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**NovaMechanics**

Cheminformatics & Nanoinformatics Excellence

## Individual Research Project

# Doctoral Researcher 3

## HORIZON EUROPE MSCA DOCTORAL NETWORK “MELOMANES”\*

Metastatic melanoma is a hard-to-treat disease and one of the most worrisome cancers. Traditional therapies (e.g., chemotherapy, radiotherapy) have limited efficacy as metastatic melanoma is resistant to them. At the same time, the use of single-target therapeutics often fails, due to the heterogeneity and dynamic nature of cancer cells, leading to the need for combination therapies.

The development of anticancer immunotherapies, and chimeric antigen receptor (CAR)-T cells in particular, has shown great promise. Nevertheless, the physical barriers represented by cellular and non-cellular components of the tumor microenvironment combined to the abnormal tumor vasculature and high interstitial fluid pressure, hamper the efficient tumor infiltration of CAR-T cells. MELOMANES is a network of 18 partners (including 10 non-academic partners) aiming to train 12 Doctoral Researchers for the development of a combined therapy. This therapy will exploit the properties of magnetic nanoparticles to induce damage on the tumor microenvironment by magnetic and optic hyperthermia to facilitate the infiltration of CAR-T cells. Research and transferable training of the doctoral researchers will be performed in a highly interdisciplinary, intersectoral, and international environment. In addition to acquiring skills related to the research project, they will be trained in open science, communication and dissemination, responsible research and innovation, circular economy, ethics, data management, entrepreneurship, marketing, intellectual property, and gender dimension in research as well. Their competences will be validated through certification and qualification examination, allowing a new generation of highly skilled doctoral researchers to emerge with high-level training in the multidisciplinary field of nanomedicine.

*\*Project funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them.*

## DESCRIPTION OF THE INDIVIDUAL RESEARCH PROJECT

The Doctoral Researcher (DR) student will develop novel computational techniques for the calculation of electrochemical, atomistic, and other types of nanodescriptors. The DR will use these to develop validated and robust predictive machine learning/artificial intelligence models for the risk assessment of iron carbide NanoParticles (NPs) used in NanoMedicine and applicable in Metastatic Melanoma therapy. Upon graduation, the DR is expected to have acquired the soft and hard skills required to solve cutting-edge machine learning and artificial intelligence problems. To achieve this, the DR will benefit from a multidisciplinary environment and collaboration between NovaMechanics Ltd (NovaM), the Swiss Federal Laboratories for Materials Science and Technology (EMPA), and the Vrije University Foundation (Stichting VU).



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## Objectives

- 1) Development of computational and in silico approaches to extract the maximal knowledge possible from experimental datasets.
- 2) Establishment of statistically significant relationships between measured biological activity profiles of the multifunctional iron carbide NPs and their physical, chemical, and biological properties.
- 3) Implementation of novel machine learning/artificial intelligence techniques for the predictive modelling and clustering of multiple applications and validation of these machine learning models by laboratory and real-world results.

## Methodology

The DR will digitally reconstruct iron carbide NPs of different sizes and calculate electrochemical, atomistic, and/or other types of nanodescriptors. In parallel, the DR will study the literature to find/extract laboratory real-world results and experimental datasets to develop validated and robust predictive machine learning/artificial intelligence models for the Risk Assessment (RA) and the Life Cycle Assessment (LCA) of iron carbide NPs in NanoMedicine (Metastatic Melanoma therapy). The DR will use the KNIME nodes and Isalos Analytics Algorithms developed by NovaM and develop novel algorithms and concepts to fully extract and exploit the knowledge from experimental datasets. Different iron carbide NPs will be digitally reconstructed to study the effects of different parameters (e.g., coatings, functionalisation) on the Metastatic Melanoma therapy, as well as the effect of the adsorption of metastatic melanoma drug molecules on the surface of iron carbide NPs.

## Expected Results

- 1) Development of novel techniques for the calculation of nanodescriptors.
- 2) Development of validated and robust predictive machine learning/artificial intelligence models for the risk assessment of iron carbide NPs.

## Supervisors and host organisations

### Main supervisors and recruiting organisation:

Dr. Antreas Afantitis, *NovaMechanics Ltd*, Digeni Akrita 51, 1070, Nicosia, Cyprus

NovaMechanics Ltd is a Cheminformatics & Nanoinformatics company that develops state of the art software and user-friendly web services to facilitate accessibility, and integration within drug discovery, materials design, and patient stratification decision-making frameworks. NovaMechanics Ltd participates as a major partner or coordinator >30 Research Projects having collaboration in the field of NanoMedicine with many universities, institutes, and companies around the world.

### Co-supervisor (academic partner):

Prof. Vangelis Harmandaris, SimEA Era-Chair, CaSToRC, The Cyprus Institute K. Kavafi 20, Nicosia, 2121, Cyprus



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Dr. Frank Kupper, *Vrije University Foundation (Stichting VU)*, De Boelelaan 1105, 1081 HV, Amsterdam, Netherlands

Dr. Roland Hischier, *Swiss Federal Laboratories for Materials Science and Technology (EMPA)*, Lerchenfeldstrasse 5, 9014, St. Gallen, Switzerland

### Planned mobility track and secondments:

1) Four (4) months (i.e., from the 12<sup>th</sup> to the 15<sup>th</sup> month of the project) at Swiss Federal Laboratories for Materials Science and Technology, Switzerland to work on an interface for a more direct/better integration of the results from toxicological investigations into the RA/LCA methodologies.

2) Six (6) months (i.e., from the 25<sup>th</sup> to the 30<sup>th</sup> month of the project) at Stichting VU, Netherlands to work on the integration of the Responsible Research and Innovation (RRI) framework to open-up innovation processes for reflection and learning to co-create solutions and new responsible business opportunities

### Enrolment in Doctoral School:

The Cyprus Institute K. Kavafi 20, Nicosia, 2121, Cyprus

## TERMS AND CONDITIONS FOR EMPLOYMENT

### Duration

36 months

### Gross Salary (total cost with Cyprus coefficient):

2635€/per month

### Other allowances

Mobility allowance 600€/per month (gross-total cost), family allowance if applicable 660€/per month (gross -total cost)

## THE CANDIDATE PROFILE

### Academic prerequisite

We are looking for a Doctoral Researcher with a 5-years Diploma (or integrated MSc) degree in Chemical Engineering (preferred) or related fields. Candidates holding less than 5-years bachelor's degree in Chemical Engineering (or related field) should hold an M.Sc. degree in Chemical Engineering (or a related field).

### Technical skills and knowledge required



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- High grades in relevant courses (Mathematics, Biology, Computer Programming, Thermodynamics, Physical Chemistry, Transport Phenomena, Process Control, etc.)
- English at least C1 level
- Strong programming skills (Python, KNIME, Fortran, MATLAB, etc.)
- Related research or working experience in the field of Nanoinformatics, Computational Mechanics, Electrochemistry, or a related field (a web hyperlink of their Diploma or Master Thesis could be included in the attached CV)
- Good knowledge of Linux operating system (i.e., writing bash scripts)
- Knowledge of KNIME, Isalos Analytics and COMSOL software
- Experience with extensive literature searches and systematic reviews and QC of the results

### Soft skills

- Great sense of thoroughness and organization
- Dynamism, problem-solving, and autonomy
- Writing skills in English and ability to summarize are essential
- Strong Motivation to invent new scientific algorithms/methodologies

### Exclusion criteria a M.Sc. degree

The candidate, at the time of recruitment, must hold a 5-years Diploma (or integrated MSc) degree in Chemical Engineering (preferred) or related fields. Candidates holding less than 5-years bachelor's degree in Chemical Engineering (or related field) should hold an M.Sc. degree in Chemical Engineering (or a related field).

The candidate must not have resided or carried out their main activity (work, studies, etc.) in Cyprus for more than 12 months in the 3 years immediately before the recruitment date. Compulsory national service, short stays such as holidays, and time spent as part of a procedure for obtaining refugee status under the Geneva Convention are not considered.

The candidate, at the time of recruitment by **NovaMechanics Ltd** (Cyprus), must not be enrolled in a doctoral school or have been awarded a doctoral degree.

## WHAT WE OFFER

- An enrolment in a PhD program;
- An international work environment, in which doctoral researchers can develop their skills and innovate within a highly-skilled team;
- An attractive 36 months' salary;
- An individual and well-structured scientific and transferable training (open science, responsible research and innovation, circular economy, ethics, data management, entrepreneurship, creativity, communication, career plans and gender balance in science) within the Melomanes network.



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## APPLICATION PROCEDURE

- Motivation letter (max. 2 pages);
- CV including the details of education/qualifications, work experience, language skills, and other relevant skills; indication of at least two Scientists for reference letters (academic and/or non-academic);
- Certified/signed copy of a recent transcript of exams taken with respective marks.
- A certified/signed copy of a Master of Science certificate or a letter from the Head of the degree course stating that the Student is going to finish before September 2023;
- A summary of relevant research projects/activities (max. 5 pages).

Applicants can apply for up to 3 projects within the consortium, indicating the order of preference.

All applications will be checked for eligibility (in particular, the adherence to the mobility rule). Incomplete applications will be ignored. Shortlisted candidates will be invited for an interview. Candidates will be notified of the outcome. Start of employment is foreseen September-October 2023.

If you are highly motivated and interested in doing research in an internationally oriented and highly successful network, you should send your application to [hr\[at\]novamechanics\[dot\]com](mailto:hr@novamechanics.com) with Ref: MarieCurie2023-NanoMedicine.

### Equal opportunities

Equal opportunities policy without distinction on the grounds of gender, racial or ethnic origin, religion or belief, disability, age, or sexual orientation will be applied.

The selection is not limited to EU citizens; therefore, candidates can be of any nationality.

**Apply for this position at [hr\[at\]novamechanics\[dot\]com](mailto:hr@novamechanics.com)  
before the 15<sup>th</sup> April 2023**