PhD@DICAM seminar

"Molecular dynamics in antibody engineering"

Lecture by Prof. Francesco Zonta, Xi'an Jiaotong Liverpool University, Suzhou, China
Date: 17/7/2023 h. 15.00
Place: Aula TA-03, Via Terracini 28, Bologna

Antibodies' primary purpose in the immune system is to discriminate between "self" and "non-self" molecules in the organism and initiate the immune response in the second case. This is done thanks of an immensely vast repertoire of possible sequences in the Complementary Determining Regions (CDRs), which allow the antibody to recognize proteins or other macromolecules. In recent years, this remarkable property has been exploited to transform antibodies into biotechnological tools and drugs. The ability to use computer simulations to design antibodies with desired biochemical properties would represent a major breakthrough for medicine and biotechnology. However, this requires the ability to sample the large space of possible antibody sequences in order to select one antibody with good affinity to its molecular target. The steady increase in computational power in the last 50 years is opening unprecedented opportunities in biology, as computer simulations of biological systems have become more accessible and can reproduce experimental results more accurately.

In this talk, I will show that it is indeed possible to use computer simulations to replace experiments in the limited but practically useful scope of improving the binding affinity of an antibody to its target by using a combination of Molecular Dynamics simulations used to sample the protein conformations, and a Monte Carlo algorithm to sample the space of sequences. The antibodies designed with this method had an affinity comparable to the best ones obtained experimentally and could be obtained within a similar timeframe. The methodology proposed here could represent a valid alternative for improving antibodies in cases in which experiments are too expensive or technically challenging and could open an opportunity for designing antibodies for targets that have been elusive so far.

Francesco Zonta, PhD

Francesco Zonta background is in Theoretical and Mathematical Physics. He got his Ph.D. in Physics in Padova University in 2007. In the following years he was Post-Doc and Researcher in the Venetian Institute of Molecular Medicine in Padova. In 2015 he moved as Research Associate Professor to the Shanghai Institute for Advanced Immunochemical Studies in ShanghaiTech University, where he was first the director of Bioinformatics and Computational platform and then Co-PI in the Laboratory of Computational Biology. He joined Xi'an Jiaotong Liverpool University (XJTLU) in 2023 as Associate Professor. His research interests are in the design of antibodies for therapeutic purposes and simulations of biological systems.