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

Newsletter 2, December 2021

The **Advanced Machine Learning for Innovative Drug Discovery** (AIDD) project is a Marie-Skłodowska-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 other countries.

Project development

The **AIDD project started on 01.01.2021** and on 21.10.2021 the first Supervisory Board Meeting took place. Due to Covid-19 restrictions, most of the associated Partners joined the meeting remotely by Zoom.

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.

In Newsletter #1, we introduced all the Beneficiaries of the AIDD Consortium. In this Newsletter we briefly describe all Associated Partners.

Associated Partners of the AIDD 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.

The Technical University of Munich (TUM) is one of the leading universities in the world, within the Top 100 worldwide and the top university in Germany. TUM organized and participated in multiple Marie Curie ITNs and ERC Grants. Fabian Theis who is director of the Institute of Computational Biology at the Helmholtz Center Munich and coordinates the Helmholtz Artificial Intelligence Cooperation Unit (HelmholtzAI), will supervise a few fellows in the AIDD Project and will help with the organization of the scientific venue of the upcoming Schools and conferences. He is a full professor at the Technical University of Munich, holding the chair 'Mathematical Modelling of Biological Systems' and associate faculty at the Wellcome Trust Sanger Institute.

Ascenion is an independent technology transfer company focussing on the life sciences. It is a partner to 30 research organizations, universities, and university hospitals in Germany and Europe, including life-science institutes of the Helmholtz and Leibniz Associations, the Charité, the Hannover Medical School, the Medical University of Innsbruck, the Institute of Molecular Biotechnology of the Austrian Academy of Sciences, and the University Medical Center Göttingen. Ascenion offers access to more than 800 commercial opportunities and closes some 60 revenue-generating cooperation and licensing agreements between research and industry per year.

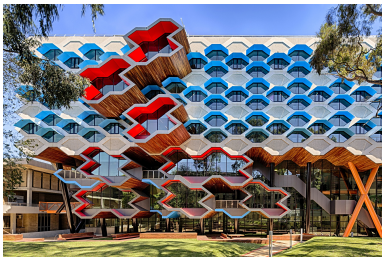
Ascenion's multidisciplinary, industry-experienced team works closely with its partners to tap the potential of their research by identifying promising results, obtaining patent protection, and turning pure science into applied technology. Particular strengths are spin-off support and project development, where early-stage projects are transformed into assets that attract potential investors and licensees. This has led to the founding of numerous new companies and the transfer of innovative medical approaches into approved drugs. Profits from Ascenion's operative business and exit proceeds flow via its parent company, the LifeScience Foundation for the Promotion of Science and Research, to fund further translational research at its partner institutes.

Novartis is reimagining medicine to improve and extend people's lives. As a leading global medicines company, Novartis uses innovative science and digital technologies to create transformative treatments in areas of great medical need. In its quest to find new medicines, Novartis consistently rank among the world's top companies investing in research and development. Novartis products reach nearly 800 million people globally and Novartis is finding innovative ways to expand access to Novartis latest treatments. About 109,000 people of more than 145 nationalities work at

Novartis around the world. Find out more at https://www.novartis.com.

NIBR (Novartis Institutes for BioMedical Research), the research organization of Novartis, is a global organization of approximately 6,000 scientists, physicians, and business professionals. Among other disease areas and platforms, NIBR has world-leading expertise in the areas of cheminformatics and the application of machine learning in drug discovery.

The University of North Carolina at Chapel Hill is ranked 33rd in the world and is 23rd in the United States among global universities, according to the 2019 Academic Ranking of World Universities (ARWU). As an integral part of the university, the UNC Eshelman School of Pharmacy is the top-ranked pharmacy school in the United States, according to U.S. News & World Report. The School is an internationally recognized leader in pharmacy practice, education, and research.



La Trobe Institute for Molecular Science (LIMS) is a translationally focused multidisciplinary research institute within La Trobe University (LTU), one of the top 1.4% of universities worldwide. LIMS brings together LTU's leading researchers to work on some of the most critical problems facing our world today. The Institute's vision is achieved through excellence in four thematic areas: Cancer, Infection and Immunity, Molecular Design, and Nanoscience.

Bar-Ilan University (BIU) is one of the largest research universities in Israel. BIU offers high-level academic studies and the development of advanced research within the framework of faculties, departments, multi-disciplinary centers, and research centers. The Chemistry Department is currently in an unprecedented growth phase. Many new faculty members have been recruited leading to new capabilities in computational chemistry, structural biology, magnetic resonance, bio-inorganic chemistry, and nano-materials and devices, alongside the more established fields of medicinal chemistry, organic, inorganic, and physical chemistry.

Guangzhou Regenerative Medicine and Health Guangdong Laboratory (Bioisland Laboratory) was founded on 22nd December 2017, it is operated as a public research institution as one of the first provincial laboratories to develop as the reserves of national laboratories in Guangdong Province. Bioisland Laboratory aims at addressing major strategic needs of Guangdong Province and the whole country through 5 research areas and is committed to become a pioneer of international scientific research in stem cell and regenerative medicine, which covers from fundamental science to translational and clinical research.

The AI drug design group in Bioisland Laboratory aims to develop novel AI algorithms to facilitate drug discovery and provide computational chemistry support for both in-house and collaborative drug discovery projects with external partners. It has state-of-the-art computational tools and high-performance computing hardware.

Istituto di Ricerche Farmacologiche Mario Negri IRCCS is a no-profit Foundation, devoted to research on human health, pharmacology, and dissemination. There are about 750 people working in three sites in Italy. The three pillars in our manifesto are: carrying scientific research projects, training young people, disseminating the results of our research.

MAX PLANCK INSTITUTE
OF MOLECULAR PHYSIOLOGY

The MPG is a non-profit organization that supports excellent fundamental research through a network of Institutes situated in Germany, as well as internationally. The Max Planck Institute of Molecular Physiology, Dortmund (MPI-MP) is one of over 80 independent Institutes of the Max Planck Gesellschaft. It consists of four Departments that combine chemical biology, biochemical reconstitution, structural biology, and advanced microscopy.

Founded in 1958 and formerly known as Beijing Institute of Chemical Technology, Beijing University of Chemical Technology (BUCT) is a national key university directly affiliated to the Ministry of Education of China, one of the Project 211 universities and 985 Project Innovation Platforms. BUCT shoulders the mission of innovative talent education, scientific research, and high-tech development.

After 60 years of continuous efforts, BUCT has developed into a multi-disciplinary institute with a solid foundation in science and engineering, along with other distinctive disciplines such as business management, economics, law, literature, philosophy, education, medical science, and etc. It has formed a complete talent development system from the undergraduate level, the postgraduate level up to the postdoctoral level. In the ESI rankings, chemistry and material science have entered the top 1‰, the disciplines of material science, engineering, biology, and biochemistry top 1%. The primary discipline of chemical engineering and technology is the 3rd place in China. The BUCT “Green Chemistry, Chemical Engineering, and Materials” discipline group was listed as a First-Class Discipline in the Double First-Class Project in 2017.

BUCT has 14 colleges/schools, 15,340 full-time undergraduate students, 7,643 full-time postgraduate students (including 953 PhD students), 3034 students of continuing education, and 341 full time international students. It has more than 2,600 faculty members and staff, including around 780 full professors and associate professors out of the 1,200 full-time faculty members. BUCT is also the host university of eight academicians from the Chinese Academy of Science and the Chinese Academy of Engineering, five international academicians, and about 60 distinguished professors.

G.A. Krestov Institute of Solution Chemistry of the Russian Academy of Sciences (ISC RAS) is a nonprofit research organization under the Ministry of Science and Higher Education of the Russian Federation. The Institute is a subdivision of the Russian Academy of Sciences and is one of the units of the Department of Chemistry and Materials Science of the Russian Academy of Sciences (DCMS RAS). The main aim of the ISC RAS is organizing and carrying out theoretical and applied research in the field of solution theory, preparation of new materials, and development of modern chemical technologies using solutions.

Coming soon

Newsletter #3 will cover the First Summer School.

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.