INSTITUTE OF BIOCHEMISTRY AND BIOPHYSICS POLISH ACADEMY OF SCIENCES



The Institute employs:

- 128 academics
- 70 technical employees
- 47 administration staff

The Institute of Biochemistry and Biophysics of the Polish Academy of Sciences, funded in 1957, is one of the leading research institutes in the field of life sciences in Poland. Our mission is to carry out basic research in various areas of biology, biophysics, biochemistry, and genetics. We also understand the need for the efficient movement of basic science discoveries into practice, and we therefore constantly increase our efforts to transfer the research results to the industry and clinic.

Research conducted at the Institute is carried out in 41 research units and 5 research facility units. Each unit (Laboratory or Department) has one leader.

IBB PAS manages the Henryk Arctowski Polish Antarctic Station on King George Island in the West Antarctic. The Station was established in 1979 and has been operating continuously since then. Its patron, Henryk Arctowski, a remarkable Polish geophysicist and geographer, was one of the first Poles who reached the Antarctic at the end of the 19th century.

Piotr Zielenkiewicz, EOSC meeting, November 25th, 2022



The Institute of Biochemistry and Biophysics of the Polish Academy of Sciences educates over 140 PhD students

More than 90 research projects are carried out at the Institute each year.

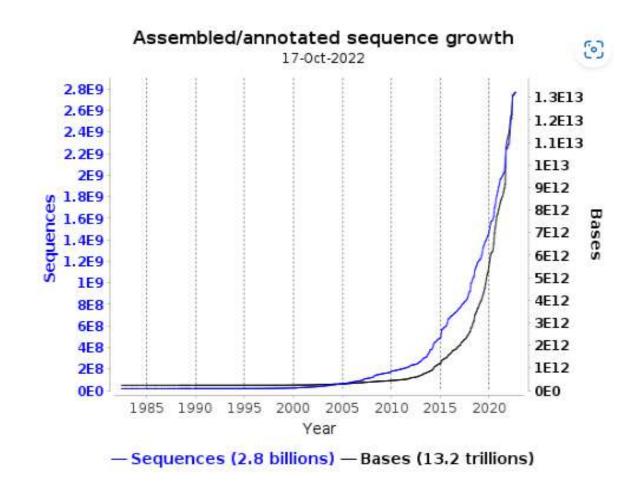
SCIMAGO institutional ranking rates IBB the 3rd best
scientific institution in Poland (after Warsaw and
Jagiellonian Universities)

The Institute is a member of 4 research infrastructures included in the Polish Research Infrastructure Map:

- PolarPOL (Polish Multidisciplinary Laboratory of Polar Research)
- ELIXIR.PL
- POL-OPENSCREEN
- E-XFEL (Free Electron Laser)



Piotr Zielenkiewicz, EOSC meeting, November 25th, 2022



eutopenscreen

eu:openscreen drive

Working in partnership in Chemical Biology and early Drug Discovery across Europe and beyond

EOSC-Life and EOSC-Future partner

European Infrastructure of Open Screening Platforms for Chemical Biology

...

...

....

4

Multinational initiative

- Distributed RI with ca. 30 partner sites
- Established in 2018
- Long-term funding from 10 member countries: CZ, DE, DK, ES, FI, LV, NO, PL, PT, SE
- 3 partner site categories:
 - Screening platforms
 - Chemistry groups
 - Database host
- 3-step partner site accreditation procedure:
 - Nomination of site by ministry
 - Evaluation by external experts
 - Approval of sites by all member countries, based on evaluation reports



European RI for Chemical Biology and early Drug Discovery

EU-OPENSCREEN provides access to

- Technologies (e.g. screening platforms)
- Resources (e.g. compound collections)
- Expertise (e.g. in medicinal chemistry)
- Data (e.g. bioactivity data)
- Training

Users from academia and industry



EU-OPENSCREEN partners



EU-OPENSCREEN Libraries

European Chemical Biology Library (ECBL) Diversity library

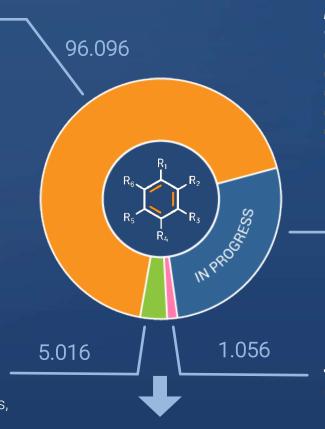
- 96.096 structurally highly diverse compounds
- Average MW=350 g/mol
- 0.0005 % of PAINS

Horvath D. et al., ChemMedChem 2014, 9, 2309

ULL PAPERS	
Design of a General-Purpose Europe creening Library for EU-OPENSCRE	
ragos Horvath, ^{4,6} Michael Lisurek, ⁵⁶ Bernd Rupp, ⁵⁶ Ron ens von Kries, ⁵⁶ Didier Rognan, ⁶⁶ C. David Andersson, ⁶⁰ likael Elofsson, ¹⁶⁹ Per-Anders Enqvist, ⁵⁰ Anna-Lena Gust vrdi Mestres, ⁷⁷ Gilles Marcou, ¹²¹ Alexander Varnek, ¹²¹ Mari onald Frank ¹⁵⁶	Fredrik Almqvist, ¹⁰ avsson, ¹⁴ Nikita Remez, ¹⁰

European Chemical Biology Library (ECBL) Pilot library

- 2.464 bioactives: active against 1039 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



European Chemical Biology Database <u>https://ecbd.eu/</u>

The European Academic Compound Library (EACL)

Novel donated compounds from chemists worldwide

- Target is 40.000 compounds
- Regulated and confidential access (e.g. MTA)
- IP stays with the chemist
- Embargo period up to 3 years
- User friendly online submission: <u>http://www.eu-openscreen-cmpds-donation.eu/login.php</u>

Fragment Library NEW!

Set of low MW and ultra-low MW fragments

 Collaboration with INSTRUCT/ iNEXT-Discovery sites

Compound submissions

Chemists make their compounds available to other international biologists.

Regulated access: Compounds tested at EU-OPENSCREEN partner sites only (not passed down to 3rd parties without consent of chemist).

Profiling of compounds: effect on cells (viability, cell painting), bacteria, fungi.

Transparency: E-mail notification to chemists when compounds tested (who, where, when, target class).

Novel IP shared between chemist, biologist and/or partner site to facilitate translation of research results.



1. One size fits nobody - it's obvious from many years of building a similar infrastructure that domain experts need to drive decisions on hardware and software that is capable of serving domain-specific data types.

2. Life sciences area is one of the biggest data producers among all scientific disciplines It requires dedicated solutions to meet FAIRification requirements (e.g. FAIR implies a decent description of metadata for a digital object - a chemist will not make a good metadata structure for data from sequencing or think of how to store this data, because he does not know what the pattern of access to them is

3. The ambition of IBB is to build a modern data management framework for life sciences on the basis of the newest approaches for distributed data management, finding and governance like data mesh or data fabric (IBM's proprietary solution of data mesh).

Thank you!

Prof. Dr. Piotr Zielenkiewicz Head, Bioinformatics Dept. Institute of Biochemistry and Biophysics PAS, Warsaw, PL piotr@ibb.waw.pl +48 225925750