WARWICK
THE UNIVERSITY OF WARWICK

CSC/WCPM joint seminar

The dynamics and flexibility of biomedically important proteins: a combined computational/experimental approach to tackle antimicrobial resistance (AMR)

Jasmine Desmond

INTEGRATE AMR Early Career Fellow, Warwick Physics

Monday, 20th February, 1 p.m.
PS0.17a Seminar room, Physical Sciences

Abstract: 700,000 people die each year from drug-resistant infections, a figure that - if action is not taken - is estimated to increase to 10 million by 2050. The drug penicillin targets essential cell wall biosynthetic enzymes that still remain attractive targets for new efforts in drug discovery. Elucidating protein dynamics and flexibility is key to understaning the selective interactions of proteins with a drug as it docks. In spite of the success of x-ray crystallography in the determination of rigid protein structures, the experimental technique is unable to provide insight into the dynamics of proteins. Such information can, however, be elucidated using molecular modelling. Important protein conformational changes often occur on microsecond-millisecond timescales and are difficult to access using traditional modelling techniques, such as molecular dynamics (MD). Here, we present the results of computationally inexpensive, geometric simulations of protein motion for a range of proteins important in antimicrobial resistance (AMR).

A buffet lunch is available from 12:45 pm.

More info: http://warwick.ac.uk/wcpm/seminars

WCPM
Warwick Centre for Predictive Modelling