

ACTIVITY AND FINANCIAL REPORT

2021

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FOREWORD

Dear colleagues and friends of
EU-OPENSOURCE,

2021 was another year heavily affected by the COVID-19 pandemic, and the work at our infrastructure, with partner sites and our scientific collaborators was no exception. However, we all learned how to make the best of this situation, and you will find several examples of this in this report.

Our office team worked mostly from home while the laboratory team continued onsite to test and ship compounds to our partners. Most notably, all our training activities switched from physical training courses to online webinars, thereby reaching out to much larger audiences.

We organised our traditional bi-yearly 'European Chemical Biology Symposium' for the first time as a completely virtual event in May. The event attracted over 1,000 registrations with nearly 170 abstracts and talks from 60

renown speakers. A planned summer training school in Spain was postponed to 2022. However, we organised a virtual autumn school in November, with a week full of lectures from speakers of our partner sites about different aspects of chemical biology and early drug discovery.

The pandemic also triggered the formation of two large emergency consortia by the European Commission. The ISIDORE project has over 150 partners and EU-OPENSOURCE will lead a transnational access work package dedicated to diagnostic and therapeutic discovery services. Meanwhile, our partner site ITMP in Hamburg is participating in the BY-COVID project to ensure that all SARS-COV-2 data can be easily found and used by the community. Team members were also engaged in the writing of several EU proposals in 2021, all of them tackling either new

technologies or important topics within health and the agrisciences.

Over 20 screening projects are now using our compound libraries and the technology platforms and expertise of our partner sites. We have gained valuable experience in the fields of chemoproteomics and fragment-based drug discovery thanks to our DRIVE project. We aim to develop additional services in these areas in the years to come.

An important milestone for us in 2021 was the start of our bioprofiling activities. Using a panel of standardised assays, we are now acquiring physicochemical, biochemical and cellular data on all of our 100,000 compounds. These data range from the measurement of compound solubility and spectroscopic properties to cellular toxicity and anti-microbial properties. They will be made

Dr. Wolfgang Fecke,
EU-OPENSOURCE Director General

accessible to users in our European Chemical Biology Database. The wide availability of the data to everyone will help scientists to identify novel chemical probes and develop better data-driven computational prediction tools. You will learn more about these and other topics in our Annual Report 2021, and I look forward to working with you in 2022.

On behalf of the whole Central Office team,
Dr Wolfgang Fecke, EU-OPENSOURCE Director General



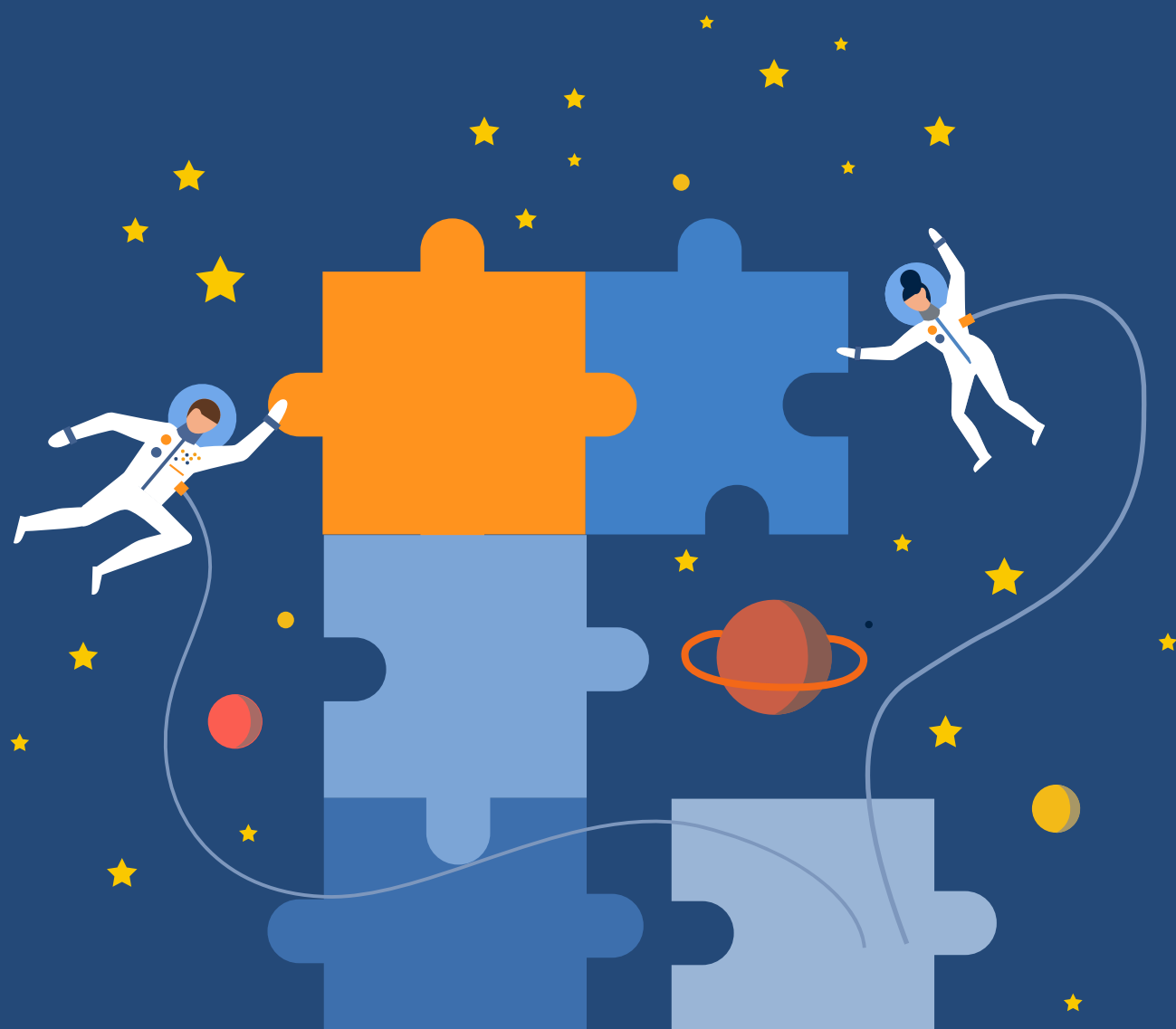

EU-OPENSOURCE TEAM 2021

OUR TEAM WAS
ABLE TO RESPOND
QUICKLY TO PANDE-
MICS-RELATED CHAL-
LENGES AND INTRO-
DUCED NEW TOOLS
AND FORMATS FOR
COLLABORATION.

Our team continued to grow in 2021 with nine people working in the central office and four working in our central compound management facility.

We could welcome three new employees to our international team: Victoria, Annegret and Robert.

Despite the pandemic we organised common activities and a great team event. Our team has shown again its good collegiality, spirit, enthusiasm and supportiveness.



Victoria Mora

joined us in March 2021 to complete the compound management team. Victoria holds a degree in Chemistry. She worked in the UK for ten years in Organic Chemistry and then worked in Analytical Chemistry in Berlin specialising in food analysis using LC MS-MS/TOF. In her new role at EU-OPENSOURCE, she is responsible for the quality control of our compounds. She also supervises the acquisition of our academic compounds and builds up a network with potential compound donors.



Annegret Haden

joined the Finance department in early 2021. She ensures the timely payment of our invoices and supports us in our day to day finance business. She also coordinates our order processes and payment transactions and acts as a key contact for our tax advisors.



Robert Harmel

joined us in autumn 2021 as our new Scientific Project & Industry Liaison Manager. Robert is responsible for establishing potential industry collaborations and acts as prime contact for scientists from research and industry who would like to work with us. Robert is an organic chemist by training and holds a PhD in Chemical Biology from the Leibniz Institute for Molecular Pharmacology (FMP), where he worked on the development of new analytical tools to study signalling of challenging small molecule messengers.



NEW LAB EQUIPMENT AND SOFTWARE

LIQUID CHROMATOGRAPHY-TIME OF FLIGHT SPECTROMETRY SYSTEM

The Quality Control laboratory of EU-OPEN-SCREEN has been expanded by the acquisition of a new liquid-chromatography tandem with a time-of-flight detector (LC-TOF).

Our new instrument is a UPLC (ultra-high-pressure liquid chromatography) instead of a common HPLC (high pressure-liquid chromatography), allowing faster analytical run and also reducing the use of solvents. The mass range of the detected samples that a LC-TOF spans from 10 to 10,000 m/z; being the range of a single-quadrupole mass detector (MSD) of 100-1,000 m/z.

This allows the measurement of a much wider range of compounds, including natural compounds.

This is a key feature considering the wide variety of chemical structures of the academic compounds that will be part of our library. And finally, LC-TOF measures accurate masses, therefore having superior precision in measurement, and a much higher accuracy that would lead to a reliable assessment of our first confirmed hit compounds.

NEW SOFTWARE FOR COMPOUND REGISTRATION AND INVENTORY

In 2021, EU-OPENSOURCE selected a powerful and intelligent software system for the management of the EU-OPENSOURCE compound collections. The MOSAIC software was developed by the company Titian and is already used by many pharmaceutical companies. EU-OPENSOURCE is working with Titian and ChemAxon to implement a Mosaic

Sample Bank with a specific configuration for the sample registration of EU-OPENSOURCE compounds. The pre-configured package of the Sample Bank will track all compounds, and our partner sites will be able to directly place orders. Our specific configuration will also include a ChemAxon registration module for newly acquired compounds.

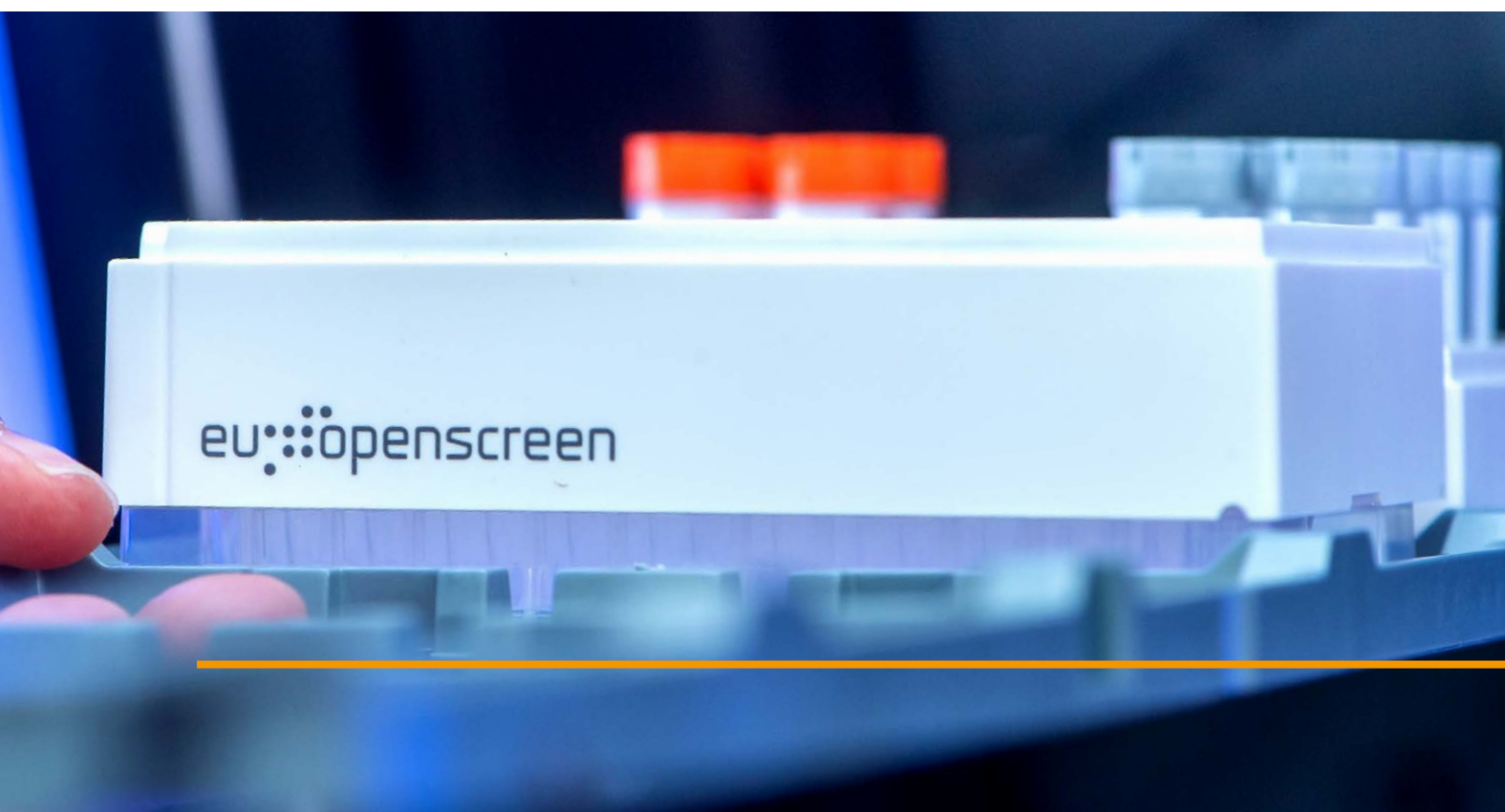
FIRST HIT PICKING CAMPAIGNS

Following the primary screening of the library at partner sites, the EU-OPENSOURCE central compound management received numerous requests for hit picking in the scope of follow up studies. With the distribution of a few microlitres per compound, projects could be supported to the next phase.

EU-OPENSOURCE could also support partner sites with the preparation of assay ready plates for primary screening with volumes distribution in the nanolitre range using the ECHO 650 instrument. The project types included EU-OS ERIC project, fragment screening and DRIVE screening.

The second unit, another but smaller STAR-let liquid handling workstation from Hamilton, passed all acceptance tests in August 2020. This unit will be used mainly to register compounds and reformat the European Academic compound library (EACL). As the name suggests, this innovative and unique library is made up of compounds provided by academic chemists from Europe and beyond. Here, the main workflow is designed to reformat the compounds from larger scale 24-well plates into 96-well plates.

By using the latest technology, we are constantly optimising our work processes and expanding our range of services.



NEW BIOPROFILING SERVICES

BIOPROFILING

All compounds in the EU-OPENSREEN compound collection are tested and characterised for a basic set of properties which are relevant for chemical biology or drug discovery projects by testing them in a standard panel termed ‘bioprotefiling’ assays. Bioprotefiling assays have been assigned to suitable EU-OPENSREEN screening partner sites after an internal tender process, during which, the screening sites have submitted their proposals following specific guidelines described in the bioprotefiling handbook (created by EU-OPENSREEN ERIC).

The bioprotefiling proposals were evaluated by independent external reviewers based on evaluation criteria

- adequate description and clarity of the assay,
- assay validation experiments/assay performance and sensitivity,
- assay cost and timelines, proven track record of the services provider,
- excellence of the provider,
- consumption of tested compounds.

Assay	Type of assay	Rationale	Performing Institute
Solubility	Physicochemical	Poor solubility can mask compound activity in bioassays including underestimated activity, reduced hit rates in HTS and variable data outputs.	University of Santiago de Compostela (USC)
Interference with common Bioluminescence reporters	Biochemical	Important readout for many cellular reporter format assays. Will identify potential screening artefacts/false positives based on modulation of reporter enzymes.	Polish Academy of Sciences, Institute of Bioorganic Chemistry (IBCH PAS)
ROS (Reactive Oxygen Species)	Biochemical	Redox active compounds are commonly found in many screens as false positives as they can oxidize disulfide bridges in proteins or react with important co-factors.	Polish Academy of Sciences, Institute of Bioorganic Chemistry (IBCH PAS)
Cell viability	Cell-based	Detection of the number of living cells by various means, e.g. measurement of ATP.	Institute for Molecular Medicine Finland (FIMM)
Antibacterial and antifungal assays	Biological	Deliver information about potential antibacterial and antifungal properties by testing compounds in a panel of growth assays.	Fundación MEDINA (MEDI) Helmholtz-Centre for Infection Research (HZI)
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.	Fundación MEDINA (MEDI) University of Santiago de Compostela (USC) Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP) Institute of Molecular and Translational Medicine, Palacky University Olomouc (IMTM)
Absorbance-Autofluorescence *	Physicochemical	Characterisation of the spectral properties of the EU-OPENSREEN compounds. The assay combines an absorbance scan and auto-fluorescence readings.	EU-OPENSREEN Compound Management Facility

Panel of EU-OPENSREEN ERIC Bioprotefiling assays



THE IMPORTANCE OF BIOPROFILING

Bioprotection of the EU-OPENSOURCE compound collection will contribute to the wealth of quantitative data on compound bioactivities and will comprehensively characterise each of the compounds before they are used by the scientific community. This process will add essential biological and physicochemical context to help interpret results from user projects. EU-OPENSOURCE's network of state-

of-the-art screening centres will offer users access to a wide range of read-out technologies. Some examples of these are absorbance, luminescence or fluorescence intensity technologies. The centres will allow users to implement assay formats such as cell-based, biochemical and even model organism-based assays.

The bioprotection data will allow the early identification of read-out interferences caused by compound properties. This makes it easier to eliminate false positive hits from screening results, which in turn improves the selection of high value compounds for further optimisation. This will ensure that results generated in

screening campaigns are reliable, reproducible and comparable. This helps to meet the objective of driving standards in preclinical research.

BENEFITS OF BIOPROFILING

- provide a maximum quality compound collection for the users
- secure reliable screening results
- identify and flag compounds with properties that could perturb specific bioassay read-out technologies (e.g. by autofluorescence, or luciferase inhibition) in order to reduce false-positive results
- provide data as an incentive for chemists to submit compounds to the EU-OPENSOURCE collection



EUROPEAN CHEMICAL BIOLOGY DATABASE (ECBD)

The central data hub for data generated within the EU-OPENSREEN network - the ECBD is developed in line with the FAIR principles ensuring Findability, Accessibility, Interoperability, and Reusability of the data.



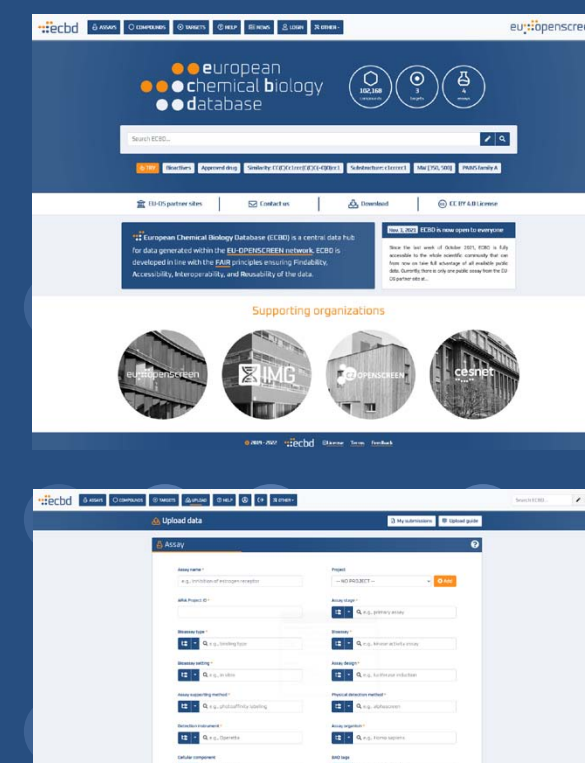
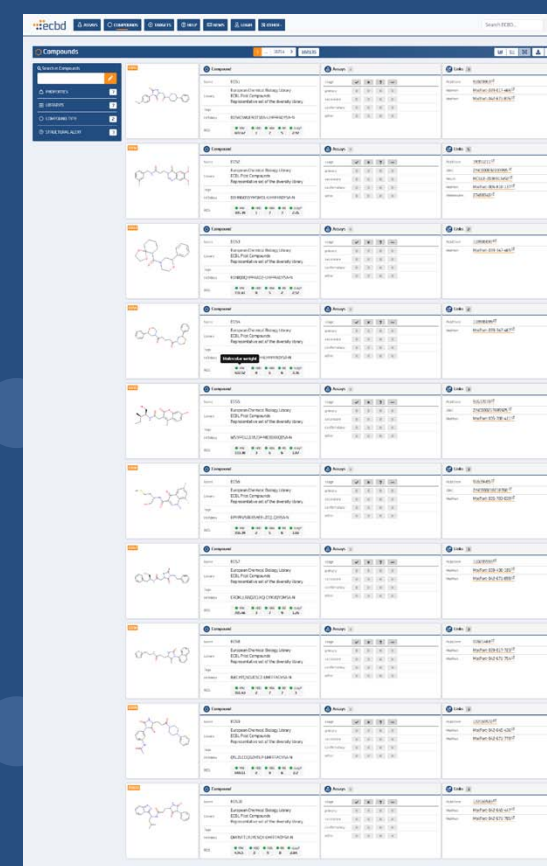
ECBD NOW ONLINE

The ECBD was developed and is hosted by our Czech partner site, the Institute of Molecular Genetics (IMG). The ECBD is a web portal with powerful search and analysis capabilities and contains validated output from partner screening sites in a public as well as pre-release environment. It was developed in line with the FAIR principles, ensuring Findability, Accessibility, Interoperability, and Reusability of the data.

The database supports curation, annotation and organisation of data and metadata. A flexible privacy model is used for rapid and safe dissemination and exploitation of data. Users

remain the owners of their data, and there is an optional hold period of 36 months for data publication. High standards of security and traceability of IP are in place, e.g., the citable indexing of data points (EUOS, DOI or URL) and links to originator laboratories for primary raw unprocessed data.

The ECBD has established links to other data resources, e.g., ChEMBL, PubChem, UniProt and BioAssay Research Database (BARD). This has been done to facilitate data reuse and to increase the reach and impact of the scientific results of EU-OPENSREEN.



Screenshot examples of the ECBD web-interface: <https://ecbd.eu>



FIRST VIRTUAL ECBS2021

Our biennial scientific conference, the 7th European Chemical Biology Symposium 2021 (ECBS2021), took place on 26– 28 May 2021 and was a great success. Overall attendees rated the conference with 8.8 out of 10 points. More than 1,000 scientists from around the world registered for this conference and we received 169 abstracts for poster and oral presentations. Seventeen speakers presented at the event and thirteen posters were selected for short, 5-min flash presentations.

The ECBS has become a renowned event in Europe, bringing together world experts, top scientists and young investigators in the field of Chemical Biology. The ECBS is jointly organised by EU-OPENSREEN and the EuChemS Division of Chemistry in Life Sciences (<http://www.euchems.eu/>). It focuses on diverse aspects of innovative chemistry at the interface with biology, material science, biophysics, and other disciplines.

Over the course of three days, 60 speakers covered a diverse range of topics: artificial intelligence in drug design, small molecules targeting nucleic acids, new pharmacological approaches: targeting protein degradation, protein aggregation and self-assembly, bio-nanotechnology and synthetic biology, natural compounds chemistry and biology, glycochemistry and glycobiology, fighting resistant pathogens, and new approaches in antiviral therapies. A special session on 'Gender & Diversity' was organised in 2021 for the first time.



Prof. Herbert Waldmann, Head of the Chemical Genomics Center of the Max Planck Gesellschaft, gave the opening lecture on "Pseudo Natural Products – Chemical Evolution of Natural Product Structure".

In conjunction with the ECBS2021 main conference, a Young Investigator Workshop (<https://yiw2021.eu>) was organised directly ahead of the ECBS on 24– 25 May. The workshop provided a platform for young investigators at an early stage of their careers to present their research and to network with potential future leaders in the field.

The ECBS 2021 also included a dedicated session on gender issues. The session mainly focused on screening and there was a discussion of the 2020 documentary film "Picture a Scientist", directed by Sharon Shattuck and Ian Cheney. The film presents several prominent female researchers and brings to light the barriers and challenges they encountered. The film enabled a discussion about discrimination and harassment between scientists and possible solutions.

Over the course of three days, 60 speakers covered a diverse range of topics:

- artificial intelligence in drug design,
- small molecules targeting nucleic acids,
- new pharmacological approaches: targeting protein degradation, protein aggregation and self-assembly,
- bio-nanotechnology and synthetic biology,
- natural compounds chemistry and biology,
- glycochemistry and glycobiology,
- fighting resistant pathogens, and
- new approaches in antiviral therapies.

Nine prizes were awarded for the best presentations in the following categories: Organic chemistry interfacing biology; Innovative hit compounds and biomaterials for drug discovery and development; Innovative approaches in life science; Chemical tools in biology; Chemical glycobiology; and Natural products in chemical biology. These prizes were sponsored by the Italian Chemical Society and the Spanish Royal Society of Chemistry (RSEQ).

An ECBS2021 special issue is currently in preparation to be published in *Molecules*, which is the leading international, peer-reviewed, open access journal of chemistry, published semimonthly online by MDPI. The manuscripts were selected from submissions by ECBS2021 attendees, with a special emphasis on contributions from early-stage researchers.

The ECBS2021 Organising Committee members were Wolfgang Fecke (Chair), Francesco Peri (Chair), Katja Herzog, and Bahne Stechmann.

The ECBS2021 conference book and the ECBS2021 abstract book are available on the ECBS2021 website: <https://ecbs2021.eu>. The next ECBS2023 will be held in May 2023 in Stockholm, Sweden, hosted by the Karolinska Institutet.



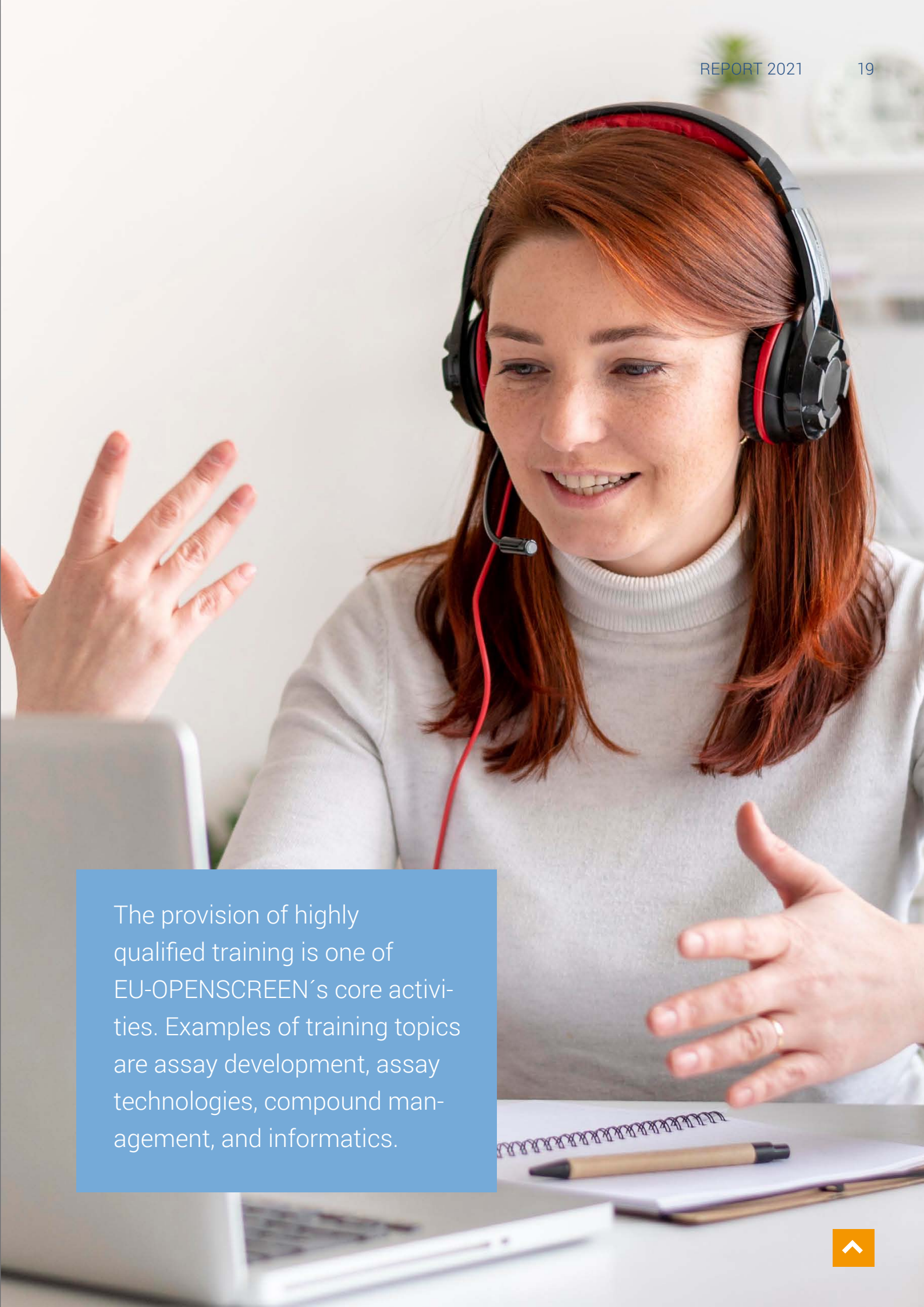
TRAINING ACTIVITIES

The second training call of EU-OPENSREEN launched in 2020 was heavily affected by Covid-19 restriction rules. Alternative online training activities were developed for EU-OPENSREEN and the DRIVE project in 2020 and 2021. Webinars, workshops, and online

training schools received positive feedback from the Partner Site Forum (PSF) and the Scientific and Ethical Advisory Board (SEAB).

The training activities offered in 2021 are listed in the table below.

Partner site	Title of the training activity	Access	Targeted audience	Date
FMP 1.Jens Peter von Kries 2.Martin Neuen-schwander 3.Katina Lazarow 4. Christopher Wolff	Machine Learning Enhanced Cell Morphology Profiling in Molecular Pharmacology: Virchow 2.0	Online, free of charge	Internal workshop for EU-OS partner sites	24 March 2021
IME Sheraz Gul	Enzyme targets and mechanism of action studies in drug discovery	Online, free of charge	Internal workshop for EU-OS partner sites	13 April 2021
USC 1.Mabel Loza 2.Pepo Brea	Phenotypic screening employing neuron-differentiated cell lines	Online, free of charge	Internal workshop for EU-OS partner sites	11 May 2021
IMTM 1.Magdalena Otrrocka 2.Jacek Kolanowski	Indicator displacement assays in identification of binders of 3D RNA structures	Online, free of charge	Internal workshop for EU-OS partner sites	8 June 2021
Attended by FIMM	Galleria Mellonella Workshop	Online and on-site	Young researchers	21 July 2021
EU-OS partner sites and external speakers	Chemical biology and drug discovery autumn school	Online, free of charge	Researchers and students	15 - 19 November 2021



The provision of highly qualified training is one of EU-OPENSREEN’s core activities. Examples of training topics are assay development, assay technologies, compound management, and informatics.



SYMPOSIA IN AFRICA, LATIN AMERICA AND AUSTRALIA

This year, EU-OPENSREEN organised, as part of the RI-VIS project, four international Research Infrastructure symposia with colleagues in different world regions: Africa, Latin America and Australia.

The symposia were held over 2 - 3 days, starting with the Africa-Europe Symposium on 1 - 2 February 2021, followed by the Latin America-Europe Symposium on 15 - 17 June (organised in collaboration with EU-LAC ResInfra) and the Australia-Europe Symposium held on 5 - 7 October.

The meetings attracted a considerable interest from the community and more than 1,300 participants registered for these events.

The symposia brought together relevant stakeholders and provided a forum to discuss partnerships between Research Infrastructures (RI) as well as common challenges and opportunities. They raised awareness of individual RIs, and identified measures to mitigate existing cooperation challenges between RIs. New ideas emerged for starting to work together and for working better together. Attendees had the opportunity to network with colleagues working in RIs in other parts of the world. Many RIs have established or are entering into new collaborations with partners outside of Europe.

Reasons to cooperate can be summarised as follows:

- harness collective global knowledge and experience,
- support leveraging of new international funding for RIs,
- promote access to and exchanges between RIs,
- facilitate the mobility of researchers,
- assist in meeting global challenges, or
- compensate each other's shortcomings.

Global challenges require openness and RIs need international collaboration to ensure the best use of limited resources. RIs share similar operational challenges and they can learn from each other. Attendees expressed an interest in exchanging experiences. Surveys after the symposia confirmed that there is a strong interest in organising similar symposia in the future to address shared challenges.



Facing global challenges together: EU-OPENSREEN launched various events to strengthen international cooperation to establish global relations in 2021.

USER PROJECTS

THE FIRST USER PROJECTS STARTED IN 2021. MORE THAN 28 PROJECTS WERE SUCCESSFULLY LAUNCHED WITHIN OUR INFRASTRUCTURE AT OUR PARTNER SITES IN THE EU-OPENSREEN MEMBER COUNTRIES.

In addition, ten pre-applications are in the pipeline from scientists whom we supported in their grant proposals. Once their projects have been approved, their projects will be able to kick off. EU-OPENSREEN works with institutions all over Europe and an increasing number of users contact us to use our services and get support for their research.

The majority of projects are about cancer and neurodegenerative disorders. Other screening campaigns target rare diseases, diabetes, antibiotics, and antivirals. As a result of the COVID-19 pandemic, EU-OPENSREEN decided to grant a fast track for SARS-CoV-2 related projects. This fast track service was used by four researchers to screen our pilot library. Two of these data sets are now openly shared and visible in the recently launched ECBD. The first two large screening campaigns of the ECBL came to an end in 2021 and were added to the ECBD. These campaigns derived from the EU-funded project EU-OPENSREEN-DRIVE. Most of the new data will be available in 2025, as the 36 month embargo period is often selected by scientists to secure intellectual property.

Two screening campaigns were awarded funding through the EU-OPENSREEN-DRIVE medicinal chemistry call. Chemical optimization of hit compounds will be granted in 2022 by our medicinal chemistry sites. One such project is presented below.

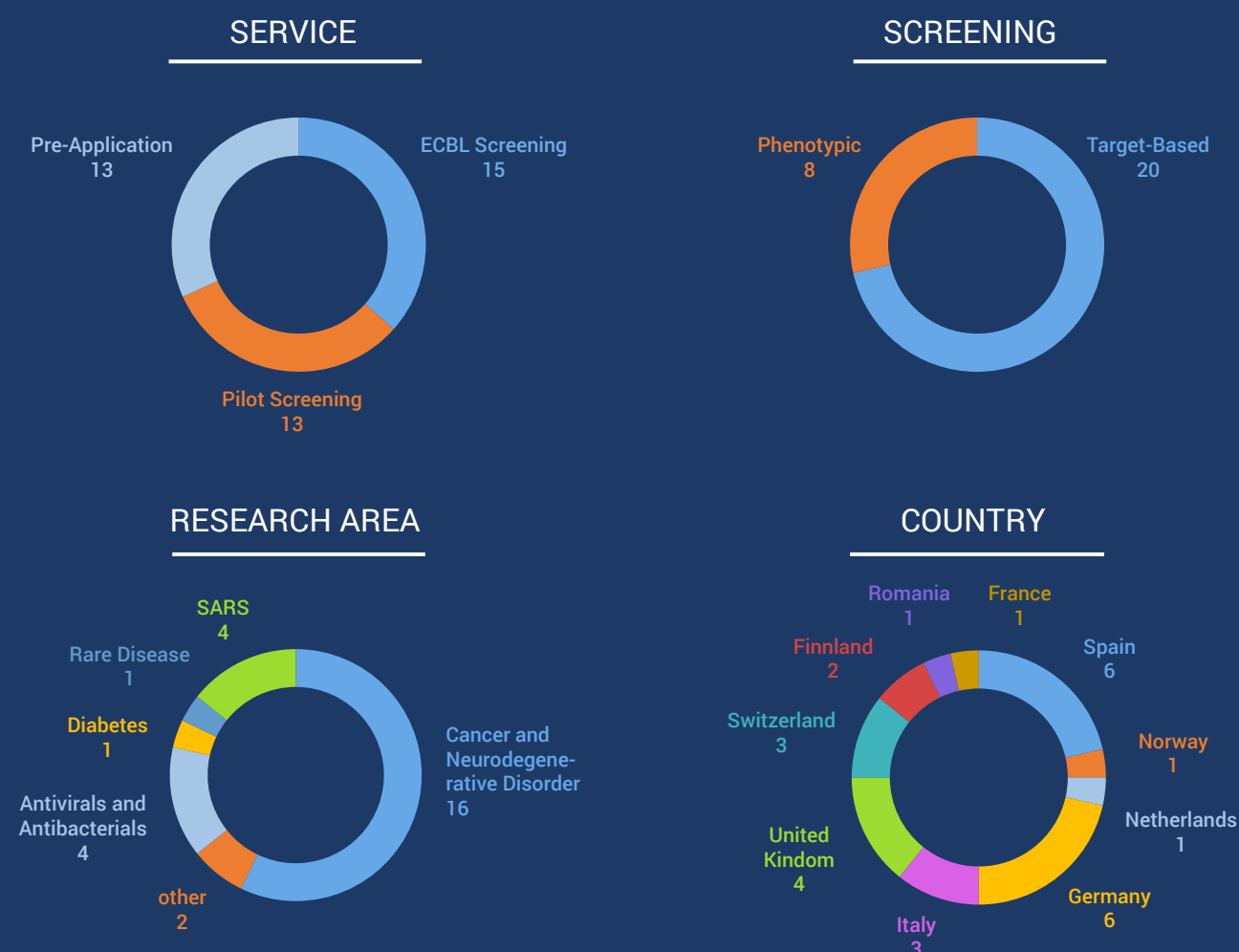


Figure1: Overview of user projects carried out at EU-OPENSREEN screening partners sites including services and technologies used, projects research area and countries distribution of users applying to our screening services



UNCOVERING MITOCHONDRIAL ER CONTACT SITES MODULATORS WITH POTENTIAL RELEVANCY IN THERAPEUTICS.

USER:

Prof. Ana Garcia Saez, University of Cologne, Institute for Genetics, Germany

EU-OPENSREEN SCREENING PARTNER:

Dr. María J. Vicent, Centro Investigación Príncipe Felipe (CIPF), Spain

EU-OPENSREEN MEDICINAL CHEMISTRY PARTNER:

Prof. Dr. Ana Martínez, Center for Biological Research Margarita Salas (CSIC), Spain (planned for 2022-2023)

Prof. Ana Garcia Saez project aims to identify small molecule compounds that selectively modulate the dynamics of contact sites between mitochondria and the endoplasmic reticulum (MERCS). MERCS influence a variety of cellular functions and show altered morphology in several human diseases including neurodegenerative disease and cancer. The development of new chemical probes, as proposed in this study, could elucidate more mechanistic details about the biological function of MERCS and its role in human pathology. Taken together, this research could create opportunities towards new pharmaceutical intervention strategies.

The Saez group has recently developed MERLIN: a stable cell line that contains a bioluminescence resonance energy transfer (BRET)-

based biosensor that allows the monitoring of changes in MERCS dynamics efficiently with small time and money consumption. MERLIN was further optimised to meet the requirements of an automated high-throughput screening campaign (Figure 2).

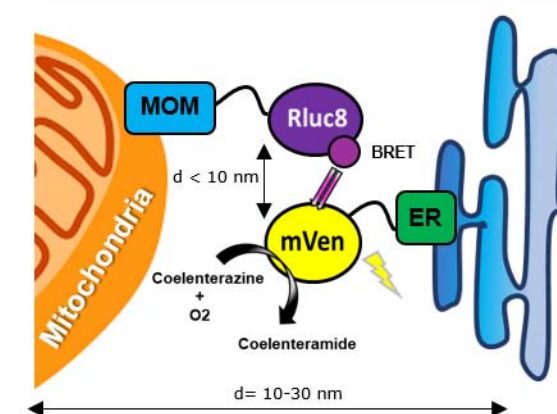
With this robust assay in place, Prof. Saez was approved for the small molecule screening call in autumn 2019. Our EU-OS partner site CIPF led by Dr María J. Vicent further refined and adapted the conditions from a 96- to a 384-well plate format to enable the screening campaign of the EU-OPENSREEN small molecule diversity library (ECBL). The identified hits were further validated in a dose-response dependent fashion where even one of the molecules showed nM potency with respect to MERCS modulation.



It was a pleasure at all levels to work with the CIPF in the context of EU-OPENSREEN. It gave us the opportunity to carry out a sophisticated chemical screening in a very efficient way, which would not have been possible otherwise and which sets the basis for a promising collaboration that still continues.

Ana Garcia Saez

Mito-ER distance by BRET



Workflow

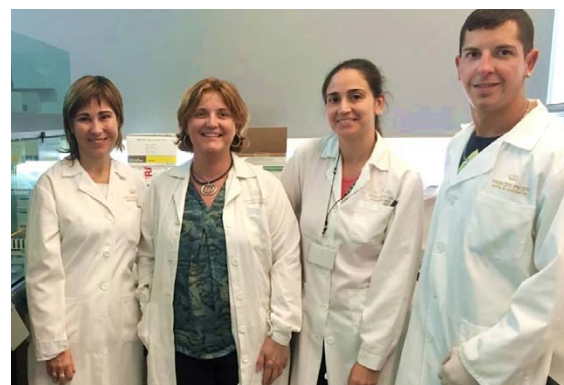
1. Cell seeding
2. Treatment
 - ↓ BRET ↑ Distance
 - ↑ BRET ↓ Distance
3. Coelenterazine addition
4. Data processing
 - BRET = $(I_A - I_0) - cf$

Figure 2: High-Throughput screening using MERLIN – Screening technology employed and project workflow.



With these hit compounds in hand, Prof. Saez applied for the medicinal chemistry call in autumn 2021 to further improve the performance and therapeutic potential of the identified molecules together with the group of Prof. Ana Martinez at CIB-CSIC. This follow-up proposal aims to better understand the chemical diversity of the obtained screening hits and to optimise the pharmacological properties of the compounds by designing derivatives with improved ADME (Absorption, Distribution, Metabolism, and Excretion).

A successful outcome of this research will help to discern the mechanism by which these compounds elicit their effect on MERCs. Additionally, it will provide safe leads structures with activity at nanomolar concentrations. Altogether, the results produced here could lay the foundation of a better understanding of MERCS biology and might identify protein components of MERCS as novel drug targets.



Pictures: 1 – Research Group of Prof. Dr. Ana J. Garcia-Saéz, University of Cologne
2 – EU-OPENSREEN ERIC screening site of Dr. Maria J. Vincent, Centro Investigación Príncipe Felipe, 3 - EU-OPENSREEN ERIC medicinal chemistry site of Prof. Dr. Ana Martinez Gil, Consejo Superior de Investigaciones Científicas

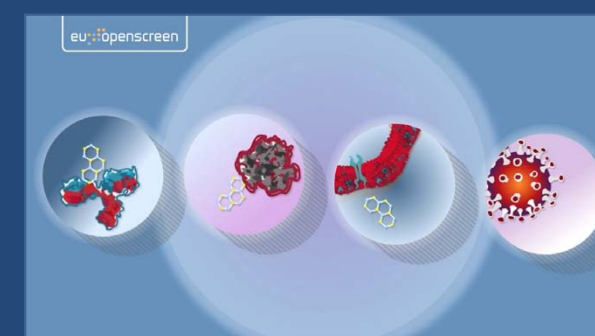
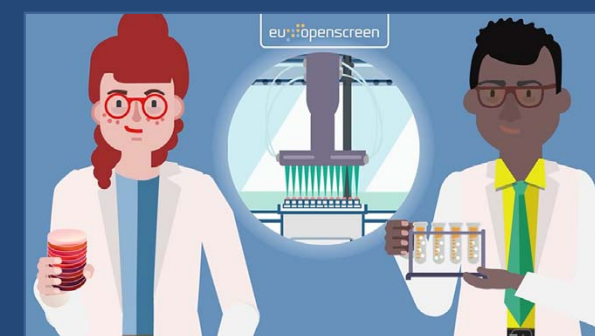
SCIENTIFIC OUTREACH

VIDEOS EXPLAINING OUR SERVICES

In 2021 we launched our first videos explaining our services in a comprehensive, attractive and easy to use and easy to understand way. Three films were produced by a professional agency specialised in science communication.

The first film is made for a general audience and explains the major pillars of EU-OPENSREEN. The short sequence gives valuable insights into our work and shows how to benefit from our services. The film takes the viewer on a journey to discover the secrets of life and to develop novel drugs to fight the grand societal challenges.

The other two films explain our services to biologists and to chemists. The films are featured in a prominent section on our website and on our YouTube channel. Shorter clips were used in social media.



Please find the explanation videos and further content on our website in the “video content” section.

[Video section](#)



GET TO KNOW OUR PARTNER SITES

EU-OPENSOURCE 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.

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-OPENSOURCE ERIC and remain embedded in their host institutions.

To showcase our complete service offer we produced a comprehensive brochure featuring all our partner sites in the respective member countries. Get to know our partner sites and see what they can offer for your research project. You will learn about their infrastructure and technical focus, their projects and their scientific track records.

FIND OUT ABOUT OUR COVID-19 RELATED SERVICES

Moreover, partners with a specific research focus on infectious diseases can provide their support in the design and development of phenotypic assays (monitoring of bacterial growth inhibition, viral replication and virus-induced cyto-pathic effects), target-based

assays with engineered bacteria or viruses cell-based high-content screening (HCS) assays and host cell response assays all implemented in Biosafety Level (BSL) 2 and 3 laboratories.

Please find the brochures and other publications on our website in the “Resource center” section.

[Ressource center](#)

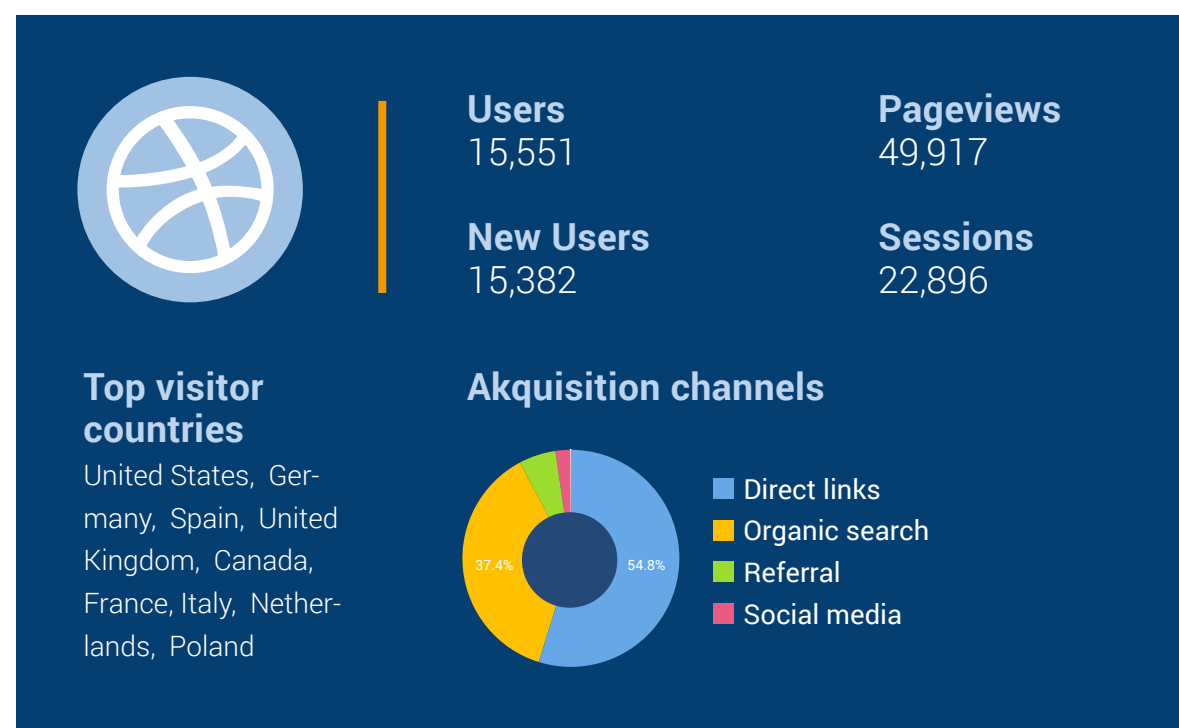


SOCIAL MEDIA AND COMMUNICATIONS

We increased our activities in our different social media channels which is clearly shown in the steadily rising number of followers: Our LinkedIn company page increased to 591 followers, our LinkedIn group "chemical keys for life's locks" increased to 318 followers and our Twitter account has now 784 followers.

In addition, we presented EU-OPENSREEN's services at several conferences and especially at our flag ship event, the ECBS 2021,

which was held in 2021 for the first time completely virtually and which was a great success. Please have a look at the separate ECBS section in this report (page 16). Our training school in autumn 2021 and several webinars helped to spread the word on our services and to attract new users to our infrastructure.



EU-OPENSREEN ERIC ECBS 2021 Announcement, 26-28 May, 2021 [View this email in your browser](#)

EU-OPENSREEN ERIC - February 2021

European Chemical Biology Symposium (ECBS) 2021

26-28 May, 2021 | Virtual conference
Free registration now open!

It's our pleasure to invite you to the virtual European Chemical Biology Symposium (ECBS) 2021, which is jointly organised by EU-OPENSREEN ERIC and the EuChemS Division of Chemistry for Life Sciences.

The meeting builds on the success of the 6th ECBS/LS-EuChemS in Madrid in 2019, the 5th ECBS in Budapest 2017 and the ICBS/ECBS joint meeting in Berlin in 2015.

Francesco Peri (Chair)
University of Milano-Bicocca, Italy
EuChemS

Wolfgang Focke (Chair)
EU-OPENSREEN ERIC, Germany
eu.openscreen

The virtual ECBS 2021 brings together scientists from Europe and overseas to present and discuss their latest achievements in cutting edge chemical sciences at the interface with biology and medicine, ranging from new

Online Autumn School Announcement - EU-OPENSREEN ERIC
Newsletter No 23, October 2021 [View this email in your browser](#)

Autumn training school - November 15 - 19, 2021

FREE OF CHARGE **This course is free to attend!**
Just register for a place beforehand - please note the registration instructions below.

We would like to invite you to the first edition of our EU-OPENSREEN AUTUMN TRAINING SCHOOL on various aspects of chemical biology from November 15 - 19

Starting with a general introduction to the field, we will continue by exploring more specific subjects such as

- hit selection,
- cheminformatics,
- medicinal chemistry,
- principles of open data and open-source tools,
- assay development and optimisation,
- data analysis.

New services of EU-OPENSREEN ERIC, such as **fragment screening** will also be presented.

Additionally, our speakers will introduce you to the EU-OPENSREEN ERIC European Chemical Biology Database (ECBD), compound libraries and specific instruments which are used during compound management and screening campaigns.

Speakers:

- Mabel Loza, University of Santiago de Compostela, ES
- Johannes Landskron, University of Oslo, NO
- Daniel Svozil, IMG Prague, CZ

We are promoting our meetings and training events via social media channels, the newsletter and our website. With a base of more than 1000 active subscribers and above average open and click rates, our newsletter is a well accepted communication and information tool to liaise with our community.

[Newsletter section](#)



EUROPEAN PROJECTS

EU-OPENSOURCE is involved in several European projects in order to ensure the long term **sustainability** and to enhance the **collaboration** with other life science research infrastructures



EU-OPENSOURCE DRIVE

EU-OPENSOURCE started in 2017 to develop the EU-OPENSOURCE-DRIVE project proposal to further strengthen the research infrastructure and to support its long-term sustainability. The INFRADEV-03-2018-2019 call from the European Commission, specifically targeting entities with international memberships such as European Research Infrastructure Consortia (ERICs), provided the necessary funding for our activities to ensure long-term sustainability. We also paid specific attention to the interaction with industry and SMEs to foster the innovation potential of our European research infrastructure.

In addition to coordinating the financial and scientific administration of all 33 partners working on 10 different work packages (WP9), EU-OPENSOURCE ERIC also leads the work package on Excellence in ERIC operations and management (WP1) and on Transnational access - demonstration of EU-OPENSOURCE'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 this type of action from the European Commission is meant for ERICs to work on and test poten-

tial new structures and processes needed for the continuous adaptation to arising research needs, EU-OPENSOURCE is also strongly involved in all other work packages. These activities include:

- completing the management processes needed for a large, distributed infrastructure
- widening the awareness of academia and industry for EU-OPENSOURCE services and data
- growing capacities and competence in the field across Europe
- supporting the establishment of a national compound ambassador network to foster and speed-up the collection of academic compounds (WP2),
- managing fragment library design and its procurement to enable joint fragment screening projects with structural biology partners from other European RIs (Instruct) (WP4),
- managing chemical proteomics services and user project applications (WP5),

eu::openscreen
drive

www.drive.eu-openscreen.eu

Grant No. 823893

Total budget:
€ 5 m

Duration
54 months



- the development of new features in the European Chemical Biology Database to increase user friendliness and data impact (WP6),
- managing newly established industry boards and their engagement (WP7)
- organising training schools and webinars (WP8).

A FRAGMENT LIBRARY FOR RESEARCHERS

In collaboration with several European partners, EU-OPENSOURCE established its own unique fragment library. This set of compounds is composed of about 1,000 low molecular weight fragments (available in 100 mM DMSO-d₆ solutions with Heavy atom count (HAC) >8) and nearly 100 ultralow molecular weight compounds (so-called 'mini-frags', available in 1M DMSO-d₆ with HAC <8). All are derived from the available fragment space of the European Chemical Biology Library (ECBL).

The fragment library has been designed to facilitate the follow-up of initial fragment hits with a rapid selection of parent molecules in the ECBL diversity library. The fragments and minifrag are substructures of this library.

It is available at six EU-OPENSOURCE-DRIVE and six iNEXT-Discovery/Instruct-ERIC sites. It was used in several fragment screening projects in 2021, using biophysical methods and structural techniques such as X-Ray and Small-angle X-Ray scattering (SAXS) to identify the binding of those small molecules to

Whereas WP4, WP5 and WP7 enlarge the EU-OPENSOURCE capacity for new services and structures, WP6 and WP8 work in a complementary manner to the established offers paid for by the ERIC membership fees.

several protein targets. EU-OPENSOURCE chemistry sites are available to support users from both chemical and structural biology communities. The sites provide their medicinal chemistry expertise to improve the fragments in promising lead compounds.

An EU-OPENSOURCE success story is the use of the fragment library in the discovery of novel SARS-CoV-2 therapeutics. The findings were published in Science Advances in 2021 by EU-OPENSOURCE collaborators at the XChem platform at Diamond.

Diamond is the iNEXT-Discovery partner that performed a crystallographic fragment screen of the macrodomain part of the Nsp3 gene product that SARS-CoV-2 uses to suppress the host cell's natural antiviral response. This study used several fragment libraries including the EU-OPENSOURCE one and discovered 234 fragment compounds that directly bind to sites of interest on the surface of the protein, and that can be used by researchers and pharmaceutical companies to design compounds that could be developed into antiviral drugs. ([doi: 10.1126/sciadv.abf8711](https://doi.org/10.1126/sciadv.abf8711))

ACADEMIC COMPOUND LIBRARY

With the implementation of the DRIVE project, we offer the opportunity to all chemists to submit their property compounds to the EU-OPENSOURCE Academic Compound Collection. We aim to collect a total of 40,000 new compounds sourced from chemists. The compound submission processes were set up in 2021. We built communication channels with chemists and we will start scheduling the distribution of the compounds to the partner sites in 2022.

During the year, 8 MTAs (Material Transfer Agreements) were signed and a total of 252 new compounds were added to the Academic Compound Library. These came from different Institutes:

- University of Bari and University of Catania (Italy),
- Czech Academy of Sciences (Czech Republic),
- University of Santiago de Compostela (Spain),

- Polish Academic of Science (Poland),
- Leibniz-Forschungsinstitut für Molekulare Pharmakologie (Germany).

We have also received an extra 478 new compounds from Karlsruher Institut für Technologie, Institut für Organische Chemie, and from the Institute of Biological and Chemical Systems (Germany) in the first quarter of 2022.

By submitting the compounds, the institutions wish to contribute to finding new biological activities of their submitted compounds.

Several virtual workshops were organised in 2021 to present this project to more chemists. For example the participation of a talk in the conference ESOC 2021. We will continue these efforts in 2022.

EU-OPENSOURCE-DRIVE TRANSNATIONAL ACCESS PROJECTS

Transnational access calls allow researchers in Europe and beyond to benefit from the expertise and the technologies offered by EU-OPENSOURCE's state-of-the-art facilities that are not necessarily available in their home countries.

Thanks to two successful transnational access calls launched in 2019, EU-OPENSOURCE ERIC provided European research-

ers with logistical, technological and scientific support needed to access the infrastructure services for small molecule screening and chemical proteomics available at EU-OPENSOURCE-DRIVE partner facilities.

In 2021, we strengthened our services by launching the first medicinal chemistry and our second chemical proteomics and MSI call for proposals. The medicinal chemistry



call invited thirteen academic groups, who accessed the European Chemical Biology Library (ECBL) at EU-OPENSREEN screening facilities, to apply for support in hit-to-lead optimisation. Call details can be found at <https://www.eu-openscreen.eu/index.php?id=130>. Two projects, out of the four applications received, will be funded. They will exploit our partners' medicinal chemistry expertise and capacities to ensure hit-to-lead process to improve specificity, activity and physicochemical properties of identified molecules. The first success story is reported above in the "first user projects" section.

Transnational access to chemical proteomics and compound disposition analyses were offered to external researchers during a second chemical proteomics and MSI call organised in 2021. These complement existing EU-OPENSREEN capabilities.

In fact, chemical proteomics and Mass Spectrometry Imaging (MSI) tools have emerged as key technologies to advance our understanding of the behaviour and the pharmacological effects of small molecule drugs within a cellular environment.

Within the call, European and international researchers were given the opportunity to harness the expertise of our EU-OPENSREEN-DRIVE partners in these areas. Selected projects will help to understand underlying mechanisms of action of small molecule hit or tool compounds.

To this end, applicants could either apply for access to MALDI MSI technologies for quantitative analysis of compound disposition in disease-relevant tissue, or apply for access to chemoproteomic tools to identify interacting

proteins partners. The chemoproteomics and MSI call 2021 attracted applicants from Germany, Italy, Poland, and Finland. The call supported three successful projects focused on neurodegenerative diseases, prion disorders and cancer.

Selected users gained access to state-of-the-art chemical synthesis facilities for the production of conjugated probe molecules to support affinity-based studies (HZI, IBCH-PAS), advanced proteomics facilities for the prosecution of affinity-based analyses (TUM) and MALDI-Imaging for compound disposition studies (MUAS, SINTEF).

In 2021, five EU-OPENSREEN-DRIVE chemoproteomics sites received experimental support for three access projects, for the characterisation of probes and advanced mass spectrometry-based proteomic analysis. The focus was on target identification in several areas such as depression and obesity, as well as inflammatory diseases and cancer.

Chemoproteomics workflows were carried out at several EU-OPENSREEN-DRIVE sites:

- Institute of Bioorganic Chemistry Polish Academy of Sciences,
- the Technical University of Munich
- the Department of Chemical Biology at the Helmholtz Centre for Infection Research,
- Department of Biotechnology and Nanomedicine at SINTEFSIN,
- University of Santiago de Compostela
- Leibniz Research Institute for Molecular Pharmacology.

NEW EU-OPENSREEN INDUSTRY BOARDS AND NEW R&D COLLABORATIONS

EU-OPENSREEN has been fostering collaboration between industry and our academic partners since 2020. We started by identifying new service models that can establish new synergies at the confluence of business and public institutions.

We have set up two industry boards, the Industry Liaison Office (ILO) and the Industry Associate Group (IAG), and introduced the first co-development projects with industry. In 2021, we further intensified our efforts towards sustainable industry engagement and gathered additional ILO partners and welcomed FAES FARMA and ELI LILLY.

We also held the first ILO workshop in April 2021, where we introduced our capabilities and co-development projects to ILO members. In a round table, we identified EU-OPENSREEN capabilities that can support other industry projects while at the same time serving our academic partners interests.

As a result, we have now defined the first access models for researchers from industry. Since 2021, we offer high-throughput screen-

ing of our libraries and technological co-developments. Our partners are either actively engaged in the development or in the validation of a new assays for high-throughput screening.

Within the framework, we have started six collaborations with five industry partners ranging from SMEs to big pharmaceutical companies and technology driven life science corporations. The tools that are developed within these projects include for example novel CETSA approaches or the application of droplet microarrays to new assay types.

The importance that an ERIC like EU-OPENSREEN can play for industry and vice versa has become more and more apparent. Consequently, we set ourselves the future mission to drive more collaborations in early drug discovery especially in working models that can benefit strongly from academic support. This support can either be in providing scientific expertise, or giving access to specific technology and material, or by working in socially highly important areas such as rare diseases or pandemics.



Various cooperations with industry partners were established in 2021.

EU-OPENSOURCE-DRIVE ANNUAL GENERAL MEETING, GENDER WORKSHOP AND MID-TERM REVIEW 2021 – ONLINE

On 27– 28 April 2021, 30 institutions met online for the EU-OPENSOURCE-DRIVE annual consortium meeting. Breakout sessions were held on topics such as:

- implementation of the transnational access screening and chemoproteomics user projects,
- compound submissions,
- shipments and usage of the fragment library,
- screening data uploads in the European Chemical Biology Database,
- industry engagement,
- training needs.

Discussions also took place on COVID-19 related measures and travel restrictions, as well as possible solutions. The upcoming mid-term review was also addressed, with a focus on the usage of the ARIA user application and project tracking platform from Instruct and gender aspects in our daily operations.

A workshop on gender equality focused on gender bias in the recruitment processes, gender issues in leadership and decision making and exploring what consortium members can do to further support gender equality in their institutions. The event was facilitated by Lucy Ferguson, an experienced trainer in EU projects on structural change for gender equality.

On 17 June, the European Commission evaluated the progress of all work packages of EU-OPENSOURCE-DRIVE during a 1-day mid-term review by an external reviewer.

AUTUMN TRAINING SCHOOL 2021

This first 5-day edition of our EU-OPENSOURCE training school in autumn 2021 presented various aspects of chemical biology and caught the attention of 345 attendees.

Starting with a general introduction to the field, sixteen speakers explored more specific subjects such as:

- hit selection,
- cheminformatics,
- medicinal chemistry,
- principles of open data and open source tools,

- assay development and optimisation,
- data analysis.

New services of EU-OPENSOURCE ERIC such as fragment screening and chemoproteomics were presented. Additionally, speakers from our partner sites introduced to the EU-OPENSOURCE ERIC European Chemical Biology Database (ECBD), compound libraries and specific instruments which are used during compound management and screening campaigns.

AUTUMN TRAINING SCHOOL 2021

eu.openscreen drive

4 organizers, 5 days
10 organisations
14 sessions
16 speakers (4f/12m)
345 registered participants

Many thanks for the excellent work of the speakers and your great response!

Participating organisations in order of sessions

Please find further info and session here:

🔗 www.eu-openscreen.eu/services/training/autumn-training-school-2021.html





IN 2021, WE ACHIEVED MANY IMPORTANT MILESTONES WITHIN THE EU-OPENSOURCE DRIVE PROJECT

- > 11 compound provision campaigns for the EU-OS Academic Compound Library
- > 100+ ongoing outreach activities
- > 53 applications for the TNA access call
- > 13 HTS screening campaigns in different stages of implementation
- > A library of about 1.000 small molecule fragments was designed and so far used in 6 fragment-based drug discovery collaborations
- > the European Chemical Biology Database (ECBD) was tested and launched
- > the Industry Liaison Office and Industry Associate Group were set up.

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-OPENSOURCE 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. Work recently reported

by the EU-OPENSOURCE 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.

Ongoing work involves 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.



<https://eoscfuture.eu>

Grant No. 101017536

Total budget:
€ 42m

Duration
30 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-OPENSOURCE 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-OPENSOURCE has actively contributed to the EOSC-LIFE project with its partner sites Fraunhofer ITMP (Hamburg) and IMG (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 > 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 EOSC-LIFE workflow Hub (<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 European 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-OPENSOURCE infrastructure.

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



www.eosc-life.eu

Grant No. 824087

Total budget:
€ 26 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.

EU-OPENSREEN was actively involved in Work Package 3 of the ERIC Forum project. It addresses the employment challenges faced by all ERICs. EU-OPENSREEN conducted an in-depth survey of employment challenges among ERICs and identified areas for best practice guidelines and common actions.

Through the survey and the in-depth interviews, the following main challenges were identified:

- secondment of personnel
- employment contracts
- payroll
- insurances
- Hiring
- keeping good personnel and

- new work for the personnel.

The most pressing issues in the field of employment were identified as being legal, contracting and payroll aspects. This was particularly the case with special employment situations when employing people outside the statutory seat of the ERIC or when working with secondments.

The following recommendations could be derived from the results of the study:

- explore possible joint framework agreements for all ERICs with international experts in the field of legal, contracting and payroll issues
- preparation of a set of best practices guidelines based on the already existing expertise of ERICs in HR and Gender policies,
- employee handbooks and workplace rules,
- regulations for remote working options,
- performance appraisals and fringe benefits.

It is also planned to establish an ERIC forum internal HR expert group for regular exchanges.



www.eric-forum.eu

Grant No. 823798

Total budget:	Duration
€1.5m	48 months

INEXT-DISCOVERY

EU-OPENSREEN is partner in the Horizon 2020 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 do this through multi-disciplinary courses, workshops and training activities.

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

On 7 May 2021, a virtual meeting was held with representatives from EU-OPENSREEN-DRIVE and iNEXT-Discovery sites to discuss the the distribution and usage of the fragment library for in-house research activities and user projects. The event focused on the transition from screening workflows (iNEXT-Discovery) to medicinal chemistry support for hit optimisation (EU-OPENSREEN).



www.inext-discovery.eu

Grant No. 871037

Total budget:	Duration
€ 10m	48 months

RI-VIS

RI-VIS is a Horizon 2020 project to increase the visibility of European research infrastructures (RIs) to new communities in Europe and beyond.

EU-OPENSOURCE co-leads Work Package 3 on “International outreach and partnering events” and co-organised global symposia in 2021 to engage with new user communities and research infrastructures (see above). Over 1,300 participants registered to the four symposia. They came from RIs, science policy organisations, and research institutions.

EU-OPENSOURCE contributed to three White Papers that provide recommendations on how to increase collaboration between European research infrastructures and counterparts from Africa, Latin America and Australia. The papers are targeted at funders, policymakers and RI managers and collate the insights of 21 experts from the respective regions.

Together with EMBRC/CCMAR and the South African Department of Science and Technology, EU-OPENSOURCE co-authored the “Com-

munication guidelines for European research infrastructures: engaging with stakeholders in African countries”, which are available on Zenodo. RI-VIS also published similar communication guidelines for Latin America.

Furthermore, RI-VIS has developed the “Communication Toolkit for European Research Infrastructures”, which provides an easy and useful set of tools, guidelines and resources to improve the communication strategy and activities of research infrastructures. Its common use is expected to increase the individual and collective visibility of research infrastructures, by aligning key-messages and improving how different stakeholders perceive them.

The Communication Toolkit can be downloaded from the RI-VIS project website (<https://toolkit.ri-vis.eu/home>)

The final meeting of the RI-VIS is being held on 17 January 2022.



www.ri-vis.eu

Grant No. 824063

Total budget:
€1.5m

Duration
36 months

MARBLES

EU-OPENSOURCE, together with our partner sites Fundación MEDINA and Fraunhofer ITMP, are partners in a new Horizon 2020 project, MARBLES. MARBLES, which is coordinated by Prof. Gilles van Wezel at the University of Leiden, aims to harness the power of marine microbes and their bioactive molecules.

MARBLES uses a novel and systematic approach to accessing and exploiting marine microbial biodiversity for sustainable bioprospecting to discover microbial consortia and bioactive molecules for application in aquaculture and agriculture and in the clinic. The research teams specifically look for new antibiotics and antifungals as well as microbes that can serve as bioprotectants in agriculture and aquaculture.

The kick-off meeting of the MARBLES project was organised as a hybrid event on 7–8 October, with project partners participating in person at the Kasteel Oud Poelgeest near Leiden.

Fundación MEDINA coordinates the discovery of new bioactive molecules against human, plant and fish pathogens in work package 4. The chemistry of potent compounds and elicitors are determined, and analogues of selected compounds generated. They are then screened in a broad panel of assays against fish, plant and human pathogens. This allows chemists to identify the best candidate compounds to be selected for further development. Pure compounds and associated data will be stored for post-project use by EU-OPENSOURCE.



www.marblesproject.eu

Grant No. 101000392

Total budget:
€ 7.5m

Duration
60 months

BY-COVID

In view of the ongoing 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 COVID-19 Data Portal, the project connects well-established data resources and delivers access to heterogeneous yet interlinked data across domains and jurisdictions. The project will provide high-level indexing of COVID-19 related knowledge from different fields. To do so, it respects the FAIR data principles and uses workflow environments fully aligned with the European Open Science Cloud (EOSC).

EU-OPENSOURCE will be most active in Work Package 2 on "Accessing heterogeneous data

across domains and jurisdictions for enabling the downstream processing of COVID-19 and future pandemic episodes data", together with its partner site ITMP Fraunhofer Hamburg. The related work will focus on non-patient related data sources and address data transfer needs associated with bioactivity studies. This will enable reuse through dataset integration across domains using both in situ and cloud-based approaches.

The generated data will be made available through dedicated repositories, e.g. the EU-OPENSOURCE European Chemical Biology Database (ECBD), considering its non-sensitive nature. Additionally, this task will build a concrete and substantial link between BY-COVID and data emerging from other projects.

ITMP Fraunhofer Hamburg is working on early detection of epidemic hotspots and a mechanistic understanding of SARS-CoV-2 variants and COVID-19 outcomes. It will do so via demonstrator projects, which will feed into further research questions.



<https://by-covid.org>

Grant No. 101046203

Total budget:
€ 12m

Duration
36 months



TALENT WINS GAMES, TEAMWORK AND INTELLIGENCE WIN CHAMPIONSHIPS.

Michael Jordan (American businessman and former professional basketball player)

A great strength of EU-OPENSOURCE is our network of experienced partners in science and industry. By bringing together multiple competences in a reliable network, we create new solutions to meet the challenges of the twenty-first century.



FINANCIAL STATEMENT



In 2021 eight member countries – Czech Republic, Denmark, Finland, Germany, Latvia, Norway, Poland and Spain – supported the ERIC through their annual memberships. The country contributions represent the main income for EU-OPENSSCREEN.

These contributions covered the operational costs of the central office as well as recurring and running costs of the Central Compound Management Facility (CCMF).

Concerning the scientific activities, the host country, Germany, contributed with an additional budget for the processing of the purchased compound collections in the year 2020 and their biological and physico-chemical characterisation. Third-party funding represents the income granted from the European Commission for the execution of Horizon 2020 and Horizon Europe projects.

The overall expenses of the central office were in line with the expectations and predictions assessed in 2020 for the year 2021. Due to the high market inflation throughout Europe, EU-OPENSSCREEN expects higher amounts in these cost categories in the near future.

Three observations must be pointed out that explain the surplus of 249,813€ at the end of 2021.

Not all planned purchases for the CCMF and scientific services provided by EU-OPENSSCREEN could be made in 2021. These costs are covered by the host country. Since the Federal Household closed its accounts in November and the unspent amount could not be shifted to the following year, the grants were transferred to the Research Infrastructure (109,365€). This amount will be spent at the beginning of 2022 as the scientific services and CCMF activities continue. Some training activities did not roll out as planned, as many courses and seminars were supposed to be in-class trainings and could therefore not be held.

Last, tax refunds from the year 2019 and 2020 that were not paid out in the concerning fiscal years, but were paid out in 2021.

EU-OPENSSCREEN ERIC BUDGET 2021

INCOME AND EXPENSES 2021

Income	Amount (€)
Regular ERIC membership fees	1,295,239
Host country contribution	1,968,619
Third party funding	387,545
Tax Refunds (VAT & Import Taxes)	384,257
Total contributions	4,035,660
Expenses	Amount(€)
Central Office	1,288,128
Laboratory	1,858,902
Third party funding	113,053
European Chemical Biology Database (ECBD)	160,000
Training	6,602
VAT & Import Taxes	359,162
Expenses total	3,785,847
Surplus/Deficit:	249,813



EU-OPENSREEN ERIC BUDGET 2021

FUNDING FROM PROJECTS

The table below shows the duration and total budget for each project active during the year 2021. The overall budget of each project can be broken down into the cost categories personnel costs, subcontracting, and direct costs. The latter are funds for travel, equipment or other goods and services necessary to seamlessly fulfill the project’s demands.

The table “Planned Project Funding and Grants” show this cost breakdown. Resources allocated for personnel costs resemble the paramount significance international Projects have at EU-OPENSREEN ERIC.

The last table in this section (Actual Third-Party Project Funding in 2021) shows the expenses assessed for each project. In the year 2021 the personnel costs represented the highest cost claimed, followed by the direct costs. In the following year EU-OPENSREEN ERIC expects an increase in this cost category, since many activities were not possible to perform in 2021 due to the pandemic.

Project	Start	End	Amount (€)
ERIC-Forum	01/2019	12/2022	44,166
RI-VIS	02/2019	07/2021	236,406
EU-OPENSREEN DRIVE	02/2019	01/2023	1,438,758
EOSC-Life	03/2019	02/2023	73,718
I-Next	02/2020	01/2024	24,375
EOSC-FUTURE	04/2021	09/2024	tbd
MARBLES	04/2021	03/2026	76,250
BY-COVID	10/2021	09/2024	28,500

PLANNED PROJECT FUNDING AND GRANTS

	DRIVE	RI-VIS	EOSC-Life	iNEXT	MAR-BLES	By-COVID	ERIC Forum
Personnel	719,606	130,625	44,975	10,000	48,000	20,800	33,333
Subcontracting	25,000	/	/	/	/	/	
Direct costs*	411,400	58,500	14,000	9,500	13,000	2,000	2,000
Indirect costs	282,752	47,281	14,744	4,875	15,250	5,700	38,833
	1,438,758	236,406	73,719	24,375	76,250	28,500	44,166

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

ACTUAL THIRD-PARTY PROJECT FUNDING IN 2021

	DRIVE	RI-VIS	EOSC-Life	iNEXT	MAR-BLES	By-COVID	ERIC Forum
Personnel	151,843	80,147	17,238	2,466	7,200	1,733	13,865
Subcontracting	/	/	/	/	/	/	/
Direct costs*	87,781	25,021	/	/	/	167	84
Indirect costs	59,906	26,292	4,310	616	1,800	475	3,487
	299,530	131,460	21,548	3,082	9,000	2,375	17,436

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



COUNTRY IN FOCUS: GERMANY

In Germany, EU-OPENSOURCE can look back at a long history. Almost twenty years ago, our German partner sites initiated the ChemBioNet, a national network of open access platforms to support academic chemical biology. The ChemBioNet served as a template for a European network, which led to the foundation of EU-OPENSOURCE in 2010.

The Leibniz-Forschungsinstitut fuer Molekulare Pharmakologie (FMP) coordinated the preparatory phase of EU-OPENSOURCE. Since the inauguration of EU-OPENSOURCE as an ERIC in 2018, the Central Office and the Central Compound Management Facility of EU-OPENSOURCE have been co-located with the FMP on the research Campus Berlin-Buch.

The FMP hosts a high-capacity screening partner site and a medicinal chemistry partner site. The other two German sites are based at the Helmholtz Centre

for Infection Research (HZI) in Braunschweig offering a specialist screening site and at the ITMP Fraunhofer Institute in Hamburg offering a high-capacity screening site.

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LEIBNIZ-FORSCHUNGSINSTITUT FÜR MOLEKULARE PHARMAKOLOGIE SCREENING UNIT

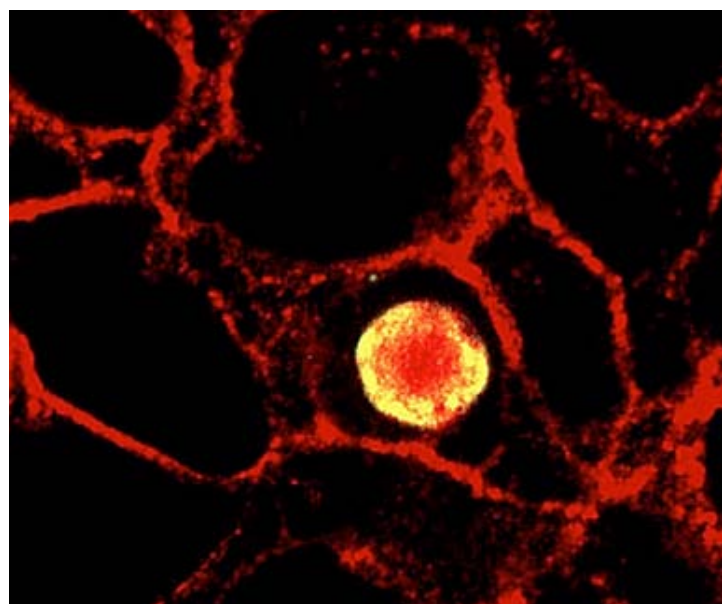
The FMP Screening Unit serves for systematic screening of large compound or genome-wide RNAi libraries with state-of-the-art equipment like automated microscopes and microfluidic systems .

The Screening Unit is part of the Chemical Biology Platform and collaborates with partners from academia and industry.

The platform aims to:

- Provide well designed screening collections (70.000 cpds) including about 3.000 FDA approved drugs, 1,280 compounds with annotated activities, and novel molecules synthesized and donated from academia (about 4.000 cpds)
- provide additional hundred thousands compounds from EU-OPENSOURCE
- identify bioactive small molecules as tools for modulation of biological functions for research
- downscale test volumes to reduce costs for expensive reagents.

Since 2004, 400 screening projects have been supported. Several of these have started clinical trials for patients suffering from cancer, rare disease, or strokes due to the malformation of blood vessels

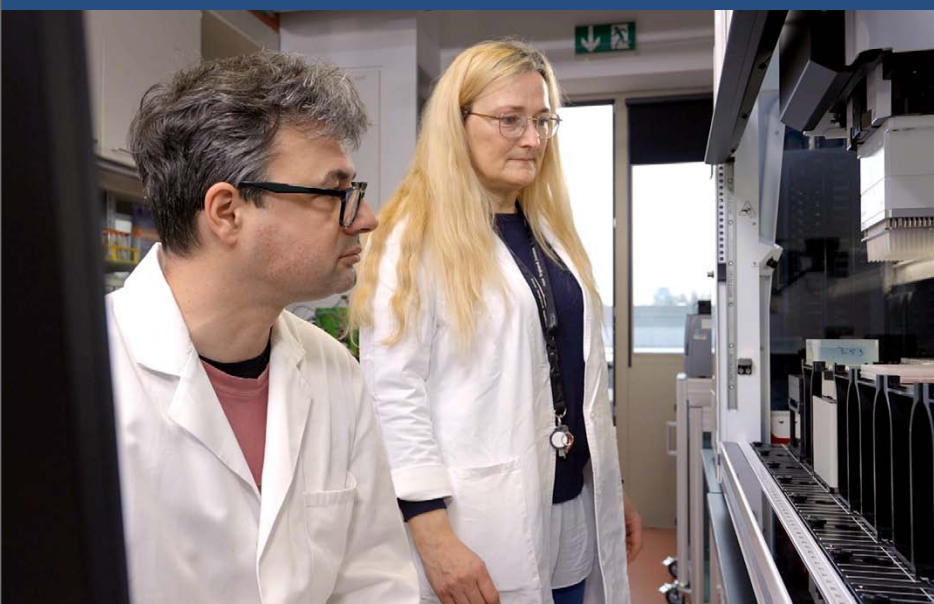


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**Dr. Jens Peter
von Kries**

EU-OPENSOURCE 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.



Location:
BiotechPark Berlin-Buch

Head of Unit:
Dr. Jens Peter von Kries

Website:
www.leibniz-fmp.de/
screeningunit



LEIBNIZ-FORSCHUNGSINSTITUT FÜR MOLEKULARE PHARMAKOLOGIE MEDICINAL CHEMISTRY UNIT

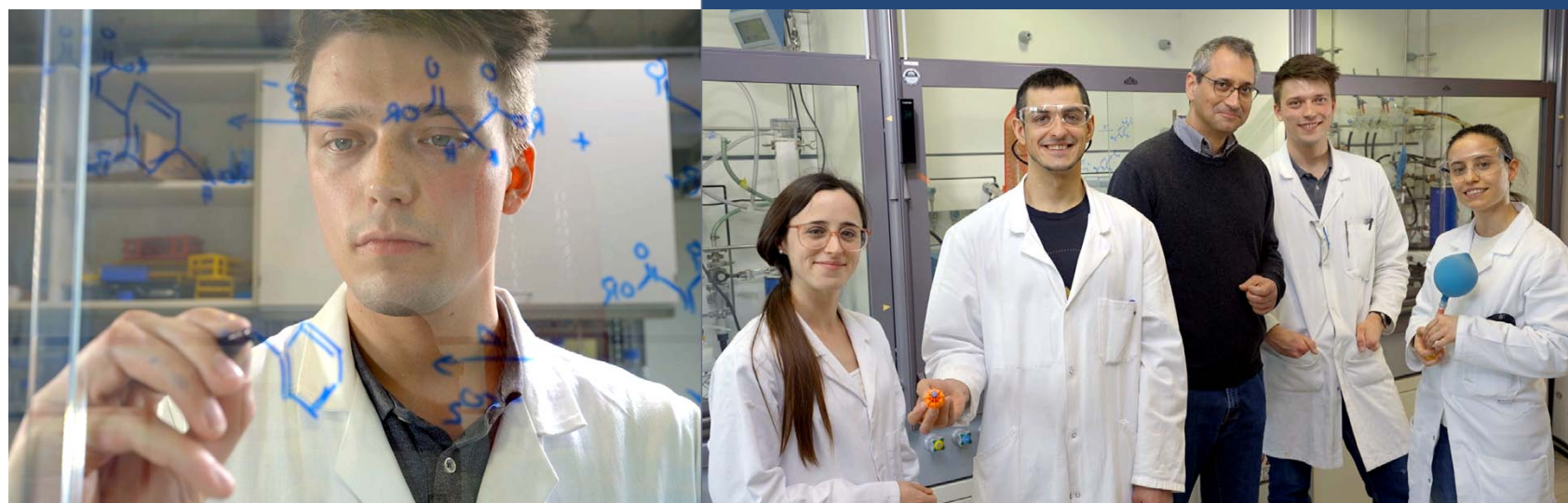
The unit focuses on “developing new chemical tools to answer fundamental biological questions”. It optimizes small molecule hits emerging from screening or from rational drug design approaches. It therefore works closely with the screening and the drug design units.

The medicinal chemistry unit is interested in developing and advancing methodologies for the investigation of unexplored biological targets. This work embraces in particular SAR studies and the molecular recognition phenomena underlying protein ligand interactions. Also of interest are synthetic methods to access privileged or novel scaffolds useful in drug discovery.

➤ New unexplored biological targets or pharmacological applications/therapeutic concepts.

Each research project is guided by at least one of the following principles:

- New chemical structures of the small molecule modulator
- New unexplored mechanisms of action for a given biological protein target, or



**Dr. Marc
Nazaré**

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

Location:
BiotechPark Berlin-Buch

Head of Unit:
Dr. Marc Nazaré

Website:
www.leibniz-fmp.de/nazare



HELMHOLTZ CENTRE FOR INFECTION RESEARCH CHEMICAL BIOLOGY DEPARTMENT

The core theme of the chemical biology department is the investigation of infection processes by the use of chemical compounds that control complex cellular mechanisms.

The three main goals of the department are:

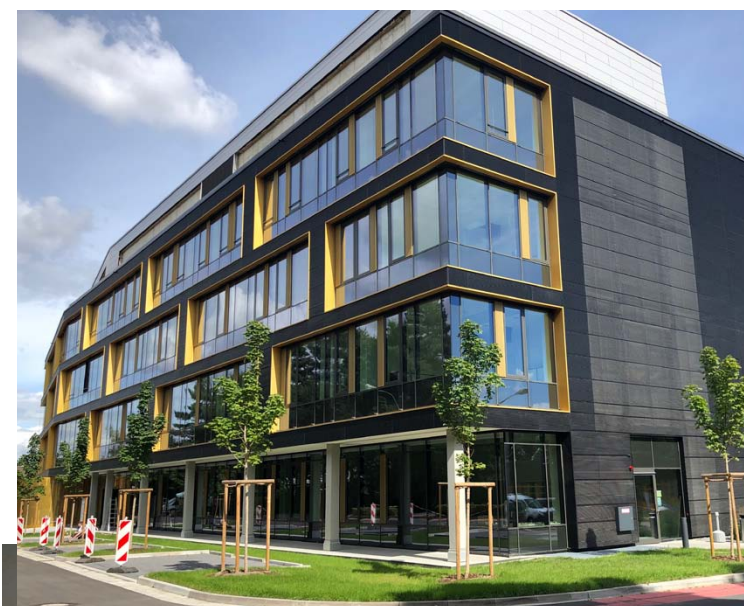
- Discovering new antibacterial and antiviral drugs
- characterising their functionality, and
- optimising their properties.

- Natural product chemistry. Examples include the cystobactamids, the amidoche-locardins, or the armeniaspirols.
- Peptide chemistry. The group hosts HZI's peptide facility and prepares both soluble peptides as well as arrays of peptides coated on planar supports.

The first goal of the department is to identify inhibitors and activators in host and pathogen interplay. This is done through screening techniques. The second objective of the department is to elucidate the molecular mode of action of bioactive compounds. To do so, profiling assays are applied to recognise patterns. In addition, the department optimises active compounds to leads and clinical candidates.

Areas of special expertise:

- Drug conjugation for targeted delivery. This concerns multifunctional antibacterial compounds, but also anticancer conjugates and more recently antiviral PROTAC conjugates.



”



**Prof. Dr.
Mark Brönstrup**

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



Location:

Science Campus Braunschweig

Head of Unit:

Prof Dr Mark Brönstrup

Website:

🔗 www.helmholtz-hzi.de/en/research/research-topics/anti-infectives/chemical-biology/our-research/



FRAUNHOFER ITMP

INNOVATION AREA DRUG SCREENING & COMPOUND REPURPOSING

The ITMP innovation area for drug screening and compound repurposing offers comprehensive High-Throughput Screening with Hit validation and profiling capability, supported by a bioinformatics and IT infrastructure to aid rapid data processing and decision making .

The primary focus is developing biologically relevant and screening compatible assays for use in biomedical research, chemical biology and drug discovery. These assays can be operated via a fully integrated robotic screening platform.

➤ Expertise in progressing compounds to industry standard Lead and Candidate milestones.

Core competencies:

- State of the art tools and technologies for developing innovative assays
- Assay readout technologies including optical, label-free and high content imaging
- Access to a variety of small molecule compound libraries
- Triaging of compounds using mechanism-of-action, selectivity and ADMET profiling
- Delivery of high quality compounds as starting points for drug discovery



**Dr. Philip
Gribbon**

EU-OPENSREEN membership is an essential way for Fraunhofer to connect and collaborate with disease biology experts across Europe helping to discover new hits, leads and chemical tools to facilitate research.

Location:
VolksparkLabs Hamburg

Head of Unit:
Dr Philip Gribbon

Website:
www.itmp.fraunhofer.de/en/innovation-areas/drug_screening_repurposing.html



KEEPING UP THE MOMENTUM

2021 was another year heavily affected by the COVID-19 pandemic. We have learned how to make the best of this situation. For example, our training activities switched from physical training courses to online webinars, reaching much larger audiences. Thank you to all of our partners!

IMPRINT

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No 823798 (ERIC Forum)
No 824063 (RI-VIS)
No 871037 (i-Next Discovery)
No 101000392 (MARBLES)
No 101046203 (BY-COVID)

RT Revisionstreuhand Berlin GmbH
Wirtschaftsprüfungsgesellschaft

Audit Report

for the

Fiscal Year

ending December 31, 2021

of

**The European Infrastructure of Open Platforms for Chemical
Biology**

EU-OPENSOURCE ERIC

Berlin

RT Revisionstreuhand Berlin GmbH
Wirtschaftsprüfungsgesellschaft

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Appendix II:	Changes of fixed assets in the year 2021
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A. Audit contract and performance of the engagement

The Director General of

The European Infrastructure of Open Screening Platforms for Chemical Biology

EU-OPENSREEN ERIC, Berlin

(hereinafter referred to as „EU-OPENSREEN ERIC“ or „ERIC“)

appointed us as auditor for the income and expense accounts for the fiscal year ending December 31, 2021.

The EU-OPENSREEN ERIC was established by seven founding members (Czech Republic, Germany, Spain, Finland, Latvia, Norway, Poland) as a European Research Infrastructure Consortium (ERIC) by statutes dated March 25, 2018. Denmark was welcomed as a member on January 1, 2019.

EU-OPENSREEN is a non-profit organization, which integrates high-capacity screening platforms across the European Union and beyond, strengthening the synergies among different partners and research facilities. It uses a rationally selected compound selection from European chemists. EU-OPENSREEN ERIC is committed to grant open access to its resources to researchers from academic institutions, small and medium-sized enterprises and industrial organizations. Moreover, the ERIC will profile all compounds delivering extensive information on physico-chemical cellular toxicity and anti-microbial properties.

The year from January 1 up to December 31, 2021, is the third complete fiscal year of the ERIC.

As the statutes do not define in Article 11 the kind of financial reports to be issued, income and expense accounts based on a cash basis (similar to those required for charitable and tax-exempt foundations) were presented to us by the EU-OPENSREEN ERIC.

We conducted our audit in accordance with the legal requirements applicable for tax-exempt institutions in Germany. An auditor conducting an audit obtains reasonable assurance about whether the financial reports are free from material misstatements. Absolute assurance is not attainable due to the inherent limitations of an accounting and internal control system and due to the sample-based test nature of an audit. There is an unavoidable risk that material misstatements in the financial reports remain undetected. Areas which are generally covered in special engagements were not included in our scope of work.

We performed the audit in April, 2022 in Berlin. The audit was completed at the date of this report.

Our responsibility and liability as auditor is guided by the „General Engagement Terms for Wirtschaftsprüfer and Wirtschaftsprüfungsgesellschaften - General Public Auditors and Public Audit Firms - as of January 1, 2017“, which are in Appendix II to this report.



Summary fo audit findings

During our audit, we obtained evidence that the requirements as described in Article 21 of the statutes of the EU-OPENSOURCE ERIC dated May 16, 2019, and generally accepted accounting principles as applied in Germany for charitable foundations have been complied with.

In line with our risk and controls based audit approach and the extent we considered necessary for the purpose to express an opinion, we considered internal controls related to sub-processes of the financial reporting process as a spart of our audit.

The ERIC's legal representative provided all evidence and explanations requested by us. We obtained a representation letter signed by the legal representative, which we included in our working papers.

During our audit we did not note any facts which indicate there could be substantial doubt about ERIC's ability to continue as a going concern, or which indicate a material deterioration of the ERIC's performance or a material offence of the ERIC's legal representative or its employees against German law.

In 2021, EU-OPENSOURCE ERIC received material prepayments for future research and development activities, which overstated the annual result.

B. Auditor's report

We have audited the financial report of

The European Infrastructure of Open Screening for Chemical Biology

EU-OPENSOURCE ERIC, Berlin.

These financial reports comprise the income and expense position fort he year ending December 31, 2021.

Based on our audit, the accompanying financial reports were prepared in accordance with the legal regulations applicable for chritable foundations and present fairly, in all material respects, the income and expense situation of the EU-OPENSOURCE ERIC as of December 31, 2021, and its financial performance for the year then ended.

Basis of Opinion

We conducted our audit in accordance with the German standards of auditing. Those standards require that we comply with the International Standards of Auditing (ISA). Our responsibilities under those regulations and standards are further described in the „Auditor's Responsibilities for the Audit of the Financial Report" section of our report. We are independent of the ERIC in accordance with the German General Accepted Accounting Principles and professional rerquirements and we have fulfilled our other ethical resposibilities in accordance with these requirements. We believe that the audit evidence we have obtained is sufficient and appropriate to provide a basis for our opinion.



Responsibilities of Management for the Financial Reports

Management is responsible for the preparation of the financial reports in accordance with General Accepted Accounting Principles and other legal or regulatory requirements, for them to present a true and fair view of the financial position and the financial performance of the ERIC and for such internal controls as management determines are necessary to enable the preparation of financial reports that are free from material misstatements, whether due to fraud or error.

In preparing the financial reports, management is responsible for assessing the ERIC's ability to continue as a going concern, disclosing, as applicable, matters related to going concern and using the going concern basis of accounting unless management either intends to liquidate the ERIC or to cease operations, or has no realistic alternative but to do so.

Auditor's Responsibilities for the Audit of the Financial Reports

Our objectives are to obtain reasonable assurance about whether the financial reports as a whole are free from material misstatements, whether due to fraud or error, and to issue an auditor's report that includes our opinion. Reasonable assurance is a high level of assurance, but is not a guarantee that an audit conducted in accordance with the International Standards of Auditing will always detect a material misstatement when it exists. Misstatements can arise from fraud or error and are considered material if, individually or in the aggregate, they could reasonably be expected to influence the economic decisions of users taken on the basis of these financial reports.

As part of an audit, we exercise professional judgment and maintain professional skepticism throughout the audit.

We also

identify and assess the risks of material misstatements of the financial reports, whether due to fraud or error, design and perform audit procedures responsive to those risks, and obtain audit evidence that is sufficient and appropriate to provide a basis for our opinion. The risk of not detecting a material misstatement resulting from fraud is higher than one resulting from error, as fraud may involve collusion, forgery, intentional omissions, misrepresentations, or the override of internal control.

obtain an understanding of internal control relevant to that audit in order to design audit procedures that are appropriate in the circumstances, but not for the purpose of expressing an opinion on the effectiveness of the internal control.

evaluate the appropriateness of accounting policies used and reasonableness of accounting estimates and related disclosures made by the management.

conclude on the appropriateness of management's use of the going concern basis of accounting and based on the audit evidence obtained, whether a material uncertainty exists related to events or conditions that may cast significant doubt on the ability to continue a going concern. If we conclude that a material uncertainty exists, we are required to draw attention in our auditor's report to the related disclosures in the financial reports or, if such disclosures are inadequate, to modify our opinion. Our conclusions are based on the audit evidence obtained up to the date of our auditor's report. However, future events or conditions may cause the ERIC to cease to continue as a going concern.

evaluate the overall representation, structure and content of the financial reports, including the disclosures, and whether the financial reports represent the underlying transactions and events in a manner that achieves fair presentation.

Berlin, April 28, 2022


Wolfgang Happich
Wirtschaftsprüfer

