SEMINAR

CIC biomaGUNE
MEMBER OF BASQUE RESEARCH & TECHNOLOGY ALLIANCE

Dra. Francesca Peccati
Scientist at CIC bioGUNE.

Computational protein design and engineering

Wednesday, 21st February
12.00 p.m.

CIC biomaGUNE - Seminar Room

De novo protein design and engineering of natural proteins have proven successful in both endowing proteins with unnatural functionality and fine-tuning the natural one. Over the last decades, the field has benefited from the interplay of rational design and directed evolution yielding multifunctional materials and highly active biocatalysts. Until now, computational approaches have been successful at installing a first seed of the desired activity or function –typically below the levels required for practical applications– to be extensively optimized with experimental techniques.

Three years ago, artificial intelligence changed the field of structural biology with tools such as AlphaFold and RoseTTAFold, which solved the long-standing problem of protein folding in globular proteins monomers and complexes (i.e. predicting the native state of proteins given their sequence). Over the next years, less known but equally transformative artificial intelligence-based tools have emerged that boost the success rate of computational design and engineering, providing highly optimized proteins straight out of the computer. In this talk, I will present examples of successful protein optimization campaigns based on these approaches.