CiQUS Lecture

Design of short peptides and peptide assemblies aided by machine learning and genetic algorithms

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More info: Research Group website

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12:15 p.m. CiQUS Seminar Room

FONDO EUROPEO DE DESENVOLVEMENTO REXIONAL
PO FEDER Galicia 2014-2020 – *Unha maneira de facer Europa*

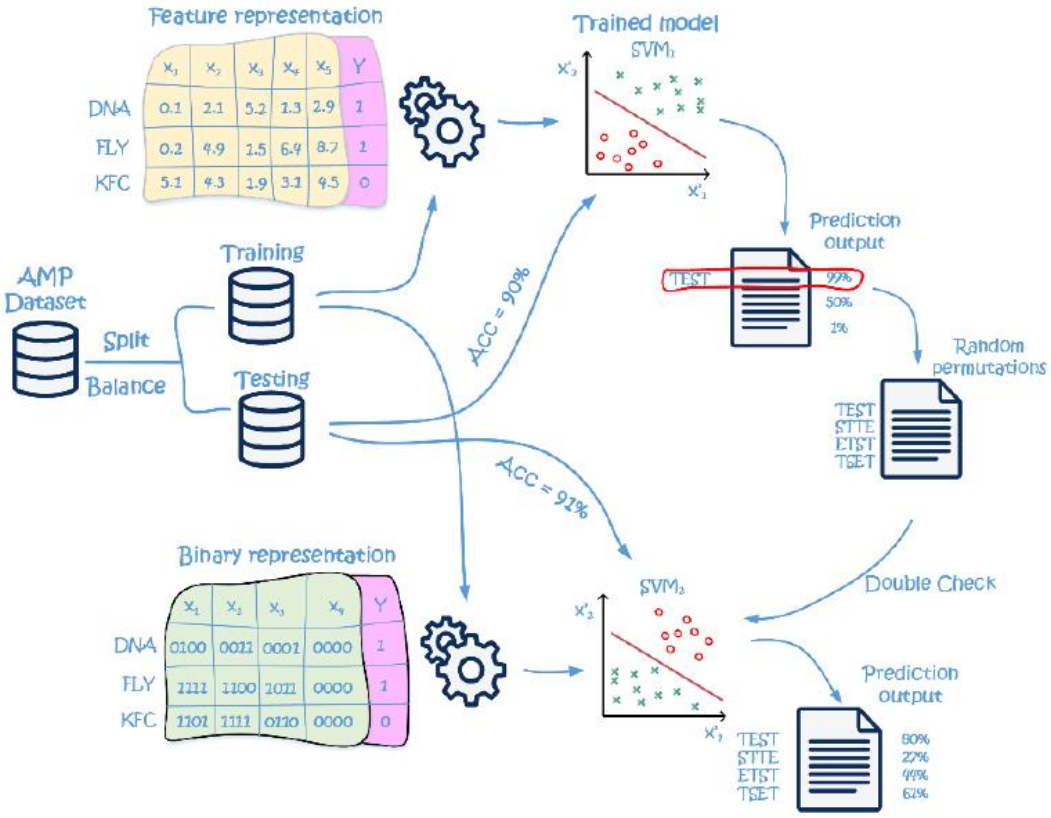
Link to personal website: https://deshpetlab.uniri.hr/

Abstract:

The discovery of new peptides (i.e., antimicrobial, antiviral, catalytic) is challenging, as they are part of a very large search space and the principles responsible for the desired activities at the sequence level are not yet fully understood. To avoid expensive and time-consuming guesswork and experimental failure, our strategy is to apply soft computing techniques 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. Machine learning 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.

Our team has already reported on a multi-objective evolutionary approach for the exploration of mass and sequence diversity-oriented random peptide libraries [1] and on the bottom-up approach for their design [2], which combines physico-chemical properties obtained experimentally and theoretically to cover larger parts of the peptide chemical space. Our current activities involve the application of machine learning to find peptides with catalytic activity, to predict their predisposition towards self-assembly [3] and to estimate their antiviral or antimicrobial activities (fig 1) [4]. For this purpose, we developed a new sequential properties representation scheme that combines physico-chemical properties with the amino acid order within the sequence. Moreover, we applied the generative adversarial network that enables the design of de-novo sequences.

[1] Kalafatovic, D.; Mauša, G.; Todorovski, T.; Giralt, E. J. Cheminform. 2019, 11 (25), 1–15.
[2] Kalafatovic, D.; Mauša, G.; Rešetar Maslov, D.; Giralt, E. Molecules 2020, 25 (15)
[3] Janković, P.; Šantek, I.; Pina, AS.; Kalafatovic, D. Front. Chem. 2021, 594
[4] Erjavac, I.; Kalafatovic, D.; Mauša, G. AI in the life sciences. 2022, https:// doi.org/10.1016/j.ailsci.2022.100034



Biosketch:

- **Work Experience**

2021 – present: Head of Medicinal Chemistry Division, Department of Biotechnology, University of Rijeka
2019 – present: Assistant Professor, Department of Biotechnology, University of Rijeka
2016 – 2018: Marie-Curie CO-FUND Postdoctoral fellow, Institute for Research in Biomedicine Barcelona, Spain 2015 – 2016: Research Associate, Advanced Science Research Centre, City University New York, USA

- **Education**

2011 – 2014: PhD, Pure and applied Chemistry, University of Strathclyde, Glasgow, UK 2004 – 2010: Mag. Pharm., Pharmaceutical chemistry and technology, University of Trieste, Italy

- **Projects**

2020 – 2025:
Design of short catalytic peptides and peptide assemblies (DeShPet: UIP-2019-04-7999) founded by the Croatian Science Fundation
2020 – 2021:
SARS-CoV-2 supramolecular mimetics for discovery of peptides that induce viral entrapment, funded by the University of Rijeka (UNIRI Covid-19)