H2020-MSCA-RISE-2019 GA 872181 – VIRTUOUS

VIRTUOUS Transfer of Knowledge (ToK) Workshop:

"Omics, Machine Learning and Molecular Modelling Targeting Taste and Nutrition"

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Nutrients modulate the key mechanisms driving cellular, tissue, organ and system level machineries in the human body. In this concern, predictive models of ligand protein interactions, protein cascades, cell activation, personalized food metabolism/taste deserve high attention being them a crucial breakthrough to provide insight in complex biological mechanisms regulating long term favorable effects to human homeostasis. Unified interdisciplinary approaches based on multidisciplinary competences will help to develop computational models in a multiscale/multiphysics fashion, moving from chemistry to structure, from structure to function. This groundbreaking vision has the capability of revolutionizing the way we understand, model and treat physiological and pathological phenomena concerning the human being toward a deeper understanding of fundamental mechanisms of life, to develop new strategies against diseases and assist us in visualizing the effects of novel treatment options, such as a diet, a nutrition supplement, a drug or a combination of them. In this context, the present Workshop explores the state of the art of omics, ontologies, bioinformatics, machine learning driven mechanistic modelling to elucidate nutrient pathways from molecular interactions to organ/system level properties and to predict long term effects of food nutrients on human homeostasis, considering also the environmental conditions.

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VIRTUOUS Transfer of Knowledge (ToK) Workshop*:*

InSyBio | Intelligent Systems Biology

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Workshop Schedule

Day 1: 9th of December 2020

VIRTUOUS ToK Workshop will be held remotely.
up to 100 attendants with registration required.

TIME	TITLE/TOPIC	SPEAKER
09*:30-09:45*	***Introductory statement by Project's Coordinator and workshop's organisers***	***Dr. Kostantinos Theofilatos, Prof. Marco A. Deriu***
09*:45-10:30*	***Profiling of Human Biological Fluids for Personalized Nutrition.*** *The lecture will provide information on proteomic methods in pre-clinical and clinical research. In detail, the developments concerning an Integrated Proteomic Toolbox for the Wet and Dry Laboratories will be described.*	***Dr. Ornella Cominetti & Dr. Loic Dayon (Nestle Research, Switzerland)***
10*:30-11:15*	***Taste and Nutrition from a Clinical Perspective*** *The lecture will introduce to the clinical perspective concerning relationships among nutritional aspects and taste with focus on Mediterranean Diet and examples considering the importance of the above mentioned relationships in clinics related to intolerances, and non communicable diseases.*	***Dr. Cinzia Myriam Calabrese (POLITO)***
11*:15-****12****:00*	***Molecular Modelling, ligand-protein interactions and application on taste receptors*** *The lecture will present main concept related to molecular modelling and applications related to the investigation of ligand protein interactions with focus on ligand-protein binding affinity and*	***Dr. Gianvito Grasso (SUPSI)***

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	ligand effects on protein activity (agonist/antagonist, etc..)	
12:00-12:45	***Bioinformatics & Machine Learning in Nutrition and Diet Research*** *The lecture will introduce participants to basic bioinformatics analysis for the application of network analytics, pathway analysis, machine learning, functional enrichment analysis and other bioinformatics tools and methods (using free and commercial tools with user friendly interfaces) with examples and emphasis given in the application of these techniques in nutrition and diet research.*	**Dr. Konstantinos Theofilatos (InSyBio)**
12:45-14:00	***An overview of Machine Learning and its applications in the field of Nutrition, Food Quality and Diet Research*** *This lecture will introduce participants to Artificial Intelligence from basic concept to applications in the field of Nutrition, Food Quality support tools and Diet Research*	**Dr Dario Piga (SUPSI)**
14:00-15:00	**break**	
15.00-15.45	***Keynote talk - Geospatial Information and Crop monitoring by smart processing of data from European Copernicus satellites.*** *The keynote will present participants the satellite technology from the Copernicus European Program and how can it be used for the agricultural sector.*	**Dr. Pablo Romero (ENGINLIFE), (also co-founder and CEO of Graniot)**
15:45-17:15	***Students Quickfire Presentations: Molecular Modelling, Protein-Protein Network, Machine Learning***	**PhD Students till 6 (15 minutes each)**
17:15-17:30	***Concluding Remarks***	

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Day 2: 10ᵗʰ of December 2020

VIRTUOUS ToK Workshop will be will be held remotely.
up to 50 attendants with registration required.

TIME	TITLE/TOPIC	SPEAKER
09:30:11:30	**Hands-on Session on Bioinformatics applications in Nutrition and Diet Research** *The hands on will allow participants to play with basic bioinformatics tools for network analytics, pathway analysis, functional enrichment analysis and other bioinformatics tools.*	**A. Korfiati, S. Mavroudi (InSyBio)**
11:30-13:30	**Hands-on Session on Machine Learning** *The hands-on session will introduce the participants into machine learning, available tools and methods to access them through Python and other scripting languages. The session will also consider nutrition and diet research related datasets.*	**Dr. Umberto Michelucci (TOELT)**
13:30-13:45	**Concluding Remarks**	**Prof. Marco A. Deriu (POLITO)**

15:00-18:30	**VIRTUOUS Executive Board Meeting (Closed to Public) All Virtuous Partners**