eu : openscreen Accelerating small molecule drug discovery by a powerful collaborative approach

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As of now, the majority of academic scientists do not have easy access to suitable drug screening platforms and compound collections which are generally expensive to purchase, operate and maintain. This represents a major limitation in the field to advance innovative drug discovery projects. With the aim to address this need, researchers from 30 institutions joined forces to launch the EU-OPENSCREEN research infrastructure which offers international scientists access to a wide range of state-of-the-art screening platforms, compound libraries and expertise. Biologist with a robust and suitable assay can access our screening platforms on a collaborative basis and screen the rationally selected compound collection. EU-OPENSCREEN also collaborates with the structural biology community to expand its capacity in fragment based drug discovery.

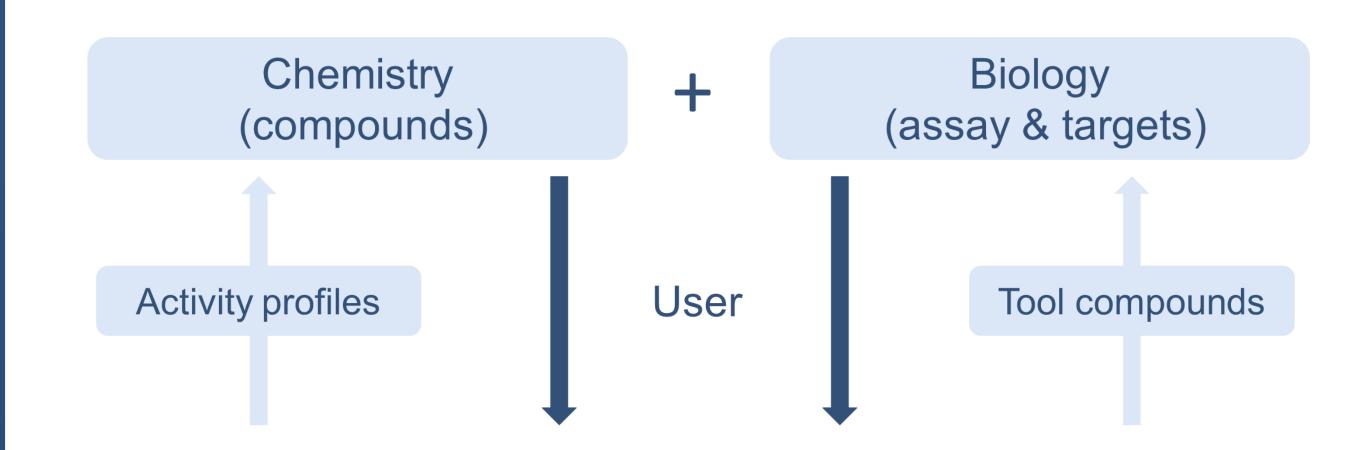
Concept

Key services



EU-OPENCREEN is a joint publicly funded European research initiative of compound screening platforms and medicinal chemistry groups at academic universities and public research institutions. EU-OPENSCREEN develops novel chemical "tool" compounds in collaboration with external scientists from all disciplines of the life sciences.

Components



EU-OPENSCREEN ERIC Shared services at host country

Central office

Central compound management facility

- access to high-throughput screening (HTS) platforms to screen your assays against EU-**OPENSCREEN's compound** collection to identify active 'hit' compounds.
- assay transfer, optimization & miniaturization.
- hit validation, hit-to-lead/probe optimization

How to apply



Submit an Expression of Interest on our website or contact us by email.

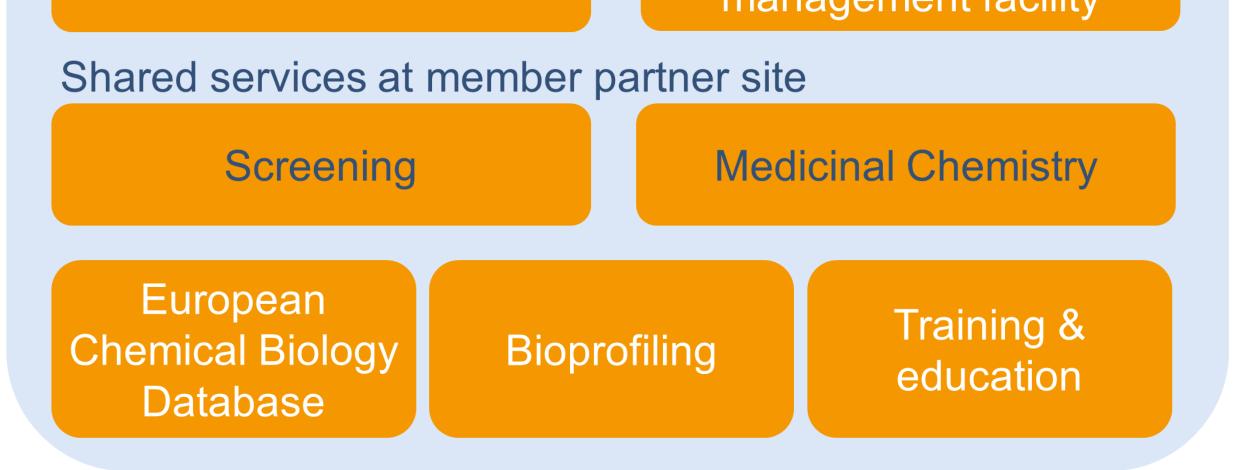
CSIC



Processing of the pre-application and organization of introductory TC.



Submit the full application trough ARIA at https://apply.eu-openscreen.eu/submit-proposal/.



 R_5



Project evaluation (scientific excellence, impact, & technical feasibility).



Discussion between applicant and partner site (requirements, IP rights, budget, timelines). Partner selection.

EU-OPENSCREEN libraries

96.096 **European Chemical Biology Library (ECBL)** Diversity library 96.096 structurally highly diverse compounds; average MW=350 g/mol; 0.0005 % of PAINS

European Academic Compound Fragment-based drug discovery

Library (EACL)

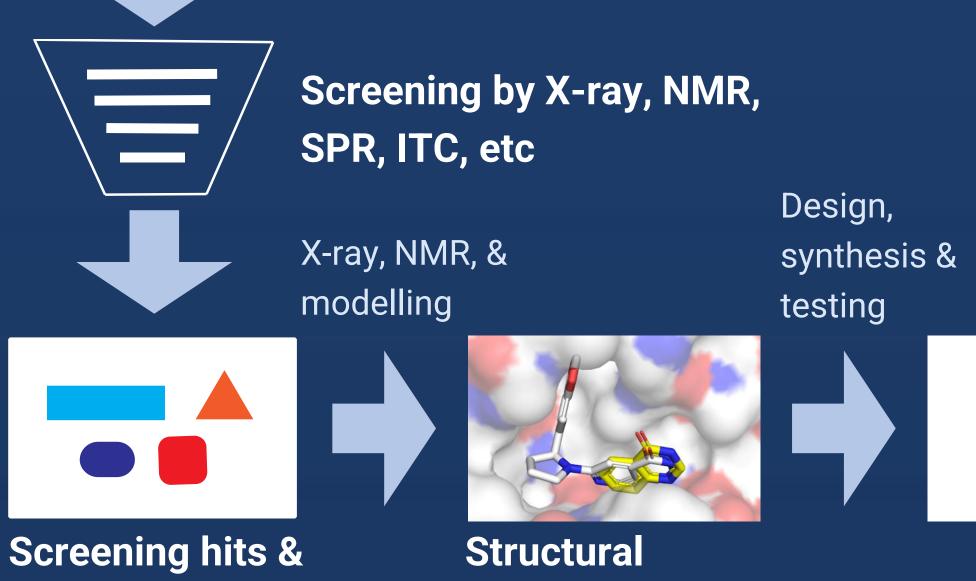
Novel donated compounds from chemists worldwide Target is 40.000 compounds User friendly online submission: <u>http://www.eu-</u> <u>openscreen-cmpds-</u> donation.eu/login.php

The fragment library is jointly used in fragment-based screening campaigns by EU-OPENSCREEN & structural biology groups of the Instruct-ERIC/ iNEXT-Discovery initiative allowing researchers to perform structural screens and subsequently use medicinal chemistry expertise to progress fragments. Example: Schuller, 2021. DOI: 10.1126/sciadv.abf8711

EU-OPENSCREEN Fragment Library

European Chemical Biology Library (ECBL) 5.016 Pilot library 2.464 bioactives (active against 1039 different targets); 2.464 representative compounds of the diversity library & 88 assay interference compounds

Fragment Library Low MW & ultra-low MW 1.056 fragments 968 fragments with HAC > 8 in DMSO-d6 (c= 100 mM) & 88 so called "minifrags" with HAC < 8 in DMSO-d6 (c= 1 M)





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https://ecbd.eu/

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