VIRTUOUS

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 872181

Machine Learning Meets Molecular Dynamics for Taste Prediction

VIRTUOUS Transfer of Knowledge Workshop: Platform Evaluation and Demo Presentation

VIRTUOUS

Scuola universitaria professionale
della Svizzera italiana

SUPSI

November 17th and 18th, 2022

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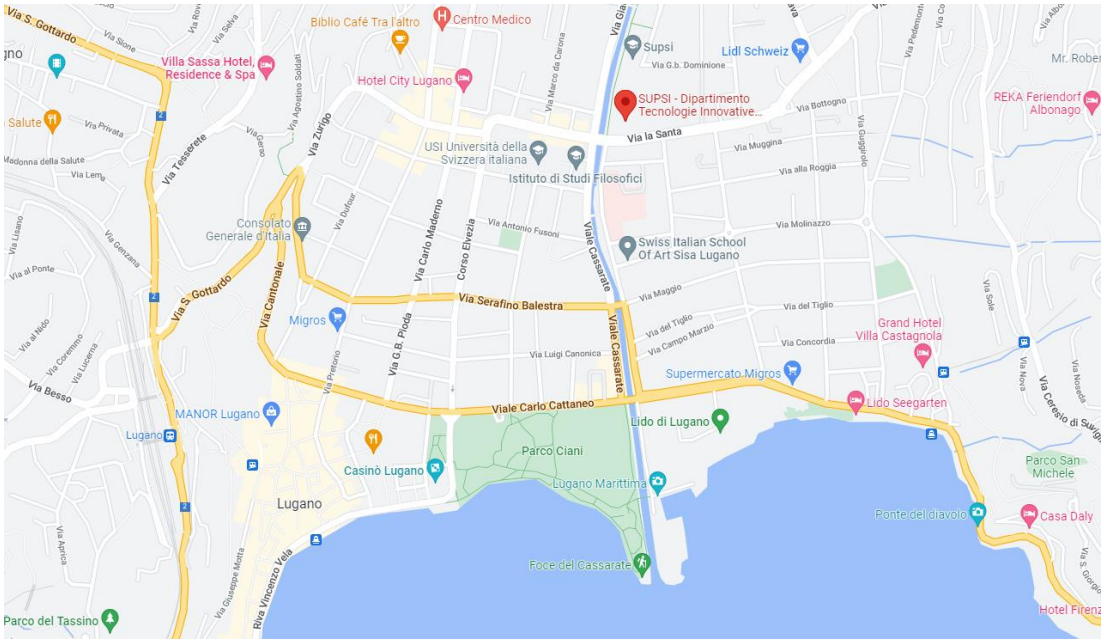
The EU MCSA VIRTUOUS project aims to create a virtual tongue through an integrated computational framework able to screen food for natural ligands targeting taste receptors. VIRTUOUS integrates drug discovery techniques, big-data and machine learning algorithms to predict the organoleptic profile of Mediterranean ingredients based on their chemical composition. Recent developments in the VIRTUOUS project will be presented in the workshop, ranging from new algorithms for advanced modelling simulation, machine learning tools to identify the most relevant descriptors affecting compounds' taste, and standardized procedures for sensory analysis of virgin olive oils. New results on application of artificial intelligence for quality assessment of extra-virgin olive oil from fluorescence spectrum will be shown. Finally, a first DEMO of the Virtuous platform will be presented.



Polo Universitario Lugano, Campus Est, Via la Santa 1, CH 6962 Lugano-Viganello, Switzerland

Rooms: C1.02 (17th November); A1.02 (18th November).

Contacts:

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Gianvito Grasso, gianvito.grasso@supsi.ch

Online participation: The workshop will be in presence. People who intend to attend the workshop remotely can write an email to dario.piga@supsi.ch to receive an MS Teams link to the workshop.

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Workshop Agenda

Day 1: November 17th, 2022, Room C1.02

Time	*Title/Topic*	*Speaker*
08:45-09:00	**Welcome**	Prof. Marco Deriu (POLITO) Dr. Dario Piga (SUPSI)
09:00-9:45	**Virtual Screening for Small Molecule Design and Discovery: from Machine Learning to Advanced Molecular Simulation Techniques**	Dr. Gianvito Grasso (SUPSI)
09:45-10:15	***Coffee break***	
10:15-11:15	**Machine learning for classification of sweeteners/bitterants compounds (methodology)**	Dr. Dario Piga (SUPSI)
11:15-12:15	**Machine learning for classification of sweeteners/bitterants compounds (hands-on session)**	Dr. Gabriele Maroni (SUPSI)
12:15-14:00	***Lunch break***	
14:00-14:30	**Sensory Analysis of Virgin Olive Oils**	Prof. Vanessa Martos (UGR)
14:30-15:15	**Taste GPCRs and their ligands: learning from data, big and small**	Prof. Masha Niv (HUJI)
15:15-15:45	***Coffee break***	
15:45-16:15	**Fluorescence Spectroscopy with Machine Learning for Rapid Quality Assessment of Extra-Virgin Olive Oils**	Dr. Manas Mejari (SUPSI)
16:15-16:45	**Advanced machine learning for Innovative Drug Discovery - the H2020 MSCA AIDD project**	Dr. Michael Wand (SUPSI)
16:45-17:15	**Feedback from the audience**	Moderator: Dario Piga
17:15	***Closure of Day 1***	

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Day 2: November 18th, 2022, Room A1.02

Time	*Title/Topic*	*Speaker*
08:45-09:30	**VIRTUOUS: where we are and where we are going**	Prof. Marco Deriu (POLITO)
09:30-10:00	**Extraction of physicochemical properties from the fluorescence spectrum with 1D convolutional neural networks: Application to olive oil**	Dr. Umberto Michelucci (Toelt)
10:00-10:30	***Coffee break***	
10:30-11:15	**Insight into the Virtuous Platform: design and implementation of a user-friendly web service to predict the organoleptic profile of the Mediterranean ingredients**	Lorenzo Pallante (POLITO)
11:15-11:45	**Feedback from the audience**	Moderator: Dario Piga
11:45	***Closure of WORKSHOP***	
12:00-13:30	**Executive board meeting**	All project partners
13:30	**Closure of Day 2**	

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Virtual Screening for Small Molecule Design and Discovery: from Machine Learning to Advanced Molecular Simulation Techniques

Speaker: Gianvito Grasso, Scuola Universitaria Professionale della Svizzera Italiana (SUPSI), Dalle Molle Institute for Artificial Intelligence (IDSIA), Lugano, Switzerland

The Virtuous project (https://virtuoush2020.com/) aims at integrating several computational methodologies applied to compound design and ligand-target interaction property prediction with the final aim of predicting the organoleptic profile of Mediterranean ingredients and their effects on human homeostasis. A major benefit of Virtual Screening is that it conducts efficient in-silico searches over millions of compounds, increasing the yield of small molecule design and discovery. As machine learning has become increasingly important in several scientific and technological fields in recent years, it has also been applied to virtual screening in various forms. This talk presents an overview of the challenges involved in utilising machine learning to perform small molecule virtual screening, a comparison of the most commonly used tools, as well as the techniques currently employed to reduce the time and cost of small molecule development. Moreover, the final considerations demonstrate the importance of using advanced molecular simulations in order to extract detailed information about the protein-ligand conformational properties and dynamics.

Speaker biography

Gianvito Grasso is researcher and lecturer at the Dalle Molle Institute for Artificial Intelligence, which is a research institute affiliated both at the University of Italian Switzerland (USI) and the University of Applied Sciences and Art of Southern Switzerland (SUPSI). He received the master's degree in Biomedical Engineering in 2015 and the Ph.D. in Computational Science in 2018 from University of Italian Switzerland. His research activities are mainly focused on computer simulations and artificial intelligence techniques applied to investigate the mechanical properties of subcellular structures such as cell membranes, protein filaments and protein aggregates. His research interests are also computational molecular biophysics, drug delivery systems, nanoparticles design, molecular mechanism of protein-protein, protein-ligand, and protein-nucleic acid interactions. He is author of more than 40 publications among international peer-reviewed papers, book chapters and conference proceedings. He serves as a Reviewer for more than 30 international scientific journals in the field of computational science and molecular biophysics. He is part of the International Editorial board of the Journal of Molecular Graphics and Modelling. His full list of publications is available at: https://www.researchgate.net/profile/Gianvito_Grasso

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Machine learning for classification of sweeteners/bitterants compounds

Speaker: Dario Piga, Scuola Universitaria Professionale della Svizzera Italiana (SUPSI), Dalle Molle Institute for Artificial Intelligence (IDSIA), Lugano, Switzerland

Speaker: Gabriele Maroni, Scuola Universitaria Professionale della Svizzera Italiana (SUPSI), Dalle Molle Institute for Artificial Intelligence (IDSIA), Lugano, Switzerland

In these two lectures, bitter-sweet taste prediction through supervised learning methodologies will be presented. In order to derive an explainable predictive model, a clustering-based algorithm aiming at identifying the most informative compounds' features will be described, and pitfalls of standard feature selection methods will be discussed. Theoretical and methodological aspects will be covered in the first lecture, while an hands-on Python session will be held in the second lecture, where the described methodologies will be implemented in a Jupyter notebook, using real datasets available in the literature.

Speakers biography

Dario Piga received the Master's degree in Mechatronics Engineering in 2008 and the Ph.D. in Computer Science and Systems Engineering in 2012 both from the Politecnico di Torino, Italy. From January 2015 to January 2017 he was Assistant Professor at the IMT School for Advanced Studies Lucca (Italy). Since 2017 he has been Senior Researcher at the IDSIA - Dalle Molle Institute for Artificial Intelligence (Lugano, Switzerland), founder and head of the "learning for optimization and control group". He has co-authored more than 140 peer-reviewed scientific papers in leading international journals and conferences in the fields of machine learning, control theory, and nonlinear optimization. He has collaborated with international companies and coordinated several research projects for the development of innovative AI-based systems in the manufacturing, transportation, biomedical and chemical industry. He is Associate Editor of the IFAC journal Automatica and of the IEEE-CSS Conference Editorial Board.

Gabriele Maroni received the Master Degree in Computer Science Engineering cum laude in 2016 and the Ph.D. in Engineering and Applied Sciences in 2019 both from Università degli Studi di Bergamo. In 2016 he worked as Data Scientist at Reply S.p.A. (MIlano, Italy), from October 2019 to November 2021 he worked as Machine Learning Engineer at Tenaris S.A. (Dalmine, Italy). Since November 2021 he is Researcher at IDSIA - Dalle Molle Institute for Artificial Intelligence (Lugano, Switzerland). He has years of experience working on both theoretical and applied research focused on Machine Learning and Control Theory techniques applied to interdisciplinary sectors such as Financial, Medical and Manufacturing. During his spare time he actively participates in data science competitions through the Kaggle platform.

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Sensory Analysis of Virgin Olive Oils

Speaker: Vanessa Martos

The evaluation of the sensory properties and determination of the importance of these properties in consumer product acceptance represent a major accomplishment in sensory analysis. Most of the sensory evaluation carried out by a trained panel involves measurement in two main areas, difference testing and descriptive analysis. Sensory difference tests are procedures used to determine whether judges can distinguish between two similar stimuli. In terms of food, the two stimuli are two very similar food samples. These evaluations are used to determine whether slight changes occur due to either product reformulation or the change in technological processing. Difference tests are particularly well adapted to the assessment of vegetable oils during their processing, being used to control refining efficiency. The introduction of the Panel Test has led to an evolution in the concept of oil quality. The necessary cognitions are set in order to carry out the sensory analysis of virgin olive oil. It tries to standardise the behaviour and procedures of the tasters, who should take into consideration not only the more general indications but also those specific for tasting olive oil. These procedures have led to an evaluation sheet being drawn up by the International Olive Oil Council (IOOC), leading to results being obtained from different Panels, in different areas of the same country as well as different countries to be compared.

Speaker biography

Vanessa Martos, Graduate in Pharmacy of the UGR (1998). Graduate thesis awarded special prize (2001). Professor of Dpto. Plant Physiology, Universidad of Granada since 2000, Teaching experience: in 5 degrees from 2000, Biology,Biotechnology, Biochemistry, Pharmacy and Environmental Science. Full Professor at the Department of Plant Physiology UGR since May, 2022. Deputy Head of the Mediterranean Centre and Deputy Head of the Centre for Development Cooperation Initiatives (CICODE) at the University of Granada. She has co-authored more than 60 peer-reviewed scientific papers in leading international journals and conferences in the fields of precision agriculture, design of state-of-the-art biofertilisers, and sensory and chemical analysis of products of interest in the Mediterranean Basin.

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Taste GPCRs and their ligands: learning from data, big and small

Speaker: Masha Niv, The Robert H Smith Faculty of Agriculture, Food and Environment, The Hebrew University of Jerusalem, Israel

Taste is a major driver of food choice and consumption. Ligands of taste GPCRs are numerous, chemically diverse and often have multiple biotargets. Extraoral expression of taste receptors suggests that yet unknown, endogenous ligands and modulators may be essential for their physiological roles. We integrate machine learning and modeling with experimental testing to obtain a deeper understanding of the bitter and sweet chemical space and its biological implications. I will present the BitterDB database of bitter molecules (*1*) and machine learning approaches BitterIntense(2) for intense bitterness prediction, and BitterMatch(3) that matches molecules to bitter taste receptors. I will share insights from applying these tools to large chemical datasets, and then introduce an iterative data-driven approach that led us towards discovery of several T2R14 antagonists. While bitter taste recognition is achieved by multiple T2R subtypes, typically via their orthosteric binding sites, the versatility of T1R2/T1R3 heterodimeric sweet taste receptor is facilitated by multiple binding sites. I will present our recent findings on T1R2 and T1R3 roles in recognition of sweet molecules.

The implications of the findings will be discussed in the context of food and drugs.

1. A. Dagan-Wiener *et al.*, BitterDB: taste ligands and receptors database in 2019. *Nucleic Acids Res* **47**, D1179-D1185 (2019).

2. E. Margulis *et al.*, Intense bitterness of molecules: Machine learning for expediting drug discovery. *Comput Struct Biotechnol J* **19**, 568-576 (2021).

3. E. Margulis *et al.*, BitterMatch: recommendation systems for matching molecules with bitter taste receptors. *J Cheminform* **14**, 45 (2022).

Speaker biography

Masha Niv received her PHD in theoretical chemistry from the Hebrew University, Israel in 2001, was a team leader in a biotech company Keryx Biopharmaceuticals 2001-2003, and a postdoctoral fellow and then instructor in Computational Biomedicine at Weill Medical College, Cornell University NY, US 2003-2007. She opened her lab at the Faculty of Agriculture, Food and Environment at the Hebrew University in 2007, where she is currently a tenured full professor. The Niv lab combines computational, cell-based and behavior approaches to study taste and develops the BitterDB database of bitter compounds, used by tens of thousands users worldwide. Prof. Niv co-initiated and co-lead the Global Consortium for Chemosensory Research (GCCR) that made key contributions to understanding COVID-19 chemosensory loss and recovery, and established the GPCRladies repository of women scientists in the field of GPCR. She serves on the Editorial Board of the Chemical Senses and on Scientific Advisory Boards of several companies.

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Fluorescence Spectroscopy with Machine Learning for Rapid Quality Assessment of Extra-Virgin Olive Oils

Speaker: Manas Mejari, Scuola Universitaria Professionale della Svizzera Italiana (SUPSI), Dalle Molle Institute for Artificial Intelligence (IDSIA), Lugano, Switzerland

In this talk, the application of fluorescence spectroscopy combined with machine learning methods to analyze the quality of extra virgin olive oils is presented. Fluorescence spectroscopy offers the advantage of being an optical non-invasive and contactless measuring technique that does not require complex and costly instrumentation and sample preparation. In this work, 24 different types of commercially available extra virgin olive oils were analyzed using the fluorescence measuring technique during accelerated ageing under controlled conditions. For the quantitative assessment of the quality of the oils, the UV-spectroscopy parameters defined by the European Commission norm No. 2568/91 were also measured at all the stages of the ageing process. The fluorescence data were analyzed to identify the most important regions of the fluorescence fingerprint to detect ageing processes in the oil and to develop models using machine learning techniques to identify from these markers whether a given oil is extra virgin olive oil or not. The developed models are able to distinguish between the EVOO and non-EVOO oils with a high classification accuracy. The obtained results highlight that it is possible to extract relevant features from the florescence fingerprints of oil and to predict with high accuracy whether a given oil is EVOO or not. The identification of the "fluorescence markers" allows the ideation of a future innovative new generation of intelligent optical sensors for the accessible and easy analysis of food quality. The methods investigated in this work are, in principle, not limited to olive oil and could be applied to other edible substances that exhibit fluorescence, like wine or honey.

Speaker biography

Manas Mejari received his M.Tech. degree in Control Systems from University of Mumbai (India) in 2013 and his Ph.D. in Control Systems from IMT School for Advanced Studies Lucca (Italy) in 2018. He held a postdoctoral position at the University of Lille (France) in 2018-2019. Currently, he is a researcher at IDSIA Dalle Molle Institute for Artificial Intelligence, SUPSI-USI (Switzerland). His research interests include system identification, machine learning and automatic control.

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Advanced machine learning for Innovative Drug Discovery - the H2020v MSCA AIDD project

Speaker: Michael Wand

In this talk, the H2020 Marie Sklodowska-Curie project AIDD (Advanced Machine Learning for Innovative Drug Discovery, https://ai-dd.eu) will be presented.

The goal of AIDD is to apply high-end machine learning techniques in the field of chemistry and pharmaceutics. Modern organic chemistry presents a variety of tasks which are frequently not straightforward and require chemical engineers with excellent knowledge; such tasks include e.g. retrosynthesis (find a way to synthesize a desired product from available ingredients), learning representations of complex molecules, or predicting the outcome of a chemical reaction, which may not only depend on the reactants, but also on environmental conditions (temperature, solvents, etc.). Solving such tasks efficiently with little or no human intervention is of utmost interest both in research and for industrial applications, since it allows faster and more efficient processes, as well as the development of new chemical products, e.g. for medical uses.

Speaker biography

Michael Wand has received his Diploma degree in Mathematics in 2007 and his PhD degree in Computer Science in 2014, both from University of Karlsruhe/Karlsruhe Institute of Technology in Germany. His field of interest is the theory and practice of applying state-of-the-art Machine Learning techniques to real-life data, in particular to biophysiological data which is recorded from the human body via a variety of sensors. Processing such data is highly relevant for applications in medicine, physiology, and rehabilitation.

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VIRTUOUS: where we are and where we are going

Speaker: Marco Agostino Deriu

In this talk, the coordinator will provide a comprehensive overview of what has been done by the consortium during the first three years of the VIRTUOUS project in terms of research carried out, collaborations activated, and dissemination and communication activities. The narrative will be an opportunity to propose the consortium's plan for the activities to be carried out in the last year, with a focus on the organization of organoleptic tests, validation of the platform, and future developments of VIRTUOUS beyond the end of the project. At the end of the presentation, the coordinator will stimulate discussion and participation of users by asking for opinions on the proposals presented and any further suggestions.

Speaker biography

Marco A. Deriu is Professor of Industrial Bioengineering at Politecnico di Torino. Coordinator of two European Projects: VIRTUOUS, H2020-MSCA-RISE-201, Grant agreement ID: 872181; PARENT, H2020-MSCA-ITN-2020, Grant agreement ID: 956394. Awarded by Telethon foundation for research on a rare infantile-onset neurodegenerative disease. His research focuses on computational modelling and data analysis applied to investigate mechanisms behind biological, physiological and pathological functions, to interpret and treat biophysical, biological and clinical data, to build prediction models in physiology and physiopathology. In this context, he employs multiscale modelling and machine learning techniques to unravel how molecular events drive cell, tissue and organ level behaviour. He teaches "Multiscale Biomechanics", "Biomechanical Design", and "Rational Drug Design: Principles and Applications" at Politecnico di Torino. He is author of several publications in International peer-reviewed Journals, book chapters and proceedings in the field of computational modelling applied to Bioengineering, Biophysics, Molecular Biology and Medicine.

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Extraction of physicochemical properties from the fluorescence spectrum with 1D convolutional neural networks: Application to olive oil

Speaker: Umberto Michelucci

One of the main challenges for olive oil producers is the ability to assess oil quality regularly during the production cycle. The quality of olive oil is evaluated through a series of parameters that can be determined, up to now, only through multiple chemical analysis techniques. This requires samples to be sent to approved laboratories, making the quality control an expensive, time-consuming process, that cannot be performed regularly and cannot guarantee the quality of oil up to the point it reaches the consumer. This work presents a new approach that is fast and based on low-cost instrumentation, and which can be easily performed in the field. The proposed method is based on fluorescence spectroscopy and one-dimensional convolutional neural networks and allows to predict five chemical quality indicators of olive oil (acidity, peroxide value, UV spectroscopic parameters K270 and K232, and ethyl esters) from one single fluorescence spectrum obtained with a very fast measurement from a low-cost portable fluorescence sensor. The results indicate that the proposed approach gives exceptional results for quality determination through the extraction of the relevant physicochemical parameters. This would make the continuous quality control of olive oil during and after the entire production cycle a reality.

Speaker biography

Umberto Michelucci is a cofounder and the chief AI scientist of TOELT LLC, a company aiming to develop new and modern teaching, coaching, and research methods for AI to make AI technologies and research accessible to every company and everyone. He's an expert in numerical simulation, statistics, data science, and machine learning. In addition to several years of research experience at the George Washington University (USA) and the University of Augsburg (DE), he has 15 years of practical experience in the fields of data science and machine learning. His first book, Applied Deep Learning—A Case-Based Approach to Understanding Deep Neural Networks, was published by Springer in 2018 and its second edition in 2022. He has published a second book, Convolutional and Recurrent Neural Networks Theory and Applications in 2019.
He's very active in research in the field of artificial intelligence. He publishes his research results regularly in leading journals and gives regular talks at international conferences. Umberto is a lecturer at the Lucerne University of Applied Sciences for deep learning and neural networks theory and applications. He is also a Google Developer Expert in Machine Learning based in Switzerland. He holds a PhD in Machine Learning.

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Insight into the Virtuous Platform: design and implementation of a user-friendly web service to predict the organoleptic profile of the Mediterranean ingredients

Speaker: Lorenzo Pallante

The Virtuous project (https://virtuoush2020.com/) aims at creating a virtual tongue able to predict the organoleptic profile of Mediterranean ingredients and their effects on human homeostasis and health status. One of the major scientific objectives of the Virtuous project is the development of a user-friendly web service as a decision-supporting tool (DST) for a wide range of experts and users. In detail, the platform is designed and implemented with the ultimate goal of allowing its usage and application not only to highly specialized personnel with powerful computational machines and extensive bionformatic expertise, but also to clinicians, dieticians or pathologists specializing in diets for patients with diabetes, food companies, and other professionals not expert in computational modelling or ICT. In the present talk, the main concept underlying the Virtuous platform design will be introduced and its first DEMO, including the latest taste predictors and functionalities, will be presented. In detail, the talk will cover the main aspects related to the implementation of the back end, i.e. the web service that runs on the cloud, and the relative easy-to-use front-end, which is the part of the application that is visible to the users and runs on their devices. Finally, the roadmap to the final version of the Virtuous platform scheduled for 2024 will be outlined.

Speaker biography

Lorenzo Pallante (Italy, born in 1994) is currently a PhD Student at the Department of Mechanical and Aerospace Engineering of Politecnico di Torino under the supervision of Prof. Marco Agostino Deriu within the Mechanistic and Machine Learning-driven Modelling in Bioengineering (M3B) group (https://m3b.it/). Mr Lorenzo Pallante received his B.Sc. in Biomedical Engineering from Politecnico di Torino (Turin, Italy) in 2016. In 2019, he received his M.Sc. cum laude in Biomedical Engineering from Politecnico di Torino (Turin, Italy). Since November 2019, he is enrolled in a joint PhD programme of the University of Turin and the Politecnico di Torino in Bioengineering and Medical-Surgical Sciences focused on the molecular basis of subcellular mechanics, investigated using computational modelling techniques, e.g. molecular dynamics, ensemble molecular docking, metadynamics, free energy calculations, rational drug design, and artificial intelligence tools, such as machine learning-based algorithms and pathway network modelling. His researches mainly focus on the understanding structure-to-function relationships in protein physiological and pathological behaviour. He is also the author of 7 papers in peer-reviewed journals and has participated in three international conferences also as a speaker.