

# The Advanced Machine Learning for Innovative Drug Discovery (AIDD) project

Newsletter 1, May 2021



The **Advanced Machine Learning for Innovative Drug Discovery (AIDD)** project is a Marie-Sklodowska-Curie Innovative Training Network (ITN) for Early Stage Researchers (ESRs) funded by the European Commission under the Horizon

2020 Programme, [Marie Skłodowska-Curie grant agreement No 956832](#). The project brings together fifteen academic and industry partners from ten European countries and the University of British Columbia (Canada) to train sixteen PhD students in close collaboration with associated partners from the USA, Australia, China, Israel and further countries.

## Project development

The **AIDD project started on 01.01.2021** and on 26.01.2021 the online kick-off meeting of the project was held, with introductory presentations of the partners. Within February 2021 the job advertisements for the ESRs were elaborated and a major recruitment campaign started. By the mid of March 2021, the job advertisements had been published on the project's website, on [CCL.net](#), [LinkedIn](#) (in several channels), twitter, [nature.com](#) and [Mendeley](#). Following the application deadline on 18.04.2021, an online interview process was set up and by 20.05.2021 all **15 ESRs had been selected**. Most of the ESRs are scheduled to start their work in September 2021.

## The AIDD consortium

[The AIDD consortium](#) consists of 15 beneficiaries (and one special Partner outside the EU) which will host and train 15 (+1) ESRs, as well as 12 associated partners that will provide additional training. The network includes the academic institutions in Europe that are currently most experienced in chemoinformatics education and investigators from leading European large pharmaceutical companies, as well as a number of innovative scientists and entrepreneurs. Thus the AIDD project brings together the leading investigators from academia and the pharmaceutical industry across Europe.

## Beneficiaries

**HelmholtzZentrum münchen**  
Deutsches Forschungszentrum für Gesundheit und Umwelt

[Helmholtz Zentrum München](#) is the **German Research Center for Environmental Health**. It investigates important

common diseases which develop from the interaction of lifestyle, environmental factors and personal genetic background, focusing particularly on diabetes mellitus and chronic lung diseases. Helmholtz Zentrum München is a research institution of the Federal Republic of

Germany and the Free State of Bavaria and is also a member of the [Helmholtz Association of German Research Centers](#).

Excellent basic research is the foundation of scientific work at Helmholtz Zentrum München to which **40 scientific institutes and departments** contribute. Their scientific competencies are linked with regard to content and thematically through strategic programs of the Helmholtz Association and are financed through program-oriented funding (POF). Thus, complex questions and problems relevant to science, society and the economy can be explored beyond the boundaries of institutions and disciplines.



The studies within this project will be performed in the [Chemoinformatics group](#), which is part of the [Institute of Structural Biology](#). Its main expertise in development of **computational tools for drug discovery, including Virtual Computational Chemistry Laboratory (VCCLAB)** <http://www.vcclab.org> and On-line CHEmical Modeling Environment (OCHEM) <http://ochem.eu>.



[AstraZeneca](#) (AZ) is one of the **leading research-driven biopharmaceutical companies** to span the entire value chain of a medicine from discovery, early- and late-stage development to manufacturing and distribution, and the global commercialization of primary care and specialty care medicines that transform lives. AZ employs around 70,000 people worldwide and operates in more than 100 countries. The Gothenburg R&D site is one of the major AZ research centers. The Molecular AI team in Discovery Sciences focuses on ML/AI applications in drug design. The team drives the science, builds platforms and impact projects through applying ML/AI to drug design. It has state-of-the-art computational tools and high performance computing resources. The team works in an interdisciplinary environment by closely interacting with experts from chemistry automation and medicinal chemistry, and have extensive experience working in EU and Swedish government funded projects, such as WASP, IMI2-MELLODDY, H2020-ExCAPE, H2020-BIGCHEM, etc.



[Bayer](#) is a **global enterprise with core competencies in the Life Science fields of healthcare and agriculture**. Its products and services are designed to benefit people and improve their quality of life. At the same time, the Group aims to create value through innovation, growth and high earning power. Bayer is committed to the principles of sustainable development and to its social and ethical responsibilities as a corporate citizen. In fiscal 2018, the Group employed around 117,000 people and had sales of EUR 39.59 billion. Capital expenditures amounted to EUR 1.5 billion, R&D expenses to EUR 5.2 billion.



[Janssen](#) is creating a **future where disease is a thing of the past**. Being a part of the Pharmaceutical Companies of Johnson & Johnson, the team is working tirelessly to make that future a reality for patients everywhere by fighting sickness with science, improving access with ingenuity, and healing hopelessness with heart. Main focus is on areas of medicine where the biggest difference can be made:

Cardiovascular & Metabolism, Immunology, Infectious Diseases & Vaccines, Neuroscience, Oncology, and Pulmonary Hypertension.



[Enamine](#) Ltd was founded in 1991 with the advent of high throughput screening in early drug discovery. After 25 years of stable growth **Enamine has become a world leading provider of Screening Compounds and Building Blocks**. It also offers integrated services of custom synthesis, lead optimization and molecular modeling. In Enamine, we pay great attention to the development of original and unique chemistry. We believe that diverse techniques and methodologies are the main contributors to the drug discovery process.



Aalto University

[Aalto University](#) is known for its world-class research in machine learning. For example, based on the Microsoft Academic Research citation counts **Aalto University ranked 1st in Europe (11th in the world) in Machine learning and Pattern recognition**, and currently Aalto is #3 in Computer Science in Europe (US News). Aalto runs the Finnish Center for Artificial Intelligence FCAI, Flagship of Research with 250M€ budget for 8 years, and will run the Finland node of the European Laboratory for Learning and Intelligent Systems ELLIS from 2020. Department of Computer Science at Aalto University is one of leading computer science research units in northern Europe, located at Otaniemi campus at Espoo, Finland. With more than 400 employees, the Department of Computer Science is the biggest department in Aalto University. Department is part of Aalto University School of Science.



[Freie Universität \(FU\) Berlin](#) was founded in 1948 in Dahlem, Berlin. Since 2007, FU Berlin has been consistently named **one of eleven "Excellence Universities"** within the German Excellence Initiative. FU Berlin offers a comprehensive range of studies and highly competitive programs at all academic levels, with a particularly strong reputation in mathematics as well as humanities, biology and physics. Regarding AI research, **FU Berlin focuses on machine learning for the sciences**, in particular natural sciences, as well as the connection between AI methods and mathematics. FU Berlin participates in the Berlin Big Data Center (BBDC), the Berlin Center for Machine Learning (BZML), and the Berlin Mathematics Center (MATH+). It has close collaborations and jointly funded projects with several non-university research organizations, such as the Fritz-Haber Institute, the Max-Planck Institute for Molecular Genetics, the Max-Delbrück and the Max Born Institute.

The logo for KU Leuven, featuring the text "KU LEUVEN" in white capital letters on a blue rectangular background.

KU LEUVEN

[KU Leuven](#) conducts fundamental and applied research in all academic disciplines with a clear international orientation. In the Times Higher Education ranking KU Leuven is ranked as the **12th European university**, while in the Reuters Top 100 of the World's most innovative institutions, KU Leuven is listed as the first European university. The STADIUS Center for Dynamical Systems, Signal Processing, and Data Analytics (ESAT-STADIUS) is a research division of the Electrical Engineering Department at KU Leuven, with 11 permanent staff members and about 100 PhD & postdoc researchers. Applied and fundamental research is performed in the area of control, system

identification, signal processing, machine learning, numerical optimization, and bioinformatics. The bioinformatics team at ESAT-STADIUS is a high-profile bioinformatics team with worldwide visibility. It is recognized for its pioneering work on data fusion for the prioritization of candidate disease-causing genes. The team has been developing innovative machine-learning methods for a wide range of problems in clinical genomics and drug discovery.



Founded in 1966, the [Johannes Kepler University \(JKU\)](#) is one of Austria's newer universities. This gives the JKU a unique opportunity to pursue innovative paths and many important areas of research began here in Austria - even Europe - such as **degree programs in mechatronics, computer science and since 2018 BSc & MSc program in AI**. The [LIT AI Lab](#) headed by Prof. Sepp Hochreiter was founded as a permanent research center of the Linz Institute of Technology (LIT). In the unique environment offered by the Johannes Kepler University (JKU) Linz, the LIT AI Lab bundles JKU's world-class expertise in artificial intelligence (AI) for shaping and advancing AI research and its industrial applications. With 20,000 students and approx. 3,000 employees, more than 60 fields of studies and 127 institutes, which are run by 130 professors, the JKU is Upper Austria's largest educational and research institution.

Scuola universitaria professionale  
della Svizzera italiana

The logo of SUPSI (Scuola Universitaria Professionale della Svizzera Italiana) consists of the letters 'SUPSI' in a large, bold, black, sans-serif font.

The [SUPSI \(University of Applied Sciences and Arts of Southern Switzerland\)](#) is one of the nine professional universities recognised by the Swiss Confederation. Its objective is **combining world-class research in key areas with high-quality teaching, uniting classical theoretical-scientific instruction with a professional orientation**. AIDD research partner is the [IDSIA \(Istituto Dalle Molle di Studi sull'Intelligenza Artificiale\)](#), a non-profit oriented research institute for artificial intelligence jointly affiliated with the SUPSI and the [University of Southern Switzerland \(USI\)](#).

[IDSIA](#) has developed state-of-the-art algorithms for artificial neural networks, sequence learning, evolutionary computation, control and robotics, data mining, complexity and generalization issues, swarm intelligence, operations research, mathematically optimal universal artificial intelligence and optimal rational agents. It was the smallest of the world's top ten AI labs listed in the 1997 "X-Lab Survey" by Business Week magazine. Four most valuable public companies in the world (Apple, Alphabet/Google, Microsoft, Amazon) are heavily using IDSIA's deep learning algorithms, billions of times per day. Google [DeepMind](#) is heavily influenced by IDSIA's former students, one of them co-founder, one of them first employees. Many other [IDSIA](#) alumni became professors.



tu technische universität  
dortmund

[TU Dortmund University \(TUDO\)](#) hosts 17 faculties ranging from natural sciences and engineering to social sciences and humanities. The university currently counts over 34,000 students – about 4,000 of those being international students - and 6,500 members of staff, including 300 professors. Research at TU Dortmund University is particularly renowned in **four profile areas: Materials, Production Technology and Logistics; Chemical Biology, Drug Research and Process Engineering; Data Analysis, Modeling and Simulation; Education, Schooling and**

Inclusion. TU Dortmund University presently participates in the Cluster of Excellence “Ruhr Explores Solvation (RESOLV)” and coordinates four Collaborative Research Centers.

TU Dortmund University awards more than 250 doctoral degrees per year. A core concern of TU Dortmund University is to promote young scientists – for example through a Graduate Center, the alliance with the Research Academy Ruhr and welcome services for international researchers.



Universiteit  
Leiden

[Leiden University](#) was founded in 1575 and is **one of Europe’s leading international research universities**. The Leiden Institute of Advanced Computer Science (LIACS) is the computer science institute of Leiden University, Faculty of Science, established in 1996.

It has a strong and vibrant research program in computer science with a good balance of core computer science and applications. Its key interests are in AI and data science. LIACS’ mission is to improve the state of the art in Computer Science methods, techniques and systems, and to guide new research areas that are of clear importance to society. The AI4LIFE initiative and especially its university wide SAILS program aims at improving other (especially life) sciences by making modern AI methods available to them and developing novel methods and approaches in tight collaboration with computer science and its AI research.



UNIVERSITÄT  
LUXEMBURG

[University of Luxembourg](#) ranks **17th** in the 2019 **Times Higher Education Young University Ranking** and is ranked **3rd worldwide in International Outlook**. Founded in 2003, ULUX now has 2800 employees, including **800 PhD candidates under employment contract** within **3 Doctoral Schools**. The Doctoral School in Science & Engineering offers disciplinary doctoral programs in Physics, Math, Computer Sci.,

Biology, Engineering, and an **interdisciplinary doctoral program in Computational Sciences**.



universität  
wien

The [University of Vienna](#) is the **largest Austrian research institution**, hosting 6,800 academics within 15 faculties and five centres, dedicated to both basic and applied research. Furthermore, 16 research platforms have been established to promote especially innovative

interdisciplinary research projects. The **Department of Pharmaceutical Chemistry** of the Faculty of Life Sciences is a **leading research hub for cheminformatics and machine learning**.



Universitat  
Pompeu Fabra  
Barcelona

[Universitat Pompeu Fabra](#) is a public, international and research-intensive university that **ranks 10th in the 2020 Times Higher Education Young University Ranking** and **1st among the Spanish Universities in the QS World University ranking** (position 28 worldwide and

position 7 in Europe). It is the top-ranked Spanish university (IUNE Report 2020) in yearly scientific output per professor, citations per professor, projects within the Spanish National R&D Plan (per 100 lecturers), in projects within the EU Framework Programme (per 100 lectures). It has about 12,000 enrolled students (nearly 1.300 of them in one of its 9 PhD

programmes), 1,500 teaching and research staff, and 700 administrative and service staff. The UPF is strategically located in the PRBB, one of the leading South European biomedical research hubs, that hosts 1300 international staff and scientists, core scientific facilities and multiple research institutes.

The student participating in this project will be enrolled in the [PhD studies in BioMedicine](#) and will join the [Computational Science Laboratory](#) (lead by Prof. Gianni De Fabritiis) whose interests are the application of computation to solve real world problems, defining intelligence as a form of computation. The research group develops machine learning models with intelligent, useful behavior using reinforcement learning and deep learning, for specific environments. Biomedicine is one environment where physics-based simulations and machine learning provide novel, innovative approaches. The group leads [GPUGRID.net](#), one of the top distributed computing projects worldwide for running molecular simulations on GPUs and the open platform [PlayMolecule.org](#) that has around a thousand registered scientists. The group and its spin-off company Acellera have collaborated with major industries worldwide like Sony, Nvidia, HTC mobile, UCB, Pfizer, Biogen and Novartis.

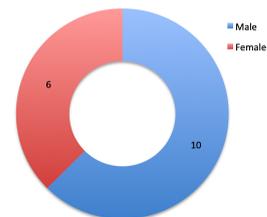
## Special 16<sup>th</sup> Partner of the Consortium



[University of British Columbia \(UBC\)](#) – is one of the most recognized universities, **ranked 2nd in Canada** and Nr 34 in the world (Times Higher Education 2020). The [Vancouver Prostate Centre \(VPC\)](#) is one of the leading subdivisions of the UBC and one of the world's most respected cancer facilities. It is a National Centre of Excellence and a designated Centre of Excellence for Commercialization and Research. The AIDD grant does not cover costs for VPC, therefore they are acting within the Consortium on their own.

## Recruitment of fellows

Following the announcement of the ESR positions, 260 (**72 females, 27.7%**) applications from 55 countries were received. All the partners were involved in scoring and pre-selecting candidates for Zoom interviews.



**43 interviews** were held and eventually **15 candidates were selected**. ESR16 is covered entirely by the partner VPC (Vancouver Prostate Center, University of British Columbia) and therefore the position was not recruited centrally. In total, **16 students (6 females, 37,5%)** will soon start working within the AIDD Consortium.

## Coming soon: Second AIDD Newsletter

In the second newsletter we will describe expertise of associated partners and will also share challenges in the search and recruitment of talented fellows for the AIDD program.

## Additional information

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie Actions, grant agreement No 956832.

Disclaimer: the newsletter reflects only the authors' view and neither the European Commission nor the Research Executive Agency are responsible for any use that may be made of the information it contains.