

Use of the EU-OPENSSCREEN fragment library – Guidelines for EU-OPENSSCREEN-DRIVE and iNEXT-Discovery/ INSTRUCT users

This document describes the general requirements and conditions set by EU-OPENSSCREEN ERIC to regulate the receiving and usage of the EU-OPENSSCREEN fragment library by interested users (i.e. EU-OPENSSCREEN-DRIVE and/ or iNEXT-Discovery/ INSTRUCT partners for internal or external projects).

General consideration

The EU-OPENSSCREEN fragment library is assembled, maintained, and distributed by EU-OPENSSCREEN ERIC central compound management facility (CCMF) in Berlin-Buch, Germany. The EU-OPENSSCREEN ERIC central office will assist the CCMF for tracking, monitoring and reporting the library usage.

Description of the library

The EU-OPENSSCREEN fragment library is composed of i) **968 fragments** available as 100 mM solution in DMSO- d_6 (1 mL), and ii) **88 smaller fragments** (minifrags) available as 1 M solution in DMSO- d_6 , separated into 25 μ L in 96- or 384-well plates for a total of 40 shipments (each can be used for a minimum of 5 screens).

Within the work carried out as part of EU-OPENSSCREEN-DRIVE (DRIVE) in work-package (WP) 4, EU-OPENSSCREEN ERIC together with DRIVE and iNEXT-Discovery partners agreed on:

- One (1) free shipment per DRIVE WP4 member
- A total of five (5) free shipments for iNEXT-Discovery/ INSTRUCT partners.

To receive the shipment, the user should indicate the following requirements:

1. expressed interest in EU-OS fragment library (*Expression of Interest* Form is available on SharePoint (link) for DRIVE partners or upon request by email for iNEXT-Discovery partners)
2. name of the person responsible for screening and feedback
3. user address
4. the expected start and end-date of the screening campaign
5. accepted conditions of the feedback (described below)

Points 2-5 can be provided to the EU-OPENSSCREEN central office by completing the *user declaration form*¹ attached to this document or available on the DRIVE SharePoint (link). The form needs to be filled in for each project implemented at the facility using the EU-OPENSSCREEN fragment library.

Both, completed *expression of interest* for the usage of the fragments and the *user declaration form*, should be sent to EU-OPENSSCREEN central office at fragment-screening@eu-openscreen.eu.

Conditions of the feedback

After each screening round of the EU-OPENSSCREEN fragment library the user provides the following feedback:*

¹This form regulates the use of the EU-OPENSSCREEN fragment library at EU-OPENSSCREEN/ EU-OPENSSCREEN-DRIVE (DRIVE) and/ or iNEXT-Discovery/ INSTRUCT and/ or others fragment screening facilities by internal or external users. The DRIVE/ iNEXT-Discovery/ INSTRUCT/ OTHER partners are responsible to ensure the delivery of internal and external projects information to the EU-OPENSSCREEN central office using this form.

- Solubility, quality and identity problems
- Biophysical method(s) used for screening
- Biological target (e.g. name of protein, RNA or other)**
- Number of hits, hit rate and the hit threshold
- Promiscuous binding alert (if observed)
- Full available information on hits (structure, ligand efficiency, structural information of binding)**

*The user of the library should note which of the data should months after the screening campaign (see below).

***EU-OPENSSCREEN ERIC will regard all project-related information disclosed by the user as confidential. Non-disclosure of confidential information will be regulated by the collaboration agreement in place between EUOPENSSCREEN ERIC and the partner.

Users will make information on hits resulting from the use of the library publicly available in the ECBD and/ or other open-access databases such as PDBe and BMRB (for structural data not supported by the ECBD). An embargo period of up to 36 months can be requested during the first 6 months (this time frame of 6 months will be deducted from the total of 36 months embargo period) after the first notification of a validated hit, to allow for publication and/ or filing patent applications to secure potential intellectual property. Data will be automatically uploaded in the public domain after 6 months passed without an embargo requested.

The feedback data will be used to monitor the performance of the library and to subsequently improve it. The feedback will be also used for the purpose of the DRIVE deliverable 4.2 on “*Publication describing the performance of the fragment library in screening campaigns*”.

Users (DRIVE and/ or iNEXT-Discovery/ INSTRUCT and or other partners including their external users) will acknowledge EU-OPENSSCREEN ERIC for providing and enabling the usage of the EU-OPENSSCREEN fragments library in publications and/ or communication activities containing data, which was generated through the usage of the EU-OPENSSCREEN fragments library using the following sentence: “*The user/ external user acknowledges EU-OPENSSCREEN ERIC for providing its fragment library for the presented scientific work. EU-OPENSSCREEN ERIC has received funding from European Union’s Horizon 2020 research and innovation programme under grant agreement No 823893 (EU-OPENSSCREEN-DRIVE).*”

When available (but not later than 12 months) after the screening campaign, the user provides the information on hit follow-up and evolution history to fragment-screening@eu-openscreen.eu.

For iNEXT-Discovery/ INSTRUCT or other partners, the usage of the EU-OPENSSCREEN fragment library in fragment screening campaigns require the signing of a collaboration agreement between the interested partner and EU-OPENSSCREEN ERIC.

User Declaration Form for the usage of the EU- OPENSOURCE fragment library

This form regulates the use of the EU-OPENSOURCE fragment library at EU-OPENSOURCE/ EU-OPENSOURCE-DRIVE (DRIVE) and/ or iNEXT-Discovery fragment screening facilities by internal or external users. The aim of this form is to ensure that i) essential user information and ii) feedback on the screening campaign for the purpose of monitoring the performance and improving the EU-OPENSOURCE fragment library are delivered to EU-OPENSOURCE ERIC.

For multiple projects please fill in separate forms. For support and questions contact us at fragment-screening@eu-openscreen.eu

User Information

Date:

Principal Investigator (Name, Surname):

Nationality of the Principal Investigator:

Email address:

Institution (including address):

Country:

Other researcher(s) involved in the screening project (Name, Surname, email address and position):

DRIVE or iNEXT-Discovery partner or other facility that will run the screen:

Name of the contact person at the at the DRIVE/ iNEXT-Discovery/ other facility (Name, Surname and email address):

Project Information

Project title:

Project abstract (please provide a short abstract of the project including scientific background and aim of the research; max. 500 characters):



Expected start and end-date of the screening campaign:

Biological target e.g. name of the protein, RNA, or other:

Screening technology envisaged for the project:

The EU-OPENSREEN fragment library will be used for COVID-19 research activities.

User statement:

I, the PI, accept the EU-OPENSREEN ERIC conditions for reporting feedback after each screening campaign that uses the EU-OPENSREEN fragment library (details on feedback conditions are enclosed in Annex I).

I, the PI, will acknowledge EU-OPENSREEN ERIC for providing and enabling the usage of the EU-OPENSREEN fragment library in publications and/ or communication activities containing data, which was generated through the usage of the EU-OPENSREEN fragment library using the following sentence: *“The user/ external user acknowledges EU-OPENSREEN ERIC for providing its fragment library for the presented scientific work. EU-OPENSREEN ERIC has received funding from European Union’s Horizon 2020 research and innovation programme under grant agreement No 823893 (EU-OPENSREEN-DRIVE).”*

I, the PI, agree to make information on hits resulting from the use of the library publicly available in the ECBD and/ or other open-access databases such as PDBe or BMRB (for structural data not supported by the ECBD).

Please notice that an embargo period of up to 36 months can be requested during the first 6 months (this time frame of 6 months will be deducted from the total of 36 months embargo period) after the first notification of a validated hit, to allow for publication and/ or filing patent applications to secure potential intellectual property. Data will automatically be uploaded in the public domain after 6 months passed without an embargo requested.

Do you agree that EU-OPENSREEN partner sites/ EU-OPENSREEN-DRIVE partners may use the general information of your project (i.e. PI name and Institution, project title etc) 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:*

Yes No

Comments (max. 500 characters):

Personal Data and Confidentiality:

EU-OPENSSCREEN commits to process personal data exchanged and received under this collaboration in line with the provisions of the General Data Protection Regulation (GDPR).

I have read and accept the EU-OPENSSCREEN ERIC privacy policy.

EU-OPENSSCREEN ERIC will regard all project-related information disclosed by the USER as confidential.

Date:

Place:

Signature:

Annex I Conditions of the feedback

After each screening of the EU-OPENSSCREEN fragment library the User needs to provide information on:

- Solubility, quality and identity problems
- Biophysical method(s) used for screening
- Biological target e.g. name of protein, RNA, other
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