eu-openscreen

EU-OPENSCREEN PARTNER SITES

SELECTED BASED ON SCIENTIFIC EXCELLENCE

Integrating Europe´s top resources and facilities in the field of chemical biology

Special focus:
EU-OPENSCREEN PARTNER SITES

www.eu-openscreen.eu

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A COMPETENCE NETWORK FOR DRUG RESEARCH AND BASIC SCIENCE

EU-OPENSCREEN is a not-for-profit European Research Infrastructure Consortium (ERIC) for chemical biology and early drug discovery with more than 20 affiliated high-throughput screening and chemistry partner sites in eight member countries. EU-OPENSCREEN operates an open-access database and a central compound management facility which stores, quality-controls and manages the EU-OPENSCREEN compound collection. We support scientists from academia and industry from countries inside and outside of the European Union, in the development of chemical tool compounds and early therapeutic candidate molecules.

Our collaborators work with peer-reviewed and experienced biological and chemical institutes by combining biological screening assays with medicinal chemistry expertise.

Build on scientific excellence, EU-OPENSCREEN strengthens innovation and competitiveness of the European Research Area by addressing some of the grand societal challenges. In this way, we also help scientists to get unprecedented opportunities to study biological processes and explore the secrets of life.

Our partner sites provide chemical biology related services including assay development, assay adaptation, screening, and medicinal chemistry (including compound design, synthesis, analytics and SAR generation).

These services are carried out in the member countries. The partner sites are organisationally independent of the EU-OPENSCREEN ERIC and remain embedded in their host institutions.

EU-OPENSCREEN in a nutshell

- Connecting the leading centres for chemical biology in Europe
- Driving innovation through collaboration
- Providing access to state-of-the-art resources in high throughput screening and medicinal chemistry
- Fostering drug discovery by providing high quality tool compounds
- Connecting academia and industry
- Providing FAIR (findable, accessible, interoperable and re-usable) data
- Bridging the gap between basic and applied research

OUR MISSION AND VISION

Mission

To progress the discovery of biologically active substances in all areas of the life sciences by providing open access to the most advanced technologies, chemical and biological resources, and scientific expertise.

Vision

EU-OPENSCREEN will become the premier European technology and expertise platform for chemical biology and the first stop for any academic researcher in the life sciences interested in developing specific chemical tools for their protein of interest.

Values

Scientific excellence: Our first priority is to strive for scientific excellence in all our offerings and procedures.

Transparency: We are clear to our partners on how we choose and distribute projects, and our open access model requires the publication of all research data so that important results can be reproduced.

Equality: We value equality as a crucial part of our work ethic because we always wish to make sure to treat our network of partners the same way.

EU-OPENSCREEN PARTNER SITES

Proven expert centres selected based on scientific excellence

EU-OPENSCREEN partner sites are leading experts in the field of chemical biology and early drug discovery in Europe. The selection of our partner sites follows a rigorous three-step procedure, which emphasises scientific excellence and technical capabilities to support user projects.

EU-OPENSCREEN partner sites have the political support of and are nominated by the ministries of their host countries. Furthermore, they are thoroughly evaluated by an independent panel of high-level experts in the field. The review process focusses on the scientific excellence of the host institution and the team; the technical capabilities of installed instrumentation and resources; the track record in project execution; the future capacities and ability to support project flow; the sustainability of the partner site operation over the long term (> 5 years); and the alignment with the EU-OPENSCREEN ERIC mission to provide open access chemical biology services to users, including a commitment to the publication of screening results in the European Chemical Biology Database (ECBD).

EU-OPENSCREEN partner sites provide chemical biology related services including assay development, assay adaptation, screening, and medicinal chemistry (including compound design, synthesis, analytics and SAR generation).

These services are carried out by the partner sites in the respective EU-OPENSCREEN ERIC member countries.

Partner sites are organisationally independent of the EU-OPENSCREEN ERIC and embedded in their host institutions.

Following a successful evaluation and confirmation process the partner sites sign legal agreements with the EU-OPENSCREEN ERIC. The format of the agreements is common for all affiliated partner sites and is aligned to the rules of the EU-OPENSCREEN ERIC. The agreement defines the procedures for handling IP rights, adherence to EU-OPENSCREEN ERIC operational standards, confidentiality, data provision and reporting.

Site selection criteria

- Scientific excellence and best practice
- Technological focus
- Long term sustainability and future potential
- Proven project and publication track record

PARTNER SITE CATEGORIES

The EU-OPENSCREEN network connects multiple competences to a seamless and efficient process

Assay Adaptation sites:

Assay adaptation groups, in close collaboration with users adapt bench-top protocols into high-throughput screening (HTS) format and optimise the assay performance under automated or semi-automated screening conditions. Typically, validated assays will then be transferred to specialist or high capacity screening sites. Assay adaptation sites may also perform compound screening on small to medium scales and will be eligible to receive copies of the EU-OPENSCREEN ERIC pilot collection for the purposes of validation of the functional performance of assays and creation of data sets to support applications to funding organisations to finance full scale screens.

Screening sites

Screening Partner sites will offer users access to assay adaptation services and automated technologies to allow large scale (>100,000 compounds for high capacity) collection of quantitative bioactivity data across a wide range of formats including cell-, biochemical- and model organism-based screens. High capacity screening sites receive and host compounds from the EU-OPENSCREEN ERIC compound collection. Specialist screening sites add expertise and technology to the EU-OPENSCREEN ERIC that is not commonly offered by screening facilities (e.g., BSL-3 capacities, radioactivity etc.) All screening sites adhere to high quality operating standards defined and monitored by the EU-OPENSCREEN ERIC

Chemistry sites

Hit-to-tool and Hit-to-lead optimisation is carried out by chemistry partner sites. The chemistry sites have a track record demonstrating expertise in chemical biology and/or medicinal chemistry. Capabilities cover the general Medicinal and Synthetic chemistry activities of SAR determination, compound design, synthesis, analytics, and structural confirmation. Chemistry sites are also sometimes closely associated or located in the same host Institution as screening partner sites.

COMPOUND COLLECTIONS

With EU-OPENSCREEN´s unique compound collections you can explore the chemical space and target biology with Europe´s only open-access chemical biology infrastructure.

The main library, the European Chemical Biology Library (ECBL), consists of about 100.000 compounds with unbiased chemical diversity, designed by five renowned academic computational chemistry groups. It is planned to add a growing number of proprietary compounds from international medicinal chemists, which will form the European Academic Compound Library (EACL)

As a fingerprint of the large library a smaller pilot library of 5000 compounds is available. Half of these compounds represent the large European Chemical Biology Library (ECBL) of 100.000 commercial compounds while the other half is made up of about 2.500 bioactive compounds. All EU-OPENSCREEN screening partner sites have access to the EU-OPENSCREEN compound collection.

The compound collection is stored in the Central Compound Management Facility (CCMF) in Berlin, Germany. The EU-OPENSCREEN compound management team quality controls and sends out the compounds in the requested formats to the EU-OPENSCREEN partner sites.

At the partner sites the compound collection can be used in different high-throughput screening projects. All compound data and the results of these projects are stored in the open-access European Chemical Biology Database (ECBD), where they are made available to a wide scientific audience.

Our pilot screening library consists of about 5.000 compounds. Half of these compounds represent our large European Chemical Biology Library (ECBL) of 100.000 commercial compounds while the other half is made up of about 2.500 bioactive compounds. A strong emphasis was put on the selection of molecules with a dedicated high target selectivity.

Visit our website for further information:
https://www.eu-openscreen.eu/services/compound-collection.html

EU-OPENSCREEN QUICK FACTS

23 Partner Sites
and 1 Database host

8 Full Member Countries

Czech Republic, Denmark, Finland, Germany, Latvia, Norway, Poland, Spain

More countries are preparing their participation.

100.000 Com-pounds

carefully selected for a wide range of research applications

EU-OPENSCREEN PARTNER SITES OVERVIEW

Screening Site | Chemistry Site | Database Site

	Abbr.	Partner-Site	Department	Address
CZ	IMG	Institute of Molecular Genetics	CZ-OPENSCREEN	Vídeňská 1083142 20 Prague 4
	IMG	Institute of Molecular Genetics	CZ-OPENSCREEN	Vídeňská 1083142 20 Prague 4
	IMTM	Palacký University Olomouc, Faculty of Medicine and Dentistry	Institute of Molecular and Translational Medicine (IMTM)	Hněvotínská 1333/5779 00 Olomouc, CZ
	MU	Masaryk University	Department of Chemistry / CZ OPENSCREEN	Kamenice 753/5, 625 00 Brno
DE	FMP	Leibniz-Institute for Molecular Pharmacology	Chemical Biology / Screening Unit	Robert-RössleStr. 10 13125 Berlin
	FMP	Leibniz-Institute for Molecular Pharmacology	Chemical Biology / Medicinal Chemistry	Robert-RössleStr. 10 13125 Berlin
	HZI	Helmholtz-Centre for Infection Research	Department of Chemical Biology (CBIO)	Inhoffenstraße 7, 38124 Braunschweig
	ITMP	Fraunhofer Institute for Molecular Biology and Applied Ecology	IME Screening Port	Schnackenburgallee 114, 22525 Hamburg
DK	BRIC	University of Copenhagen, Biotech Research and Innovation Centre	Biotech Research and Innovation Centre	Jagtvej 124 2200 Copenhagen N
	DTU	Technical University of Denmark	Chemical Biology	Ørsteds Plads, Building 345C DK-2800 Kgs. Lyngby
ES	CIPF	Prince Felipe Research Center	Advanced Therapies Program	Eduardo Primo Yúfera 3, 46012 Valencia
	CSIC	Consejo Superior de Investigaciones Científicas – Madrid	Translational Medicinal and Biological Chemistry Laboratory	Ramiro de Maeztu 9, 28040 Madrid, Spain
	MEDI	Fundación MEDINA	Screening and target validation, Microbiology and Chemistry	Avda del Conocimiento s/n., 18016, Granada
ES	USC	University of Santiago de Compostela	BioFarma Research Group	Av. Barcelona, 31, 15706 Santiago de Compostela, La Coruña
FI	FIMM	Institute for Molecular Medicine Finland	High Throughput Biomedicine (HTB) unit	P.O. Box 20FI-00014 University of Helsinki
	UH	University of Helsinki, Faculty of Pharmacy	Division of Pharmaceutical Biosciences	Viikinkaari 5 E (P.O.Box 56) 00014 Helsinki
LV	OSI	Latvian Institute of Organic Synthesis	Organic Synthesis Methodology Group	Aizkraukles 21, LV-1006 Riga
NO	SIN	SINTEF	Department of Biotechnology and Nanomedicine	P.O. Box 4760 Torgarden, NO-7465 Trondheim
	UiB	Faculty of Medicine and Dentistry, University of Bergen	Department of Biomedicine	Postbox 7804, N-5020 Bergen
	UiO-NCMM	University of Oslo, Faculty of Medicine	Biotechnology Centre of Oslo (BiO) and Centre for Molecular Medicine (NCMM)	P.O.Box 1137, Blindern 0318, Oslo
	UiT	Arctic university of Norway	Faculty of Biosciences, Economics and Fisheries	Hansine Hansens veg 17, 9019 Tromsø
PL	IBB PAS	Polish Academy of Sciences, Institute of Biochemistry and Biophysics	Department of Bioinformatics	Pawinskiego 5a, 02-106 Warszawa
	IBCH PAS	Polish Academy of Sciences, Institute of Bioorganic Chemistry	Department of Molecular Probes and Prodrugs	Noskowskiego 12/14, 61-704, Poznań
	IMB PAS	Polish Academy of Sciences, Institute of Medical Biology	Screening laboratory for anti-viral and anti-bacterial compounds	106 Lodowa St., 93-232, Łódź

CZ

CZECH REPUBLIC

Member-Country
since

2018

CZ | High-capacity screening site

Institute of Molecular Genetics of the Czech Academy of Sciences (IMG)

Vídeňská 1083, 142 20 Prague 4, Czech Republic

At a glance

- High capacity screening site with access to unique collections of chemical compounds
- Platform for nuclear receptors: Receptor X – a portfolio of cellular and biochemical assays for nuclear receptors and enzymes
- Drug sensitivity profiling platform for systematic chemosensitive profiling of libraries of small molecules on the panel of cell lines of various histological origin
- Assay adaptation to the 384- and 1536-well format for High-throughput screening (HTS) campaigns
- Probes & Drugs portal (www.probes-drugs.org)

Infrastructure and technical focus

- Integrated robotic HTS stations
- Integrated system for compound storage and sample preparation
- Laboratory Information Management System (LIMS) for compound management with an incorporated ScreenX database
- High-capacity zebrafish facility for in vivo bioactivity/toxicity studies of lead compounds from HTS and High-content screening (HCS) projects
- Excellent cheminformatics supports with a broad range of in-house developed new analytical tools and database systems

Dr. Petr Bartůněk (Head of Unit)

„IMG is proud to be a part of EU-OPENSCREEN, which connects laboratories around Europe. All data generated by this consortium will be stored in the European Chemical Biology Database and will be accessible to the scientific community based on open access principles.“

Projects past and present

2021 | ALGAE4IBD Horizon 2020 project From Nature to Bedside- Algae Based Bio Compound for Prevention and Treatment of Inflammation, Pain and IBD

2020 | EXPRO Czech grant agency project Uncovering of missing genetic components and new chemical regulators of juvenile hormone signalling

2020 | CZ-OPENSCREEN Ministry of Education Youth and Sports project National infrastructure for Chemical Biology

2019 | EXPLORE JPI-EC-AMR project Exploration of the TPP riboswitch as a new target for antibiotics

Our science in selected publications

Probes & Drugs portal: an interactive, open data resource for chemical biology
Nature Methods 2017, 14, 759–760

Estradiol dimer inhibits tubulin polymerization and microtubule dynamics
The Journal of Steroid Biochemistry and Molecular Biology 2018, 183, 68-79

Cell-Based Reporter System for High-Throughput Screening of MicroRNA Pathway Inhibitors and Its Limitations
Frontiers in Genetics 2018

Heterocyclic sterol probes for live monitoring of sterol trafficking and lysosomal storage disorders
Scientific Reports 2018, 8, 14428

Further info and site-contact

Dr. Petr Bartůněk: bartunek@img.cas.cz | +42 (0) 296 443 117

Website: https://www.img.cas.cz/en/

CZ | Database site

European Chemical Biology Database (ECBD)

Vídeňská 1083, 142 20 Prague 4, Czech Republic

EU-OPENSCREEN´s Database

The ECBD represents the central data hub designed to accommodate and disseminate data that are generated within the EU-OPENSCREEN network. As one of the EU-OPENSCREEN core services, the ECBD was developed in line with the FAIR principles ensuring Findability, Accessibility, Interoperability, and Reusability of data.

Findability and Interoperability build upon the integration of commonly used ontologies and vocabularies in combination with established identifiers and data formats, while Reusability will be ensured by the open access to data and metadata following every step of each single screening campaign under the Creative Commons license, Attribution 4.0 International (CC BY 4.0).

There are several ways to access the ECBD data, serving the needs of different types of users. Common users accessing the ECBD through a web interface can view, visualize, filter, and export data, or any of their subsets, while data scientists preferring programmatic access using data for machine learning campaigns can take advantage of the REST API or download a full database for local use.

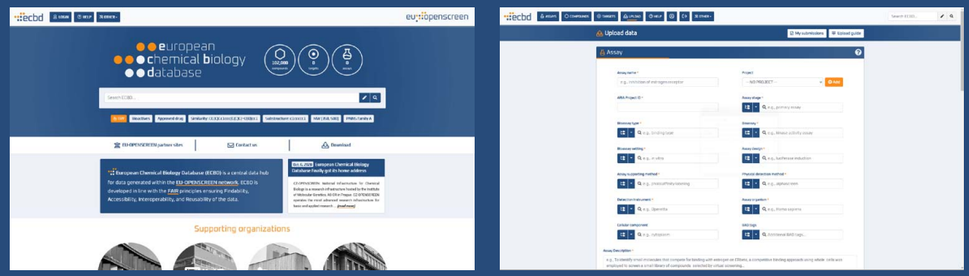
While EU-OPENSCREEN clearly promotes open access and FAIR data principles, it also pays attention to the protection of the IP interests of our collaborators and partners by offering an optional embargo period on the uploaded experimental data.

During the embargo period of up to 36 months, data are accessible only by the EU-OPENSCREEN partner site which generates the data, and by the collaborators themselves, giving them sufficient time for the publication of the results in peer-reviewed journals, for patent filing, or for follow-up studies to advance their previous findings.

Dr. Petr Bartůněk (Head of Unit)
„The ECBD is one of the key components of EU-OPENSCREEN and makes the data generated within the EU-OPENSCREEN network available to the large research community.“

Technical infrastructure

The ECBD is developed and maintained by the Institute of Molecular Genetics (IMG) in Prague, Czech Republic, led by Petr Bartůněk, Director of CZ-OPENSCREEN, the National Infrastructure for Chemical Biology. To ensure high stability, scalability, and security of the system, IMG collaborates with CESNET, the developer and operator of the national e-infrastructure for science, research, development, and education in the Czech Republic. CESNET provides the technological background of the ECBD, including cloud-based hosting with a robust backup strategy and state-of-the-art data security.



Screenshot examples of the ECBD web-interface

Further info and site-contact

Dr. Petr Bartůněk: bartunek@img.cas.cz | +42 (0) 296 443 117

Website: https://ecbd.eu/

CZ | High-capacity screening site

Palacký University Olomouc, Faculty of Medicine and Dentistry (IMTM)

Masaryk University, Kamenice 5, Brno, Czech Republic

At a glance

- High content analysis platform providing screening and high volume biology data on a broad diversity of assays and detection systems
- Industry strong, modular and flexible screening technology
- Testing in BSL3 and BSL2+ environment
- Screening in combination with ionizing radiation (X-rays), mass spectrometry, high content analysis and others
- Screening assays provide leads for downstream drug research and development
- Automated chemical library, capacity about 1.000.000 compounds

Infrastructure and technical focus

- The HTS/HCA screening platform is based on a state-of-art robotic system provided by HighResBiosolutions Ltd. The system consists of three robotic arms, automatic incubators, liquid handlers for microliter and nanoliter volumes, sealers, de-sealers, centrifuges and readers for fluorescence, luminescence, absorbance and ionizing radiation (LumijetBeta, FLIPR-PENTA, Envision, Viewlux).
- Also integrated with the system are wide-field or spinning disc confocal microscopes (Operetta, Yokogawa CV8000) equipped with software tools (Collumbus, CellProbiler) for image analysis and data evaluation.

Dr. Marian Hajdúch (Head of Unit)

„We support the challenges of biological research with state-of-the-art technology in medicinal chemistry.“

Projects past and present

2020 - 2022 | CZ-OPENSCREEN National infrastructure for chemical biology Link

2018 - 2022 | PERMED Personalised Medicine - Diagnostics and Therapy Link

2018 - 2023 | ENOCH Molecular, cellular and clinical approach to healthy ageing Link

Our science in selected publications

Steroid Glycosides Hyrcanoside and Deglucohyrcanoside: On Isolation, Structural Identification, and Anticancer Activity
Foods, 2021, 10, 136

Fluorinated derivatives of 2-phenyl-3-hydroxy-4(1H)-quinolinone as tubulin polymerization inhibitors
European Journal of Medicinal Chemistry, 2020, 192, 112176

Alcohol-abuse drug disulfiram targets cancer via p97 segregase adaptor NPL4
Nature, 2017, 552, 194

Metallacarborane Sulfamides: Unconventional, Specific, and Highly Selective Inhibitors of Carbonic Anhydrase IX
Journal of Medicinal Chemistry, 2019, 62, 9560

Synthesis and Cytotoxic and Antiviral Profiling of Pyrrolo- and Furo-fused 7-Deazapurine Ribonucleosides
Journal of Medicinal Chemistry, 2018, 61, 9347

Further info and site-contact

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Website: https://www.imtm.cz/high-throughput-screening-and-high-content-analysis-core

CZ | Medicinal chemistry site

Masaryk University (MU) – Laboratory of Organic Synthesis and Medicinal Chemistry

Masaryk University, Kamenice 5, Brno, Czech Republic

At a glance

- History of successful collaboration within chemical biology projects
- Long-term expertize in identification of new (patentable) organic compounds with targeted biological activity
- Strong track record in identification of new kinase inhibitors

Infrastructure and technical focus

- Facilities in new campus
- More than 20 fully equipped workplaces for organic synthesis
- State-of-the-art technology for purification and structural characterization of organic compounds

Dr. Kamil Paruch (Head of Unit)

„We support the challenges of biological research with state-of-the-art expertise in medicinal chemistry.“

Projects past and present

2020 - 2022 | CZ-OPENSCREEN National infrastructure for chemical biology Link

2019 - 2023 | EU-OPENSCREEN DRIVE Ensuring long-term sustainability of chemical biology services within Europe and beyond Link

2018 - 2022 | PRECLINPROGRESS Preclinical progression of new compounds with targeted biological activity Link

Our science in selected publications

Novel Chk1 inhibitor MU380 exhibits significant single-agent activity in TP53-mutated chronic lymphocytic leukemia cells
Haematologica 2019, 104, 2443

Furo[3,2-b]pyridine: A novel privileged scaffold for highly selective kinase inhibitors and effective modulators of the Hedgehog pathway
Angewandte Chemie 2019, 58, 1062

A concise synthesis of forskolin
Angewandte Chemie 2017, 56, 12586

The CHK1 inhibitor MU380 significantly increases sensitivity of human docetaxel resistant prostate cancer cells to gemcitabine by induction of mitotic catastrophe
Molecular Oncology 2020, 14, 2487

Further info and site-contact

Dr. Kamil Paruch: paruch@chemi.muni.cz | +42 (0) 549 49 5477

Website: http://orgsyn.sci.muni.cz/

DE

GERMANY

Member-Country since

2018

DE | High-capacity screening site

Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP) – Screening Unit

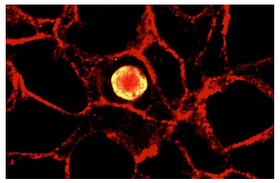
Robert-Roessle-Str. 10, 13125 Berlin, Germany

At a glance

- Since 2004, the site has supported more than 300 projects with academia and Small and Medium Enterprises
- Experience in screening of bacteria, primary and iPS cells, organoids, nematodes
- Know-how in assay development, process automation and automated analysis, combinatorial analysis of primary and counter-screens
- Know-how in assay development, process automation and automated analysis, combinatorial analysis of primary and counter-screens
- Experience in high-content screening from image to parameter conversion, to machine learning analysis
- Visiting scientists may contribute in our team and guide the process
- Additional project support by medicinal chemistry experts from the FMP for hit selection and optimization

Infrastructure and technical focus

- Morphological profiling of cellular responses by confocal imaging and pattern recognition in the context of toxicity profiling with HepG2-cells, iPS-cell differentiation and organoid cultures
- Support in assay optimization for HTS and professional assay acceptance testing
- Broad portfolio of screening technologies established for cellular systems and for protein, protein-ligand interaction or enzyme screens



Dr. Jens Peter von Kries (Head of Unit)

„EU-OPENSCREEN provides a unique chance to set European standards in Chemical Biology across platforms for systematic and open access of academic research teams to professional high-throughput screening technologies in Europe.“

Projects past and present

We supported projects for interference with Wnt-induced colon tumors, with Met-induced metastasis and with therapy resistant aggressive B-cell lymphoma. Two of these projects made it to clinical trials, one is still ongoing. Furthermore, we identified drugs which potentially interfere with vessel malformation and head strokes in teenagers in a rare disease. These are still in validation for specific interference, but are approved drugs which can be directly tested for this new application.
The platform actually serves for the Helmholtz-Initiative for Drug Research, EU-OPENSCREEN and provides open access towards academic research.

Our science in selected publications

High-Throughput Screening for Modulators of CFTR Activity Based on Genetically Engineered Cystic Fibrosis Disease-Specific iPSCs
Stem Cell Reports (2019), 12, 6, 1389–1403

Small-molecule inhibition of STOML3 oligomerization reverses pathological mechanical hypersensitivity
Nature Neuroscience (2017), 20, 2, 209–218

Systematic pharmacological screens uncover novel pathways involved in cerebral cavernous malformations
EMBO Molecular Medicine (2018), 10, 10, e9155

Pharmacological restoration and therapeutic targeting of the B-cell phenotype in classical Hodgkin lymphoma
Blood (2017), 129, 1, 71–81

Further info and site-contact

Dr. Jens Peter von Kries: kries@fmp-berlin.de | +49 (0) 30 9406 2982

Website: https://www.leibniz-fmp.de/screeningunit

DE | Medicinal chemistry site

Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP) – Medicinal Chemistry

Robert-Roessle-Str. 10, 13125 Berlin, Germany

At a glance

- Medicinal Chemistry based hit identification and evaluation as well as hit-to-chemical tool and lead optimization
- State-of-the art medicinal chemistry laboratory equipment for solution-phase chemistry, parallel synthesis and automated purification
- Access to co-localized resources for screening (EU-OPENSCREEN partner site), computational chemisty, chemoinformatics, cellular imaging, NMR, peptide synthesis
- Tailor-made probes based on chemical tools e.g. for target deconvolution, fluorescent labeling for assay development and imaging studies

Infrastructure and technical focus

- State-of-the-art medicinal chemistry lab equipped to industry standards
- Hit-triage and chemical optimization of small molecule modulators
- Fragment-based drug discovery approaches
- Structure-based design, scaffold hopping and hybridization
- Consultancy and support for developing chemistry strategies for projects

Dr. Marc Nazaré (Head of Research Group)

„Developing a chemical tool is a very collaborative approach. EU-OPENSCREEN is essential for us to network and join forces to develop new chemical tools and leads together with our partners.“

Projects past and present

2021 - 2024 | ALOOD - Allostery in Drug Discovery (EU)

2021 - 2023 | Battling Drug Resistance of Tumors using novel SHP2 Inhibitors (DFG)

2021 - 2023 | Design of ligand-based targeted delivery vehicles for the murine C-type lectin receptor Langerin (DFG)

2017 - 2021 | Tumor-targeting SMART imaging agents (DFG/NSF)

Our science in selected publications

From Pyrazolones to Azaindoles: Evolution of Active-Site SHP2 Inhibitors Based on Scaffold Hopping and Bioisosteric Replacement
Med. Chem. 2020, 63, 14780 - 14804

An Activatable Lanthanide Luminescent Probe for Time-Gated Detection of Nitroreductase in Live Bacteria
Angew. Chem. Int. Ed.2020, 59, 8728

Probing 2H-Indazoles as Templates for SGK1, Tie2, and SRC Kinase Inhibitors
ChemMedChem 2019, 14, 1514-1527

Allosteric Inhibition of a Mammalian Lectin
J. Am. Chem. Soc. 2018, 140, 14924-14934

Mutant KRAS-driven cancers depend on PTPN11/SHP2 phosphatase
Nat. Med. 2018, 24, 954-960

Further info and site-contact

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Website: https://www.leibniz-fmp.de/nazare

DE | Specialist screening site

Helmholtz Centre for Infection Research (HZI) – Chemical Biology Department

Inhoffenstr. 7, 38124 Braunschweig, Germany

At a glance

- Screening site with access to the EU-OPENSCREEN European Chemical Biology Library and the European Academic Compound Library
- Focused on viral and bacterial infectious diseases including host defense reactions
- Cell-culture based infection models
- Screens and animal infection models with Biosafety level (BSL) -3 pathogens
- *In vivo* pharmacokinetic and - dynamic studies
- Medicinal chemistry facility and expertise for hit selection and compound optimization
- Chemical biology facility and expertise for mode of action studies
- Close cooperation with clinical experts
- Member of the German Centre for Infection Research (DZIF)

Infrastructure and technical focus

- Fully equipped microbiological and cell culture laboratories up to biosafety level 3, including real-time cell culture monitoring and semi- (BSL3) and fully automated screening platforms (BSL2) supporting all major optical detection technologies
- Assay development and adaptation
- State of the art mass spectrometry for metabolomics, compound uptake and PK / PD studies
- Modern, and fully equipped (prep HPLC, LC/MS, NMR, etc) chemistry labs
- Access to NGS, Proteomics, FACS, electron microscopy

Prof. Dr. Mark Brönstrup (Head of Unit)

„We are happy to be part of EU-OPENSCREEN, as it provides a perfect setting for combining our expertise in chemical biology with innovative approaches to tackle infectious diseases across Europe.“

Projects past and present

2021| DZIF Antiinfective screening and hit identification Link

2021 | COFONI Corona Research in Lower Saxony

2021 | Breitbandwirkstoffe gegen SARS-CoV-2 (Lower Saxony)

2020 | CARB-X Optimization of Hla-Inhibitors Link

2020 | LABoVIR LAByrinthopeptins against VIRal infections

2020 | IMI-GNANOW Novel Gram-negative antibiotics now Link

Our science in selected publications

Synthetic studies of cystobactamids as antibiotics and bacterial imaging carriers lead to compounds with high in vivo efficacy
Chemical Science (2020), 11, 1316-1334

Multivalent Siderophore DOTAM Conjugates as Theranostics for Imaging and Treatment of Bacterial Infections
Angewandte Chemie Int. Ed. (2017), 56, 8272-8276

Inhibition of type IV secretion activity and growth of Helicobacter pylori by cisplatin and other platinum complexes
Frontiers in Cellular and Infection Microbiology (2020), 10:602958

Labyrinthopeptins exert broad-spectrum antiviral activity through lipid-binding-mediated virolysis
Journal of Virology (2020), 94, e01471-19

Further info and site-contact

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Website: https://www.helmholtz-hzi.de/broenstrup / https://www.helmholtz-hzi.de/bilitewski

DE | High-capacity screening site

Fraunhofer Institute for Translational Medicine and Pharmacology (ITMP)

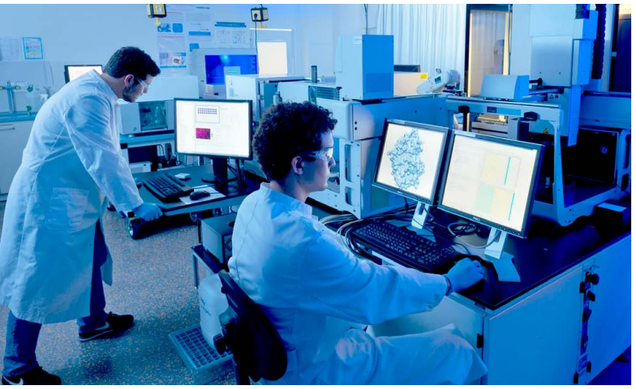
Schnackenburgallee 114, 22525 Hamburg, Germany

At a glance

- High capacity screening site with access to the EU-OPENSCREEN European Chemical Biology Library and the European Academic Compound Library
- Over 300 biochemical and cellular assays developed in past 10 years
- Level 1 and 2 biosafety laboratories including dedicated microbiological screening
- *In-vitro* toxicity and ADME profiling (cell viability to gene-tox)
- Visiting scientists can work with our team to adapt and screen assays
- Cheminformatics and structure expertises for compound selection and prioritisation

Infrastructure and technical focus

- Assay developement laboratory for minuaturisation and transfer
- Two large scale automated screening platforms, able to support all main optical and image based assay endpoints
- FACS and live cell imaging screening
- Surface plasmon resonance and target engagement assay for hit characterisation
- Advanced informatics workflows for imaging based projects
- Dedicated iPS laboratory for disease model development and testing



"We offer state-of-the-art infrastructure, an extensive expertise in assay development, HTS and structure-based drug design."

Dr. Philip Gribbon (Head of Unit)

„EU-OPENSCREEN membership is an essential way for Fraunhofer to connect and collaborate with disease biology experts across Europe. We look forward to working with you and helping discover new hits, leads and chemical tools to facilitate your research."

Projects past and present

2020 | Compound repurposing for new COVID-19 treatments Link

2020 | NEURIMS (Validation of the ion channel TRPM4 as a neuroprotective target in Multiple Sclerosis) Link

2020 | conSCIENCE (Cap snatching endonucleases as broad spectrum anti-viral targets) Link

2019 | FAIRplus (Make life science data FAIR - Findable, Accessible, Interoperable, Reusable - and improve data management) Link

Our science in selected publications

An automated and high-throughput-screening compatible pluripotent stem cell-based test platform for developmental and reproductive toxicity assessment of small molecule compounds.
Cell biology and toxicology, 2020, 1-15

Activation of caspase-6 is promoted by a mutant Huntingtin fragment and blocked by an allosteric inhibitor compound.
Cell chemical biology, 2019 26 (9), 1295-1305. e6

In vitro and in silico analysis of the effects of D_2 receptor antagonist target binding kinetics on the cellular response to fluctuating dopamine concentrations.
British journal of pharmacology, 2018, 175 (21), 4121-4136

A high-content small molecule screen identifies novel inducers of definitive endoderm.
Molecular metabolism, 2017, 6 (7), 640-650

Further info and site-contact

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Website: https://www.itmp.fraunhofer.de/de/institut/DrugDiscovery.html

DK

DENMARK

Member-Country since

2019

DK | Specialist screening site

University of Copenhagen – Biotech Research & Innovation Centre (BRIC)

Ole Maaløes Vej 5, 2200 Copenhagen, Denmark

At a glance

- Partner site specialized in high content screening
- Medium throughput capacity for smaller commercial or academic libraries (10k) and phenotypic validation libraries
- More than 10 years of experience with a variety of phenotypic readouts (autophagy, ribosome modifications, cell cycle regulation, DNA damage, neuronal homeostasis, cancer cell proliferation, protein degradation pathways)
- Advanced image analysis on physiologically relevant 3D cultures

Infrastructure and technical focus

- High content imaging in 2D and 3D
- Advanced image analysis of complex phenotypes
- Live-cell imaging
- Advanced in-house developed data analysis pipelines
- Screening platform, including liquid handling stations and flexible acoustic liquid transfer in nanoliter scale
- Full support during assay development and screening process

Prof. Krister Wennerberg (Head of Core Facility)

„EU-OPENSCREEN connects resources and technologies in a common effort to provide top-notch screening possibilities for European researchers. BRIC is looking forward to contribute to this community with our expertise on high content screening.“

Projects past and present

siRNA screen of the DDR pathway to investigate drug effects

Drug screen on the rescue of radiation response in astrocytes

Drug screen of patient derived tumor organoids co-cultured with fibroblasts

Arrayed CRISPR screen of DDR pathway genes in breast cancer cells

siRNA screen on autophagy mechanisms in cancer

siRNA screen on effect of DDR and nuclear localization genes on nucleoli in response to damage

Our science in selected publications

A high-throughput screen identifies the long non-coding RNA DRAIC as a regulator of autophagy
Oncogene. 2019; 38:5127-5141

High-throughput siRNA screening applied to the ubiquitin-proteasome system
Methods in Molecular Biology: Proteostasis 2016; 1449:421-39

eIF5A is required for autophagy by mediating ATG3 translation
EMBO Rep. 2018; 19:e46072

Further info and site-contact

Elin Pietras: elin.pietras@bric.ku.dk | +45 (0) 353 35005

Website: https://www.bric.ku.dk/core-facilities/ht-cell-based-screens

DK | Medicinal chemistry site

Technical University of Denmark (DTU) – Chemistry

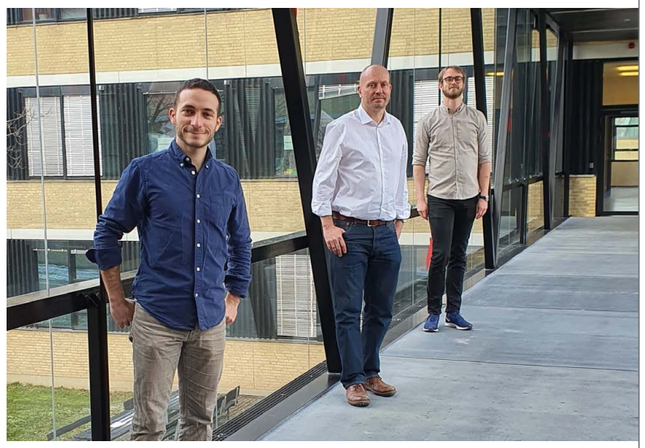
DTU Department of Chemistry, Building 207, 2800 Lyngby, Denmark

At a glance

- Medicinal chemistry site with more than 15 years of experience and access to state of the art analytical equipment
- Previous work is diverse and includes method development, analogue synthesis, structure based drug development (SBDD), and pro-drug synthesis
- Can provide computational chemistry approaches including qSAR and virtual screening
- Initial ADME profiling of analogues: Solubility, LogP, Caco-2, PAMPA, Microsomal stability, and toxicity

Infrastructure and technical focus

- Modern research labs for both synthetic- and analytical chemistry with 600 MHz and 800 MHz NMR, GC-MS, UPLC-MS, and preparative HPLC-MS equipment.
- Microwave synthesizer, parallel synthesis carousels and reaction blocks, automated peptide- and oligonucleotide synthesis, and photochemical reactors
- Facilities with fully automated biochemical and cell-based assays for screening of analogues



Prof. Mads H. Clausen (Head of Unit)

„For DTU Chemistry, our membership of the Danish research infrastructure for chemical biology and being a medicinal chemistry partner site with EU-OPENSCREEN enable us to interact with potential collaborators in chemical biology across Europe.“

Projects past and present

2020 | DZIF Blocking cholesterol production through specific protein degradation

2021 | ROS Reactive Oxygen Species in inflammatory disease Link

2019 | Argonaut Immuno-oncology Link

2018 | FBDD Design and screening of fluorinated fragments Link

Our science in selected publications

The 3F library – Fluorinated, Fsp3-rich Fragments for Expedious 19F NMR Based Screening
Angewandte Chemie Int. Ed. (2019), 59, 2204-2210

Image based morphological profiling identifies a lysosomotropic, iron sequestering autophagy inhibitor
Angewandte Chemie Int. Ed. (2020), 59, 5721-5729

Auxiliary in vitro and in vivo biological evaluation of hydrogen peroxide sensitive prodrugs of methotrexate and aminopterin for the treatment of rheumatoid arthritis
Bioorganic & Medicinal Chemistry (2020), 28, 115247

The cholesterol transfer protein GRAMD1A regulates autophagosome biogenesis
Nature Chemical Biology (2019), 15, 710-720

Further info and site-contact

Dr. Faranak Nami: fnam@kemi.dtu.dk | +45 (0) 22 79 23 57

Website: https://www.kemi.dtu.dk/english/research/organic-inorganic-chemistry/kemisk_biologi/madshclausenintro

ES

SPAIN

Member-Country
since

2018

ES | Specialist screening site

Centro de Investigación Príncipe Felipe (CIPF)

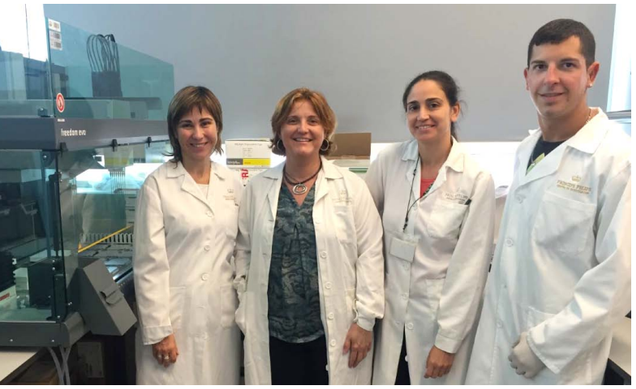
Av. Eduardo Primo Yúfera 3, 46012 Valencia, Spain

At a glance

- Screening site specialized on phenotypic assays in complex cellular systems including primary cultures and patient-derived models with access to the European Chemical Biology Library and the European Academic Compound Library
- Expertise from biochemical up to complex cellular assays
- Deep understanding of cellular trafficking and intracellular interactions by different molecular and imaging techniques
- Deep understanding of molecular mechanisms of cell death and metastasis
- Visiting scientists can work with our team to adapt and screen assays

Infrastructure and technical focus

- Assay development laboratory for miniaturisation and transfer
- Co-cultures, 3D spheroids and organoid models from different solid tumors including patient-derived samples
- Screening of exosome biogenesis/release inhibitors by combining AlphaScreen and immunofluorescence assays together with NTA
- HCS live cell imaging screening by confocal microscopy including Cytomics approach by InCell analyzer
- Cell painting approaches (2D and 3D)
- Advanced informatics and data processing workflows for imaging-based projects



Dr. María J. Vicent (Head of Unit)

„Being part of EU-OPENSCREEN broadens our possibilities to contribute towards the solution of unmet clinical needs. With our expertise in complex cellular systems we will work with you to find the best assay to answer your key scientific questions.“

Projects past and present

2020 - 2023 | SynVerPPC -PID2019-108806RB-I00 (Synergistic Approach for Metastatic Tumor and Neurodegenerative Disorder Treatments using Versatile PolyPeptide-based Conjugates)

2019 - 2021 | H2020 EU (Deep-Learning and Hpc To Boost Biomedical Applications For Health)

2018 - 2020 | SAF2017-84689-R (Understanding and drugging the Bcl-2 transmembrane interactome for tumor treatment)

2015 - 2020 | ERC Consolidator Grant 2014 Designing Personalised Polymer-based Combination Nanomedicines for Advanced Stage Cancer Patients (Acronym: MyNano)

Our science in selected publications

Polypeptide-corticosteroid conjugates as a topical treatment approach to psoriasis.
Journal of Controlled Release 2020, (318), 210-222

Mcl-1 and Bok transmembrane domains: Unexpected players in the modulation of apoptosis.
PNAS 2020,117(45), 27980-27988

High Throughput Screening (HTS) to Identify Exosome Biogenesis and Release Inhibitors,
5th Geivex Symposium, 2019

R & D Cloud CEIB: Management System and Knowledge Extraction for Bioimaging in the cloud.
Advances in Intelligent and Soft Computing 2012, 151, pp.331-338

Further info and site-contact

Esther Masià: emasia@cipf.es | +34 (0) 963 289 681

Website: www.vicentresearchlab.com

ES | Medicinal chemistry site

Center for Biological Research Margarita Salas (CSIC)

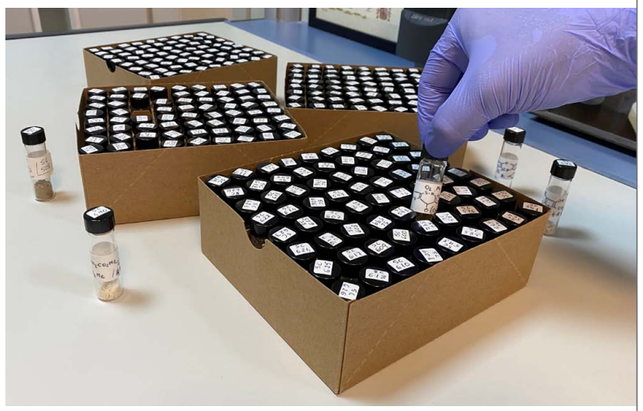
Ramiro de Maeztu 9, 28040 Madrid, Spain

At a glance

- EU-OPENSCREEN medicinal chemistry site with wide experience in structure based drug design (SBDD) and chemical genetics mainly for small heterocylcic compounds
- Synthetic chemistry designed to scale up the final pathways
- Hit-to-lead optimization beyond biological activity: looking for increase drug-like properties
- Virtual screening, computational chemistry and QSAR analysis included in our programs (drug discovery and drug optimization)
- More than six successfull programs from the bench to the clinical trials

Infrastructure and technical focus

- Synthetic and analytical capacity: hoods, lab space, microwave synthesizer, flash chromatography system, NMR, MS, HPLC/MS, elemental analysis
- ADME profile portfolio: solubility, PAMPA (BBB and oral absorption prediction) and microsomal stability
- Binding kinetics: Standard assays for kinases
- Chemoinformatics: work stations, computing clusters, and access to supercomputers clusters and scientific softwares



Prof. Dr. Ana Martínez (Head of Unit)

„Being part of EU-OPENSCREEN reinforces the internationalization of CSIC and allows our laboratory to achieve relevance beyond our borders. We contribute with our knowledge in the field and help to find drug candidates that can reach clinical phases.“

Projects past and present

2020 - 2021 | CoV2Drugs Target-and ligand-based drug repurposing to control SARS-CoV-2 pandemic Link

2018 - 2021 | ELA Madrid Design and development of innovative drugs for the treatment of ALS Link

2017 - 2021 | DRIVE Driving next generation autophagy researchers towards translation Link

Our science in selected publications

COVID-19: Drug Targets and Potential treatments
Journal of Medicinal Chemistry (2020), 63, 12359–12386

Motor neuron preservation and decrease in vivo of TDP-43 phosphorylation by protein CK-1δ kinase inhibitor treatment
Scientific Reports (2020), 10, Article number: 4449

Benzothiazole-based LRRK2 inhibitors as Wnt enhancers and pomoters of oligodencrocytic fate
Journal of Medicinal Chemistry (2020), 63, 2638-2655

Deciphering the enzymatic target of a new family of antischistosomal agents bearing a quinazoline scaffold using complementary computational tools
Journal of Enzyme Inhibition and Medicinal Chemistry (2020), 35, 511-523

Further info and site-contact

Prof. Dr. Ana Martinez: ana.martinez@csic.es | +34 (0) 91 8373 112

Website: https://www.cib.csic.es

ES | High-capacity screening site

Fundación Centro de Excelencia en Investigación de Medicamentos Innovadores en Andalucía (MEDI)

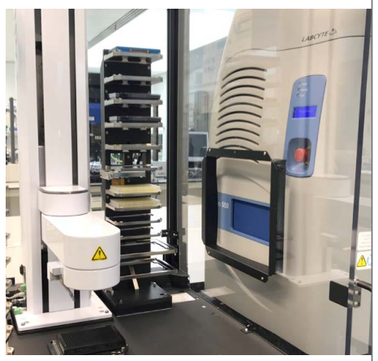
Avda. Conocimiento 3, Parque Tecnológico Ciencias de la Salud, 18100 Granada, Spain

At a glance

- High capacity screening center with core expertise in natural products drug discovery
- Access to EU-OPENSCREEN European Chemical Biology Library and the European Academic Compound Library
- Access to the MEDINA 200K natural products library
- Automated screening platforms with cutting edge assay technologies
- Biosafety Level 2 containment facilities for cell culturing and antimicrobial assays
- Chemical analytics and metabolomics
- Natural products chemistry and bioassay-guided isolation

Infrastructure and technical focus

- Development, miniaturization and validation of HTS screening assays
- Broad range of assay formats (96/384) and readouts
- Large scale HTS platform for cell based phenotypic and enzymatic assays
- Protein-protein interaction screening technologies
- High-content imaging screening
- Spheroids-3D cell culturing and anti-tumor screening
- Integrated informatics tools for assay data analysis
- Early ADME/safety platform and bioanalytics



Dr. Olga Genilloud (Scientific Director)

„As EU-OPENSCREEN partner, MEDINA is expanding its network of collaborators interested in accessing our screening platforms. We support early discovery programs from assay design and validation to preclinical evaluation of new hits and lead compounds.“

Projects past and present

2020 | NP4NTD Discovery of new antiparasitic drug candidates and innovative modes of actions from Microbial Natural Products Link

2020 | LISSA Alternatives to the use of disinfectants in the food industry aimed at reducing the survival of Listeria monocytogenes and Salmonella enterica on surfaces Link

2019 | TRIDs4DEB Driving next generation autophagy researchers towards translation Link

2017 | IIMENA Integration of informatics and Metabolic Engineering for the Discovery of novel antibiotics Link

Our science in selected publications

Strasseriolides A-D, a family of antiplasmodial macrolides isolated from the fungus Strasseria geniculata CF-247251
Organic Letters (2020), 22, 6709–6713

A high-throughput screening platform of microbial natural products for the discovery of molecules with antibiofilm properties against Salmonella.
Frontiers in Microbiology (2017), 8, 326

Design of high-throughput screening of natural extracts to identify molecules bypassing primary coenzyme Q deficiency in Saccharomyces cerevisiae
SLAS Discovery (2020), 25, 299-309

Cacaoidin, first member of the new Lanthidin RiPP family
Angewandte Chemie Int. Ed. (2020), 59, 12654-12658

Further info and site-contact

Dr. Olga Genilloud: olga.genilloud@medinaandalucia.es | +34 (0) 958 993 965

Website: https://www.medinadiscovery.com

ES | High-capacity screening site

University of Santiago de Compostela (USC)

CIMUS Research Center, Avda de Barcelona S/N – 15706, Santiago de Compostela Spain

At a glance

- High capacity pharmacogenomics platform with access to the EU-OPENSCREEN European Chemical Biology Library and the European Academic Compound Library
- Biochemical and cell-based assays including label-free technologies and High Content Imaging
- Early ADME-Tox profiling
- Vast experience in assay development and assay adaptation to HTS with more than 300 assays available
- Long track record in drug discovery and chemical biology with 15 NCE entering clinical trials
- Collaborative framework with visiting scientists working with our team for assay transfer

Infrastructure and technical focus

- Assay development laboratory for miniaturization
- Fully automated robotic platform for HTS for both biochemical and cell-based assays
- High Content Screening with automated analysis workflows
- DNA-encoded libraries technology
- Biochemical and cell-based label-free screening
- High capacity for biological reagent production using disposable bioreactors
- Translational assays for target engagement and patient stratification

Prof. María Isabel Loza (Research Manager)

„EU-OPENSCREEN membership is the way of USC-Innopharma platform to collaborate with the best science and knowledge in early drug discovery and chemical biology across Europe.“

Projects past and present

2021 | DRUGtrain Drug repurposing and discovery multidisciplinary training network Link

2019 | Pharmaceutical development of fast-track and innovative therapies targeting ACE2 for COVID-19

2020 | CANCER INNOVA Business Factory Medicines. Incubator of projects in the field of cancer drug discovery Link

2018 | Joint I+D Unit ESTEVE – USC Developing new medicines to treat chronic pain Link

Our science in selected publications

Identification of ABA Receptor Agonists Using a Multiplexed High-Throughput Chemical Screening Methods
Mol Biol. 2021;2213:99-111

Identification and characterization of Cardiac Glycosides as senolytic compounds
Nat Commun. . 2019 Oct 21;10(1):4731

Fibrates as drugs with senolytic and autophagic activity for osteoarthritis therapy
EBioMedicine. 2019 Jul;45:588-605

A New Model of Sensorial Neuron-Like Cells for HTS of Novel Analgesics for Neuropathic Pain
SLAS Discov. 2019 Feb;24(2):158-168

Further info and site-contact

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Website: https://www.usc.es/cimus/en/research/research-groups/pharmacology-applied-drug-discovery

FINLAND

Member-Country since

2018

FI | High-capacity screening site

High Throughput Biomedicine Unit, Institute for Molecular Medicine Finland (FIMM)

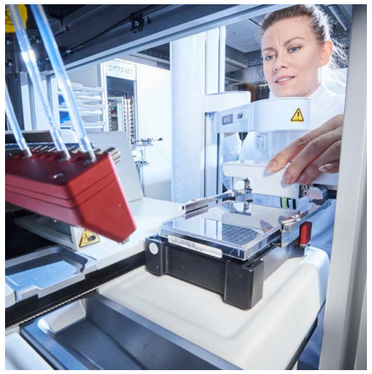
University of Helsinki, Tukholmankatu 8, 00290 Helsinki, Finland

At a glance

- High-end integrated laboratory automation with versatile liquid handling and signal detection instruments
- Access to the EU-OPENSCREEN European Chemical Biology Library and the European Academic Compound Library as well as to local libraries
- Cell-based and biochemical HTS projects utilizing small molecules and/or genome-wide siRNA library
- Established practices for ex vivo testing of patient samples against oncology drugs
- Visiting scientists are welcome to work with our team

Infrastructure and technical focus

- Expertise in screening project planning, assay development, and miniaturization
- HighRes Biosystems automated A-cell robotic platform for fully automated screening projects
- BeckmanCoulter Access platform and ECHOs for acoustic dispensing of liquids at nanolitre scale
- Optical, imaging, RT-qPCR and HT flow cytometry based signal detection modalities
- Data analysis tools and pipelines



Prof. Päivi Tammela (Head of Unit)

„As a member of the EU-OPENSCREEN network, our FIMM HTB Unit is looking forward to building exciting new collaborations and to supporting screening projects stemming from your research with our expertise and infrastructure for high-throughput screening.“

Projects past and present

2020 | Drug repurposing for SARS-CoV-2 with an open high throughput drug screening platform

2020 | Multiplexed and miniaturized immunofluorescence assay for SARS-CoV2 immunity measurement with AI-assisted image analysis

Our science in selected publications

Therapeutic targeting of KSP in preclinical models of high-risk neuroblastoma
Science Translational Medicine (2020), 12: eaba4434

Breeze: an integrated quality control and data analysis application for high-throughput drug screening
Bioinformatics (2020), 36, 3602-3604

Network pharmacology modeling identifies synergistic Aurora B and ZAK interaction in triple-negative breast cancer
NPJ Systems Biology and Applications (2019), 5, 20

Methods for high-throughput drug combination screening and synergy scoring.
Methods in Molecular Biology (2018), 1711, 351-398

Further info and site-contact

Dr. Jani Saarela: jani.saarela@helsinki.fi | +358 50 3175 485

Website: https://www2.helsinki.fi/en/infrastructures/drug-discovery-chemical-biology-and-screening/infrastructures/fimm-high-throughput-biomedicine-unit

FI | Specialist screening site

University of Helsinki, Faculty of Pharmacy (UH)

University of Helsinki, Viikinkaari 5E, 00790 Helsinki, Finland

At a glance

- Specialised screening site
- Target- and cell-based antimicrobial assay development and screening, incl. biofilm, advanced 3D and host-pathogen co-culture models
- Computational and ***in vitro*** ADMET profiling
- Development of tailored assays e.g. for novel materials
- Expertise on utilizing natural products in screening
- Organotypic cell models, cellular and vesicular drug transport assays and predictive pharmacokinetic models

Infrastructure and technical focus

- Expertise in antimicrobial screening, assay development, and miniaturization
- Biosafety level 1 and 2 microbiology and cell culture facilities
- Platform designed for antimicrobial screening workflows and follow-up assays
- Expertise in natural product discovery
- Predictive computational ADMET models
- Chem-/bioinformatics resources, access to supercomputing facilities

Prof. Arto Urtti (Head of Unit)

„The Faculty of Pharmacy EU-OPENSCREEN site has expertise on specialised screening, for instance for antimicrobials, as well as on in silico and in vitro ADMET evaluations, and hosts international level expertise and infrastructure for these studies.“

Projects past and present

2020 | SPRINGBOARD for excellence in advanced development of antibacterials Link

2019 | NO-ESCAPE Evolving the next generation of Gram-negative antimicrobials through a synergetic approach encompassing medicinal chemistry, microbiology and nanomedicine tools Link

2019 | RESET-ME Restoring *E. coli* sensitivity for antibiotics by blocking TolC-mediated efflux Link

Our science in selected publications

Ocular barriers to retinal delivery of intravitreal liposomes: Impact of vitreoretinal interface
Journal of Controlled Release (2020), 328, 952-961

Defining conditions for biofilm inhibition and eradication assays for Gram-positive clinical reference strains
BMC Microbiology (2018),18, 173

Binding Site Interactions of Modulators of Breast Cancer Resistance Protein, Multidrug Resistance-Associated Protein 2, and P-Glycoprotein Activity
Molecular Pharmaceutics (2020), 17, 2398-2410

A New Cell-Based AI-2-Mediated Quorum Sensing Interference Assay in Screening of LsrK-Targeted Inhibitors
ChemBioChem (2020), 21, 1918-1922

Further info and site-contact

Prof. Päivi Tammela: paivi.tammela@helsinki.fi | +358 50 4480 886

Website: https://www.helsinki.fi/en/infrastructures/drug-discovery-chemical-biology-and-screening/infrastructures/faculty-of-pharmacy

LV

LATVIA

Member-Country
since

2018

LV | Medicinal chemistry site

Latvian Institute of Organic Synthesis (OSI)

Aizkraukles 21, Riga LV-1006, Latvia

At a glance

- **Focus areas:** Antiinfective, cardiovascular, anticancer and Central Nervous System (CNS) drug discovery and development
- **Lead discovery and optimization:** Synthetic hit-to-lead & lead optimization; Structural biology; Biochemical & biophysical screening; Fragment based lead discovery; Natural product inspired lead discovery; *In silico* drug design
- **Pharmacology:** New drug targets, mode of action; *In vitro*, *ex vivo*, *in vivo* efficacy models; *In vitro* ADMET; *In vivo* PK and toxicity; Bioanalytical assays
- **Process chemistry:** Route scouting; Process scale-up; Kg-scale synthesis; Impurity profiling

Infrastructure and technical focus

- More than 5000 m^2 of fully equipped labs for medicinal/organic chemistry, pharmacology, and protein expression. EU-compliant animal facility
- Biophysical chemistry equipment including high-field NMRs, SPR and ITC
- Centrally operated analytical equipment including open access NMRs; X-ray; HRMS; tandem MS; microanalysis, FT-IR, and various chromatography equipment
- Kilo-scale facility including reactors (up to 63 L) and necessary auxiliary equipment

Dr. Osvalds Pugovičs (Director)

„EU-OPENSCREEN membership offers us a unique opportunity to contribute our drug discovery expertise addressing major health challenges. This platform enables networking with leading experts comprising state-of-the-art knowledge and infrastructure.“

Projects past and present

2020-2025 | ERA4TB European Regimen Accelerator for Tuberculosis

2020-2023 | SPRINGBOARD Springboard for excellence in advanced development of antibacterials

2020-2023 | InterTAU Integrative Structural Biology of Pathological tau Protein, an Appealing Therapeutic Target for Alzheimer´s Disease Modifying Drugs

2019-2022 | FAT4BRAIN Networking for excellence in functional pharmacology to study the role of fatty acid metabolism in neurological disorders

Our science in selected publications

Development of oxathiino[6,5-b]pyridine 2,2-dioxide derivatives as selective inhibitors of tumor-related carbonic anhydrases IX and XII
European Journal of Medicinal Chemistry 2020, 200, 112300

Fused isoselenazolium salts suppress breast cancer cell growth by dramatic increase in pyruvate-dependent mitochondrial ROS production
Scientific Report 2020, 10, 21595

Bacterial Sortase A with Covalent Inhibitors: 27 New Starting Points for Structure-Based Hit-to-Lead Optimization
ACS Infectious Diseases 2020, 6, 186-194

Exploiting Structural Dynamics to Design Open-Flap Inhibitors of Malarial Aspartic Proteases.
Journal of Medicinal Chemistry 2019, 62, 8931−8950

Further info and site-contact

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Website: https://www.osi.lv/en/

NO

NORWAY

Member-Country
since

2018

NO | Specialist screening site

SINTEF – Department of Biotechnology and Nanomedicine

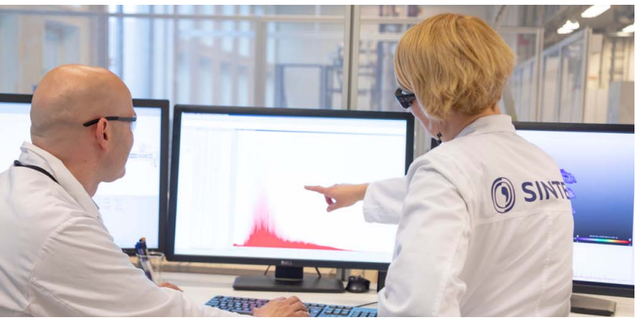
Richard Birkelands vei 3, 7034 Trondheim, Norway

At a glance

- Independent non-profit research organization welcoming academic and industrial collaborations
- Research within bioprocess development, biomaterials, immunotherapy, vaccines, gut health, drug delivery and nanomedicine
- Biochemical, microbial and mammalian cell-based high-throughput screening
- Advanced cell models (incl. spheroids, barrier, biofilm), coupled to advanced reporter assays
- Functional screening of patient cells for personalized medicine
- High-sensitivity and in-depth analysis including transcriptomics, metabolomics, proteomics and lipidomics

Infrastructure and technical focus

- Four automated liquid handling robots, fully integrated with FACS, high-content confocal imaging, and all available detection technologies
- Fully automated cell cultivation robotics with image-based readouts
- Biosafety Level 1 and 2 laboratories, specialized for viruses, eukaryotic and microbial cell-based screening
- High-throughput mass spectrometry
- Bioreactors for bioproduction from micro- to pilotscale



Geir Klinkenberg (Research Manager)

„We offer state-of-the-art infrastructure and extensive experience in assay development and high throughput screening including toxicity, and antibacterial- and antifungal activity. We also offer activity assays towards a range of mammalian cell lines.“

Projects past and present

2020 | Novel treatment for neuronal reoxygenation injuries (Development of inhibitors to undrugged DNA repair enzymes)

2019 | PRESORT Functional drug screening as clinical decision support in colorectal cancer

2017 - 2021 | H2020 REFINE Risk-benefit assessments of medical products and devices based on nanomedicines and biomaterials Link

EU-NCL The European nanomedicine characterisation laboratory Link

Our science in selected publications

High-throughput screening reveals higher synergistic effect of MEK inhibitor combinations in colon cancer spheroids
Science Reports (2020), 10, 11574

A high-throughput drug combination screen of targeted small molecule inhibitors in cancer cell lines
Scientific Data (2019), 6, 237

Identification of Regulatory Genes and Metabolic Processes Important for Alginate Biosynthesis in *Azotobacter vinelandii* by Screening of a Transposon Insertion Mutant Library
Frontiers in Bioengineering and Biotechnology (2020), 7, 475

Engineering chitinolytic activity into a cellulose-active lytic polysaccharide monooxygenase provides insights into substrate specificity)
. Journal of Biological Chemistry (2019), 294, 50, 19349-19364

Further info and site-contact

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Website: https://www.sintef.no/en

NO | Specialist screening site

Biorecognition unit & BiSS / Biophysics, Structural Biology and Screening (UiB)

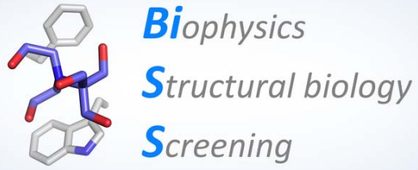
Jonas Lies vei 91, 5009 Bergen, Norway

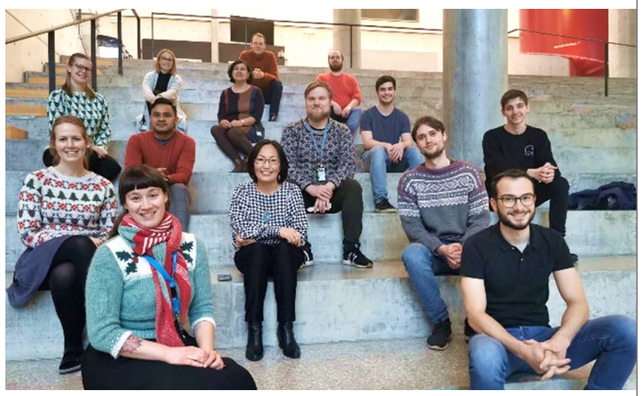
At a glance

- Notable expertise in developing therapies for misfolding disorders and infectious diseases
- Managed by the core facility for Biophysics, Structural Biology and Screening (BiSS)
- Access to European Chemical Biology Library, European Academic Compound Library and Fragments
- Chemoinformatic services for hit follow up
- Determination of binding modes using X-ray crystallography
- Self-service access to instrumentation possible after training

Infrastructure and technical focus

- Molecular-based screenings of small molecules with isolated biomolecular targets
- High throughput screening using thermal shift assay (differential scanning fluorimetry)
- Surface plasmon resonance (SPR) and bio-layer interferometry (BLI) for fragment screening and hit validation
- Instrumentation for liquid handling
- Crystallization facility in house with automated monitoring of crystal growth





Prof. Aurora Martinez (Head of Unit)

„EU-OPENSCREEN is a crucial collaborative network for the Univ. of Bergen lowering the access barrier to chemical biology facilities and drug discovery. In the Biorecognition unit, we are specialized in molecular and biophysical screens.“

Projects past and present

2018 - 2021 | BIOTEK2021, RCN (A corrective therapy for acute intermittent porphyria)
Link

2020 - 2024 | PRIME (Prevention and Remediation of Insulin Multimorbidity in Europe / H2020-SC1-2019-Two-Stage-RTD EU) Link

2018 - 2021 | BEDRE HELSE project (Structure-based exploration of targets for antibiotics)

2019 - 2023 | DLN project RESPOND[3] (Towards better computational approaches and responsible innovation strategies in early drug discovery) Link

Our science in selected publications

Differential scanning fluorimetry in the screening and validation of pharmacological chaperones for soluble and membrane proteins Protein Homeostasis Diseases
Academic Press, 2020, pp 329-341

Targeting the Class A Carbapenemase GES-5 via Virtual Screening
Biomolecules 2020, 10(2), 304

Levalbuterol lowers the feedback inhibition by dopamine and delays misfolding and aggregation in tyrosine hydroxylase
Biochimie 2020, S0300-9084(20), 30322-9

A Pharmacological Chaperone Therapy for Acute Intermittent Porphyria
Molecular Therapy 2020, 28(2), 677-689

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NO | Specialist screening site

University of Oslo – Centre for Molecular Medicine Norway (UiO NCMM)

Forskningsparken, Gaustadalléen 21, 0349 Oslo, Norway

At a glance

- Specialized screening site within EU-OPENSCREEN and managing node for the national Research Infrastructure NOR-OPENSCREEN
- Core facility for the University of Oslo and Oslo University Hospital
- Access to the EU-OPENSCREEN European Chemical Biology Library and European Academic Compound Library
- Visiting researchers can develop assays with our team
- Access to a variety of local core facilities like Genomics, Proteomics and Bioinformatics
- Competence in biochemical / cell-based assays and precision medicine

Infrastructure and technical focus

- Laboratory for assay development and transfer
- Large scale, fully automated screening platform for optical readouts (Access Workstation acoustic and classic liquid handling)
- Automated sample preparation for advanced high throughput flow cytometry assays
- Biosafety Level 2 cell culture for primary human cells
- Competence in immunology, characterization of immune cells and intra cellular signaling

Dr. Johannes Landskron (Research Manager)

„EU-OPENSCREEN connects chemical biology experts across Europe in an exceptional infrastructure. Together with the comprehensive compound library, this opens unique possibilities for our users. We are looking forward to the collaboration.“

Projects past and present

2020 | BioMedData Implementation of FAIR (Findable, Accessible, Interoperable and Reusable) data management / coordinated by ELIXIR Norway Link

2020 | FUCOMED Characterization and utilization of Fucoidan from Seaweed Link

2016 | NOR-OPENSCREEN Managing partner of the national Norwegian RI for Chemical biology and bioprospecting Link

Our science in selected publications

An in vitro assay for biomarker discovery and dose prediction applied to ibrutinib plus venetoclax treatment of CLL
Leukemia (2020), 34, 478–487

Identification of small molecule NPR-B antagonists by high throughput screening — potential use in heart failure
Naunyn-Schmiedeberg's Arch Pharmacol (2014), 387, 5–14

A Cell-Based High-Throughput Assay for Gap Junction Communication Suitable for Assessing Connexin 43–Ezrin Interaction Disruptors Using IncuCyte ZOOM
SLAS Discovery (2017), 22, 77–85

Assay development for the discovery of small-molecule inhibitors of YadA adhesion to collagen
The Cell Surface (2019), 5, 100025

Further info and site-contact

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NO | Specialist screening site

Marbio, an analytical platform for natural products (UiT)

Siva innovasjonssenter, 9037 Tromsø, Norway

At a glance

- Experience in screening complex mixtures (i.e. natural product extracts and fractions) for biological activity in biochemical and cell-based assays
- Dereplicating (identifying) known compounds in complex mixtures using chromatography and high-resolution mass spectrometry
- Isolation of bioactive natural products from crude extracts using a combination of classic techniques such as liquid-liquid extractions and flash chromatography, as well as state of the art mass guided fractionation based on HPLC
- Structural elucidation of complex natural products using high resolution MS as well as spectroscopic techniques such as NMR, IR and UV

Infrastructure and technical focus

- An analytical platform for biodiscovery
- A screening unit that tests for various applications: automated liquid handlers, multimode readers (absorbance, fluorescence, luminescence)
- A microbiology unit that isolate and cultivate marine microorganisms: shake incubators, automated colony picker
- A chemistry unit that identify and purify the bioactive natural products: Flash, HPLC, UPLC, LC-MS, MS-MS, IMS

Prof. Jeanette Hammer Andersen (Head of Unit)

„EU-OPENSCREEN gives us the opportunity to connect with laboratories across Europe. The collaboration will enhance the opportunities for identifying novel bioactive natural products.“

Projects past and present

2020 - 2023 | SuReMetS Developing novel marine ingredients using underutilized material from fisheries as well as microalgae to target management of metabolic syndrome

2020 - 2022 | TackAML Targeting drug resistant acute myeloid leukemia with a next-generation FLT3 inhibitor

2018 - 2022 | Digibiotics Digital discovery of antimicrobial molecules from marine Arctic resources with reduced risk of triggering resistance Link

Our science in selected publications

Bioactivity of serratiochelin A, a siderophore isolated from a co-culture of Serratia sp and Shewanella sp
Microorganisms 2020, 8(7), 1-17

Kinase chemodiversity from the Arctic: The Breitfussins
Journal of Medicinal Chemistry 2019; 62(22), 10167-10181

Dendrobeaniamine A, a new alkaloid from the Arctic marine bryozoan Dendrobeania murrayana
Natural Product Research 2019, 34(14), 2059-2064

Metabolomic profiling reveals the N-acyl-taurine geodiataurine in extracts from the marine sponge Geodia macandrewii (Bowerbank)
Journal of Natural Products 2016, 79, 5, 1285-1291

Further info and site-contact

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PL

POLAND

Member-Country since

2018

PL | Specialist screening site

Institute of Bioorganic Chemistry, Polish Academy of Sciences (IBCH PAS)

Uniwersytetu Poznańskiego str. 10, 61-614 Poznań, Poland

At a glance

- Specialist screening site with access the European Chemical Biology Library and the European Academic Compound Library
- Expertise in biochemical and cellular assays including high-content screening and image analysis (biological models include proteins, nucleic acids, mammalian cell lines, iPS, primary as well as plant cells and 3D spheroids)
- Employing Artificial Intelligence for high-throughput combinatorial screening
- Close collaboration and consulting on development of fluorescent and bioluminescent probes and assays

Infrastructure and technical focus

- Fully automated AGAMEDE™ screening platform to support a wide range of readouts
- Laboratory for assay development, miniaturization and assay transfer
- High-throughput imaging for live and fixed cells with confocal microscopy
- Combinatorial screening with Artificial Intelligence Algorithm
- Bioinformatic support for large volume data analysis
- Ultraresolution (<5 nm) fluorescent confocal nanoscopy in live cells (MINFLUX) & superresolution microcopy (STED, STED-FLIM)
- Unique additional focus: binders of nucleic acids
- Development of assays based on fluorescent probes for simultaneous detection of multiple parameters

Dr. Jacek Kolanowski (Head of Unit)

„We look forward to collaborating with the users from around the world, developing new screening technologies and assays, carrying out exciting projects for the identification of biologically active molecules and deconvolution of their mechanisms of action.“

Projects past and present

2020 - 2021 | SARS-CoV-2 RNA, target for inhibition of virus replication Link

2020 - 2021 | TMPRSS2 – a potential new drug target and a determinant of COVID19 outcome Link

2018 - 2023 | POL-OPENSCREEN (Polish Screening Infrastructure Platform for Chemical Biology) Link

2018 - 2021 | MultiGATE (Dual-analyte responsive fluorescent probes for a real-time multi-parametric sensing in cellular models) Link

Our science in selected publications

High-throughput evolutionary optimization of the induction medium towards recombinant protein production in BY-2 tobacco
Biotechnology and Bioengineering 2020

Small molecule PGC-1α1 protein stabilizers induce adipocyte Ucp1 expression and uncoupled mitochondrial respiration.
Molecular Metabolism 2018, 9, 28-42

Sensitive ADAR editing reporter in cancer cells enables high-throughput screening of small molecule libraries. Nucleic Acid Research 2019, 28, 47(4), e22.

A fluorescent probe for investigating metabolic stability of active transplatin analogues.
Sensors and Actuators B: Chemical 2018, Volume 255, Part 3, 2721 - 2724

Further info and site-contact

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Radosław Pilarski: rapil@ibch.poznan.pl | +48 61 829 18 65

Website: https://portal.ichb.pl/en | http://agamede.ai

PL | Medicinal chemistry site

Institute of Biochemistry and Biophysics (IBB PAS)

Pawinskiego 5a, 02-106 Warszawa, Poland

At a glance

- Bioinformatics platform for optimization of lead compounds structure
- A wide range of bioinformatics services provided by experienced scientists
- Methodology for the construction of protein-protein interaction peptide inhibitors
- Design of small molecule-, peptide- as well as peptidomimetic- inhibitors, and miRNAs as modulators of metabolism
- Physicochemical and ADME profiling (State of the art equipment and highly qualified staff performing experimental measurements)

Infrastructure and technical focus

- NEST computing cluster based on Intel and AMD processors, professional graphic computing cards and programmable coprocessor cards
- Large-scale in silico screening system, based on our molecular fitting solutions and machine learning based assessments
- Tools for the analysis and visualization of the results of large scale screening experiments, both experimental and in silico
- Systems biology tools, including reactome analysis and FBA/FVA
- Cheminformatics and Target Modelling Course

Prof. Dr. Piotr Zielenkiewicz (Head of Unit)

„I hope our involvement in EU-OPENSCREEN will not only increase the participation of Polish researchers in screening tests, but will also show the added value of in silico studies in search for the new drugs.“

Projects past and present

2021 | Speeding up discovery for mutation diagnostic therapies in cystic fibrosis: an approach based on Artificial Intelligence and Systems Biology (VERTEX Innovation Award) Link

2019 | Integrated laboratory for large-scale gene and protein analyses

2018 | POL-OPENSCREEN (Polish Platform of Screening Infrastructure for Biological Chemistry) Link

Our science in selected publications

Development and evaluation of a deep learning model for protein-ligand binding affinity prediction
Bioinformatics, 2018, 34(21), 3666-3674

DeCAF-Discrimination, Comparison, Alignment Tool for 2D PHarmacophores
Molecules, 2017, 22 (7), 1128

Performance of machine-learning scoring functions in structure-based virtual screening.
Scientific Reports, 2017, 7, 46710

Open Drug Discovery Toolkit (ODDT): A new open-source player in the drug discovery field.
Journal of Cheminformatics, 2015, 7, 26

DiSCuS: An Open Platform for (Not Only) Virtual Screening Results Management
Journal of Chemical Information and Modeling, 2014, 54(1), 347-354

Further info and site-contact

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PL | Specialist screening site

Institute of Medical Biology Polish Academy of Sciences (IMB PAS)

Lodowa 106, 93-232 Łódź, Poland

At a glance

- The research is focused on the body-environment relationships at the interface of pathogen, and the host at the molecular, cellular and body level with emphasis on infectious diseases, both viral and bacterial. Level 1, 2, and 3 biosafety laboratories are available.
- Expertise in microbiology, particularly host-pathogen interactions
- Biological chemistry and pharmaceutical sciences focus on chemical synthesis and testing of chemical compounds aimed at identifying new derivatives exhibiting antiviral, antimicrobial, and anticancer activity.

Infrastructure and technical focus

- National Library of Chemical Compounds with a target collection of more than 10,000 original molecules from academic institutions
- Specialized Screening Laboratory Bacteriology-Virology
- Automated platform for microbiological screening (Gramm-negative and -positive bacteria as well as tubercle bacilli)
- Huge collection of mycobacterial directed mutants available - http://ibmpan.pl/images/pracownie/pgifm/tabela_DCO_PGiFM.htm
- Development of biochemical assays for automatic screening
- Assessment of antiviral activity of chemical compounds against HCMV, HSV-1, EMCV, HPIV-3 and selected other BSL2 category viruses; real-time cell analysis (RTCA).

Prof. Jarosław Dziadek (Head of Institute)

„The close collaboration with experts from the EU-OPENSCREEN network allows for effective and mutually beneficial know-how transfer, development of personnel in R&D area and facilitates the discovery of innovative bioactive compounds.“

Projects past and present

2020 | Epigenetic immunomodulation dependent on elements of the microbiome. Model of direct and indirect interactions of Th17 and Treg cells with *Staphylococcus aureus* in the course of psoriasis

2020 | The course of COVID-19 disease in the aspect of immune response and genetic variability of the host and SARS-CoV-2

2019 | The use of evolutionary patterns in the optimization of chemotherapy of tuberculosis

2018 - 2023 | POL-OPENSCREEN (Polish Screening Infrastructure Platform for Chemical Biology)

Our science in selected publications

Novel Isoniazid-Carborane Hybrids Active in Vitro against *Mycobacterium tuberculosis*
Pharmaceuticals (Basel). 2020, 13:465

1H-benzo[d]imidazole derivatives affect MmpL3 in *Mycobacterium tuberculosis*
Agents Chemother. 2019, pii: AAC.00441-19

Synthesis of naphthalimide-carborane and metallacarborane conjugates: anticancer activity, DNA binding ability
Bioorg. Chem., 2020, (94), 103432

Comparative study of the effects of *ortho*-, *meta*- and *para*-carboranes ($C_2B_{10}H_{12}$) on the physicochemical properties, cytotoxicity and antiviral activity of uridine and 2'-deoxyuridine boron cluster conjugate
Bioorg. Chem., 2019

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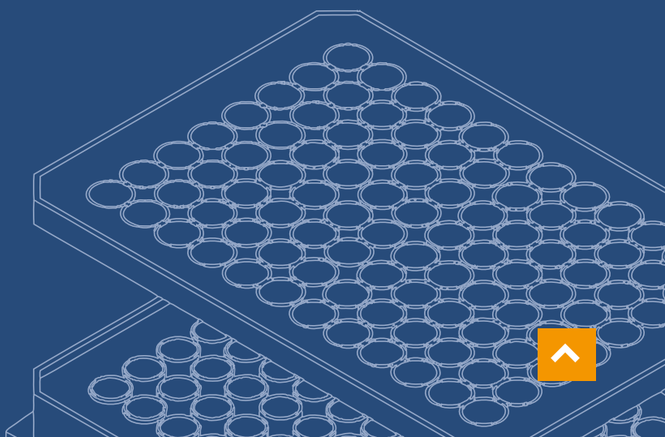

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