ALMA MATER STUDIORUM
UNIVERSITÀ DI BOLOGNA

DIPARTIMENTO
DI FARMACIA
E BIOTECNOLOGIE

AVVISO DI SEMINARIO

Il giorno **25 marzo 2025**
alle ore **14:30**

Dr. Fabio Parmeggiani

Lecturer at the Cardiff University, School of Pharmacy and Pharmaceutical Sciences
(ospite della Prof.ssa Barbara Zambelli)

terrà un seminario in lingua inglese dal titolo:

Tools for and from protein design: from modular proteins to carbohydrate recognition

Area tematica: Drug discovery and development

in presenza:
AULA II, Ciamician, via Francesco Selmi 2, Bologna BO

e in streaming:
https://teams.microsoft.com/l/meetup-join/19%3aN09c0NIyEssBnF7ObCyDOQwkgDWm1qdd9f7F2nJV9fw1%40thread.tacv2/1631519544944?context=%7b%22Tid%22%3a%22e99647dc-1b08-454a-bf8c-699181b389ab%22%2c%22Oid%22%3a%225a941351-ef41-4aa4-8771-fa50a6d62ca1%22%7d

Il seminario è organizzato nell'ambito del Corso del Dottorato in BCM.
Colleghi e studenti sono cordialmente invitati

ABSTRACT

The advances in protein structure prediction and computational protein design in the last decade, culminated with the 2024 Nobel prize in Chemistry, have provided opportunities for the development of new tools for research, diagnostics and therapeutics.
In my group we have focused on modular protein design, developing software to combine structural building blocks into proteins with custom shapes (ELFIN) and predict dynamics of these structure at design time (Dynamo) to simplify and speed up design of complex protein architectures to be used as scaffolds for novel functional nanomaterials and nanoparticles.
Additionally, we have pursued the design of novel proteins for carbohydrate recognition. Protein-carbohydrate interactions are ubiquitous, but prediction of specificity, validation of docking models and design of protein binders are still poor, due to low affinity and similarity between carbohydrates.
We have developed a 3D graph neural network (CLIMBS) that process geometry and interactions of protein-sugar interfaces, using curated sets of high-resolution structures, as well as synthetic data augmentation. CLIMBS is highly accurate in recognizing native interfaces and generalizes to carbohydrates not included in the training set, making it an invaluable tool for discrimination of docking and design models of protein-carbohydrate interactions.

BIOGRAPHICAL SKETCH

Fabio Parmeggiani is a lecturer at the Cardiff University, School of Pharmacy and Pharmaceutical Sciences since 2024. He graduated in Biotechnology at the University of Bologna, and then obtained his Ph.D. in Biochemistry from the University of Zurich working in the group of Andreas Pluckthun on design of armadillo repeat proteins for peptide recognition. He joined the group of David Baker at the University of Washington to work on computational protein design and then became group leader and EPSRC early career research fellow at the University of Bristol, before joining Cardiff University. He has worked at the forefront of experimental and computational protein engineering and design, and he is currently developing new methods to design proteins with modular structures, evaluating protein dynamics during design, and designing new proteins to recognize carbohydrates, both as cell surface antigens and in bacterial biofilms. The goal is to apply these tools for the development of new diagnostics and therapeutics.