Università degli Studi di Padova

DiSC

Lunedì **13 gennaio 2025** alle ore **10:00** presso l'aula C

la **Prof. Daniela Kalafatović**

Faculty of Biotechnology and Drug Development
University of Rijeka, CROATIA

terrà il seminario dal titolo:

Pushing the boundaries of peptide discovery using machine learning-guided generative models

The discovery of new active peptides (i.e., antimicrobial, antiviral, catalytic) is challenging, as they are part of a very large search space and the correlation between the peptide sequence and the desired activities and/or functions is not yet fully understood. To avoid expensive and time-consuming guesswork and experimental failure, our strategy is to apply machine learning (ML)-based predictions in combination with genetic algorithm-based optimizations to accelerate peptide discovery. Search-based algorithms allow for a faster exploration of peptide permutation space which grows exponentially with peptide length and whose amount and dimensionality is too overwhelming to rationally comprehend. ML can find patterns or regularities in data, build mathematical models based on the theory of statistics and make up for the lack of knowledge. To date, both strategies have been applied to a variety of chemical problems to maximize the chance of successful and rapid solving of complex issues. One of these complex combinatorial problems is the prediction of peptide self-assembly and the assignment of potential new functions to new identified sequences deriving from unexplored regions of the peptide search space.

La presenza della S. V. sarà molto gradita

Il Direttore del Dipartimento
Prof. Stefano Mammi

Prof. Marta De Zotti