EU-OPENSCREEN Medicinal Chemistry Application Guidelines

Access

EU-OPENSCREEN offers access to medicinal chemistry support for hit-to-lead, fragment-to-lead and lead optimization phases of drug discovery. In addition, researchers can access services for the design and synthesis of target degraders (PROTACs, RIBOTACs).

Detailed list of EU-OPENSCREEN chemistry groups is available on https://www.eu-openscreen.eu/services/medicinal-chemistry.html.

For information and support in the application process please contact us at scientific-projects@eu-openscreen.eu.

Who can apply?

- Researchers from academia, non-profit organisations and industry (including SMEs) can request access to EU-OPENSCREEN screening services.

- Within the frame of EU funded transnational access (TNA) calls (e.g. EU-OPENSCREEN-DRIVE, ISIDORe, etc) user access is transnational only. Users are not allowed to access facility(ies) in their home country.

General criteria for application

- Applicants commit to having obtained legal and ethical consent regarding their research, their samples and/ or their data prior to submitting their application.

- Applicants must agree to comply with the access, IP and dissemination policies described in the statutes of EU-OPENSCREEN ERIC (available at https://www.eu-openscreen.eu/fileadmin/user_upload/newsroom_and_downloads/201210_Statutes_V3_FINAL.pdf)

- Applicants must agree to comply with the EU-OPENSCREEN privacy policy and terms of submission (available at https://drive.eu-openscreen.eu/index.php?id=137).

Publication

Open access (gold or green, more details here: https://en.wikipedia.org/wiki/Open_access#Colour_naming_system) is required for any publication of access results. In case your proposal is funded by an EU grant (e.g. EU-OPENSCREEN-DRIVE, ISIDORe, etc) funding must be clearly acknowledged by: "This project has received funding from the European Union´s Horizon 2020 research and innovation programme under grant agreement No XXXXX."

How to submit a proposal:

Applicants can submit their proposals through a 2-step procedure:

1. By submitting their project idea to the EU-OPENSCREEN project management team via a dedicated Contact Form at https://www.eu-openscreen.eu/contact.html OR using the pre-application form at https://isidore-project.eu/services/diagnostic-therapeutic-development/ if applying to the ISIDORe open call.

2. Suitable applicants will then be contacted and asked to complete a full application form by connecting to the ARIA online submission platform (for the

full application template please see below "**Error! Reference source not found.**".

To create an account in ARIA please click on https://apply.eu-openscreen.eu/submit-proposal/.

Applications for access can be submitted at any time and will be evaluated on a rolling basis.

Users will receive an email confirmation through ARIA after their proposal submission, and also after completion of the review process.

Proposal evaluation

The review process of applications consists of two steps of evaluation (1. scientific and 2. technical). The application will remain strictly confidential throughout the review process. Reviewers will be bound by a non-disclosure agreement.

Two independent external experts in the field of chemical biology will evaluate the scientific excellence of the proposal. Innovation potential and gender aspects of the project-specific research questions and method will also be considered.

Technical feasibility will be assessed by the EU-OPENSCREEN ERIC chemistry partner of interest. Herein, technical reviewers will assess whether appropriate resources for the technical implementation of the projects are available at the partner sites.

The complete evaluation is carried out online in ARIA, and evaluation results are visible on the applicant's dashboard (at https://apply.eu-openscreen.eu/dashboard/).

Incomplete proposals and those that haven't passed the minimum threshold/ criteria for acceptance, will be returned to applicants for amendments according to the reviewer's comments. Users will be able to re-submit their revised proposals which will be re-evaluated.

Costs and funding

- EU-OPENSCREEN does not provide funding for the services offered by the partners sites. These costs (e.g. personnel, machine time, consumables, labware *etc*) are discussed with the relevant partner site and depend on the complexity and duration of the project.
- If you apply for an open call funded by an EU grant (e.g. EU-OPENSCREEN-DRIVE, ISIDORe, etc) costs of successful projects for instrumentation time, consumables, reagents, and personnel required at the facilities are funded.
- Current funding is available for Infectious Disease Outbreak Research within the framework of the Horizon Europe project ISIDORe (grant agreement number 101046133). Visit https://isidore-project.eu/calls/ for more information about the open calls.
- Please get in touch with us at scientific-projects@eu-openscreen.eu for grant writing support and/ or help with funding opportunities.

Application step by step:

Click on "Begin a new proposal" and follow the instructions.

1. **Proposal Details** (*required fields).

Complete the fields with details of the desired research. Please notice that instructions/ help text is available for each question pointing the mouse cursor on the question mark related to the field of interest.

Research Project title provide a title for your project

Click or tap here to enter text.

If you are applying with hits obtained in a screening previously performed at an EU-OPENSCREEN screening site, please indicate your small molecule screening project PID number. Please provide the PID number assigned in ARIA for your screening project

Click or tap here to enter text.

Are you applying for the ISIDORe open call? If yes, please enter your ISIDORe pre-application ID number

☐ Yes (enter ISIDORe pre-ID), ☐ No

Please select the medicinal chemistry support required: please select one or multiple options from the drop-down menu (multiple choices are possible)

☐ Drug design and evaluation in silico

☐ Hit-to-lead development following HTS of small molecules

☐ Fragment-to-lead development following fragment screening

☐ Optimization of potency, selectivity and in vitro ADMET properties of small molecule drug candidates

☐ Design and synthesis of target degraders (PROTACs, RIBOTACs)

☐ other (please specify)

Abstract of the scientific background, project overview and main objectives of the proposed research:* provide a concise project overview including target relevance, significance of proposed research and objectives including the expected impact of the research and the potential contribution of a new small molecule for further scientific investigation (e.g. information whether the identified molecules shall be used as probe or to build a starting point for a drug discovery project) (max. 5000 characters)

Click or tap here to enter text.

Relevant publications and patents, if any: * please report the relevant literature (up to 5 publications) including literature describing the screening target. For patents, please provide relevant information in the text box below and/ or as additional attachment.

Search by DOI, PMID, PMC, Title, Author – upload CSV/ search

Comments: please report here patent relevant information, if any (max. 3000 characters)

Click or tap here to enter text.

Attachments: please upload attachments here.

Choose file (maximum file size: 100 MB)

Please indicate the partner site of preference, if any. A detailed list and description of EU-OPENSCREEN chemistry partner sites is available at https://www.eu-openscreen.eu/services/medicinal-chemistry.html. Please select one or multiple options from the drop-down menu (multiple choices are possible). In case of multiple choices please comment below your order of preference. If you are applying for the ISIDORe open call, please select between ISIDORe service providers

☐ Masaryk University (MU), Laboratory of Organic Synthesis and Medicinal Chemistry
☐ Technical University of Denmark (DTU), Department of Chemistry (ISIDORe)
☐ Latvian Institute of Organic Synthesis (LIOS) (ISIDORe)
☐ Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP) – Medicinal Chemistry (ISIDORe)
☐ Center for Biological Research Margarita Salas (CSIC) (ISIDORe)
☐ Institute of Biochemistry and Biophysics (IBB PAS) (ISIDORe)
☐ no preference

Comment: In case of multiple sites selected, please indicate your preference here.

Please provide a brief description of yours/ PI's CV:* please include in this section a brief overview of your education, professional background, and expertise that supports the proposed research.

Click or tap here to enter text.

Please provide information about collaborators (other than the PI and her/ his research team) on this proposal:* please include name, surname, position, affiliation and reason for collaboration within this proposal and the expertise each collaborator will contribute. (max. 5000 characters)

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Click or tap here to enter text.

Are there any known technical challenges related to the implementation of the project?* If yes, please comment (max. 3000 characters)

☐ Yes (comment), ☐ No

Please outline the scientific work including a detailed description of your previous and current work relating to the proposed project and planned follow-up experiments:* (max. 5000 characters)

Click or tap here to enter text.

Please specify the target:* please specify (if possible) the target using the identifiers derived from following databases depending on the target type: (max. 1000 characters)

Target TYPE	Where to find 'IDENTIFIER'
Protein	http://www.uniprot.org
Protein Complex	http://www.uniprot.org
Nucleic Acid	http://www.ncbi.nlm.nih.gov/genbank/
Cell line	http://www.lgcstandards-atcc.org
Tissue	http://bioportal.bioontology.org/ontologies/BTO?p=classes
Organism	http://www.ncbi.nlm.nih.gov/taxonomy
Pathway	http://www.reactome.org
	OR
	http://www.geneontology.org
None	-

Click or tap here to enter text.

Please specify the disease areas in which the target is involved.* Please select one or multiple options from the drop-down menu (multiple choices are possible):

☐cancer, ☐neurodegenerative diseases, ☐infectious diseases, ☐inflammation and immunology, ☐respiratory diseases, ☐cardiovascular diseases and haematology, ☐metabolic diseases, ☐gastrointestinal diseases, ☐rare diseases (please specify), ☐other (please specify).

Specify: Click or tap here to enter text. (max 100 characters)

Please indicate already known molecules reported in the literature that are active against the proposed target (including CAS-Number (if available)) if known/ any:*
(max. 1000 characters)

Click or tap here to enter text.

Please provide a detailed description of your screening campaign including experimental data.* Please include screening technology, description of the primary assay, and primary screening data (max 5000 characters)

Click or tap here to enter text.

Attachments: please upload attachments here.

Choose file (maximum file size:100 MB)

Please report on results of the screening campaign providing the list of validated hits*: please include chemical structures of hits, if possible (in the attachments field below), counter-screen, IC50s/ EC50s established (if applicable), confirmation of compounds purity and identity etc. (max. 5000 characters)

Click or tap here to enter text.

Attachments: please upload here chemical structures of hits and any other relevant attachment.

Choose file (maximum file size:100 MB)

Please provide information about selectivity profile of the compounds and other secondary assays. Please describe assays available/ used to test selectivity, and comment on which in vivo models are available. Please include protocol details or literature references for mentioned assays (max. 5000 characters)

Click or tap here to enter text.

Attachments: please upload here any attachment relevant to provide information about selectivity profile of the compounds and other secondary assays.

Choose file (maximum file size:100 MB)

Do you have the capacity for testing/validating the activity of the newly synthesized compounds? Please justify your answer in the comment section below.

☐ Yes, ☐ No
Comment:

Please provide any requirement for PK profiling including PK assays (max. 5000 characters)

Click or tap here to enter text.

Please comment on the capacity of your team to support the project:* please refer to the capacity in terms of FTEs (Full Time Equivalent to measure work time) and number of compounds tested.

Click or tap here to enter text.

Please comment on the scientific challenges and innovative potential of the proposed research.* (max. 5000 characters)

Click or tap here to enter text.

Please describe gender aspects of the proposed research.* Please address the gender aspects both, in the group/ team and in the research content (max. 5000 characters)

Click or tap here to enter text.

Additional attachments: please upload any additional document relevant for the evaluation of this proposal.

Choose file (maximum file size: 100 MB)

Who else needs to be considered when looking at the IP of the project? (max 3000 characters)

Click or tap here to enter text.

Ethics: does the research activity proposed within this call involve research on animals or any research requiring ethical approvals?

☐ Yes (if yes, please specify) ☐ No

Specify: Click or tap here to enter text.

<u>User statement:</u>

☐ I agree to be the principal investigator of the submitted project as it is described in the present application*.

☐ I confirm that all relevant authorizations, declarations and accreditation from competent authority(ies) have been obtained in order to process the above mentioned samples and data, for the requested purposes, in full compliance with the applicable EU and National laws.

☐ All publications resulting or including data obtained through EU-OPENSCREEN-DRIVE will be published under Open Access.

☐ Legal requirements for exporting/importing materials to/from other countries have been met.*

☐ I agree that EU-OPENSCREEN partners can exploit general information of my project for outreach and reporting purposes (respecting confidentiality of project specifics): in case that you do not agree, please give your explanation in the comment section below.

Comments: please add any additional relevant comment and/or information.

How did you hear about EU-OPENSCREEN ERIC? (multiple choices available)

☐EU-OPENSCREEN website, ☐EU-OPENSCREEN-DRIVE website, ☐EU-OPENSCREEN newsletter, ☐NKS newsletter, ☐other newsletters (please specify in the box below); ☐ via institutional email, ☐via other European research infrastructures (e.g. INFRAFRONTIER, Instruct, BBMRI, EuroBioimaging, etc), ☐at conferences/ meetings/ scientific events (please specify in the text box below), ☐LifeScience RI webpage, ☐ISIDORe webpage ☐Twitter, ☐ LinkedIn, ☐other social media channels (please specify in the text box below), ☐other (please specify).

Comments: please specify the conference/ meeting/ scientific event or social media channels (max. 1000 characters)

2. Your Research Team

Choose which local researchers from your lab will be involved in the project.

Principal Investigator: the principal investigator is a scientist eligible by their institution to apply for grants. Please note that the user profile will be the reviewer's main source of information about the PI, applicant and team.

Note: If you select a Principal Investigator other than yourself they will be contacted by email to verify this submission.

Home Lab Colleagues: in addition to the applicant, please indicate other members of your home institution that will be part of the research project. Only scientists mentioned in this section will be eligible to access facilities (if applicable) if the proposal is approved. Please note that the user profile will be the reviewer's main source of information about the applicant and the team.

Note: Applicants (including PI and home lab colleagues which are mentioned in the proposal) should register for an ARIA account prior to the submission of the proposal or login directly if they are already registered with an ARIA account. Once registered, the applicants are required to follow ARIA instructions. Please note that the user profile will be the reviewer's main source of information about the applicant and the team. Please make sure to provide adequate information for evaluation.

3. Exclude Reviewers

Feel free to exclude reviewers that may have a conflict of interest.

4. Confirm Proposal

Review the information you have entered and submit your proposal for moderation and review.

5. Accept terms and conditions of submission

Accept terms and conditions of the access routes you have selected.

6. Proposal submitted

Your proposal has been successfully submitted. You will receive a notification about acceptance or rejection of your proposal within 8-10 weeks after submission.