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ACTIVITY AND FINANCIAL REPORT 2022

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FOREWORD

by Director General Dr Wolfgang Fecke

Dr. Wolfgang Fecke, EU-OPENSCREEN Director General

Dear partners, colleagues and friends, 2022 has been an exciting year for EU-OPENSCREEN. Despite the adverse social and economic conditions caused by the remnants of the global pandemic and by Russia's war on Ukraine, EU-OPENSCREEN succeeded in overcoming these challenges and moving forward with its operations, thanks to the flexibility and strong commitment of its team and partners.

Staying true to its mission in serving the scientific community, EU-OPENSCREEN has increased its overall volume of activity and enlarged its number of countries and partner sites. Our portfolio of screening and technology collaborations grew over the year to a total of more than 30 active projects. This was accompanied by the initiation of our first five medicinal chemistry projects.

Together with our scientific offerings in the fragment screening and chemoproteomics fields, EU-OPENSCREEN is now in a position to fulfill its core mission of developing novel small molecule chemical probes, and to fully support chemical biology and early drug discovery projects.

Our two new member countries, Portugal and Sweden, added highly experienced partner sites to our network and gave us additional capacity and flexibility to serve the needs of our growing user community. Several successful grant applications allowed us to establish EU-OPENSCREEN as an important service provider. Among them the emergency pandemic response project ISIDORe and the canSERV project which serves users in the cancer area. In addition, the launch of the AgroSERV project in late 2022 gave us, for the first time, the opportunity to gain experience in agrochemical research. Overall, the number of EU-funded projects increased significantly, from eight in 2021 to thirteen in 2022.

Existing workflows were optimized, compounds were analysed with increasing efficiency, and novel compounds were sourced from academic groups. Our academic compound library grew significantly from a few hundred compounds to now about 4.000 molecules, many of them displaying also exciting new chemistry. Additional team members were recruited, and strategically important grant applications were written. Thanks to the generous support from the German Ministry of Research and Education, large compound bioprofiling campaigns delivered important experimental data on all our 100.000 compounds. Most of this data is already submitted to our open access European Chemical Biology Database (https://ecbd.eu). Collaborations with like-minded infrastructures intensified on many levels, culminating in the signing of a 'Memorandum of Understanding' between EU-OPENSCREEN ERIC, Instruct ERIC, and Euro-Bioimaging ERIC at the ICRI conference in October.

While the organization of our annual virtual training school and webinar series became almost a routine activity, I would like to point out two additional highlights of the year. In the framework of our EU-OPENSCREEN-DRIVE project, we discussed in a very fruitful meeting in Santiago de Compostela with industry leaders from pharmaceutical companies, Life Sciences technology providers and Biotech companies, realistic opportunities for future collaborations. And, using our first bioprofiling data set as a basis, we kicked-off our first computational modelling challenge on Kaggle in collaboration with the US-based Society of Laboratory Automation and Screening (SLAS).

Most of these activities will continue in 2023, confirming the role of EU-OPENSCREEN as a true facilitator and enabler of chemical biology research in Europe.

On behalf of the whole team,

TIMELINE OF KEY HIGHLIGHTS

01/2022

Portugal joins EU-OS as new member country

02/2022

Our training webinar series 2022 started off in February with Anna-Lena Gustavsson, Director of Chemical Biology Consortium Sweden

06/2022

Webinar with Mads Hartvig Clausen, Technical University of Denmark (DTU) and Director of DK-OPENSCREEN

07/2022

Sweden joins EU-OPENSCREEN as new member country

Webinar on July 26 with Jonathan Baell, Director of the Australian Translational Medicinal Chemistry Facility

09/2022

Start of our EU-OPENSCREEN/SLAS Data challenge

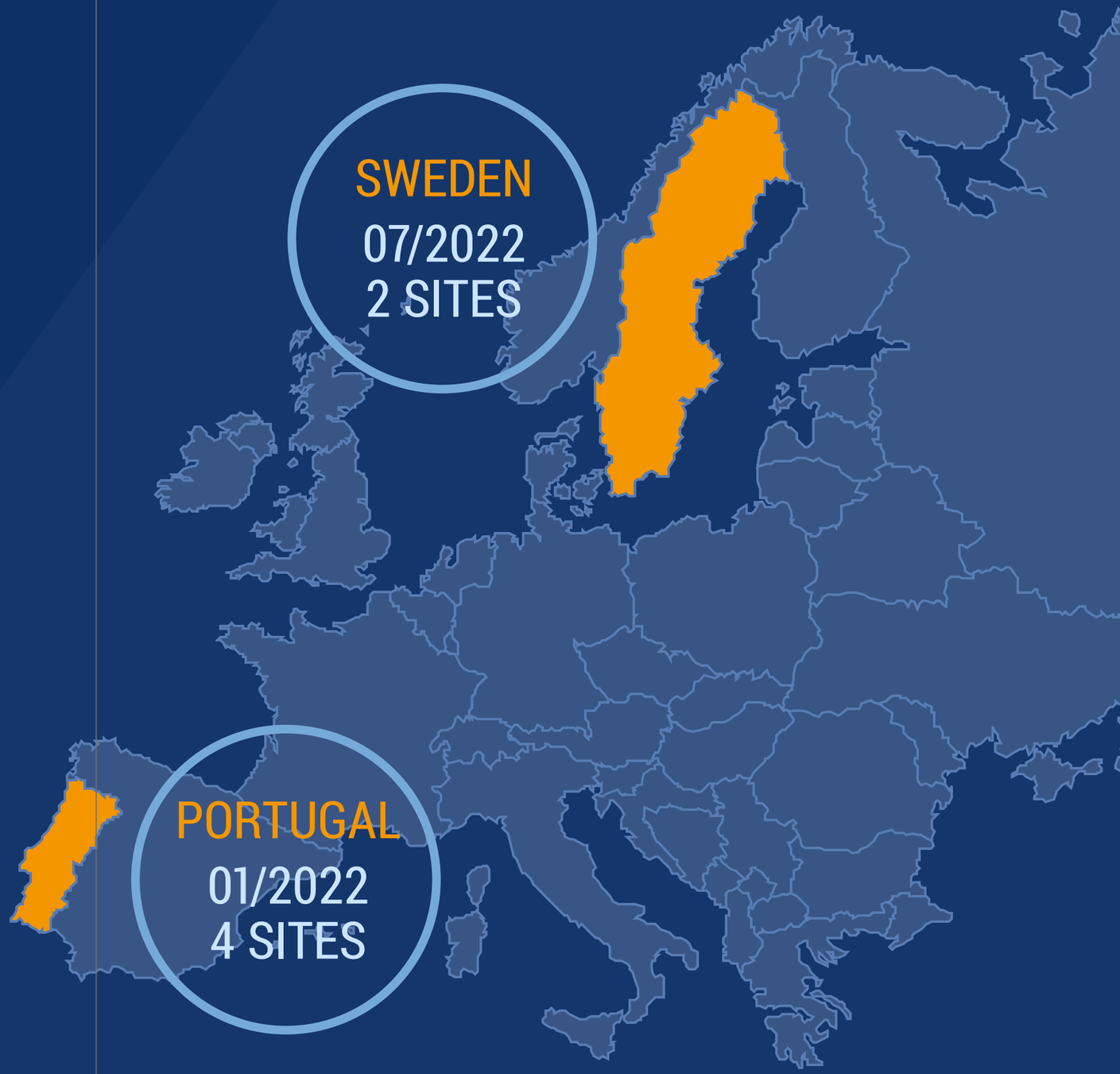
Kick off meeting of canSERV project in Brussels

11/2022

Autumn training school 2022: five-days virtual training event

NEW MEMBER COUNTRIES AND PARTNER SITES

We are constantly working to expand our network and add additional skills and capacity to our infrastructure. We are very proud to welcome two new partner countries and several new Partner sites to our community in 2022.



NEW MEMBER COUNTRY

PORTUGAL - 01/2022

Portugal joined the EU-OPENSCREEN ERIC as a new member country in January 2022. The National Infrastructure for Chemical Biology and Genetics in Portugal (PT-OPENSCREEN) has been included in the 2020 Portuguese Roadmap of Research Infrastructures. PT-OPENSCREEN, which is coordinated by the Institute for Health Research and Innovation of the University of Porto (i3S), brings together the main research centers in the areas of chemistry and biology across the country and coordinates the participation of Portugal in EU-OPENSCREEN.

The representing entity is the Fundação para a Ciência e a Tecnologia (FCT, I.P.). Portugal will be represented in the Assembly of Members by Marta Abrantes (FCT) and Dr. António Pombinho (i3S).

These are really exciting times for Portuguese chemical biology research. We were able to establish a dynamic national infrastructure and now join forces with the best European institutions in the field.

Dr. António Pombinho / Institute for molecular and cell biology, University of Porto

PT-OPENSCREEN

All Portuguese sites are members of PT-OPENSCREEN the nationwide network of Portuguese chemistry and biology research institutes bridging chemistry-based research areas (organic and medicinal chemistry) and molecular and structural biology. Across its partners PT-OPENSCREEN provides Open Access to synthesis of chemical tools and probes, cellular and biochemical assays for screening, as well as hit to lead optimization and follow-up studies. A common goal is to build a library of Portuguese chemical compounds. In addition, PT-OPENSCREEN coordinates the participation of Portugal in EU-OPENSCREEN.

New specialist screening site

i3S-LA / UNIVERSIDADE DO PORTO

i3S (Instituto de Investigação e Inovação em Saúde da Universidade do Porto) is a Portuguese Research Institute with 74 research groups. i3S is dedicated to research and innovation in basic, applied, and translational Health and Life sciences.

It focuses on research programs addressing major challenges as cancer, infectious diseases, neurologic disorders, and regenerative medicine. The BioSciences Screening platform at i3S is the coordinating institution of PT-OPENSCREEN. i3S BioSciences Screening platform as an EU-OPENSCREEN screening partner site offers access to facilities and expertise in assay development and screening of phenotypic and homogeneous assays, image and data analysis and 3D organoids culture.

New specialist screening site

CNC-UC / UNIVERSITY OF COIMBRA

The High-Throughput/High-Content Screening Platform at CNC-UC was the first screening platform implemented in Portugal and is equipped with state-of-the-art instrumentation to perform large-scale loss- and gain-of-function screenings using siRNA/microRNA/CRISPR libraries, as well as screenings using libraries of chemical compounds.

The focus of the platform is on functional genomics screenings using libraries of siRNAs (ca. 70,000 individual + 20,000 pools; genome-wide and focused screenings), microRNAs (ca. 2,500 mimics/inhibitors) and small libraries of FDA-approved chemical compounds (ca. 1,200 compounds). The research activities focus on the study of host-pathogen interactions and the development of assays to study different aspects of bacterial, viral and parasitic infections. CNC has a strong expertise in functional genomics screening, high-content microscopy and host-pathogen interaction and infection assays in human cells (BSL2).

New medicinal chemistry site

iMed.ULisboa / UNIVERSIDADE DE LISBOA

The Chemical Biology and Medicinal Chemistry (CBMC) Scientific Hub is coordinated by Prof. Dr. Rui Moreira and located at the Research Institute for Medicines (iMed.ULisboa) in Lisboa. The Hub provides support in bioorganic chemistry, chemical biology, computational chemistry and medicinal chemistry.

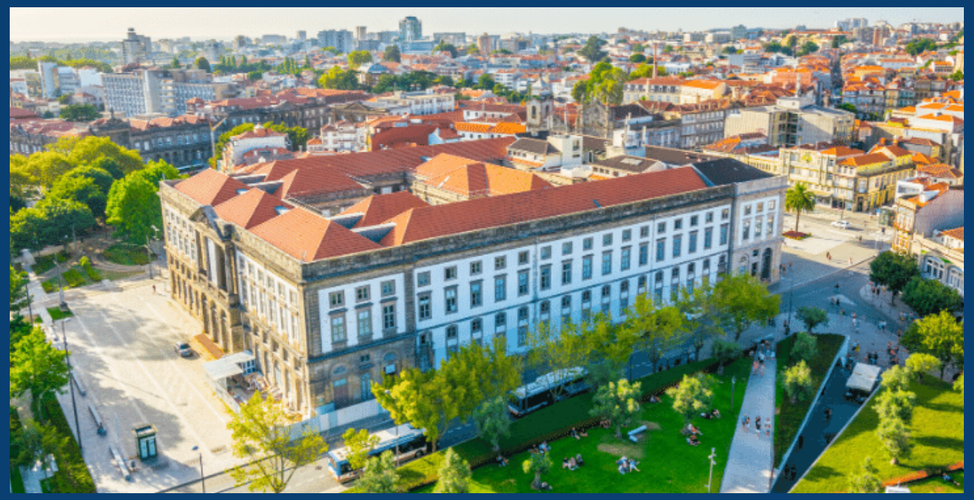
The expertise available for EU OPENSCREEN projects includes screening of large chemical libraries (200K compounds), hit expansion and hit-to-lead optimisation, development of chemical probes for cell imaging and chemoproteomics, target identification, computer assisted drug design, development of synthetic methodologies, in vitro and in vivo ADME profiling, and development of animal models of disease for efficacy studies.

New medicinal chemistry site

FCUP / UNIVERSIDADE DO PORTO

The Drug Discovery Research Group is located at the Faculty of Sciences of the University of Porto (FCUP) and working at the chemistry–biology interface in R&D areas related with human health and well-being.
The team has an extensive experience in organic synthesis, creating an in-house library of more than 3000 compounds, and in optimizing hits/leads emerging from phenotype or target-based screenings or from other type of rational drug design approaches.

The group projects are mainly related to the rational discovery of new chemical entities (NCEs) to feed the pipeline of diseases with unmet needs for therapeutic solutions. The R&D is focused on the discovery of NCEs with drug-like and ADMET properties and ultimately in proof-of-concept in in vivo disease models. The core expertise of the group covers 4 big areas: 1) Drug Discovery & Drug Delivery; 2) Biological screening; 3) In vitro evaluation of ADMET properties and 4) Analytical Chemistry.



NEW MEMBER COUNTRY

SWEDEN - 07/2022

From July 1st, 2022, Sweden expands the circle of EU-OPENSCREEN member countries from 9 to 10 countries. As a partner of EU-OPENSCREEN since the preparatory phase, our Swedish colleagues played an important role in developing EU-OPENSCREEN over the past 10 years.

The representing entity is the Swedish Research Council. Sweden will be represented in the Assembly of Members by Helena Berglund (VR) and Professor Fredrik Almqvist (Umeå University).

THE CHEMICAL BIOLOGY CONSORTIUM SWEDEN (CBCS)

The Chemical Biology Consortium Sweden (CBCS) was formally established in 2010 through the joint efforts of academic and industrial researchers within small-molecule discovery, and Swedish public funding agencies. CBCS originated as a VR-funded national infrastructure (2010-2017) and has since 2013 been a SciLifeLab platform. By 2022, CBCS is again a VR-funded national infrastructure and has expanded to include 6 nodes. Today, CBCS is represented at all Sweden's larger universities; from north to south: Umeå, Uppsala, Stockholm, Linköping, Gothenburg, and Lund, which have different focus areas reflecting the local strong research environments.

CBCS has a long track record in screening projects with different model systems ranging from enzymatic assays and cell-based phenotypic screens up to pathogens in biosafety level 2 (BSL-2) and biosafety level 3 (BSL-3) environment. CBCS will offer assay development support, compound screening services, and hit-to-lead guidance in BSL-2 and BSL-3. The BSL-2 and -3 laboratories are equipped with instruments that allow medium- to high-throughput screening campaigns and liquid-handling solutions combined with various assay read-outs as well as automated time-lapse microscopy.

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New high-capacity screening & medicinal chemistry site

CBCS-KI / KAROLINSKA INSTITUTET

Karolinska Institutet is Sweden's single largest centre of medical academic research. The chemical biology infrastructure at the Department of Medical Biochemistry and Biophysics and within SciLifeLab provides access to a range of pioneering technologies in molecular biosciences. As an EU-OPENSCREEN partner site, the Karolinska Institutet will provide assay development, screening and medicinal chemistry support. CBCS is a core part of the Chemical Biology and Genome Engineering (CBGE) platform at SciLifeLab, which also includes the CRISP Functional Genomics and Chemical Proteomics units, thereby complementing the expertise of EU-OPENSCREEN in these important areas.

Dr Anna-Lena Gustavsson, Director Chemical Biology, Chemical Biology Consortium Sweden (CBCS), SciLifeLab, Karolinska Institutet already looks back on a long and successful cooperation with EU-OPENSCREEN and is looking forward to intensifying this cooperation as a future partner site.

The collaboration with EU-OPENSCREEN is a decisive step in the right direction for the Swedish Chemical Biology Consortium and opens up new opportunities for us to contribute our expertise in new projects and to advance research in Europe.

Dr Anna-Lena Gustavsson / Director, Chemical Biology Consortium Sweden, SciLifeLab, Karolinska Institutet

New specialist screening & medicinal chemistry site

CBCS-UMU / CBCS-UMEÅ

CBCS-Umeå is situated at the Department of Chemistry and has dedicated facilities for assay development, high throughput and high content screening, synthetic chemistry facilities and medicinal chemistry support. CBCS Umeå also has advanced cell biology and infection labs (BSL-2 level) and long experience of screening with infection disease models.

It has significant expertise with different infection models, co-culturing, organoid culturting, as well as whole-organism screening (e.g., C. elegans) and microbiology screens (e.g., E. coli, Mycobacteria, Chlamydia etc.).
As one of the two founding nodes in CBCS, the CBCS Umeå chemistry team has gained extensive experiences in screening hit evaluations, lead identification and optimization, scaffold hopping, and structure-based design as well as hit evaluation from cell based phenotypic screens. The team also has experience in probe development for mechanism of action (MoA) elucidations.

CBCS has assisted Swedish researchers in the field for over a decade and the membership in EU-OPENSCREEN will now open new avenues for Swedish researchers and will also be open for European researchers to access the expertise built up within CBCS.

Associate Professor Erik Chorell / Co-Director, Chemical Biology Consortium Sweden, Umeå University

NEW PARTNER SITES IN FINLAND AND GERMANY

New specialist screening site

BIOCITY TURKU DEPARTMENT (BCT)/ UNIVERSITY OF TURKU, FINLAND

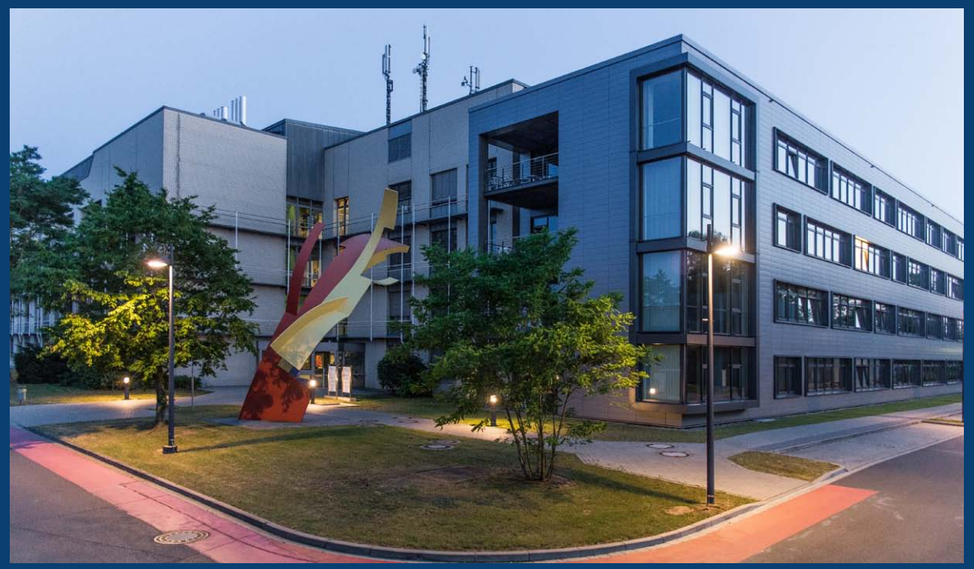
Along the expertise in small molecule HTS, the University of Turku (UTU) brings onboard a specialised expertise in screening and validation in complex cell models and animal models (zebrafish embryos). The High Content Screening Laboratory at the Institute of Biomedicine combines advanced 3D organotypic culture models for oncology with tailored high-content analysis solutions to extract biologically relevant parameters indicative of tumour progression and invasion. The Turku Screening Unit is affiliated with four laboratories from across the bioscience campus in Turku, to provide services spanning from virtual screening, structure determination and medicinal chemistry through protein, cell and organoid screens to small animal model screens.

New medicinal chemistry site

HELMHOLTZ-CENTRE FOR INFECTION RESEARCH (HZI) / GERMANY

The Helmholtz-Centre for Infection Researchin Germany, which is already a screening partner site, now also joined us as a new medicinal chemistry group.

The core theme of the chemical biology department is the investigation of infection processes by the use of chemical compounds. Complex cellular mechanisms are decoded by the individual analysis of cellular components, such as signaling proteins or enzymes that are inhibited or induced by chemical compounds. Subsequently their impact on the cellular phenotype can be described.



NEW COLLABORATIONS AND PARTNERSHIPS

COLLABORATIONS WITH INDUSTRY: 2ND INDUSTRY LIAISON OFFICE WORKSHOP IN SANTIAGO DE COMPOSTELA

On October 5-6, 2022, within the frame of EU-OPENSCREEN-DRIVE we held the 2nd Industry Liaison Office (ILO) workshop in Santiago de Compostela at our partner site University de Santiago de Compostela (USC). Representatives from pharma companies, large biotech companies, small start-ups and SMEs were discussing together with us how to shape future industry engagements in our consortium. The workshop forms the next stage for innovative partnerships between academia and industry.
Following fruitful discussions during the ILO workshop, EU-OPENSCREEN will intensify its efforts in this area and provide dedicated access opportunities for biotech and pharmaceutical companies to support precompetitive, exploratory science and disruptive technologies that can accelerate chemical biology and early drug discovery.

PARTNERSHIPS WITH OTHER RESEARCH INFRASTRUCTURES: EU-OPENSCREEN SIGNED A MEMORANDUM OF UNDERSTANDING WITH EURO-BIOIMAGING AND INSTRUCT-ERIC

A new, collaborative agreement among the life science research infrastructures EU-OPENSCREEN ERIC, Euro-BioImaging ERIC and Instruct-ERIC was signed during the International Conference on Research Infrastructures (ICRI 2022) in Brno, Czech Republic, on October 21, 2022. The trilateral Memorandum of Understanding is designed to benefit the life science research community by building common pipelines for user access, and joining forces in training, external communication, FAIR data management, and funding opportunities.
The three ERICs have successfully collaborated in the past, particularly in the European Commission-funded projects BioMedBridges, CORBEL, RI-VIS, and EOSC-Life, as well as in the ongoing RI services ISIDORe project. The new agreement will strengthen our existing collaboration and will allow for extended outreach and synergies, project funding, training, user access and data management.

EU-OPENSCREEN TEAM 2022

During 2022, our team continued to grow. We welcome three new employees to EU-OPENSCREEN: Charlotte Wit as Junior Scientific Project Manager, David Garcia Lopez as Laboratory Automation Technician and Edgar Specker as Interim Compound Manager.

Charlotte Wit

Charlotte studied Molecular Biology in Leiden (the Netherlands) and she holds a doctor's degree from the Freie Universität Berlin. She joined the Scientific Projects Team in August 2022 to manage the INFRASERV projects ISIDORe and CanSERV, in which she focuses on supporting transnational user access to EU-OPENSCREEN facilities.

David Garcia Lopez

David studied IT at the University of La Laguna, Biology at the University of Granada, and Molecular Biology Research at the University of Valencia. He works alongside Edgar Specker (Interim Compound Manager) and is responsible for handling the compounds of our library and ensuring that the databases are updated, synchronized, and backed up. Additionally, David works on developing new instructions for the machines; enabling them to perform better, or adding required new functions, such as new controls. He also monitors any software or hardware-related issues that may arise to ensure the smooth operation of the lab.

Edgar Specker

Edgar Specker is an experienced Compound Manager who is seconded to us from our partner site the Leibniz Institute for Molecular Pharmacology (FMP) in Berlin. Edgar has already been working for EU-OPENSCREEN before and supports us since October 2022 while our Laboratory Automation Manager Sophie Brusseau is on maternity leave. Edgar works on the preparation of screening and hit-picking plates for the EU-OPENSCREEN partner sites.

NEWS FROM OUR LABORATORY

Refined techniques, expanded service offerings and more accumulative results - we have continued to improve laboratory processes in 2022.

HIT PICKING

Since the delivery of the ECBL to the different partner sites, a constant demand for hit picking requests was registered. In 2022 the hit picking request raised to 25 and is constantly increasing. We were able to improve the hit pickings data files with the software knime® (www.knime.org) and optimise the workflows for hit picking and reformatting with the Hamilton Venus software. We are now prepared to deliver the incoming requests much faster and with high reliability and precision.

With the arrival of the two new member countries Portugal and Sweden into the consortium, two copies of the complete ECBL were prepared and be delivered to their partner sites. Furthermore, a set of 1408 academic compounds in 4 plates was sent to all partner sites for bioprofiling and screening in future user projects. The structural data of these compounds were published in the ECBD. The academic compound library perfectly complements the structural diversity of the commercial library and adds new structural motifs to the already existing library. It will play an integral role in the ECBL library and gives EU-OPENSCREEN the opportunity to expand its visibility in the field of organic and medicinal chemistry approaching various academic institutes as well as in the academic screening sites across Europe (see interview with Victoria Mora).

QUALITY CONTROL OF THE EUROPEAN CHEMICAL BIOLOGY LIBRARY

In June 2022 the identity, purity and position of ca 100,000 compounds from the European Chemical Biology Library (ECBL) was assessed, using Liquid-Chromatography-Mass Spectrometry detector (LCMSD) and Liquid Chromatography-Time of Flight detector (LC-TOF) instruments. All plates were checked for the position of the samples on the plate to ensure that the reformatting had been carried out correctly and no misplacement of compounds occurred. Each result was carefully checked and evaluated by a set of criteria in alignment with the European Chemical Biology Database (ECBD). Identity is confirmed through the mass to charge ratio (m/z) observed through the LC-TOF detector and the purity (set as a threshold of 90%) is assessed by the area of the major peak (corresponding to the compound as seen in the mass spectrum) in the UV spectra using diode-array detector (DAD).

About 5-15% of our compounds have no chromophores, therefore UV data on the purity for these compounds were inconclusive. An evaporative light scattering detector (ELSD), used in tandem with a mass spectrometer, was installed, optimized and validated as a straightforward and simple alternative to assess the purity of those compounds that cannot be measured by UV detection.

BIOPROFILING

IMPORTANCE OF BIOPROFILING

Bioprofiling of the EU-OPENSCREEN compound collection has been contributing to the wealth of quantitative data on compound bioactivities and has added essential biological and physicochemical context to help interpret results from user projects. EU-OPENSCREEN's network of state-of-the-art screening centers is offering users access to a wide range of read-out technologies. The bioprofiling data allow the early identification of read-out interferences caused by compound properties making it easier to eliminate false positive hits from screening results, which in turn improves the selection of high value compounds for further optimisation. This ensures that results generated in screening campaigns are reliable, reproducible and comparable and helps to meet the objective of driving standards in preclinical research.

BIOPROFILING PROGRESS AND SUCCESS STORIES

The majority of the bioprofiling assays have been performed successfully and completed by selected EU-OPENSCREEN´s high throughput screening partner sites who have tested the EU-OPENSCREEN 100,000 compounds library (Table 1 summarises the progress ofeach assay). The data generated from these screening campaigns, after being validated, have been uploaded and published in the EU-OPENSCREEN open-access database (ECBD). These well-annotated, standardised, and controlled data sets complement existing public bioactivity data sets (e.g., Molecular Libraries Program-MLP). Large-scale open access data also provide the basis for computational data integration to allow for prediction of drug-target interactions as well as adverse effects. EU-OPENSCREEN has been provided bioprofiling budget to the selected partner sites which sums up to approximately 1,318,000 Euros up to now. Additionally, the EU-OPENSCREEN Compound Management has tested the EU-OPENSCREEN compound library (100.000 compounds) in autofluorescence and absorbance assays adapted to the bioprofiling screening campaign. The analysis of these results will be completed in 2023. Another great success of the bioprofiling project is the participation of EU-OPENSCREEN bioprofiling solubility assay results in the 1st EUOS/SLAS Joint Challenge where EU-OPENSCREEN ERIC provided a high-quality data set of experimentally measured aqueous solubility of about 100,000 small molecules which was produced at the high throughput screening partner site at the University of Santiago de Compostela (USC). 70,000 of these molecules are available for download on Kaggle database, and the residual 30,000 compounds will be withheld for prediction. EU-OPENSCREEN´s academic library (with currently approximately 4000 compounds provided by chemists all around the world) will also be bioprofiled in the same assays and at the same partner sites. The testing is on-going.

Assay	Partner site	Status
Solubility	USC	The assay has been completed (primary screening, validation of hit compounds).
Luminescence reporters	IBCH PAS	The assay has been completed (primary screening, validation of hit compounds).
ROS (Reactive Oxygen Species)	IBCH PAS	The assay has been completed (primary screening, validation of hit compounds).
Cell viability	FIMM	The assay has been completed (primary screening, validation of hit compounds).
Antibacterial and antifungal assays	MEDINA HZI	Deliver information about potential antibacterial and antifungal properties by testing compounds in a panel of growth assays. 4 bacteria expected end June 2023
Cell-painting	Cell-based	Multiplexes many readouts based on the use of several fluorescent dyes to reveal broadly relevant changes of cellular components or organelles.
Absorbance-Autofluorescence*	FMP, USC, IMTM, MEDINA	Issues with comparing results for reference compounds, fault parameters have been detected. 2500 bioactives will be tested in parallel.

Table 1: List of EU-OPENSCREEN ERIC Bioprofiling assays
*) EU-OPENSCREEN is responsible for performing the Absorbance-Autofluorescence assay by screening the EU-OPENSCREEN compound library and delivering the results.

THE EU-OPENSCREEN ACADEMIC LIBRARY

Our Academic Compound Collection is growing: More than 2600 compounds have already been collected. A short interview with our Academic Comound Manager Vitoria Mora.

Hello Victoria, who can participate in the EU-OPENSCREEN Academic Compound collection?

Basically, any chemist in the world is invited to add their compounds to the EU-OPENSCREEN Academic compound collection.

Are there any specific requirements?

All compounds should be provided with proof of identity (either mass or NMR) and the purity should be 90%. The structure of each compound will undergo computational filters to assess physicochemical properties (i.e., solubility, molecular weight), reactivity and diversity.

Have you already received compounds from Academia?

Our approach has raised considerable interest in the community and we are proud to have received already 2600 compounds from chemists all around Europe.

What is my advantage in adding my compound to the EU-OPENSCREEN Academic Compound collection?

You will get the great opportunity to learn more about the biological activities of your compounds and to make them available to a much larger research community.

By adding your compounds to our academic compound collection you will benefit from new collaboration options and contribute to the generation of tool compounds and novel leads for drug development.

How would you like to develop your Academic Compound Collection?

The objective of EU-OPENSCREEN is to collect unique compounds from the chemistry community which might not always be ‘drug-like’ in the classical sense but often represent innovative chemistry.

If I am interested to participate how should I proceed?

If you are interested to collaborate with us and to add your compound to our European Academic Compound Library I am happy to talk to you on the phone or answer your questions via my dedicated email compound-submission@eu-openscreen.eu or you can fill out the expression of interest form on our website: https://www.eu-openscreen.eu/compound-submission.html. Anyway do not hesitate to contact me if you would like to know more about this great opportunity.

Please contact our Analytical Chemist Victoria Mora if you are interested to add your compounds to the EU-OPENSCREEN Academic Compound Collection.

Send an email to compound-submission@eu-openscreen.eu or fill out the expression of interest form on our website: www.eu-openscreen.eu/compound-submission.html

TRAINING

The success of our training activities in 2022 can be attributed to their strategic focus on diverse audience groups, yielding positive outcomes across various levels. These training events, conducted both virtually and on-site, catered not only to EU-OPENSCREEN employees and partner sites but also extended their reach to the global scientific community, encompassing scientists from different backgrounds and career stages.

The training activities and events involved webinars, on-site courses, the annual EU-OPENSCREEN online Autumn training school and the annual training call specifically dedicated to EU-OPENSCREEN partner sites.

On top of that, EU-OPENSCREEN dedicates 10% of the annual training budget for appropriate training and skills development for the RI staff at the various levels, from top management to technicians and supportive personnel.

COMPOUND LOGISTICS COURSE IN PRAGUE (MARCH 2022)

In the frame of EU-OPENSCREEN-DRIVE training, the EU-OPENSCREEN partner site, the Institute of Molecular Genetics of the ASCR (IMG) in Prague offered an on-site training course on compound logistics in Prague, Czech Republic. The course was intended mainly for staff in charge of compound collection management and specifically dedicated to EU-OPENSCREEN and prospective EU-OPENSCREEN partner sites.

The two-day training course also raised the interest of external researchers who were attracted by the state-of-the art technologies available at IMG and the high-quality training offered. Experienced scientists from IMG contributed interesting lectures as well as hands-on training focused on compound management workflows, automated liquid handling workstations and storage systems, as well as compound quality control.

AUTUMN ONLINE TRAINING SCHOOL

The Autumn training school 2022 already running for the second year was a great online event hosted and organised by EU-OPENSCREEN under EU-OPENSCREEN-DRIVE. A five-days virtual training event with almost 35 hours of live discussions with Q&As and 426 registrants from all around the world (approx. 15% of non-European countries including Brazil, Korea, US, India, Mexico, Africa). The EU-OPENSCREEN Autumn training school with 20 sessions and 22 speakers from academia, industry and other Research infrastructures involved topics from various scientific areas such as chemical biology, chemoproteomics, cheminformatics, assay development, high-thruput screening, compound libraries, hit selection, lead optimisation, fragment screening, screening automation, probes and drugs, medicinal chemistry, open data, databases and many more.

According to the analysis of the feedback survey results the majority of the attendees were PhD students and post-docs between 20-30 years old. This fact shows that EU-OPENSCREEN training school succeeded in its goal of attracting and engaging mainly young scientists. The survey also revealed that 90% of the participants were very satisfied with the organisation and moderation of the event while approx. 80% would very likely attend another EU-OPENSCREEN training activity in the future.

You can find the Autumn training school 2022 recordings here:

https://www.eu-openscreen.eu/newsroom/autumn-school-2022-webinar-recordings.html

WEBINARS

Monthly training webinars with prestigious speakers from academia, industry and other research infrastructures were organised by EU-OPENSCREEN for the first time. Attendees from different countries and career stages had the opportunity to watch live presentations for various scientific topics and have fruitful discussions while asking their questions to the experts during the live Q&A sessions.

The preparation, organisation and outreach campaign was organised by EU-OPENSCREEN. Feedback surveys were also prepared by EU-OPENSCREEN and collected answers were used for statistical purposes, evaluation and preparation of future webinars.

The analysis of the survey results showed that EU-OPENSCREEN monthly webinars provide a forum for access to experienced scientists and their expertise mainly for young scientists (PhD students and early career stage scientists) who want to be informed about the latest technologies and scientific advances and engage with experts.

Due to the important interest in our webinars, EU-OPENSCREEN will continue with the organisation of monthly webinars in 2023, covering the breadth of topics in chemical biology and early drug discovery.

Webinars 2022

- Anna-Lena Gustavsson
- Dr Davide Danovi (Senior Lecturer at King's College London
- María J. Vicent , CIPF Principe Felipe Research Center, Valencia
- Harald Schwalbe, Director Instruct ERIC
- Mads Hartvig Clausen, Technical University of Denmark (DTU) and Director of the DK-OPENSCREEN
- Jonathan Baell, Monash Institute of Pharmaceutical Sciences (MIPS) of Monash University.
- Brinton Seashore-Ludlow, Karolinska Institutet / Chemical Biology Consortium Sweden
- Olga Genilloud, Fundación MEDINA in Granada, Spain

You can find these and other webinars on our website:

www.eu-openscreen.eu/newsroom/webinar-recordings

EU-OPENSCREEN TRAINING CALL FOR PARTNER SITES

In 2022 the fourth EU-OPENSCREEN training call for our partner sites was launched. These training calls are dedicated to our partner sites with a proven track record/expertise in one of the areas of interest and wanting to offer training courses and to the scientific staff at the EU-OPENSCREEN partner sites and at the central office wishing to participate in staff exchanges, international practical workshops or external courses in the field of chemical biology.

EU-OPENSCREEN ERIC provides training funds for four training categories: training courses, external courses, staff exchanges and international practical workshops. For the training courses, EU-OPENSCREEN funds dedicated training programs belonging to the areas of process automation, assay development, high-throughput screening, screening data analysis and data transfer, database usage and linked IT processes, medicinal chemistry strategies and project management (organised by our partner sites).

External courses are planned to give training opportunities to young scientists (MSc and PhD students) who are performing their studies at EU-OPENSCREEN partner sites helping them to acquire knowledge, techniques and procedures that will help them to be globally competitive.

The external courses offered in the frame of the EU-OPENSCREEN training calls can include but are not limited to seminars, conferences, workshops in Europe and internationally. EU-OPENSCREEN also offers travel grants for staff exchanges especially to those scientists working at an EU-OPENSCREEN partner site who want to acquire or extend skills needed for their work which are not yet available at their home site.

This way the exchange will additionally improve the co-operation among EU-OPENSCREEN partner sites. In line with EU-OPENSCREEN's efforts to reach out to global user communities and following the recommendation of the EU COM High Level Expert Group to strengthen its international outreach, EU-OPENSCREEN ERIC training call 2022 also included an international practical workshop. The aim of this practical training is to train and raise awareness of EU-OPENSCREEN and its services among international researchers. We have received six applications for the 2022 training call, one for a training course, two for staff exchanges and three for external courses. The proposals were evaluated by external reviewers according to specific criteria and rules. All of them were successful and funded with approx. 21,000 Euros in total.

USER PROJECTS

19 NEW PROJECTS WERE SUCCESS-FULLY LAUNCHED in 2022 WITHIN OUR INFRASTRUCTURE.

Starting 2019, 68 projects have been handled by EU-OPENSCREEN partner sites of which 31 were ongoing in 2022. Access has been requested for a variety of services and resources offered within the network: screening technologies (37 projects), medicinal chemistry support (6 projects), chemoproteomics expertise (6 projects), co-development activities (6 projects) and usage of the fragment library (13 projects). In 2022, 19 new projects have started at EU-OPENSCREEN and 19 projects were completed and results have been delivered to the users for further exploitation. Access costs were either covered through grants acquired by the user or funded through EU projects such as ISIDORe and EU-OPENSCREEN-DRIVE. From 2019 and through 5 open calls, EU-OPENSCREEN-DRIVE funded a total of 24 user projects (screening, medicinal chemistry and chemoproteomics), of which 5 medicinal campaigns were initiated and progressed during 2022.

As expected, many users are interested to find new tools and drugs to study cancer. and, due to the pandemic state since 2020, we face an increased interest in infectious diseases, which is visible from the user requests received in 2022 to access EU-OPENSCREEN services via ISIDORe (e.g 5 full applications for screening services and 1 application to medicinal chemistry services). EU-OPENSCREEN contributed in the past to the coronavirus crisis by publishing two SARS-CoV-2 data sets from the pilot library in 2021 within the ECBD. New screening data sets on SARS-CoV-2 are currently produced within our facilities. This effort is paralleled by the first project run and funded by ISIDORe in 2022 bringing together EU-OPENSCREEN and the European Lead Factory in a cooperation to strengthens the European role to discover and develop novel antivirals against SARS-CoV.This marked a milestone in our aim to increase public-private collaborations. The hit-to-lead campaign submitted by researchers at Pivot Park Screening Centre (PPC) is carried out by the Latvian Institute of Organic Synthesis (LIOS) under the supervision of Prof. Aigars Jirgensons, Scientific Director at LIOS (see also: https://www.europeanleadfactory.eu/newsroom/cross-consortium-cooperation-strengthens-european-efforts-discover-and-develop-novel).

While EU-OPENSCREEN is active in multiple service areas, the core business remains to be screening services. Roughly half of the users screen the full European Chemical Biology Library (ECBL, 96.096 compounds). The other half screens the ECBL pilot library (approx. 5,000 compounds including 2,464 bioactives) or the bioactives (2,464 compounds). The ECBL pilot library, which includes the bioactive compound library, is still offered without replenishment fees with the intention to provide users with the possibility to test their assay and to support them with initial screening data. This continuous support from EU-OPENSCREEN is meant to strengthen the user's funding applications and raise their chances in running a follow up screen for the full ECBL.

Beyond traditional screening, there is a large interest in fragment screening; which can be performed at EU-OPENSCREEN and iNEXT-Discovery/Instruct-ERIC sites using the EU-OPENSCREEN fragment library. The latter was designed and assembled within the frame of EU-OPENSCREEN-DRIVE in 2020 thanks to the cross-RI collaboration between EU-OPENSCREEN and Instruct-ERIC. Similar to the ECBL pilot library, fragments are offered in-kind by EU-OPENSCREEN and together with the funded access through the iNEXT-Ddiscovery/Instruct-ERIC sites this service is an attractive and fast road for user projects.

With the start of the EU-OPENSCREEN-DRIVE project in 2019, the ERIC started to explore public-private collaborations. As a new service, co-development projects with companies were pursued. In 2022, the first two collaborations with Promega on their nanoBRET technology have been finalized and the results were presented on the 2nd Industry Liaison Office Workshop. The resulting products were taken into the commercial catalogue of Promega. The outcomes will be published in a scientific journal in the near future and followed up by a user story on the EU-OPENSCREEN website. Another private-public partnership user story is already available since 2022. Together with the user Felix Torres from ETH Zürich, the EU-OPENSCREEN partner site LIOS supported the launch of the start-up NexMR. Please read more on Felix' project below.

COLLABORATION BETWEEN ETH ZÜRICH AND EU-OPENSCREEN PAVED THE WAY FOR ULTRAFAST NMR SCREENING AND SUPPORTED THE LAUNCH OF A PROMISING START-UP COMPANY

USER:

Dr. Félix Torres, ETH Zürich, Laboratory of physical chemistry, Switzerland

EU-OPENSCREEN MEDICINAL CHEMISTRY PARTNER:

Prof. Kristaps Jaudzems, LIOS, Riga, Latvia

In August 2021, Félix Torres, together with Prof. Roland Riek and Matthias Bütikofer, filed a patent on “target-ligand interaction detection and characterization by photo-CIDNP NMR”. To extend the chemical space of compatible molecules with the newly developed screening method, Félix had to explore which molecules are susceptible to yield photo-CIDNP polarization.

BACKGROUND

Félix and his colleagues from the group of Prof. Roland Riek at ETH Zürich developed new NMR screening methods to overcome the poor sensitivity of NMR spectroscopy. They combined photo-CIDNP hyperpolarization to enhance the NMR signal and flowthrough approach to reach unprecedented screening rates while using low micromolar concentrations. Moreover, photo-CIDNP screening is applicable to NMR spectrometers of much humbler fields (< 600 MHz).

COLLABORATION WITH EU-OPENSCREEN

To collect data to design photo-CIDNP compatible fragment libraries, Félix visited the group of Prof. Kristaps Jaudzems at our medicinal chemistry partner site, the Latvian Institute of Organic Synthesis in Riga, Latvia(LIOS), to test a selection of molecules offered by EU-OPENSCREEN. The photo-CIDNP NMR spectra of 917 molecules were recorded, of which 137 showed strong and 202 showed moderate signal enhancements.

A subset of 102 best-polarized compounds was screened against PIN1, an important target in oncology. PIN1 is involved in solid tumors and is regarded as a challenging target due to its shallow active site. Although this sub-selection contained fragments in a diverse range of molecular weight (200-600 Da), the screening campaign identified two hits. The first hit, 5-methyl-indole-2-carboxylic acid, was already reported in the literature with an affinity of 20 µM. The second hit, a hydroxy-benzofuran derivative, is currently being validated. Initial results show structural similarity to the first hit. Thus, the screening with the ECBL sub-library is the first strong proof-of-concept data set for successful photo-CIDNP screening of diversified libraries.

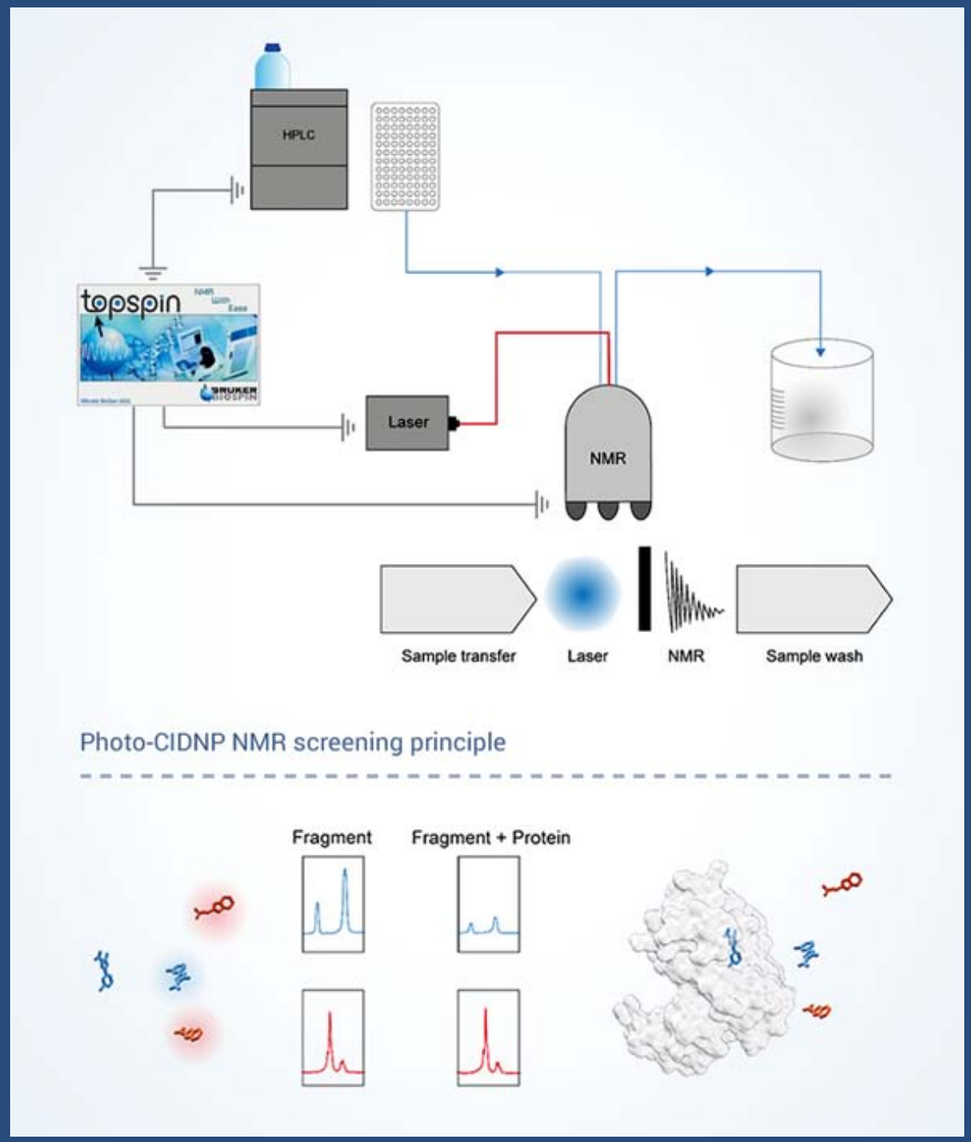
To collect data to design photo-CIDNP compatible fragment libraries, Félix visited the group of Prof. Kristaps Jaudzems at our medicinal chemistry partner site, the Latvian Institute of Organic Synthesis in Riga, Latvia(LIOS), to test a selection of molecules offered by EU-OPENSCREEN. The photo-CIDNP NMR spectra of 917 molecules were recorded, of which 137 showed strong and 202 showed moderate signal enhancements.

FUTURE RESEARCH

The analysis of the EU-OPENSCREEN library CIDNP resulted in the identification of around 60 new molecular features which can serve as a molecular frame to design fragment libraries. A subset of 49 aromatic features is now used to generate a pilot library of 287 fragments. This new library has been screened against PIN1 and identified 39 hits, it will be screened in the future against K-Ras, and other hot targets to support drug discovery efforts. The photo-CIDNP fragment libraries will be upgraded at the end of 2022 to reach a phase II pilot of >1000 fragments.

Thanks to the EU-OPENSCREEN collaboration, we can design libraries compatible with hyperpolarization containing an unprecedented chemical diversity.

Félix Torres

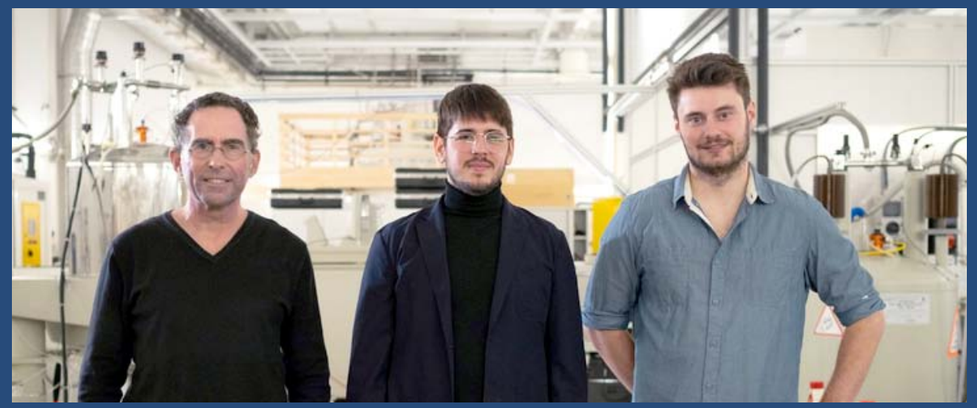


Top: Schematic setup of the photo-CIDNP NMR system. Bottom: Schematic representation of the photo-CIDNP NMR screening principle. Ligands that bind to the protein will show a reduced intensity within the NMR spectrum.

Please read the full story here: "Ultrafast Fragment Screening Using Photo-Hyperpolarized (CIDNP) NMR" | Journal of the American Chemical Society
https://pubs.acs.org/doi/10.1021/jacs.3c01392

COLLABORATION WITH NexMR

Currently, Félix Torres runs the start-up company NexMR, which offers access to the photo-CIDNP screening technology and provides customers with fragment libraries specially designed to accelerate fragment-based drug design. NexMR forecasts to be able to provide photo-CIDNP overlaying technology on any Bruker instrument by the end of 2023 and to diversify its photo-CIDNP fragment library to 100'000 compounds within the next 3 years.



Prof. Roland Riek, Dr. Félix Torres, Matthias Bütikofer in their labs at the ETH Zürich.

SCIENTIFIC OUTREACH

PARTICIPATION IN SCIENTIFIC CONFERENCES AND EVENTS

EU-OPENSCREEN actively participated in various scientific conferences and events to promote its infrastructure and services, as well as to foster collaborations with other research organizations. We presented our research findings and showcased the capabilities of EU-OPENSCREEN at major international conferences, such as the International Conference on Research Infrastructures ICRI 2022 in October 2022, in Brno, Czech Republic. ICRI provided a platform for high-level debates of research infrastructure policymakers, operators and users, and research stakeholders from around the world to address the most pressing research infrastructure topics. EU-OPENSCREEN co-organised the side event at ICRI on "International Cooperation of Research Infrastructures". The successful signing of the Memorandum of Understanding with our partner research infrastructures Euro-BioImaging and Instruct-ERIC at ICRI 2022 reflects this process. EU-OPENSCREEN also organized presentations and sessions at various international conferences to highlight the latest developments in chemical biology and screening technologies and to reach out to existing and new user groups.

EU-OPENSCREEN / SLAS DATA CHALLENGE

On September 19th, 2022, EU-OPENSCREEN teamed up with the Society for Laboratory Automation and Screening (SLAS) and launched the 1st edition of the EU-OPENSCREEN/SLAS joint data mining challenge on the Kaggle competition platform. High quality unpublished data, obtained from our partner sites, have been provided to the data scientist community to benchmark current prediction models and to facilitate the development of better computational models. Participants were called upon to predict capabilities on real, high-quality data sets provided by academic partner sites from EU-OPENSCREEN ERIC to foster forward-thinking scientific research. 100 teams entered their predictions into our first Kaggle competition. The competition helped us to significantly increase our visibility among computational scientists and to foster collaboration with the SLAS.

OUTREACH TO INDUSTRY

In 2022, we significantly strengthened our outreach activities towards pharmaceutical and biotech companies. We developed a new industry-focused brochure that outlines the infrastructure, services, and benefits of collaborating with EU-OPENSCREEN for industrial research projects. The brochure highlights our expertise and capabilities in supporting the discovery and development of new drugs, agrochemicals, and other bioactive compounds. It also showcases case studies of successful collaborations between EU-OPENSCREEN and industry partners, demonstrating the value and impact of utilising the consortium's resources in industrial research endeavors. The industry brochure can be downloaded here.
We also included a dedicated section on industry on our website (https://www.eu-openscreen.eu/participate/access-for-industry.html). The new section serves as a one-stop resource for industrial researchers to learn about the infrastructure, access services, and initiate collaborations with EU-OPENSCREEN highlighting our commitment to engaging with the industry and fostering collaborative research.

NEW WEBSITE SECTION: SUCCESS STORIES

EU-OPENSCREEN's new website section on success stories from user projects is a valuable platform for showcasing the impactful research outcomes and collaborations enabled through our screening resources and services. The stories highlight the diverse range of projects that have benefited from our capabilities and serve as an inspiration to our user community and the broader scientific community. We will continue to update and expand this section to share more success stories and demonstrate the value of EU-OPENSCREEN's resources in advancing research and innovation in the field of chemical biology and drug discovery.

EUROPEAN PROJECTS

In order to ensure long-term sustainability and to enhance collaboration with other life science research infrastructures, EU-OPENSCREEN actively participates in several projects/initiatives funded by the European Commission.

EU-OPENSCREEN DRIVE

EU-OPENSCREEN-DRIVE (2019-2023) coordinated by EU-OPENSCREEN is an H2020 funded project that further strengthens the ERIC and supports its long-term sustainability by bringing together 33 partners across 15 European member and associated states. The core of the consortium consists of EU-OPENSCREEN partner sites, who provide access to their services and expertise in the field of small-molecule screening and medicinal chemistry. This group is complemented by several key institutions granting expertise and excellence in scientific areas such as chemoproteomics and fragment-based screening for extending the ERIC´s capacities and competences in those fields with the aim to provide European and international users access to a comprehensive offer of services across the whole early drug discovery pipeline.

In addition to coordinating the financial and scientific administration of all 33 partners working on 10 different work packages (WP9), EU-OPENSCREEN ERIC also leads the work package on Excellence in ERIC operations and management (WP1) and on Transnational access - demonstration of EU-OPENSCREEN's integrated Screening and Medicinal Chemistry capacities through external user projects (WP3) with a resource of 96 person months over a duration of 57 months. As of the INFRADEV action from the European Commission is meant for ERICs to work on and test potential new structures and processes needed for the continuous adaptation to arising research needs, EU-OPENSCREEN is also strongly involved in all other work packages.

During the last 4 years, EU-OPENSCREEN-DRIVE supported 23 user projects from hit identification to chemical proteomics and compound disposition (see section on "User Projects").

In 2022, within the frame of EU-OPENSCREEN-DRIVE, the EU-OPENSCREEN team and its partner sites have

- completed the management processes needed for a large, distributed infrastructure
- enlarged its member countries with Sweden and Portugal joining the consortium in summer 2022 (for more details see section "New Member Countries and Partner Sites")
- completed the access procedures needed for the access to the medicinal chemistry sites and run the first five medicinal chemistry campaigns progressing hits from successful screening projects in WP3 (for more details see section "User Projects"). Managed chemical proteomics services and run additional 3 user project applications in WP5.

- prepared a Handbook and defined user workflows for a new category of partner site (e.g. chemoproteomics and MSI) with the aim of its integration in EU-OPENSCREEN portfolio in the upcoming 2023 (WP1, WP5)
- widened the awareness of academia and industry for EU-OPENSCREEN services and data. We also paid specific attention to the interaction with industry and SMEs to foster the innovation potential of our European research infrastructure (for more details see section “Scientific outreach”)
- continued supporting the national compound ambassador network to foster and speed-up the collection of academic compounds and enlarged the European Academic Library (WP2) (for more details see section “Our academic compound collection”)
- organised training activities and webinars (WP8) (for more details see section “Training”)
- promoted and managed the usage of the newly established fragment library in fragment screening projects in collaboration with structural biology partners from other European RIs (Instruct-ERIC/ iNEXT-Discovery) promoting synergies between the two life science consortia (WP4) (for more details see section “User Projects”).

Whereas WP4 (Fragment screening), WP5 (chemoproteomics & MSI) and WP7 (industry) enlarge the EU-OPENSCREEN capacity for new services and structures, WP6 (database) and WP8 (training) work in a complementary manner to the established offers paid for by the ERIC membership fees and are described in dedicated sections.

www.drive.eu-openscreen.eu

Grant No. 823893

Total budget: € 5 m

Duration 54 months

ERIC FORUM

The ERIC Forum Implementation Project is a Horizon2020 project that brings together the ERIC community to strengthen its coordination and enhance collaborations between the partners. One of the major goals of the ERIC Forum project is to support ERICs in preparation with the knowledge and experience of the existing ERICs. In 2022 EU-OPENSCREEN was part of the Gender Equality Working Group. The group had the aim to exchange good practices and support the implementation of the gender equality plan. EU-OPENSCREEN successfully published its first Gender Equality plan in 2022. In October 2022 the General Assembly and the final meeting of the ERIC Forum was held in Brussels, where the ERIC community met with key stakeholders and policy makers. The final meeting in Brussels was also the starting point for the follow-on project ERIC Forum II.

ERIC FORUM Final Project Meeting in Brussels in October 2022.

www.eric-forum.eu

Grant No. 823798

Total budget: € 1,5 m

Duration 48 months

EOSC-Life

An open collaborative space for digital biology was opened by the European Commission through the funding of European Open Science Cloud (EOSC) projects. EU-OPENSCREEN participates in the EOSC project for Life Sciences: EOSC-LIFE. It involves the development of FAIR compliant data resources published in the cloud. The project provides policies and guidelines for processing secure and ethical data reuse and for creating an ecosystem of innovative tools.

Through open hackathons and bring your-own-data events, EOSC-LIFE implements workflows from across disciplines and addresses the needs of interdisciplinary science. The consortium brings together thirteen research infrastructures and 47 additional partners, all coming from 23 European countries. EU-OPENSCREEN has actively contributed to the EOSC-LIFE project with its partner sites ITMP (Fraunhofer Institute for Translational Medicine and Pharmacology, Hamburg) and IMG (Institute of Molecular Genetics of the Czech Academy of Sciences, Prague).

ITMP are co-leaders of WP1, which focuses on the deployment of FAIR cloud services. The work of Fraunhofer has focused on managing the implementation and providing technical support to more than 20 projects which have been selected as demonstrators and open calls.

This has led to multiple collaborations and to the development of resources with research infrastructures such as BBMRI and EuroBioimaging. Primary high-content screening data related to COVID-19 has been repurposed in the Image Data Resource (https://idr.openmicroscopy.org/webclient/?show=screen-2603) along with associated analysis workflows in the EOSCLIFE workflow Hub (q https://workflowhub.eu/workflows/238). Collaborations with EATRIS resulted in the development of resources to enable the FAIRification of drug sensitivity data (https://doi.org/10.1093/bib/bbab350).

As a part of the EOSC-life Demonstrator project 1 (European Open Science Cloud resources for Chemical Biology and Structure-Based Drug Discovery workflows), the full FAIRification of the Europen Chemical Biology Database (ECBD) was employed. Apart from the integrated tools (ontologies, established identifiers) and data access routes (web UI, database and API), a user-friendly interface for the data description and deposition was developed.

The user interface integrates all underlying ontologies and provides a system of focused fields working only with their specific parts. There is also a possibility to introduce custom values as well as define any field inapplicable in a given context.

In combination with the Creative Commons License (CC BY 4.0), ECBD is a fully-fledged FAIR data repository for chemical biology that enables a wide community to take advantage of data generated within the EU-OPENSCREEN infrastructure.

Ongoing work is focussed on dissemination of EOSC-LIFE associated activities and ensuring sustainable operation of the developed resources over the long term.

EOSC-*Life*

www.eosc-life.eu

Grant No. 824087

Total budget:
€ 26 m

Duration
54 months

EOSC FUTURE

The European Open Science Cloud (EOSC) forms an ecosystem of research data and related services that enable and enhance access and reuse of FAIR research outputs (i.e., data and other digital objects). The European Commission further amplified its open science efforts by launching the EOSC Future project. The project will promote the EOSC portal development by integrating, consolidating, and connecting e-infrastructures, research communities and initiatives in the field of open science. The test science projects (TSPs) in EOSC Future will serve as examples of how joint projects can address major, if not global, challenges for Europe's societies and how research infrastructures can align to support Horizon Europe's missions within the EOSC.

The EU-OPENSCREEN partner site Fraunhofer ITMP is responsible for a TSP to integrate phenotype and chemotype multi-omics open COVID-19 data to aid the identification of therapeutic targets of phenotypic hits from COVID-19 repurposing.

Previous work reported by the EU-OPENSCREEN team (https://www.nature.com/articles/s41598-021-90296-2) demonstrates the power of this approach by making use of public data sets that were available at the beginning of the pandemic. Work in 2022 involved a deeper integration of the data with complementary data sets in ChEMBL covering primary and secondary targets of the hit compounds. Advanced work would involve integrating public proteomic and transcriptomic data sets in a Knowledge Graph. These data sets are associated with virus-host interactomes held in the COVID-19 data portal.

EOSC Future

https://eoscfuture.eu

Grant No. 101017536

Total budget: € 42m

Duration 30 months

iNext-DISCOVERY

EU-OPENSCREEN is partner in the H2020 project iNEXT-Discovery (Infrastructure for transnational access and discovery in structural biology). The project brings together 26 partners and aims to make structural biology key facilities for X-rays, NMR, cryo-EM and macromolecular biophysics accessible to new user communities. It will also develop methods further exploiting joint research efforts, and integrate different scientific fields into structural biology. It will also develop methods further exploiting joint research efforts, and integrate different scientific fields into structural biology. It will do this through multi-disciplinary courses, workshops and training activities.

The project started in February 2020 and the collaboration between EU-OPENSCREEN and iNEXT-Discovery sites enables the connection of structural biology with screening and medicinal chemistry. EU-OPENSCREEN contributes to the project through networking activities, such as the organisation of meetings to discuss collaboration opportunities. EU-OPENSCREEN contributes to the project through networking activities, such as the organisation of meetings to discuss collaboration opportunities

iNEXT DISCOVERY

inext-discovery.eu

Grant No. 871037

Total budget: € 10m

Duration 48 months

MARBLES

EU-OPENSCREEN, together with our partner sites Fundación MEDINA and Fraunhofer ITMP, are partners in the Horizon 2020 project, MARBLES.

MARBLES project aims to provide sustainable products such as microbiomes, microbial strains and pure compounds identified from the marine environments. As an example of a typical approach, MARBLES is identifying the most promising ecosystems for natural product discovery in sponges by linking global sponge biodiversity patterns to both overall microbial diversity and biosynthetic gene cluster (BGC) diversity. One of MARBLES strategies is to mimic the natural host-microbiome system, together with studying the evolution of the microbial diversity, at multiple cultivation conditions.

In order to make these valuable compounds (and the rich associated data) produced by MARBLES available to the wider scientific community after the end of the project, they will be integrated into the EU-OPENSCREEN compound collection. Pure compounds and associated data will be stored for post-project use by EU-OPENSCREEN.

The annual meeting was organized in Wageningen, The Netherlands on the 17-18th of October 2022 with project partners participating in person. Fundación MEDINA coordinates the work package 4 for the generation of small molecules for chemical diversity.

MARBLES
HARNESSING MARINE MICROBES FOR DRUG DISCOVERY AND SUSTAINABLE PRODUCTION OF FISH & CROPS

www.marblesproject.eu

Grant No. 101000392

Total budget: € 7,5 m

Duration 60 months

ISIDORe

ISIDORe is a rapid-response project to the SARS-CoV-2 pandemic that brought the world to a halt in 2019-2020. The Horizon Europe-funded project of 21 m Euro, launched in early 2022, aims to respond to immediate health threats and prepare for possible upcoming disease outbreaks.

ISIDORe is coordinated by Prof. Jonathan Ewbank (ERINHA). EU-OPENSCREEN is a beneficiary within the extended consortium of 154 partners coming from research infrastructures and other networks from 32 countries. ISIDORe therefore represents the largest and most diverse research and service-providing instrument to study infectious diseases in Europe, with expertise from structural biology to clinical trials broadcasted in a catalogue of services exceeding 300 services.

After the kick-off meeting early 2022, the outbreak of Mpox outside of endemic countries was the first rapid response that tested ISIDORe's flexible response to immediate threat. ISIDORe was the first European project to respond. An open call for proposals was launched within 2 months and this received much praise from the European Commission.

Within ISIDORe, EU-OPENSCREEN leads WP10 on 'Support for diagnostic & therapeutic development'. In 2022, we launched several COVID-19-related research projects at our partner sites and WP10 partners offering services in antibody discovery and diagnostic. Over the year, four additional calls were opened to open the gate for 'preparedness research' for epidemic-prone diseases that might form a human health risk in the future. Data resulting from collaborations and service provisions through ISIDORe will be shared with the BY-COVID portal.

For more details about ISIDORe fudned user project see section on "User Projects".

ISIDORe

www.isidore-project.eu

Grant No. 101046133

Total budget: € 21 m

Duration 36 months

BY-COVID

In response to the COVID-19 pandemic, the European Commission launched an emergency call in 2021. The call aimed to enable researchers, health care professionals and society at large scale to access, share and analyse research data across borders and disciplines. Together with 27 partners, the BY-COVID project tackles data challenges hindering effective pandemic response. The main goal of the endeavour is to ensure that data on SARS CoV-2 and other infectious diseases can be found and used by everyone.

Via the established BY-COVID Data Portal, the project connects well-established data resources and delivers access to heterogeneous yet interlinked data across domains and jurisdictions. The project thereby provides high level indexing of COVID-19 related knowledge from different fields. It respects the FAIR data principles and uses workflow environments fully aligned with the European Open Science Cloud (EOSC). EU-OPENSCREEN contributed in 2022 to a publication on Data Management Plans in European projects, like BY-COVID and ISIDORE, and on how to enable data sharing in large consortia. “Umbrella Data Management Plans to integrate FAIR data: lessons from the ISIDORe and BY-COVID consortia for pandemic preparedness” was submitted and accepted to DSJ for the special issue, Data Management Planning across Disciplines and Infrastructures https://codata.org/call-for-papers-data-management-planning-across-disciplines-and-infrastructures.

Part of making data publicly available via the BY-COVID poral is finding ways to instruct researchers to make high quality data findable. EU-OPENSCREEN, together with its partner site ITMP Fraunhofer, Hamburg, contributed to the establishment of the FAIR cookbook, which is an online repository providing guidance per topic on how to make research data openly accessible.

The data generated in the ISIDORe project will be made available through dedicated repositories, e.g. the EU-OPENSCREEN European Chemical Biology Database (ECBD) and BY-COVID, considering its non-sensitive nature. This task builds on the substantial link between BY-COVID and data emerging from ISIDORe.

BY-COVID

https://by-covid.org

Grant No. 101046203

Total budget: € 12 m

Duration 36 months

canSERV

CanSERV is a Horizon Europe-funded programme, coordinated by Prof. Jens K. Habermann (BBMRI-ERIC) that provides cutting edge, interdisciplinary and customised oncology services across the entire cancer continuum. The project unites a multidisciplinary consortium of 19 European partners (https://www.canserv.eu/partners), consisting of Research Infrastructures, key organisations in the field of oncology, project management, and sustainability.

The aim of the project is to make a collective effort for a single catalogue and user-friendly Transnational Access (TNA) process as a foundation for prospective development of cancer research in Europe. Defragmenting technological development strategies, sharing knowledge and training, and testing future technological breakthroughs will define the identity of canSERV. canSERV will form essential support to the ERA in providing effective solutions to the cancer patient community.

The kick-off meeting for the project took place in September 2022 in Brussels where amongst representatives of EU-OPENSCREEN, other RIs, and the European commission, there was a strong feel of synergy and willingness to unite forces in this project.

In canSERV, EU-OPENSCREEN leads (together with EATRIS) WP4 on ‘New therapeutic solutions’ and is involved in WP1, WP2, and WP3, where our partners will provide services related to ‘Disease models’, ‘Advanced technologies for personalized oncology’, and ‘Biomarker research, development, and validation’, respectively. The data resulting from services provided through canSERV in the future, will be made available through EOSC4Cancer.

canSERV
providing cutting edge cancer research services across europe

www.canserv.eu

Grant No. 101058620

Total budget: € 14,9 m

Duration 36 months

EOSC4Cancer

EOSC4Cancer is the latest addition to the Horizon Europe-funded EOSC ecosystem. Specifically, EOSC4Cancer is the European-wide initiative to accelerate data-driven cancer research. It brings together a consortium of 29 organizations from 13 countries, including cancer research centres, research infrastructures, leading research groups, hospitals, supercomputing centres, and patient/survivor associations.

Through five use-cases, EOSC4Cancer organizes research and cancer patient's data into systematically organised and relevant formats for use in translational research, medical practice, and related health outcomes. Colorectal cancer was chosen as a working case for representing a tumour type with abundant data and ample cross border collaborations.

The EOSC4Cancer kick-off meeting took place in October 2022 in Barcelona. EU-OPENSCREEN is represented in EOSC4Cancer to assist and upload any data coming out of the canSERV project.

eosc | cancer

eosc4cancer.eu

Grant No. 101058427

Total budget: € 7,8 m

Duration 30 months

AgroServ

EU-OPENSCREEN is a beneficiary in the Horizon Europe project "Integrated SERvices supporting a sustainable AGROecological transition" (AgroServ), which is coordinated by AnaEE. AgroServ was launched in October 2022, and over the next 5 years will offer researchers access to a wide range of customized and integrated services to support them to conduct experiments at different scales (i.e., from the molecular level to ecosystems) across many scientific disciplines, from plant and animal phenotyping, bioengineering, experimental ecology, microbiology, bioimaging, metrology, data modelling, to socio-economics.

The diversity of the AgroServ consortium with 11 RIs and 73 affiliated partners enables researchers to conduct interdisciplinary and transdisciplinary studies to better address the underlying challenges of transitioning to sustainable and resilient agriculture and agroecology practices.

EU-OPENSCREEN and its partners Fundación MEDINA, Granada (Spain), Instytut Chemii Bioorganicznej Polskiej Akademii Nauk, Poznan (Poland), University of Santiago de Compostela (Spain), Consejo Superior de Investigaciones Científicas (CSIC), Madrid (Spain), the Weizmann Institute of Science, Rehovot (Israel) and the Vlaams Instituut voor Biotechnologie (VIB) in Ghent (Belgium) will support users to identify novel biologically active compounds for crop protection from pests or as physiological agents to promote crop productivity in changing environments or for veterinary drugs. Open calls for users are expected in 2023.

AgroServ

agroserv.eu

Grant No. 101058020

Total budget: € 15 m

Duration 60 months

FINANCIAL STATEMENT 2022

In 2022 ten member countries – Czech Republic, Denmark, Finland, Germany, Latvia, Norway, Poland, Portugal, Spain and Sweden – supported the ERIC through their annual memberships.

EU-OPENSCREEN ERIC BUDGET 2022

INCOME AND EXPENSES 2022

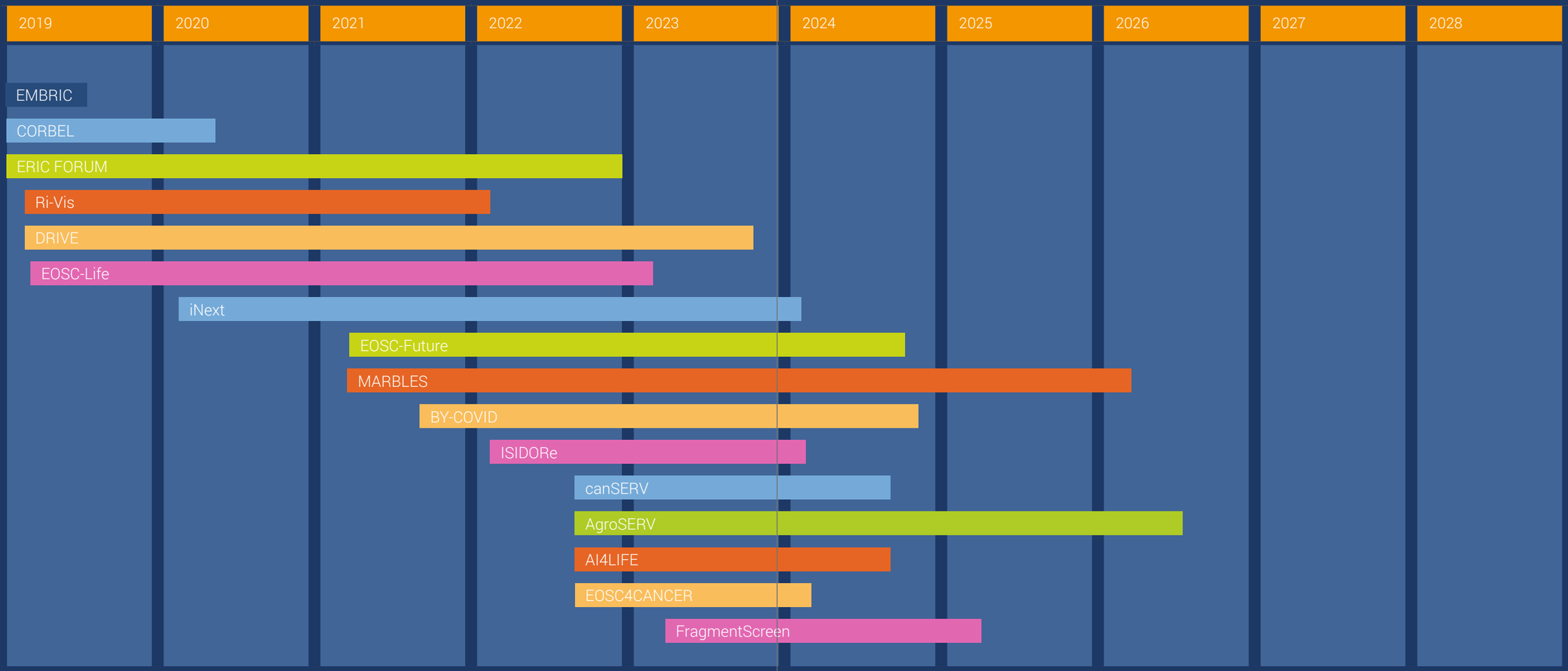
Income	Amount (€)
Regular ERIC membership fees	1,415,710
Host country contribution	1,031,984
Third party funding	540,520
Tax Refunds (VAT & Import Taxes)	118,665
Income total	3,106,879

Expenses	Amount(€)
Central Office	1,378,361
Laboratory	1,037,295
Third party funding	256,564
European Chemical Biology Database (ECBD)	160,000
Training	15,296
Long-term Central Compound Management Facility sustainability	86,000
VAT & Import Taxes	113,835
Expenses total	3,047,351

Surplus	59,528

EU-OPENSCREEN ERIC BUDGET 2022

FUNDING FROM PROJECTS (DURATIONS OF THE CURRENT AND EXPIRED PROJECTS)



In order to ensure long-term sustainability and to enhance collaboration with other life science research infrastructures, EU-OPENSCREEN actively participates in several projects/initiatives funded by the European Commission.

EU-OPENSCREEN ERIC BUDGET 2022

PLANNED PROJECT FUNDING AND GRANTS (FULL PROJECT CYCLE)

	DRIVE	CanServ	ISIDORe	RI-VIS	AgroServ	A4Life	EOSC-Life	ERIC Forum	Fragment Screen	iNEXT	MARBLES	By-COVID	EOSC4 Cancer
Personnel	734,984	231,840	106,039	130,625	97,744	24,000	44,975	33,333	93,860	10,000	48,000	20,800	24,000
Subcontracting	25,000	/	/	/	/	/	/	/	/	/	/	/	/
Direct costs*	412,846	900,867	224,117	58,500	35,971	3,600	14,000	2,000	20,200	9,500	13,000	2,000	2,000
Indirect costs	286,957	283,177	82,539	47,281	31,798	6,900	14,744	38,833	28,515	4,875	15,250	5,700	6,500
	1,459,787	1.415,884	412,695	236,406	165,513	34,500	73,719	44,166	142,575	24,375	76,250	28,500	32,500

ACTUAL THIRD-PARTY PROJECT FUNDING IN 2022

	DRIVE	CanServ	ISIDORe	RI-VIS	AgroServ	A4Life	EOSC-Life	ERIC Forum	iNEXT	MARBLES	By-COVID	EOSC4 Cancer
Personnel	141,421	25,760	32,401	9,076	6,516		2,667	21,956	13,876	2,562	9,589	6,933	3,200
Subcontracting	24,000	/	/	/	/		/	/	/	/	/	/	/
Direct costs*	127,542	/	/	96	2,398		/	/	451	/	571	/	/
Indirect costs	/	/	/	/	/		/	/	/	/	/	/	/
	292,963	25.760	32,401	8,980	8,914		2,667	21,956	14,328	2,562	10,160	6,933	3,200

*) Travel, equipment, goods and services / all amounts in (€)

COUNTRY IN FOCUS: NORWAY

Norway became a founding member of EU-OPENSCREEN in 2018, showcasing its commitment to advancing scientific research. The country hosts four specialized screening sites strategically distributed across its regions. These include the Biorecognition unit & BiSS/Biophysics, Structural Biology and Screening (UiB) in Bergen; the Centre for Molecular Medicine Norway at the University of Oslo; Marbio, an analytical platform for natural products at the University of Tromso; and SINTEF's Department of Biotechnology and Nanomedicine in Trondheim.

Specialist screening site

THE ARCTIC UNIVERSITY OF NORWAY

MARBIO – AN ANALYTICAL PLATFORM FOR NATURAL PRODUCTS

Marbio prepares and screens fraction libraries from extracts provided by Marbank and provides technology and competence within the area of high-throughput screening and natural products drug discovery.

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

Site 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 isolates and cultivate marine microorganisms: shake incubators, automated colony picker
- A chemistry unit that identifies and purify the bioactive natural products: Flash, HPLC, UPLC, LC-MS, MS-MS, IMS

Prof. Jeanette Hammer Andersen

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

Location:
Arctic University of Norway, Tromsø

Head of Unit:
Prof Jeanette Hammer Andersen

Website:
https://en.uit.no/forskning/forskningsgrupper/gruppe?p_document_id=380005

Specialist screening site

SINTEF

DEPARTMENT OF BIOTECHNOLOGY AND NANOMEDICINE

SINTEF has a strong operation in the fields of microbial molecular biology, bioprocess- and medical technology, biopolymers/polymers, biopharmaceuticals and nanomedicine, and is operating a state-of-the-art research infrastructure including advanced mass spectrometry.

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

Site 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
- BSL 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

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.

Location:
SINTEF, Trondheim

Head of Unit:
Geir Klinkenberg

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

Specialist screening site

UNIVERSITY OF OSLO

CENTRE FOR MOLECULAR MEDICINE NORWAY (NCMM)

The Centre for Molecular Medicine Norway is an international biomedical research centre, with the overall objective of translating basic medical research into clinical practice. It is a part of UiOs interdiciplinary focus on Life Sciences.

At a glance:

- Specialized screening site within EU-OPENSCREEN and managing node for the national RI NOR-OPENSCREEN
- Core facility for the University of Oslo and Oslo University Hospital
- Access to the 100K EU-OPENSCREEN commercial and academic libraries
- 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

Site 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
- BSL 2 cell culture for primary human cells
- Competence in immunology, characterization of immune cells and intra cellular signaling

Dr. Johannes Landskron

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.

Location:
University of Oslo

Head of Unit:
Dr. Johannes Landskron

Website:
https://www.med.uio.no/english/research/core-facilities/chemical-biology-screening

Specialist screening site

UNIVERSITY OF BERGEN (UIB)

BIOPHYSICS, STRUCTURAL BIOLOGY, AND SCREENING (BISS)

Biophysics, Structural Biology, and Screening (BiSS) is a core facility of the Faculty of Medicine. BiSS offers expertise and access to a range of instrumentation to study the interactions of small molecules with macromolecules, protein biophysics, and for crystallization.

At a glance:

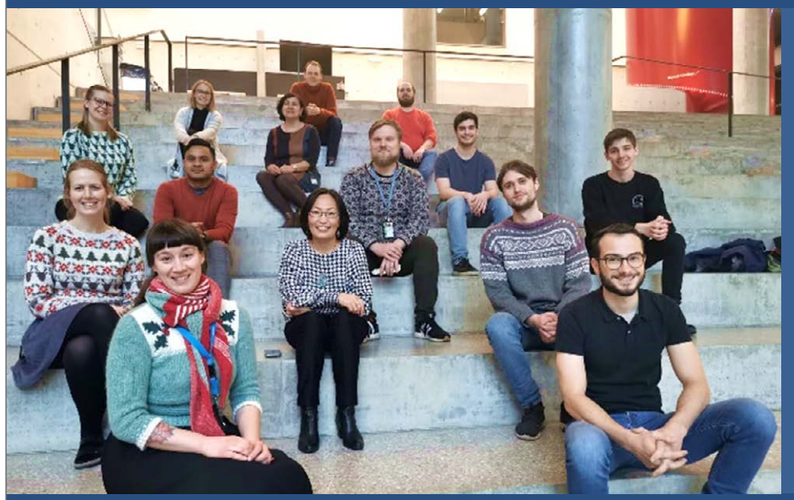
- Specialist screening site with skills in combination of biophysical techniques - experimental and computational
- Notable expertise in developing therapies for misfolding disorders and infectious diseases
- Managed by the core facility for Biophysics, Structural Biology and Screening (BiSS)
- Chemoinformatic services for hit follow up
- Determination of binding modes using X-ray crystallography
- Self-service access to instrumentation possible after training

Site 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

EU-OPENSCREEN is a crucial collaborative network for the University 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.



Location:
University of Bergen

Head of Unit:
Prof. Aurora Martinez

Website:
https://www.uib.no/en/rg/biss

WE SUCCESSFULLY EXPANDED OUR NETWORK AND COMMUNITY THROUGH THE ADDITION OF NEW MEMBER COUNTRIES, PARTNER SITES, COLLABORATIONS WITH INDUSTRY PARTNERS, RESEARCH INFRASTRUCTURES, AND EXCITING NEW USER PROJECTS.

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