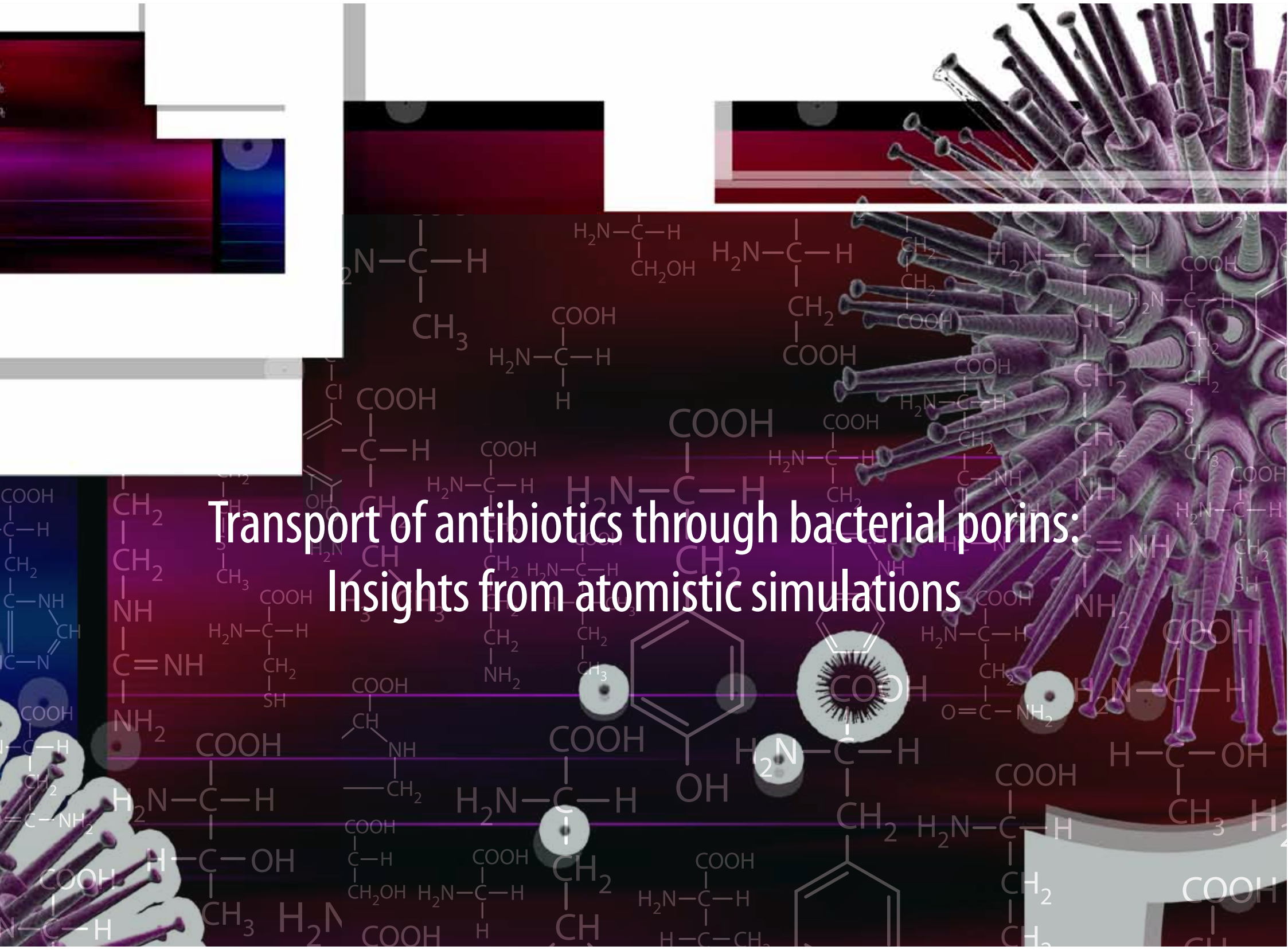
23.05.2011

Seminar 11:00

CRS4 - BUILDING 1 - ROOM D130

Loc. Piscina Manna - Building 1 - 09010 Pula (CA) - Italy



Transport of antibiotics through bacterial porins: Insights from atomistic simulations

Speaker

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The aim of the study is to investigate antibiotic transport through porins, which is based on passive diffusion at a molecular scale. To do so, we use accelerated molecular dynamics calcuations to simulate the antibiotic transport through the porin.

The talk will present a complete analysis of the translocation of an antibiotic (ampicillin) through the bacterial porin outer membrane protein F, providing insight into the key determinants (preorganization, solvation, entropy-enthalpy compensation) and molecular mechanism for the transport process.

The information gathered from our simulations could be used as an input toward designing antibiotics with optimal physicochemical properties, allowing them to translocate with a higher rate through porins.