



ALMA MATER STUDIORUM
UNIVERSITÀ DI BOLOGNA

DIPARTIMENTO
DI FARMACIA
E BIOTECNOLOGIE

AVVISO DI SEMINARIO

Il giorno **3 Maggio 2024**
alle ore **14:00**

Prof. Carmen Domene-Núñez

Professor of Computational Chemistry, University of Bath, United Kingdom
(ospite di Prof. Matteo Masetti)

terrà un seminario dal titolo:

Computational studies of GLUT transporters: some insights into the glucose transport machinery of human cells

in presenza:

Aula A Farmacologia, via Irnerio 48, Bologna BO

Collegli e studenti sono cordialmente invitati

ABSTRACT

Glucose is a vital source of energy for cells, and its transportation into cells is crucial for various physiological processes, including cellular respiration and metabolism. GLUT transporters, a family of membrane proteins also known as glucose transporters, facilitate the passage of glucose across cell membranes. These transporters have different affinities for glucose and exhibit different tissue distributions. The most well-known member of this family is GLUT1, which is found in various tissues and plays a fundamental role in glucose uptake, particularly in cells that have a constant need for glucose, such as red blood cells and the blood-brain barrier. Through selected examples from our work carried out using computer simulation, I will provide an overview of the current knowledge we have about transport and selectivity in this family of transporters.

BIOGRAPHICAL SKETCHES

Prof. Carmen Domene-Núñez is a professor of Computational Chemistry at the University of Bath (United Kingdom) and she has been recently visiting the Harvard and Oxford Universities. She has a PhD in Chemistry (University of Exeter) and more than 120 publications in internationally refereed journals. She has been recently awarded by the Royal Society of Chemistry Corday-Morgan Prize. Her research uses computational techniques to study the structure and dynamics of biological systems, for understanding biochemical and biophysical processes from a microscopic perspective. Matching methods to problems is necessary and requires development, implementation, and optimization of novel simulation tools. Pursuit of this has taken her into a number of branches of theoretical chemistry including quantum chemistry, the theory of electronic structure and intermolecular interactions, statistical mechanics, ab initio and classical computer simulation and spectroscopy.