## SCIENTIFIC SEMINAR



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Computational Chemistry Lab CIC bioGUNE

## Novel AI-Driven Approaches for Protein Design

Proteins are truly the most amazing machines in Nature. Yet despite their varied talents, all proteins start out with the same basic form: a linear chain of amino acids. After being assembled in cellular factories called ribosomes, each chain folds into a unique, exquisitely complex 3D shape. Those shapes, which determine how proteins interact with other molecules, define their roles in the cell. De novo protein design explores the full sequence space, guided by the physical principles that underlie protein folding. Computational methodology has advanced to the point that a wide range of structures can be designed from scratch with atomic-level accuracy. Whilst almost all classic protein engineering has involved the modification of naturally occurring proteins, it is now possible to design new functional proteins from the ground up to tackle current challenges in biomedicine, chemical synthesis and nanotechnology.

In this lecture, we will summarize our recent contributions to the exciting field of protein design and engineering, boosted by revolutionary AI tools which now provide the long-awaited speed and accuracy necessary for fast validation in the wet lab. Applications of in-house developed methodology include the thermostabilization of pathological mutants of proteins involved in iron metabolism, development of biosensors and discovery of biocatalysts for new-to-Nature reactions.

CIC bioGUNE MEMBER OF BASQUE RESEARCH & TECHNOLOGY ALLIANCE



Friday June 16 <u>Atrio 800</u> <u>12.00H</u>

