

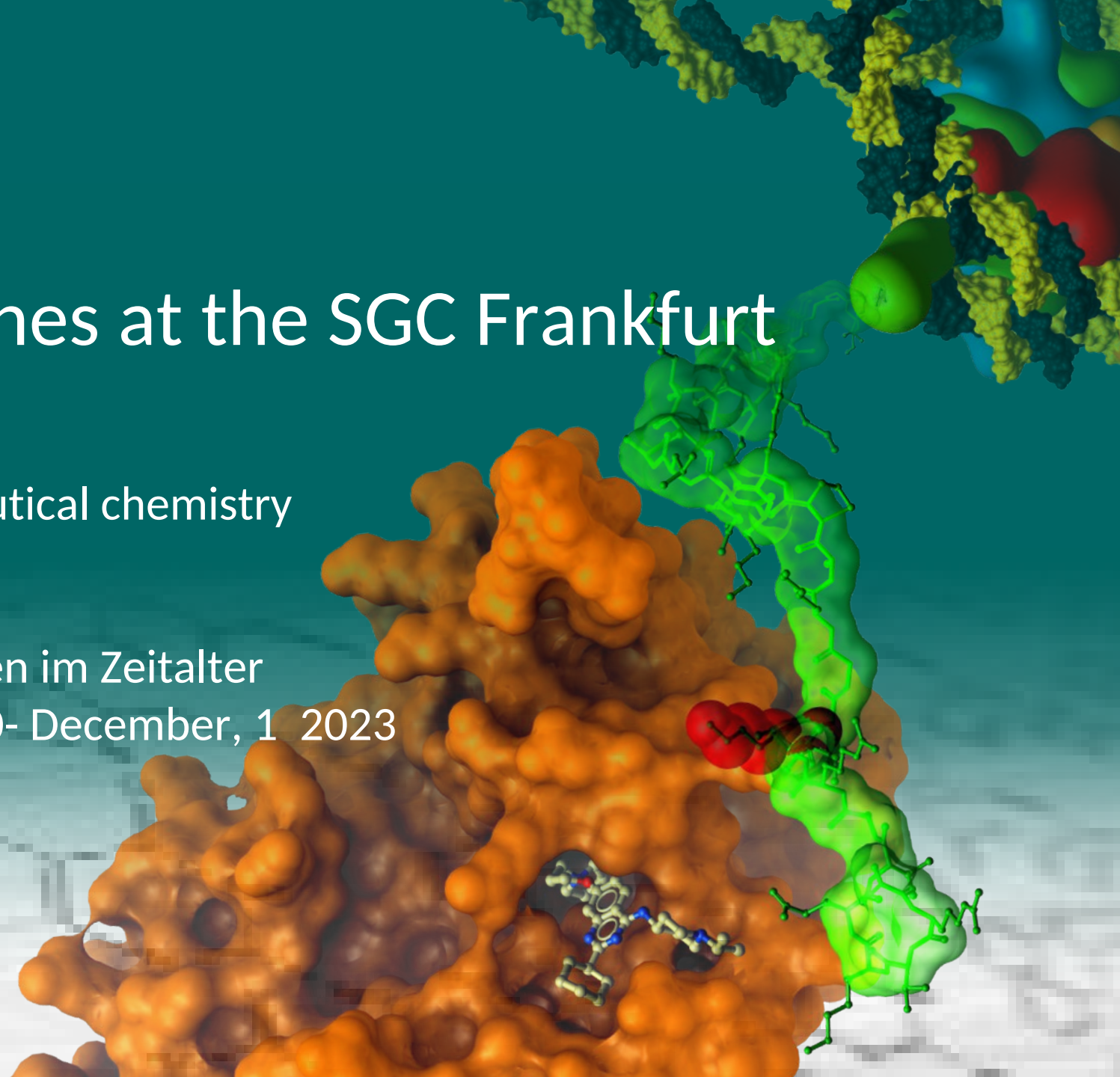
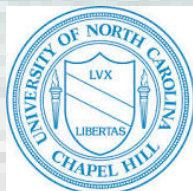


Open Science approaches at the SGC Frankfurt

Dr. Susanne Müller-Knapp

SGC Frankfurt, Institut für pharmaceutical chemistry
Goethe University Frankfurt

Wissenschaftliche Publikationskulturen im Zeitalter
von Open Access, Jena November, 30- December, 1 2023



THE STRUCTURAL GENOMICS CONSORTIUM (SGC) IS A GLOBAL PUBLIC PRIVATE PARTNERSHIP DEDICATED TO OPEN SCIENCE



- **International public-private partnership (PPP)** with a mission to accelerate the discovery of new medicines through precompetitive, open science.
- **SGC supports a network of scientists in 6 universities in 5 countries** plus a network of 300+ collaborators.
- **Global network of partners, funders for 20 years**, including pharmaceutical companies, charities, and government agencies.
- **SGC co-authors ~25 peer-reviewed papers each year with industry.**

➤ **SGC is a charity** incorporated in the UK, **SGC Head Office is in Canada.**



Our Ethos: Open Access

Promptly placing results,
reagents and know-how
in the public domain



We agree **not** to file for
patent protection on any
of our research outputs
(and encourage our collaborators to do the same)



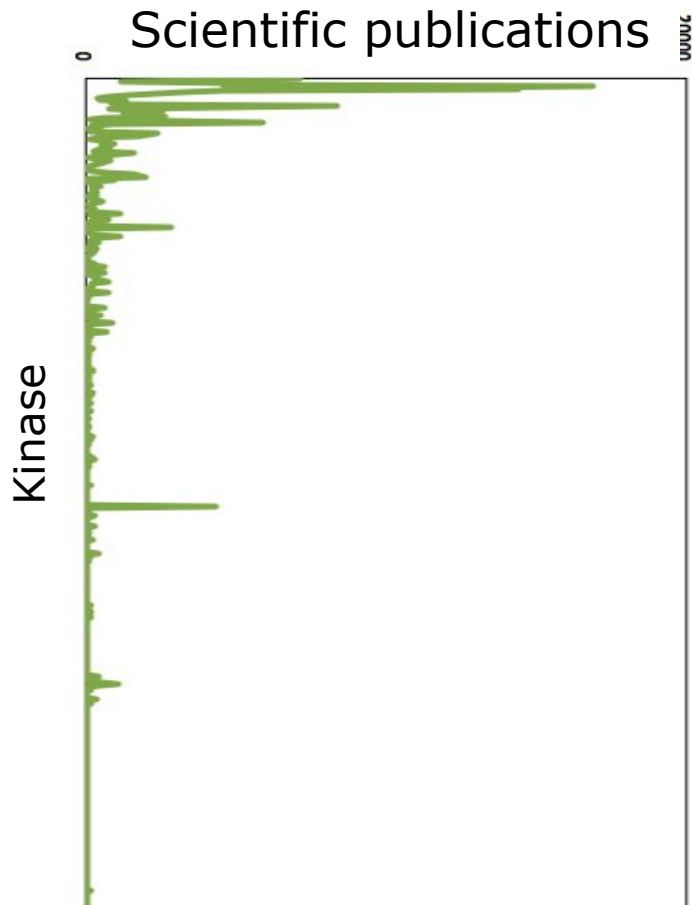
www.thesgc.org

- > \$250B a year invested in biomedical research
 - No new medicines for schizophrenia since 1950's
 - No new treatment for Alzheimer's since early 80's

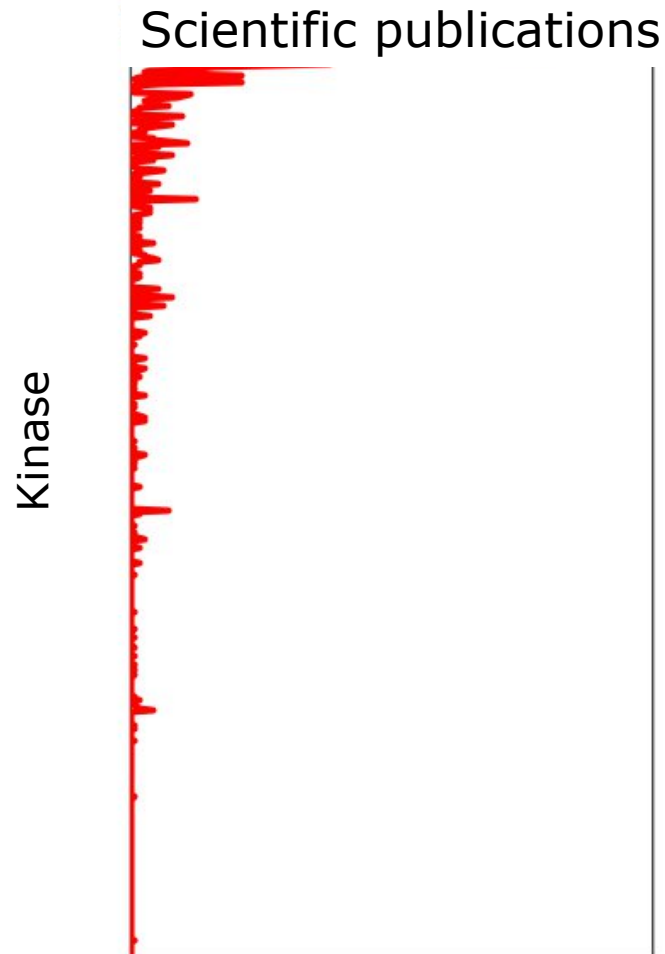
Medicines are not affordable for most people in the world

MOST SCIENCE IS REDUNDANT

Global Effort (2019)



German Effort (2019)



COMMENT

ANTHROPOLOGY Call for unity in the science of human beings [p.168](#) | **GENETICS** Reviewed: two primers on personal genomics [p.169](#) | **POLICY** Sanitation, not vaccination, is most important in Haiti [p.175](#) | **OBITUARY** Jack Oliver, key player in proof of plate tectonics, remembered [p.176](#)



Too many roads not taken

Most protein research focuses on those known before the human genome was mapped. Work on the slew discovered since, urge **Aled M. Edwards** and his colleagues.

When a draft of the human genome was announced in 2000, funders, governments, industry and researchers made grand promises about how genome-based discoveries would revolutionize science. They promised that it would transform our understanding of human biology and disease, and provide new targets for drug discovery. Yet more than 75% of protein research still focuses on the 10% of proteins that were known before the genome was mapped — even though many more have been genetically linked to disease.

We performed a bibliometric analysis to assess how research activity has altered over time for three protein families that are central in disease and drug discovery: kinases, ion channels and nuclear receptors. For all three, we found very little change in the pattern of research activity — which proteins are associated with the highest number of publications — over the past 20 years*. Even those proteins that have been directly associated with disease remain 'hidden in plain sight', with scientists proving very reluctant to study them.

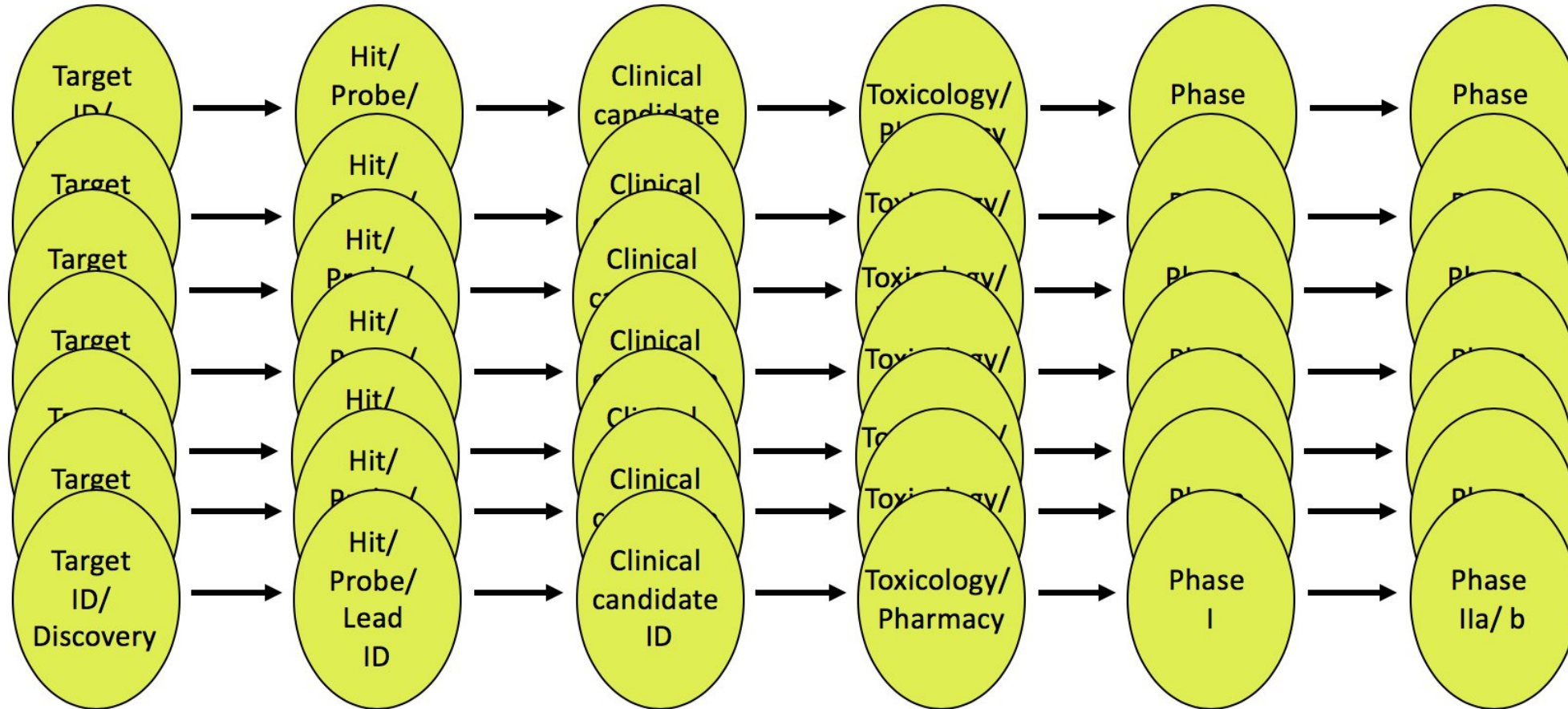
Where there has been a shift in research activity, it was often spurred by the emergence of tools to study a particular protein, not by a change in the protein's perceived importance. We believe that ensuring high-quality tools are developed for all the proteins discovered may be all that is needed to drive research into the unstudied parts of the human genome — even within funding and peer-review systems that are inherently conservative.

We searched for mention of every human

[NATURE.COM](#)
Protein mapping gains a human focus: [ga.nature.com/tybjeff](https://www.nature.com/tybjeff)


10 FEBRUARY 2011 | VOL 470 | NATURE | 163

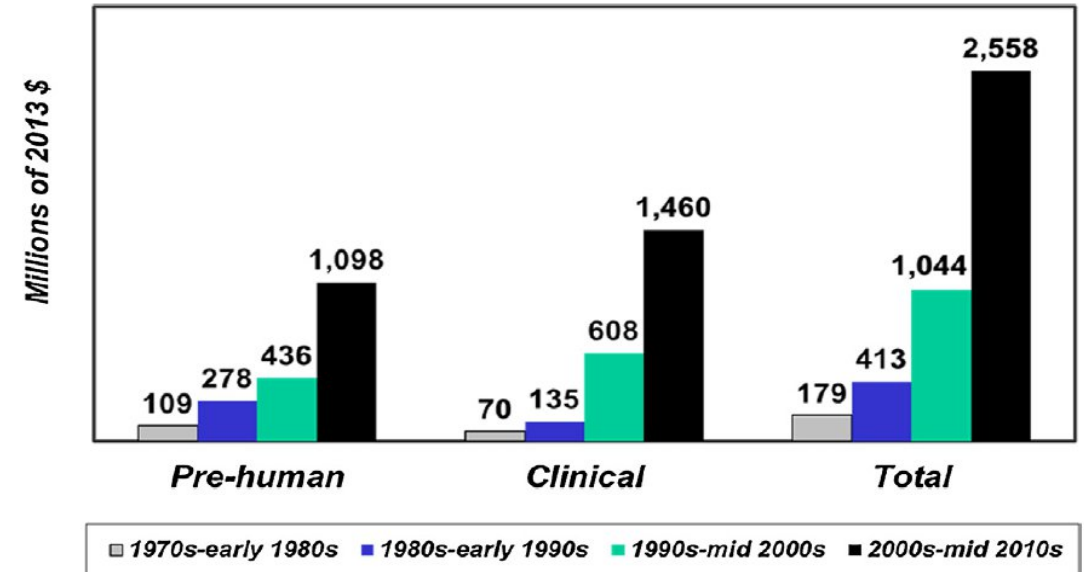
SILOED PROPRIETARY DEVELOPMENT LEADS TO REDUNDANCY



Examples of failed parallel late-stage clinical programs: NK1 receptor antagonists for analgesia; matrix metalloproteases and farnesyltransferase inhibitors for cancer; cholesterol ester transfer protein for CVD; beta-amyloid for AD; aurora kinase inhibitors for breast cancer

WHAT DOES INDUSTRY GAIN?

- New medicines are exorbitantly expensive
- >\$2.5B in private sector R&D costs per approved new drug
- # new drugs approved per \$1B halved every 9 years since 1950s
- clinical attrition rates 



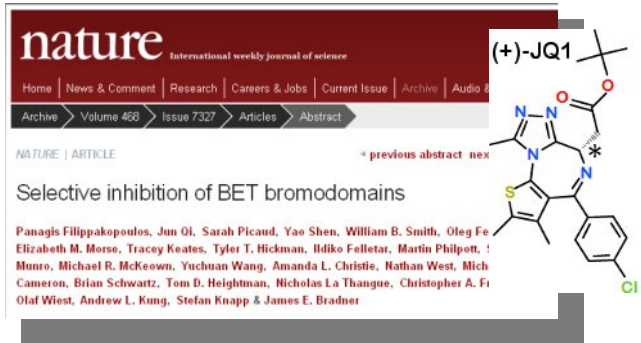
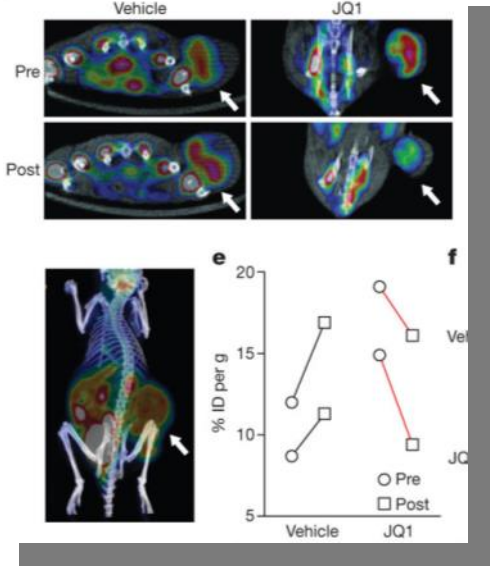
- Launches at \$100,000's per patient per year the new normal
- Trends exacerbating pricing:
- Sustainability for public and private payers?

Precompetitive Research – from lab to patients?

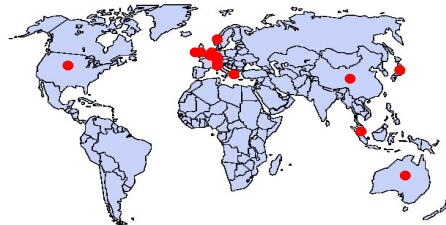


July 2009
GSK
collaboration starts

SGC and Harvard start collaboration
RET /NMCC



Co-publication of JQ1 probe (SGC; cancer) and I-BET probe (GSK; inflammation) JQ1 distributed to

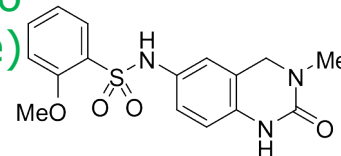


GSK carries out first in man study (open)

Booming interest in Academia and Industry
Pfizer BET probe announced



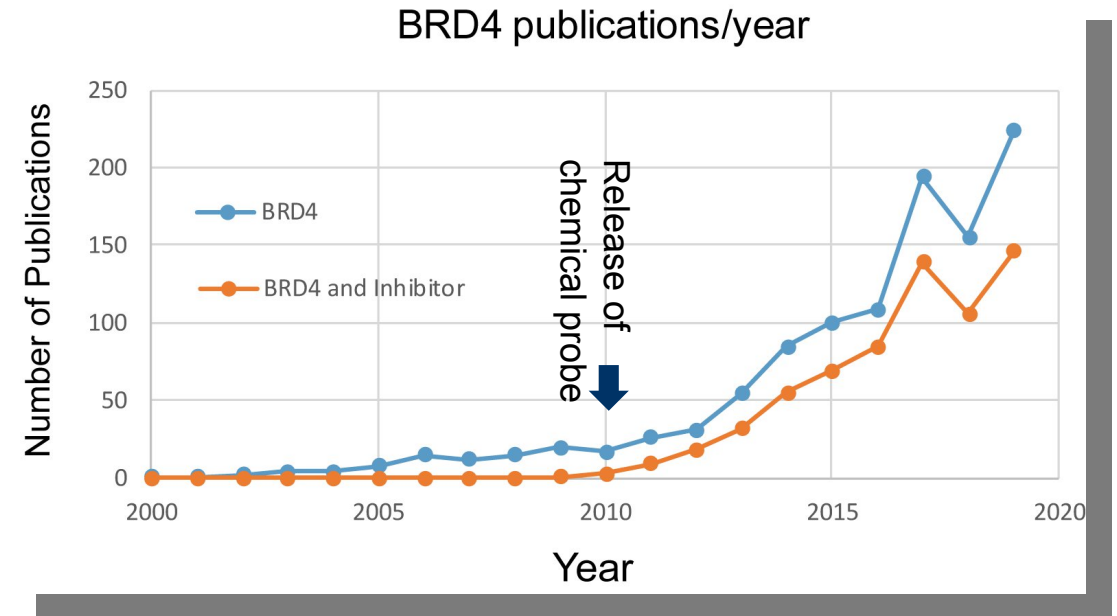
d4 linked to 1L (Nature) 1 (Cell)



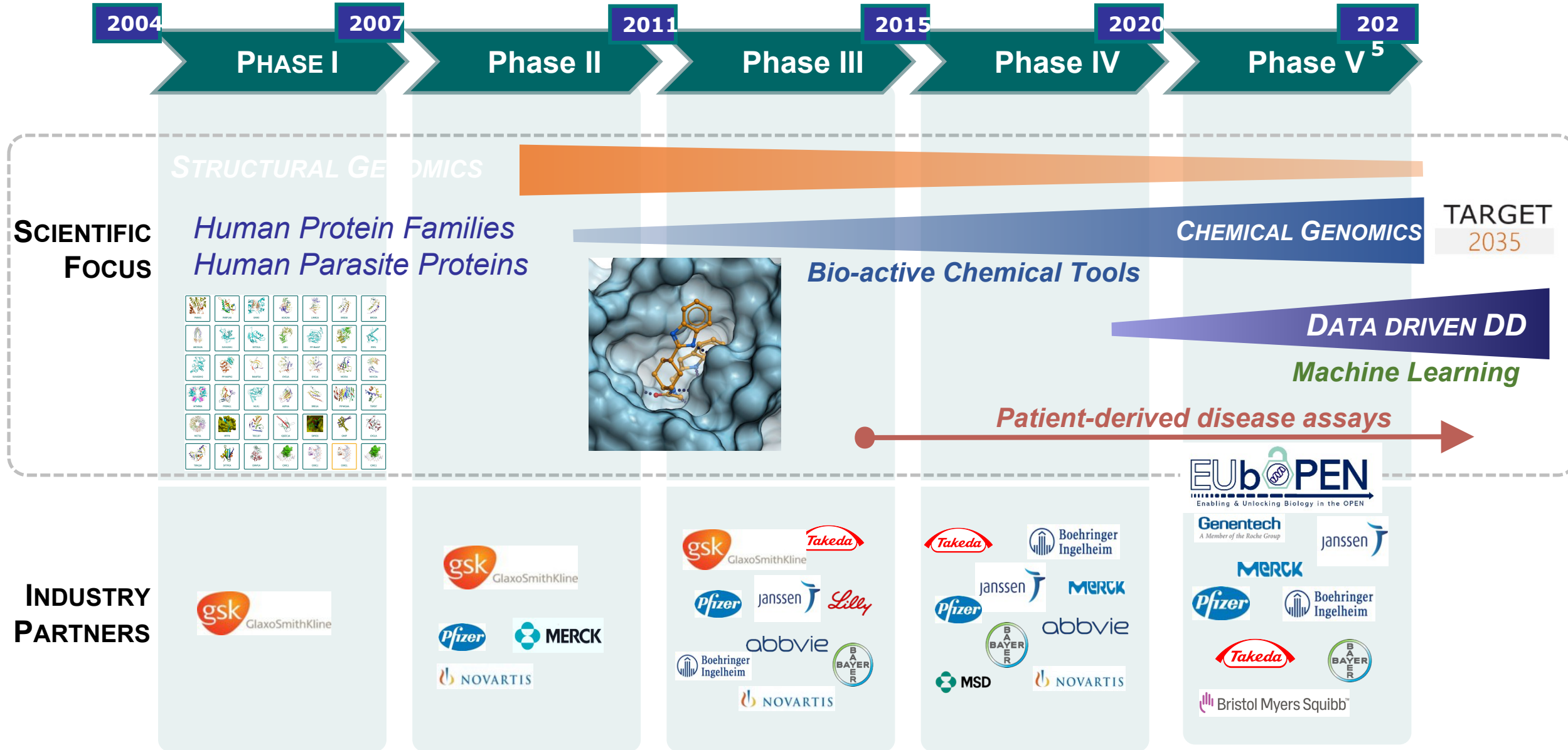
Currently >30 clinical trials

OPEN SCIENCE AS SOLUTION

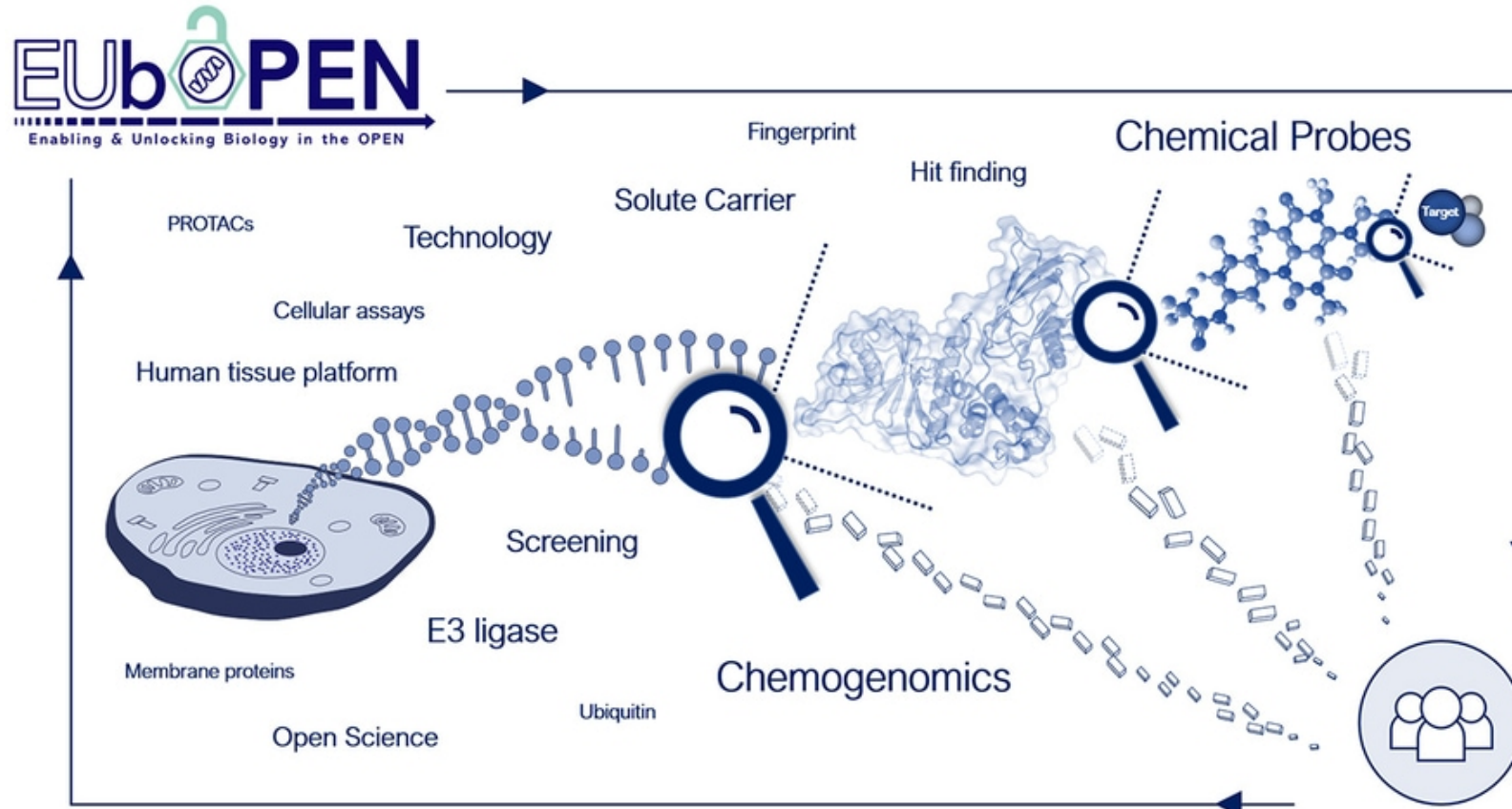
- Encourage innovation
- Engage industry
- Accelerate science
- Increase reproducibility
- Reduce redundancy
- Engage patients
- Mobilize funding
- Develop new technologies through crowd sourcing



Evolving science and partners to address pressing global needs

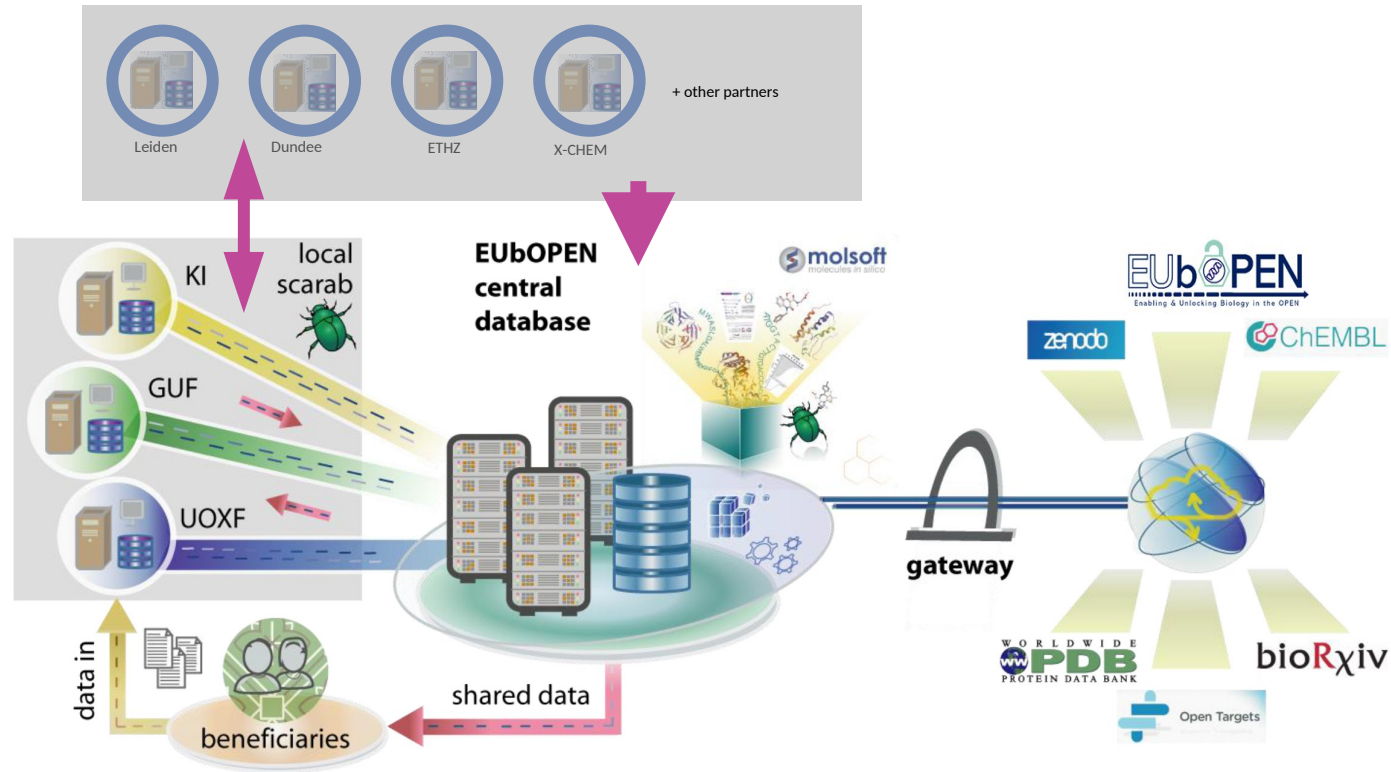


EU_BOPEN



- The EU_BOPEN consortium is an **Innovative Medicines Initiative** (IMI) funded project to **enable and unlock biology in the open**.
- **22 partners** from academia and industry; five years (2020-2025)
- **Total budget of 65.8 million euros** covered by a grant from the IMI and cash and in-kind contributions from the EFPIA companies, IMI Associated Partners and non-EU partners.
- **Open Science Policy**

DATA ACCESSIBILITY



- Open access requirement for **all** EUBOPEN and SGC publications
- Depositing publications in repositories
- Subject-based/thematic repository (e.g., [arXiv](#), [Europe PMC](#)), **OR**
- [Zenodo](#) the OpenAIRE repository hosted by CERN
- [FAIR Guiding Principles](#)
Findable, Accessible, Interoperable, Reusable

DATA REPOSITORIES

Development and update of Data Management Plan

- DMP has been established and updated on annual basis
- Deposition of DMP in Zenodo

Providing Open Access Research data in sustainable repositories e.g.,

- Protein structures in PDB (315)
- Proteomics sets in Pride (15)
- Images in BioImage Archive (~1.4M images)
- Compounds to ChEMBL and EUBOPEN Gateway



In addition to data

- Plasmids in Addgene



After publication of data, 70% of reagents remain not accessible

- Reproducibility of results?
- Quality control?

Open Science Probes

Chemical probes are validated, biologically active small molecule probes with their associated data, control

The probes meet the following criteria:

- ✓ Potency < 100 nM (IC₅₀ or K_d)
- ✓ Selectivity within target family >30-fold
- ✓ Extensive off-targets profiling outside target family
- ✓ Cellular on-target activity < 1 μM (IC₅₀ or EC₅₀)
- ✓ 100 x less potent control compound available
- ✓ No PAINS elements

Probe search: Enter search keyword, Probe category search (kinase)

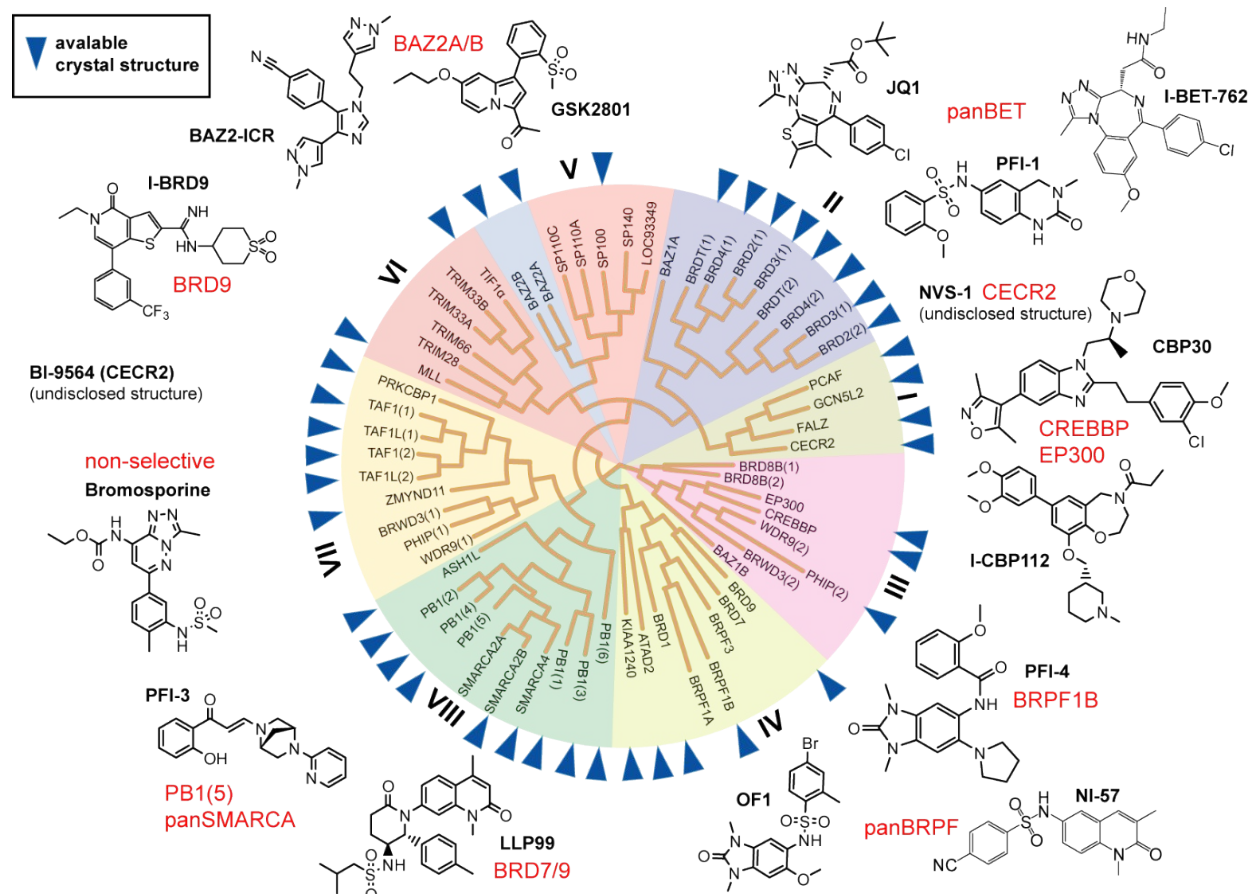
All probes can be used by the research community without restriction! If you would like to join the project and donate a probe, please contact the SGC Frankfurt.

Contact: SGC Frankfurt

Other chemical probes from SGC: ChemicalProbes.org

Probe contribution: abbvie, Bayer, Boehringer Ingelheim, janssen, MSD, Pfizer, Takeda

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Open Science Probes

<http://www.sgc-ffm.uni-frankfurt.de/>

<https://www.thesgc.org/chemical-probes>



SCIENCE FORUM

Donated chemical probes for open science

Abstract: Potent, selective and broadly characterized small molecule modulators of protein function (chemical probes) are powerful research reagents. The pharmaceutical industry has generated many high-quality chemical probes, but the lack of data and guidance makes it difficult for researchers to decide which chemical tools to choose. Several pharmaceutical companies (AbbVie, Bayer, Boehringer Ingelheim, Janssen, MSD, Pfizer, and Takeda) have therefore entered into a pre-competitive collaboration to make available a large number of innovative high-quality probes, including all probe-associated data, control compounds and recommendations on use.

SUSANNE MÜLLER*, SUZANNE ACKLOO, CHERYL H. ARROWSMITH, MARCUS BAUSER, JEREMY L. BARTZA, JULIAN BLAGO, JARK BÖTTCHER, CHAS ESKINETS, PETER J. BROWN, MARK E. BURNINGE, ADRIAN J. CARTER, DAVID DAMERELL, VOLKER DÖTSCH, DAVID H. DREWRY, ALED M. EDWARDS, JAMES EDWARDS, JON M. ELKINS, CHRISTIAN FISCHER, STEPHEN V. FRYE, ANDREAS GÖLLNER, CHARLES E. GURMESHAU, ADRIAN UZZERMAN, THOMAS HANKE, INGO V. HARTUNG, STEVE HITCHCOCK, TREVOR HOWE, TERRY V. HUGHES, STEFAN LAUFER, VOLKHART MULL, SPIROS LIKAS, BRIAN D. MARDEN, HISANORI MATSUO, JOHN MATTHIAS, ROYAN C. O'HAGAN, DAVID R. OWEN, VINEET PANDI, DANIEL RAJAN, SAUL H. ROSENBERG, BRYAN L. ROTH, NATALIE S. SCHNEIDER, CORA SCHOLTEN, KUMAR SINGH SAHATELONI, ANTON SIRENOV, MASAYUKI TANGAWA, CHIH-TSEI PAUL K. THOMPSON, DANIEL K. TREIBER, AMELIA YI VIANA, CARROW J. WELLS, TIMOTHY M. WILSON, WILLIAM J. ZUERCHER, STEFAN KNAPP AND ANKE MUELLER-FAHRNOW*

- Lack of tools, which help understand biology and disease-relevant processes
- In a bibliometric analysis, we found that chemical probes were the most impactful tools to enable researchers to work on new genomics targets
- Freely available probes to human proteins will enable discovery of new medicines
- Collaboration with vendors for sustainability

Chemical probe = a drug-like small molecule that selectively modulates the activity of a specific protein in cells



DISCOVERED

190+

Chemical probes discovered by SGC or with pharma or academics



DISTRIBUTED

42,662+

Samples of chemical probes distributed globally by SGC and trusted vendors



CITATIONS

7,285+

SGC chemical probes used by scientists around the world



CLINICAL TRIALS

25+

Clinical trials and late-stage preclinical programs based on therapeutic hypotheses generated with SGC chemical probes

HUNDREDS OF PAPERS USING SGC PROBES RESULTING IN THERAPEUTIC HYPOTHESES

Tissue Assays

Within EubOPEN, our aim is to develop open access cell assay protocols and data from well-characterised human disease tissue and blood-profile chemical probes and chemogenomic libraries, guiding identification of biomarkers and novel targets to drive drug discovery. To this end, our human tissue and blood-derived assays within areas of high medical need in inflammatory diseases, fibrosis, oncology and neurodegenerative diseases. Our current network of collaborations consists of hospitals, research institutes and universities in Toronto and Montreal (Canada), Frankfurt (Germany) and Stockholm (Sweden).

EubOPEN Tissue Assay data sets:

[Hepatotoxicity screening in primary human hepatocyte spheroid cultures](#)

[Viability screening in matched tumor and normal organoids from colorectal cancer patients](#)

[Therapy re-sensitization of drug resistant organoids](#)

[Toxicity screen in isolated B cell assay](#)

[Cytokine secretion screen in isolated B cell assay](#)

[NASH model to assess anti-steatosis effects of chemical probes](#)

[NASH model to assess fibrosis effects of chemical probes](#)

[NASH model to assess inflammatory effects of chemical probes](#)

[Targeting of CAF-induced therapy resistance in CRC organoid-stroma co-cultures](#)

[Identification of compartment-specific drug sensitivities in CRC organoid-stroma co-cultures](#)

Protocols and results

Therapy re-sensitization of drug resistant organoids



Preliminary version (25th April 2022)

Disease area

Colorectal cancer (CRC) is among most lethal malignancies in the world and is often diagnosed at an advanced stage when the tumor cell dissemination has already started. Chemo- and targeted therapies provide only a limited increase of overall survival for these patients. The major reason for clinical failure remains therapy resistance. New combination strategies that target cellular pathways that are rewired in tumor cells could help to overcome therapy resistance but the identification of actionable drivers for personalized therapy remains challenging.

Rationale

Patient-derived tumor organoids have recently emerged as preclinical models that faithfully recapitulate the molecular and phenotypic characteristics of CRC. We have established a CRC organoid biobank and have molecularly characterized 29 patient-derived organoids (PDOs). To model the response to chemotherapy, we have exposed all tumor organoids to 5-FU, Oxaliplatin, SN-38 and Gefitinib and measured individual sensitivities. This allowed us to identify resistant tumor samples providing an opportunity to study underlying mechanisms.

Aim

In order to identify strategies for therapy re-sensitization we will subject resistant CRC organoids to sub-toxic doses of therapeutic drugs in combination with chemical probe libraries.

Methods

Cell culture condition: PDOs were established and cultured as previously described (van de Wetering et al., 2015). For detailed information on organoid handling and culturing refer SOP. Tumor cells are cultured for three days in 50 µl/well medium containing advanced DMEM/F12 supplemented with 10 mM Hepes, 1x Glutamax, 1x penicillin/streptomycin, 2% B27, 12.5 mM N-acetylcysteine, 500 nM AB3-01, 10 µM SB202190, 20% R-spondin 1 conditioned medium, 10% Noggin conditioned medium, 50 ng/ml human EGF.

General protocol: Colony formation assay was performed in n=29 CRC organoids to standardize the input cell number. Organoids were transduced with Luciferase2-P2A-EGFP lentivirus as described (Schmalzer et al., 2019). In a 96 well format, single cells were seeded in 15 µl 90% Matrigel, grown for 3 days in full organoid medium. On day 3, cells were washed and cultured in growth factor-reduced medium in presence of therapeutic drug for 6 days. Sensitivity to 5-FU, Oxaliplatin, SN-38 or Gefitinib was tested at 7-point dilution using a digital dispenser (Tecan De300).

Combination screens of tumor organoids will be performed in 384-well plates. Cells will be enzymatically dissociated, seeded in 10 µl 50% Matrigel and let recover for 3 days before culture in growth factor reduced medium. 5-FU, Oxaliplatin, SN-38 or Gefitinib will be added at fixed a sub-toxic concentration (determined above) and combined with chemical probe library that will be screened at a 4-point dilution for 4 days.

Readout: Luciferin Live Cell Substrate will be performed as readout on day 3 and the viability was measured after 7 days of culture by One-Glo 2X Luciferase assay system. To correct for seeding differences the data will be normalized in each well to the initial measurement.

Results

Colony formation assay in 29 lines showed different growth potential of single cells. Therefore, we standardized the input cell number to assure similar colony number for all lines (Fig. 1A). Treatment of organoids with the chemotherapeutic drugs 5-FU, Oxaliplatin, SN-38 and the EGFR inhibitor Gefitinib, revealed a heterogeneous response. Drug sensitivity is plotted as normalized Area Under the Curve (AUC) (Fig. 1B).

The resistant lines for each individual drugs (marked in red) will be subjected to chemical probe libraries to identify chemotherapy sensitizers. In 384-well plates, organoid cell will be subjected to either compound libraries alone or in combination with a sub-lethal dose of therapeutic drug. We will identify chemical probes that only show toxicity only in combination combined (Fig. 1C). In preparation of the screens, seeding consistency in 384-well plates was confirmed (Fig. 1D). For quality control (Z-factor and Z-Prime factor) each screening plate will contain positive and negative controls. Viability data after single agent and combination



treatment will be fitted analysed to determine IC₅₀, AUC and Drug Scoring Sensitivity (DSS). To score for synergistic combinations, we will use Bliss independence model that compares observed and the predicted combinatorial responses.

Conclusions

We present a powerful personalized platform to screen chemogenomic drug libraries to overcome therapy resistance. Screening data will be updated as available.

Figure

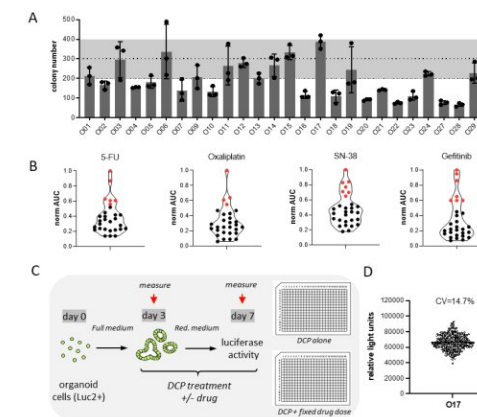


Figure 1. Therapy re-sensitization of drug resistant organoids. (A) Colony formation assay for 29 CRC organoids. (B) Sensitivity to different chemotherapies and the targeted compounds (Gefitinib). Resistant lines are marked in red. (C) Schematic representation of experimental design of therapy re-sensitization assay. (D) Seeding consistency of untreated 384-well plate. Dot plot of raw data (relative light units). Coefficient of variation (CV) is shown.

References

- van de Wetering et al., 2015, Cell 161, 933–945.
- Schmalzer et al., 2019, EMBO 238(12): e100928

EUBOPEN - FAIRPLUS COLLABORATION ENABLED DATA UPLOAD OF METADATA TO BIOIMAGE ARCHIVE



Home About Datasets Making the data FAIR Get involved Impact Resources News & Events

EUBOPEN case study: Open by design saves time

The EUBOPEN project is an international consortium of 22 partners from academia and industry, funded by IMI/IHI.

The goal of EUBOPEN is to create a library of compounds binding to 1,000 proteins. The goal of EUBOPEN is to create a library of compounds binding to 1,000 proteins. These ~5,000 compounds will be well characterised for their ability to interact with human proteins within their native environment, the cell.

To achieve its goal, EUBOPEN is fully committed to Open Science and aims to publish all its generated data open and fully accessible to everyone. The project has been working with experts from the FAIRplus project to organise the project's data to be accessible and interoperable for end users.

This case study details how EUBOPEN's commitment to Open Science allowed the FAIRplus squad teams to quickly and efficiently gain an overview of the data available, and the data to be generated over the course of the project.

The FAIRplus squad teams have summarised their work on this in the FAIR Cookbook. The recipe gives background on the current data standards for high-content multiplex screening, and proposes a pragmatic way to organise the data with minimal effort on the researcher's side.

Read/download/share the EUBOPEN case study, openly available on Zenodo

For more information on the EUBOPEN case, visit the FAIR Cookbook applied example

CASE STUDY

FAIRplus
FAIRplus use case IMI EUBOPEN:
Open by design saves time

Challenge

Background

Challenges & Goals

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Replying to @ELIXIRcloud_aai

Finally, project

#BioHackEU22 focus

#FAIRCookbook, #f

#systembiology, #f

#diseases & Workfl

@FAIRplus_eu @mybioinformatics

@nutano

2022 BioHackathon Europe

Number	Project name
31	The SH&H in data management: Improving connectivity between RDM and FAIR Cookbook
32	Training booster: developing FAIR training materials and Learning Paths
33	Training Systems biology curators in building interoperable and



About Collaborate Data Gateway Protocols Chemical Tools Chemogenomics Antibodies Tissue Assays News & Events Publications

Successful collaboration with FAIRplus

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Innovative Health Initiative @IMI · 33m

Great to see two IMI projects (@EUBOPEN & @FAIRplus_eu) working together like this to advance the principles of FAIR data and #OpenScience 🙌🙌🙌

FAIRplus @FAIRplus_eu · 1T

@EUBOPEN is fully committed to #OpenScience and aims to publish all its generated data open and fully #accessible to everyone. Read our case study on EUBOPEN to find out our collaboration on making data #FAIR: fairplus-project.eu/news/eubopen-c...

CASE STUDY

FAIRplus
FAIRplus use case IMI EUBOPEN:
Open by design saves time

Case Study
IMI EUBOPEN:
Open by design saves time

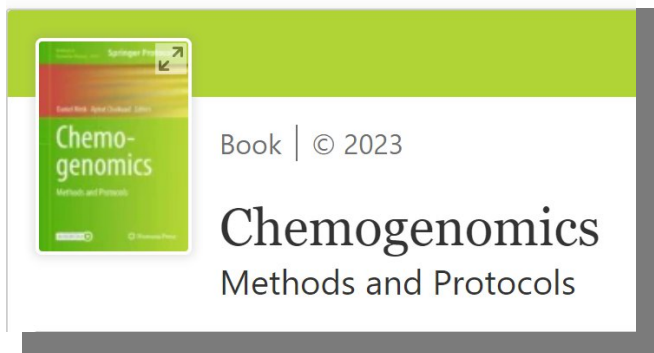
Availability of metadata

TB of data

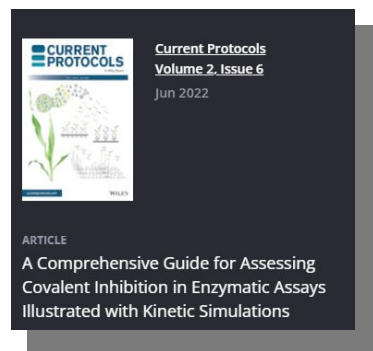
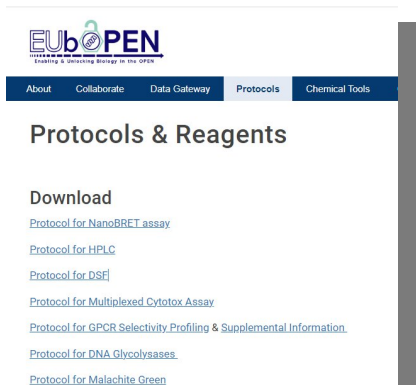
LONG-LIVED ASSAY PLATFORMS



- Protocols and methods established for Chemogenomic published in articles and as book
- Protocols on EUBOPEN Website
- All tools available
- Company founded offering established assay platform



Merk, D., Chaikuad, A. (eds) Chemogenomics. Methods in Molecular Biology, vol 2706. Humana, New York, NY https://doi.org/10.1007/978-1-0716-3397-7_1



CELLinib GmbH – a Frankfurt based fee-for-service CRO for your cellular selectivity profiling needs

CELLinib128
Selectivity Screen

CELLinib
Half-life

CELLinibEC50
Dose-response

We want to speed up your drug discovery project by quickly and accurately characterizing your small molecule inhibitor in living cells using the Promega NanoBRET technology. Let's illuminate science together!

Dr. B.-T. Berger, CEO CELLinib GmbH, Altenhöferallee 3, 60438 Frankfurt, 12.09.2023 CELLinib – illuminate science together using the Promega NanoBRET technology 1



Protocol
Single tracer-based protocol for broad-spectrum kinase profiling in live cells with NanoBRET



Protocol
High-content live-cell multiplex screen for chemogenomic compound annotation based on nuclear morphology



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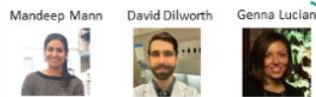
Open Lab Notebooks

Extreme Open Science Initiative: SGC scientists around the world are starting to post their lab notebook online in real time.

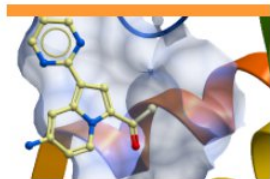
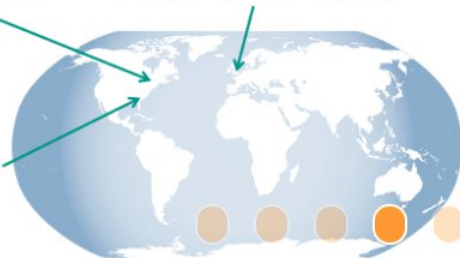
University of Toronto, Canada



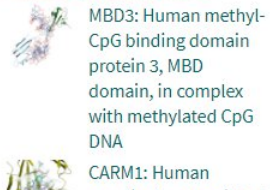
University of Oxford, U.K



University of North Carolina, U.S.A.



Latest Structures



MBD3: Human methyl-CpG binding domain protein 3, MBD domain, in complex with methylated CpG DNA

CARM1: Human



New Publications

Structural basis for the ability of MBD domains to bind methyl-CG and TG sites in DNA. *J. Biol. Chem.*

Structural and functional analysis of the DOT1L-AF10



Chemical Probes

SGC3027 - for PRMT7
22nd March 2018

SGC-GAK-1 - a chemical probe for GAK
27th February 2018

SGC-AAK1-1 - a dual inhibitor of AAK1 and PRMT7/PRMT8



News from SGC

Conference announcement: BMP Signalling in Cancer II
Posted on 16th March 2018

ALS Reproducible Antibody Platform: Open Science to enable consistent data and accelerate

scientificdata updates

a blog from *Scientific Data*

[Scientific Data](#) [Blog](#) [Post](#)

Previous post
[Data Matters: Interview with Ben Lehner](#)

Next post
[Expanding our generalist data repository options](#)

SCIENTIFIC DATA | SCIENTIFIC DATA

An open approach to Huntington's disease research

[October 19, 2016 | 1:11 pm](#) | Posted by [Andrew Hufton](#) | Category: [Featured](#), [Guest Posts](#)

Guest post by [Rachel Harding](#), postdoctoral fellow at the [Structural Genomics Consortium](#), University of Toronto, Canada

Huntington's disease (HD) is a fatal neurodegenerative disorder caused by a mutation in the *huntingtin* gene¹. The progressive break down of brain neuronal cells in HD patients leads to deteriorating mental and physical abilities over a 10-20 year period prior to death, the symptoms often described as having Parkinson's disease, Alzheimer's disease and amyotrophic lateral sclerosis (ALS) simultaneously². At the start of the *huntingtin* gene there is a CAG trinucleotide repeat region that encodes a stretch of poly-glutamine residues in the amino-terminus of the encoded protein. This repeat tract is expanded in HD patients. The repeat length of this region correlates with the age of symptom onset³. Affecting approximately 1 in 10,000 of the population⁴, rare juvenile forms of the disease exist in patients with the longest CAG expansions, although adult-onset HD patients typically have between 40-50 CAG repeats with symptom onset beginning between the ages of 35-50.



RACHEL HARDING

What interests many scientists most in the field, and would be imperative to developing targeted and effective

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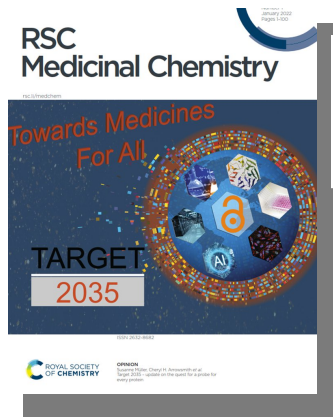
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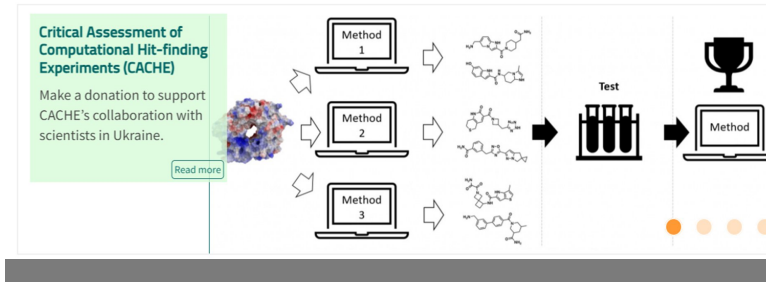
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OPINION

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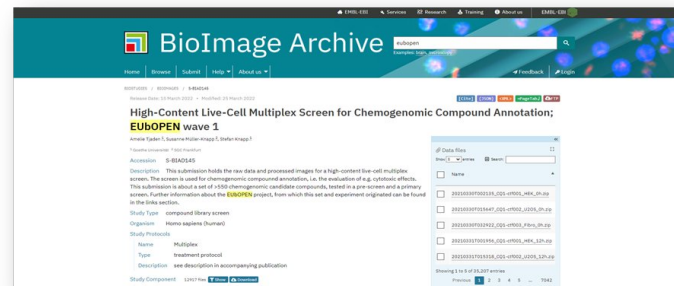
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