



# *GTR-IRCCS-RCMS Seminar*

## **Leveraging Computational Approaches for Innovations in Protein Engineering and Enzyme Design**



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**August 21, 2023 15:30 ~ 17:00**

***Noyori Materials Science Laboratory  
Chemistry Gallery***

The rapidly evolving field of protein engineering and enzyme design has paved the way in groundbreaking advancements, promising transformative applications across industries ranging from biotechnology to pharmaceuticals. A key driving force behind these accomplishments is the integration of computational methods, which have expanded our understanding of protein structures, dynamics, and interactions with unprecedented depth.

In this seminar, I will delve into the pivotal role of computational approaches in expediting the design, optimization, and discovery of novel enzymes and engineered proteins. I will explore the remarkable potential of combining computational chemistry and machine learning techniques to advance and accelerate protein engineering and enzyme design. This integrative approach has the ability to revolutionize our understanding of complex protein structures, predict enzymatic behavior. Furthermore, this synergistic combination can unlock the full potential of protein engineering methodologies and contribute to a future where computational approaches drive transformative innovations in biotechnology and medicine.

Keywords: protein engineering, enzyme design, computational methods, molecular modeling, directed evolution, machine learning.

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