D8.3 Report on co-ordination of joined training with other BMS ESFRI projects and establishing new collaborative links

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Table of Contents

1. Introduction 4
2. ESFRIs training activities 6
2.1 Training activities with other ESFRIs 6
2.1.1 EU-OPENSCREEN as partner in iNEXT-Discovery 6
2.1.2 ECBD training involving ChEMBL 7
2.1.3 Common platform of the European Life Science Research Infrastructures 7
2.2 The Research Infrastructure Training Programme (RITrain) 8
3. New collaborative links established to organise summer schools/ courses 10
3.1 One-week summer course on advances in selected areas of biomedicine for students of medical faculties 10
3.2 6th Prague-Weizmann Summer School Advances in Drug Discovery – DRUG discovery and development from basic research through preclinical to clinical phases 11
3.3 Summer course in cooperation with Menendez Pelayo International University in Santander 12
4. Conclusions 14

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1. Introduction

EU-OPENSCREEN is the European Research Infrastructure for Chemical Biology, which was established as a European Research Infrastructure Consortium (ERIC) by seven countries (the Czech Republic, Finland, Germany, Latvia, Norway, Poland, Spain) in April 2018. Denmark joined as the 8th ERIC member country in 2019.
The aim of EU-OPENSCREEN is to develop novel chemical compounds that exhibit specific biological responses on organisms, cells or cellular components in a defined, well-understood and specific manner, in collaboration with external researchers. These chemical compounds can be used by researchers as research tools (or 'probes') to study fundamental cellular processes, such as signalling or metabolic pathways in immune responses, tissue repair etc. EU-OPENSCREEN applies screening of collections of >100,000 compounds, by using robotics-based high-throughput screening platforms in an automated process, and subsequent hit-to-probe optimisation to develop these chemical probes.

The three main user communities of EU-OPENSCREEN are:

- Biologists, who wish to develop suitable assays that are amenable to screening and who are interested in developing 'tool' compounds for their research of interest.
- Organic chemists, who seek to make their compounds readily available through EU-OPENSCREEN and thereby to expose them to a wide range of different biological targets in order to uncover potential biological activities of their compounds.
- Users of the EU-OPENSCREEN database who access the screening datasets, which EU-OPENSCREEN makes publicly available without restrictions on use.

The EU-OPENCREEN-DRIVE (DRIVE) project unites 34 partners from 16 different European member or associated states aiming at accelerating the implementation of EU-OPENSCREEN services and extending its capacities and competences in the fields of chemoproteomics and fragment-based screening.

A prerequisite for the successful operation of the EU-OPENSCREEN ERIC is an expert staff including scientists, engineers and technicians trained in the state-of-the-art technologies needed to deliver screening and medicinal chemistry services to users. In addition, the training dedicated work-package (WP) adds the following main objectives:

- to identify training gaps and develop a **suitable training program for external users** to reduce the barrier to enter projects and increase readiness and quality of incoming projects
- to promote and integrate **service-oriented** operations
- to use **modern training tools** as part of training delivery (eLearning etc.)
- to improve **integration into existing European training programs**.

Intended to users, researchers and industrial representatives, the EU-OPENSCREEN-DRIVE proposed training program will *i*) bring together specialised partner sites and their excellent knowledge, and *ii*) build up an educational platform to create new training opportunities for users and potential users. By linking different expertise from different partner sites, the proposed program will overcome educational gaps at single sites. The more experienced users will gain better awareness of chemical biology, infrastructure services, and their future requests and applications for infrastructure services will be more appropriately formulated. Researchers from future partners of ERIC non-member/observer countries will gain valuable knowledge by participating in webinars and on-site courses during their stays in the highly equipped and experienced partner sites in ERIC member countries.

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The overall EU-OPENSCREEN-DRIVE training program for users and EU-OPENSCREEN staff (detailed in deliverable 8.2) will include:

- **Web-based activities** such as live web-based video courses (webinars) or web-based theoretical courses. EU-OPENSCREEN intends to develop and offer web-based platforms for training and education, which will allow maximum flexibility for communities to be trained (by matching the individual schedules of trainees), and will be less prone to capacity limitations. Very importantly, students, teachers and researchers taking care of small children, can easily complete such courses. In fact, this will allow to prioritise the gender balance during the design and resourcing of courses.
- **On-site practical courses**: the theoretical web-based courses will be complemented by on-site practical courses at one or more EU-OPENSCREEN partner sites. Typically, practical courses will be condensed into 2-3 days, to allow students and researchers with limited time capacities to attend the courses.
- **Staff exchanges** for scientists coming from prospective partner sites in member and non-member countries.
- **Links to international training networks, graduate programs, summer schools** with the aim to coordinate the training activities with other Biological and Medical Sciences Research Infrastructures (BMS RIs) and other national and international training initiatives.

Deliverable 8.3 'Report on co-ordination of joined training with other BMS RI projects and establishing new collaborative links' relates to Task 8.3 'Establish links to international training networks, graduate programs, summer schools and develop synergies' of WP8. This is an ongoing task from month 6 (M6) until month 36 (M36). As such, this report summarises the result of the work from M6 to M18 of the EU-OPENSCREEN-DRIVE project, while the planning and implementation of synergies through joined training programs with other Life Science Research Infrastructures (LS RIs, previously called Biological and Medical Research Infrastructures (BMS RIs)) will continue.
Therefore, this deliverable describes: i) the joint training activities with other ESFRIs and the ESFRIs training opportunities (e.g. RITrain) and ii) new collaborative links established to organise summer schools.

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2. ESFRIs training activities

The European Strategy Forum on Research Infrastructures (ESFRI, https://www.esfri.eu/) aims to develop the scientific integration of Europe and to strengthen its international outreach. Research Infrastructures (RIs) from various scientific areas invest significant resources in education and training programs leveraging European researchers to build knowledge in multi-disciplinary fields of science and advanced technologies to drive forward the European research landscape.

Aiming at sharing the best practice in the area of training, EU-OPENSCREEN ERIC, in the framework of EU-OPENSCREEN-DRIVE, intends to establish solid links with targeted LS RIs complementing the chemical biology expertise of our community with other disciplines crucial for the overall drug discovery pipeline.

In fact, alongside the courses reported in deliverable 8.2 on "Report on newly developed courses organized by EU-OS-DRIVE" the training program prepared in WP8 will also coordinate and link to training activities with other RIs such as ELIXIR, which organizes bioinformatics and data science-related workshops and courses; INSTRUCT-ERIC, which offers hands-on workshops in cryo-EM, NMR and X-ray approaches; and with Euro-BioImaging, which is a European leader in organising workshops, courses and external meetings related to light and electron microscopy as well as image and data analysis (sections 2.1, 2.3).
Moreover, to ensure scientific and financial sustainability of the ERIC, advanced training of the ERIC managers is ongoing: the EU-OPENSCREEN Director General and the Scientific Strategy Officer have undertaken a dedicated master course offered by the Research Infrastructure Training Programme (RITrain) with a focus on the training of management and leadership staff in research infrastructures (RIs) (section 2.2). Where it could benefit users, staff exchange between EU-OPENSCREEN and other RIs will be supported (considering that due to the current coronavirus pandemic staff exchanges in year 2020 are hampered).
New collaborative links will be established with medicinal chemistry summer schools organised by the Royal Society of Chemistry in Spain (SEQT) or by the European School of Medicinal Chemistry (ESMEC) in Urbino, Italy. One summer course will be organized in cooperation with Menendez Pelayo at the International University in Santander (section 3.2).

2.1 Training activities with other ESFRIs

Training activities planned and/ or organised in collaboration with other LS RI partners are detailed below.

2.1.1 EU-OPENSCREEN as partner in iNEXT-Discovery

EU-OPENSCREEN ERIC is a partner in the EU funded Horizon 2020 project iNEXT-Discovery (Infrastructure for transnational access and discovery in structural biology; Grant Agreement No.: 871037), that combines the requisite instrumentation and expertise accumulated by experts in structural biology, medicinal chemistry, translational medicine, biological imaging and food research, and makes it available to scientists across Europe. It offers joint research activities building on cross-disciplinary mentorship to enhance the growth and development of new communities and accelerate discoveries. iNEXT-Discovery brings together 26 partners of which key Life Science Research Infrastructures (LS RIs) will strategically identify the best approaches for outreach to their respective communities. In this context, EU-OPENSCREEN ERIC will develop specific plans to involve the broader chemical biology community with the aim to connect structural biology with screening and medicinal chemistry.

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Capitalising on an already ongoing collaboration within the DRIVE project, in WP4 EU-OPENSCREEN's medicinal chemistry sites collaborate with iNEXT-Discovery partners on the extension of EU-OPENSCREEN ERIC capacities and the service portfolio through the integration of fragment-based drug discovery (FBDD) and the provision by EU-OS of a bespoke fragment library, which is structurally related to the jointly-used EU-OPENSCREEN small molecule diversity collection.

Within iNEXT-Discovery, EU-OPENSCREEN **will organise together with INSTRUCT-ERIC (pan-European research infrastructure in structural biology), a focused meeting to discuss opportunities for further collaboration with other RIs** and other stakeholders to maximize the impact of future lead discovery initiatives.

2.1.2 ECBD training involving ChEMBL

Data management and the development, implementation, and operation of the open access European Chemical Biology Database (ECBD) resource is a core service funded and implemented under the agreed operational plan of the EU-OPENSCREEN ERIC. EU-OS partner sites will generate substantial amounts of data covering a variety of information on chemicals, proteins, cellular pathways, assays, screens and chemical optimisation programs, and the ECBD will contain validated output from screening centres in a public as well as pre-release environment. The ECBD is hosted by the Institute of Molecular Genetics (IMG) in Prague (Czech Republic) and is currently in its implementation phase. It will support curation, annotation and organisation of data and metadata. Data will be deposited with a flexible privacy model for rapid and safe dissemination and exploitation, where data ownership stays with the user. There will also be links to published structure–activity relationships (SAR) (e.g. ChEMBL), Chemical Structure (e.g. PubChem), and Target (e.g. UniProt) resources.

The IMG team will provide support and training services for users and the EU-OPENSCREEN staff through i) the implementation of webinars on common topics related to the ECBD (e.g., data deposition, data search, data visualisation, data analysis) and ii) the **organisation of workshops at IMG to demonstrate all capabilities of the ECBD and share best practices in the community**. Within this training program, one workshop will be organised in collaboration with EMBL-EBI's ChEMBL staff (EMBL-EBI is founding member of Euro-BioImaging ERIC – the European Research Infrastructure for Imaging Technologies in Biological and Biomedical Sciences and an ELIXIR node), which works in close contact with the IMG staff on data transfer from ECBD to ChEMBL. EU-OPENSCREEN users and staff will benefit from the extensive experience of EMBL-EBI in providing trainings of scientists at all levels with focus on biological data.

2.1.3 Common platform of the European Life Science Research Infrastructures

EU-OPENSCREEN was also partner in the CORBEL project,[1] which brought together 13 LS RIs and ended in May 2020 translating its achievements into a common platform of the European Life Science Research Infrastructures as a pillar for the long-term collaboration between them and serving as presentation point of LS RIs common activities (e.g. offering cross-RI service pipelines to European researchers) (Figure 1).

[1] "Coordinated Research Infrastructures Building Enduring Life-science services"; grant agreement No. 654248, duration: from 1 October 2018 to 31 May 2020; CORBEL aimed at establishing a framework of shared services between the ESFRI Biological and Medical Research Infrastructures (BMS RI, now Life Science Research
Infrastructure, LS RI). More information about the project can be found here.

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CORBEL demonstrates that the joint support of different RIs and collaborative activities including training of scientists and facility staff is crucial and of great impact to the European life science research landscape. Beyond access to specific resources and cutting-edge technologies, researchers and facility staff received technical support and training from experts in different fields of the life sciences, and acquired new skills in the use of advanced technologies and data analysis. Also, RI managers benefitted from the project through exchanges of working experiences and common practices.

With the aim to continue and strengthen the cooperation and synergies between LS RIs initiated within CORBEL, several bilateral collaboration agreements were developed and/ or signed (e.g between EU-OPENSCREEN and Euro-BioImaging), while plans for collaborative trainings, staff exchanges and cross-promotion campaigns are under discussion and will be continued in the future. EU-OPENSCREEN ERIC will strongly engage to promote interdisciplinary trainings with other RIs for the benefit of the common life science community.

Figure 1List of shared services of LS RIs offered by CORBEL and beyond. The image is taken from online sources (https://www.corbel-project.eu/about-corbel/participants.html).

2.2 The Research Infrastructure Training Programme (RITrain)

Distributed research infrastructures have a unique governance and organisational model, funding structure, various stakeholder groups (ERIC staff, funders, partner sites, user community) and therefore have specific managerial requirements. The Horizon2020-project RItrain (http://ritrain.eu/) aimed to improve the training of management and leadership staff in research infrastructures and developed an international 'Executive Masters in Management of Research Infrastructures' (EMMRI) programme that is tailored to the specific needs of research infrastructures (https://emmri.unimib.it/).

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The international EMMRI programme is delivered by University of Milano Biccoca and is composed of eleven core modules and one optional module, including Governance and organisation; Financial Management; Leadership and team building; Service provision; Strategic Management of RIs; Business Development and innovation in the RI context; Developing a sustainable funding model for RIs; International law and compliance; Raising awareness; and Infrastructure and resource management.

EMMRI is designed to give experienced science professionals the skills and knowledge they need to take on greater managerial responsibilities. One member of the EU-OPENSCREEN ERIC office team (Bahne Stechmann), who has been working for EU-OPENSCREEN since November 2010, has been selected among 115 applications to participate in the first Master class of the EMMRI programme and was among the first to graduate with an MBA in March 2019 (see Figure 2). Currently, a second member of the EU-OPENSCREEN ERIC office team (Wolfgang Fecke) is enrolled in the EMMRI programme and will graduate in late 2020.

Figure 2 Bahne Stechmann (EU-OPENSCREEN ERIC) MBA graduation in March 2019.

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3. New collaborative links established to organise summer schools/ courses

The DRIVE training program includes several summer schools/ courses aiming at improving the integration of our chemical biology expertise into existing European training programs involving and/ or exploiting other RIs and other national and international training initiatives. We report here below the schools/ courses that have been successfully organised in year 2019 (sections 3.1, 3.2) and the upcoming summer course planned for 2021 (section 3.3). Further joint training activities will be planned in the future to benefit the life science community. As example, we plan to establish new collaborative links with medicinal chemistry summer schools organized by the Royal Society of Chemistry in Spain (SEQT) and/ or by the European School of Medicinal Chemistry (ESMEC) in Urbino, Italy, to mention a few.

3.1 One-week summer course on advances in selected areas of biomedicine for students of medical faculties

This course is organised annually in July by the 2nd Faculty of Medicine Charles University within the project of the Ministry of Education, Youth and Sports entitled "*Increasing the quality of education at Charles University and its relevance to the need of labour market*". Reg. No. CZ.02.2.69/0.0/0.0/16_015/0002362. The course focuses on acquiring new knowledge and practical experience with biomedical research. The aim is to increase the qualification of graduates of medical faculties of the Charles University in Prague in the field of biomedical research and to increase their interest in postgraduate education. The course takes place in three Institutes of the Czech Academy of Sciences in Prague (Institute of Physiology, Institute of Molecular Genetics (IMG) and Institute of Organic Chemistry and Biochemistry) and it has both a theoretical (lectures) and a practical part (demonstration). The course is primarily, but not exclusively, intended to first and second year students, it is held in English and its capacity is limited to 20 participants.

In 2019, our IMG team in Prague contributed to this course. One day of the course was dedicated to Chemical Biology and Advanced Imaging for Biomedical Research. During the morning session, Petr Bartůněk gave a lecture "*Introduction to Chemical Biology*", which included the following topics:

- Chemical biology in Academia what is probe and what is drug?
- Drug repurposing, biochemical
- Cell-based and model-organism-based assays
- Signalling pathways, target ID
- Big data and how to make sense out of it.

During the afternoon demonstration session, Martin Popr and Ctibor Škuta introduced High-Throughput Screening (HTS) and demonstrated the laboratory automation including High-Content Screening (image based and label-free). The attendees were also introduced to the compound workflow from the point of arriving to its usage in the screen. The advanced microplate reformatting and in-house developed LIMS database was demonstrated to the course attendees as well.

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In 2019, 20 students from several medical schools in the Czech Republic participated into this national initiative. Although this summer course is organised every year in July, this year the course is postponed until September 2020 due to the coronavirus pandemic. Details about the course can be found here.

3.2 6th Prague-Weizmann Summer School Advances in Drug Discovery – DRUG discovery and development from basic research through preclinical to clinical phases

The 6th Prague-Weizmann Summer School Advances in Drug Discovery took place in Prague, Czech Republic in September 2019 (http://www.praguesummerschool.cz/index.php) and it was organised by the University of Chemistry and Technology, Prague (www.uct-prague.eu), Institute of Organic Chemistry and Biochemistry of the CAS, Prague, (www.uochb.cz) and the Weizmann Institute of Science (www.weizmann.ac.il), Rehovot, Israel. The summer school gives a broad view on the advances in drug discovery process from the basic science up to the production process development.

The Summer School was intended mainly for PhD students and postdocs. Expert speakers from major international pharma and biotech companies and academia covered the following broad areas:

- Target discovery
- General chemical approaches – medicinal chemistry
- Structure and *in-silico* based drug design
- Lead structure characterization
- Preclinical and clinical development
- Principles and examples of commercial drug development cycle.

A travel prize of 650 € for the participation in the 6th Prague-Weizmann Summer School Advances in Drug Discovery in Prague was awarded for the best poster during the poster session of the 16th Annual Meeting of the Medicinal Chemistry Section of the Israel Chemical Society (MCS-ICS) 2019 in Rehovot, Israel. The winner of the travel award was Abed E. Saady, a third year Ph.D Student at Prof. Fischer's Lab at Bar-Ilan University, with his poster entitled *"Fluorescent Oligonucleotide probes for the Detection of HER-2 mRNA Breast Cancer Marker"* (Figure 3). Since Abed was unable to attend the Prague – Weizmann Summer School, Helaneh Salameh from the same laboratory participated instead. The meeting involved the Weizmann Institute of Science (www.weizmann.ac.il), an EU-OPENSCREEN-DRIVE partner, as one of the organizers. EU-OPENSCREEN ERIC representatives participated in this meeting promoting EU-OPENSCREEN activities to the local Israel community.

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Figure 3 Haim Barr (Weizmann Institute), Eylon Yavin (the Hebrew University of Jerusalem), Abed E.Saady (Bar-Ilan University), Wolfgang Fecke (EU-OPENSCREEN ERIC) - from left to right.

3.3 Summer course in cooperation with Menendez Pelayo International University in Santander

Menéndez Pelayo International University (UIMP in Spanish) has a special summer school program of Advanced Courses. This program is opened for external institutions and entities, and UIMP offers budget and location for such courses. These courses are organised and located in Santander and other places in Spain.

UIMP opens calls for courses proposals every year. The proposals may be submitted by lecturers, researchers, professionals or senior officers of entities and institutions and must comply with UIMP rules. Within WP8, EU-OPENSCREEN-DRIVE submitted one proposal in the form intended for that purpose, which includes the main details (title, campus, dates, sponsor, etc.), director or contact person, a draft of the programme (Table 1), summary of the content and a profile of the audience the course is aimed at.

The proposal will be analysed by the Programming Team in terms of i) scientific, technical or humanistic suitability, ii) fitting in with the programming and iii) sufficient sponsorship, and subsequently submitted to their Governing Board for approval.

The following program has been submitted to UIMP for the organisation of the EU-OPENSCREEN-DRIVE summer activity with a tentative date of Summer 2021:

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- **Schedule:**

Table 1 Tentative EU-OPENSCREEN-DRIVE program submitted to the UIMP call for proposals

Date/ Session	MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY
Morning					
1st Session	*General introduction to chemical biology*	*Hit selection*	*Cheminformatics*	*Medicinal chemistry I*	*Principles of open data and open source tools**
2nd Session	*Assay development and optimization*	*Data analysis*	*Probes & Drugs*	*Medicinal chemistry II*	*ECBD and other successful EU-OS projects and initiatives**
Afternoon					
3rd Session	*Compound libraries*	*Instruments/ equipment*	*Trip*	*Round tables*	*End*

*planned invitation of other LS RIs to contribute to the session

- **Summary:**

The seminar is intended for PhD students interested in chemical biology and drug discovery. The participants will be introduced to basic principles of drug discovery from target gene to candidate molecule. That will include assay development with the overview of the most common types of assays used in the drug discovery process. The composition of compound libraries, their criteria and properties together with the compound logistics will be discussed. The morning session of the second day will be dedicated to the hit selection and confirmation and the subsequent data analysis. The participants will get the basic knowledge of a typical workflow from developing and carrying out an assay to the identification of a lead compound. Main principles of screening data analysis will be part of these sessions as well. During the afternoon session, the instrumentation and equipment used in the drug discovery process will be shown by means of short videos. Wednesday morning sessions will be focused on cheminformatics and data mining with the presentation of in-house developed tools. During the Thursday morning sessions basic principles of medicinal chemistry will explained to the audience. This scientific field is important for optimization of newly identified biologically active compounds to obtain pharmacologically usable compounds with selective-active properties. The students will have the opportunity to discuss all gained knowledge during the afternoon round tables. The Friday morning sessions will introduce the basic principles of open data and open source tools. Our Open Access ECBD and other successful projects and initiatives will be presented. These sessions will be joined by researchers from ELIXIR/INSTRUCT-ERIC/Euro-Bioimaging infrastructures. The lectures from these other infrastructures will give examples of their successful projects and the general practices used in other ESFRIs. For instance, presentations might include an introduction to the Image Data Resource (IDR: https://idr.openmicroscopy.org/about/) consisting of Cell-IDR and Tissue-IDR is an online resource generated by Euro-BioImaging, which stores, integrates and serves highly annotated image datasets from published scientific studies. Large reference datasets are made publicly available, allowing searching, viewing, mining, processing and analyzing complex multidimensional life sciences image data.

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4. Conclusions

During the first 18 months of the EU-OPENSCREEN-DRIVE project we have developed collaborative links with national and international initiatives and envisaged the cooperation with several LS RIs for targeted training activities and workshops. This work will continue in the future as standard training assets of EU-OPENSCREEN ERIC and as part of our involvement in the European scene for basic and advanced trainings of scientist of all levels. The newly developed common platform of the European Life Science Research Infrastructures will serve as basis for future engagement in cross-RI training activities and staff exchanges.

In order to train our infrastructure's management, further educational support was granted to the EU-OS management team by educational activities mediated via RItrain. A dedicated EU-OPENSCREEN-DRIVE summer seminar on Chemical Biology is envisaged for 2021 aiming to bring together experts in the field of chemical biology and drug discovery and researchers of RIs of various interrelated disciplines of the life sciences.

The co-ordination of joined training with other ESFRI LS RIs projects and the establishment of new collaborative links will actively continue in the future. The long-term collaborations of EU-OS with other ESFRI projects will allow to establish new collaborative courses as well as to open existing courses to a broader audience.

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