eu:openscreen

UNCOVER NEW BIOACTIVITIES OF YOUR COMPOUNDS

EU-OPENSCREEN'S OPEN COMPOUND SHARING INITIATIVE

A NEW COMPOUND SHARING INITIATIVE

The quality of a screening collection is one of the most critical factors for successful drug discovery. Compound collections often predominantly consist of compounds that are commercially available, but both compounds synthesised by academic chemists and natural products represent a rich, untapped source of chemical diversity. EU-OPENSCREEN aims to make them better accessible.

Organic chemists produce numerous compounds, often designed for specific activities against specific targets or phenotypes. Typically, only a few of the most promising compounds are used in further studies, while the vast majority are ultimately stored on shelves and in fridges unused, despite the significant resources invested in their production. Furthermore, compounds with a low activity against the initially intended target may be active against another target or be useful in an unrelated assay.

Unfortunately, chemists who synthesise these compounds often have limited ability to systematically test them against a wide variety of biological targets and uncover such hidden biological activities. The consequences are therefore twofold: these compounds remain untested, and they are often rendered inaccessible to other researchers.

To address these gaps, the publicly funded open-access initiative EU-OPENSCREEN offers chemists the opportunity to make their compounds available, in a regulated and transparent framework, to a wider community of biologists for testing in suitable bioassays. By doing so, chemists can expose their compounds to a broad range of biological and drug targets, which would otherwise not be practical through individual one-to-one collaborations. If a compound is identified as a validated hit compound, a research collaboration can be initiated between the submitting chemist and the biologist who developed the bioassay.

Your compounds are kept in our advanced, fully automated system for easy and accurate handling.

BENEFIT FROM SHARING YOUR COMPOUNDS

REGULATED ACCESS

Compounds are tested only at official EU-OPENSCREEN partner sites and are not passed on to third parties without consent.

TRANSPARENCY

You will be promptly notified when one of your compounds has been identified as a validated hit compound and continuously updated on the usage of your compounds.

FAIR AND EQUITABLE SHARING OF BENEFITS

Measures are in place to ensure that any benefits arising from the utilisation of your compounds and all subsequent applications and commercialisations are shared equitably.

RICH ANNOTATION OF YOUR COMPOUNDS

Submitted compounds are initially annotated in a suite of cell-based, biochemical, and physicochemical assays to analyse their physicochemical and biological properties ('bioprofiling') before being continuously tested and annotated in our screening campaigns.

FREE STORAGE

Your compounds are kept in our advanced, fully automated system for easy and accurate handling. We offer free storage, quality control, bioprofiling, and screening services for chemists who submit compounds.

EU-OPENSCREEN's open compound sharing initiative represents a great opportunity for chemists to make their compounds available to a broad scientific community – while retaining full ownership rights.

BIOPROFILING IN DETAIL

Bioprofiling generates a wealth of quantitative data and enables a rich annotation of your submitted compounds.

Submitted compounds are characterised in a suite of cell-based, biochemical, and physicochemical assays to analyse their key properties and to identify potential interferences with assay readouts.

This panel ensures that the results generated from screening campaigns are reliable, reproducible, and comparable.

Our precise bioprofiling ensures the best possible application of the submitted compounds.

INTERFERENCE WITH COMMON BIOLUMINESCENCE REPORTERS (BIOCHEMICAL)

Interference with bioluminescence reporters, which are routinely used as readouts in many cellular assays, is the main cause of false positives in screening campaigns.

Compounds are tested at the Institute of Bioorganic Chemistry (IBCH PAS) for their ability to activate or inhibit luciferase (Firefly, Renilla and Nano-Luc) in a 384-well plate format.

SOLUBILITY (PHYSICOCHEMICAL)

Poor solubility can mask compound activity in bioassays, leading to underestimated activity, reduced hit rates in HTS, and variable data outputs.

Kinetic solubility measurements are performed at the University of Santiago de Compostela (USC) using laser nephelometry in a 384-well plate format.

CELL VIABILITY (CELL-BASED)

Unspecific cellular toxicity of compounds is a common reason for false positives in cellular assays, especially in the cancer field.
Compounds are tested at the Institute for Molecular Medicine (FIMM) for their effect on cell viability by measuring the amount of intracellular ATP (measurement type: luminescence) in 384-well plate format using HepG2 cells, initially at a concentration of 10 µM.

ANTIBACTERIAL AND ANTIFUNGAL ACTIVITY (CELL-BASED)

Compounds are tested for antibacterial and antifungal activity at Fundación MEDINA and the Helmholtz-Centre for Infection Research (HZI). These institutions conduct growth assays with four Gram-negative bacteria, two Gram-positive bacteria, two yeast strains, and one fungal strain.

IDENTIFICATION OF REACTIVE OXYGEN SPECIES (ROS) (BIOCHEMICAL)

Redox-active compounds in screens are commonly found as false positives, as they can oxidise disulfide bridges in proteins or react with important cofactors.

Two assays are performed at the Institute of Bioorganic Chemistry (IBCH PAS) in a 384-well plate format: the first assay identifies redox-active compounds by monitoring the conversion of resazurin to resorufin, while the second assay identifies H2O2-producing compounds by monitoring the oxidation of phenol red with horseradish peroxidase.

PROCESS OF SUBMITTING COMPOUNDS FOR THE ACADEMIC LIBRARY

If you are interested in learning more about EU-OPENSCREEN's compound submission model and sharing your compounds, please contact us.. Our team will gladly guide you through the submission procedure step-by-step.

Please also see our explanation video on this topic in our video section:

www.eu-openscreen.eu/videos

1 Review and sign the Material Transfer Agreement, which regulates the rights and obligations of the contracting parties involved, including policies on data and compound usage.

2 Submit information (e.g., structure, ID) on your compounds via our web portal with login details provided by us.

3 Ship your compounds to us in 24-rack tubes (ideally 5-10 mg each and 90% minimum purity), which we will provide to you free of charge.

4 We will reformat and transfer your compounds to 384-well plates, quality control and distribute them to our official EU-OPENSCREEN partner sites for screening and bioprofiling.

5 All compound-related data (including structural data, quality control, bioprofiling and bioactivity data) will be disclosed after an embargo period in EU-OPENSCREEN's public European Chemical Biology Database (ECBD).

6 Your compounds will be integrated into EU-OPENSCREEN's European Academic Compound Library (EACL) and exposed to a wide range of biological/drug targets. If a compound is identified as a validated hit, EU-OPENSCREEN will promptly notify you and facilitate the next steps.

We look forward to your enquiry!

✉ compound-submission@eu-openscreen.eu

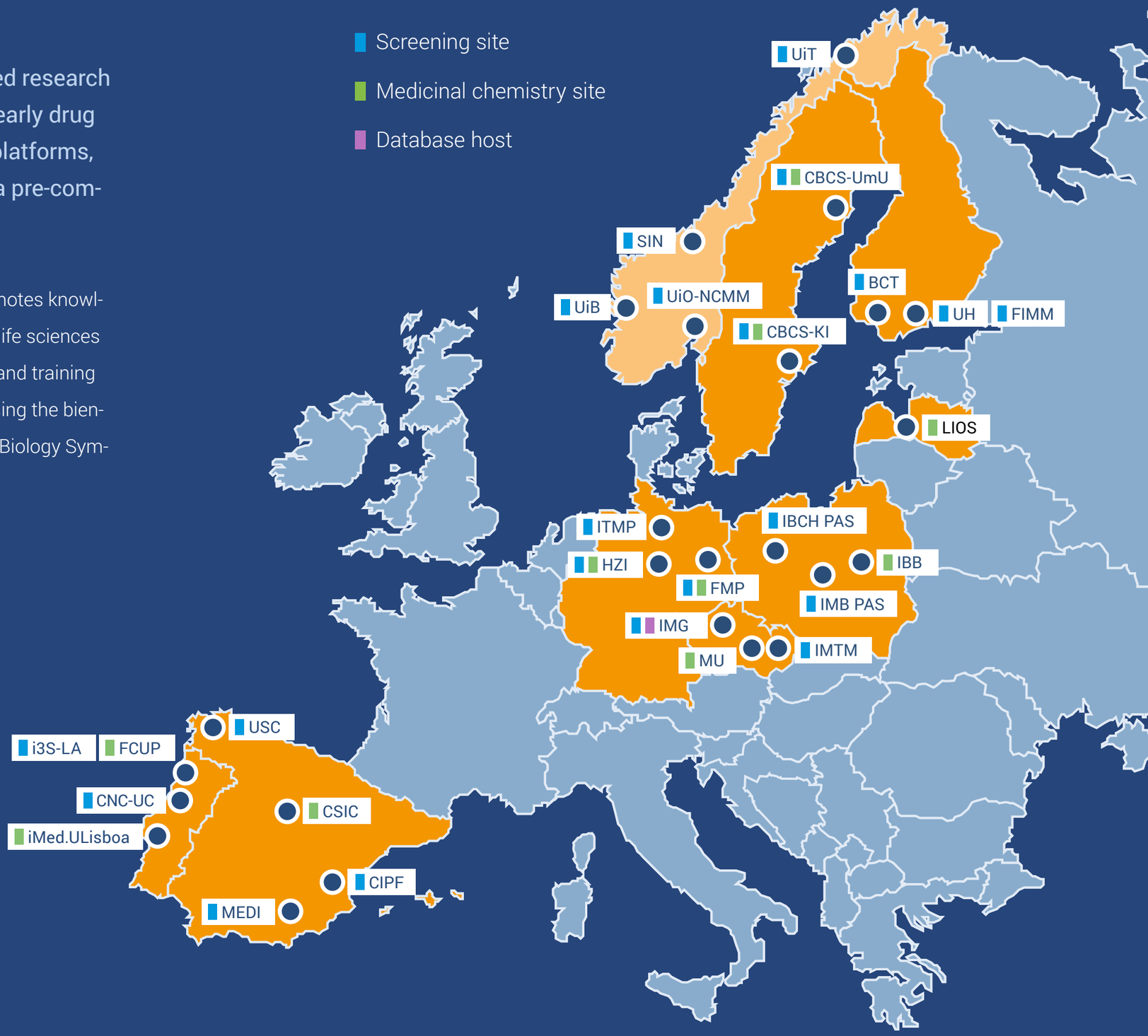
ABOUT EU-OPENSCREEN

EU-OPENSCREEN is an international, publicly funded research infrastructure initiative which supports projects in early drug discovery by democratising access to technology platforms, expertise, and compound collections and creating a pre-competitive network of like-minded researchers.

EU-OPENSCREEN's ca. 30 academic partner institutions offer expertise and instrumentation to collaboratively develop novel chemical probes for the life sciences community. Primary screening data are made available to the scientific community through the open-access European Chemical Biology Database (www.ecbd.eu). EU-OPENSCREEN also promotes knowledge sharing within the life sciences by organising webinars and training activities and co-organising the biennial European Chemical Biology Symposium.

For a fast look at what we're about and what we offer, watch our explanation videos on our website:

www.eu-openscreen.eu/videos



LIBRARIES OVERVIEW

European Chemical Biology Library (ECBL)

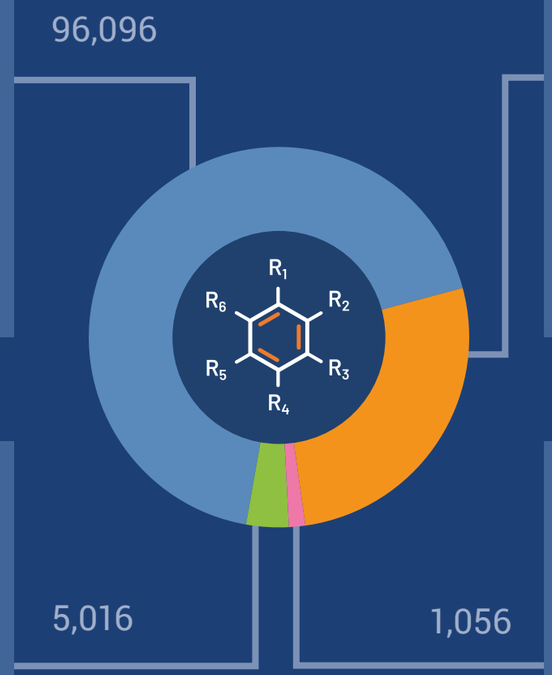
Diversity library

- 96,096 structurally highly diverse compounds
- Average MW=350 g/mol
- PAINS free
- Designed by renowned european academic computational chemistry groups

European Academic Compound Library (EACL)

Novel submitted compounds from chemists worldwide

- Regulated and confidential access (e.g. MTA)
- IP stays with the chemist
- Embargo period up to 3 years
- Constant support from our Central Compound Management Facility (CCMF) for submitting Chemists inquiries



European Chemical Biology Library (ECBL)

Pilot library

- 2,464 bioactives: active against 1,039 different targets, contain 654 approved drugs and 368 highly selective probes
- 2,464 representative compounds of the diversity library
- 88 assay interference compounds in 4 dilutions

Fragment Library (FDBL)

Set of low MW and ultra-low MW fragments

- 968 fragments with HAC > 8 in DMSO-d6
- 88 so called “minifrags” with HAC < 8 in DMSO-d6
- Derived from the fragment space of the ECBL, collaboration with INSTRUCT/ iNEXT-Discovery sites