialty training : Research X Professional ☐

a few key words to describe the subject of training :

The use of supercomputer to model and simulate, via molecular dynamics simulations, proteins and their processes at the molecular scale

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Title of internship:

- Simulation of transport properties of porins from the Outer Membrane of Gram-negative bacteria

this subject is a first step towards a thesis: **Yes** - No

Short texte describing your project

Gram-negative bacteria are protected by an additional outer membrane, which represents a true barrier for the passage of any molecule. Polar molecules can overcome this barrier using some water-filled channels, called porins. These porins, used to exchange non-specific molecules, represent also the main entry for polar antibiotics in their way to reach the internal targets. Many examples of resistant bacteria have shown how porins can be modified, either in their expression or in their structure, to avoid the entry of antibiotics. Therefore porins represent an intrinsic resistance mechanism against antibiotics. To date it does not exist yet a theory explaining how polar molecules can permeate porins. Within the perspective to identify novel scaffolds as antibacterials, information gathered at the molecular scale on the process by which molecule translocate through porins would help to design new compounds with improved permeability for Gram-negative bacteria. A possible project would explore the structural/dynamical properties of porins and the interactions of antibacterials during their permeation through porins.
