Data-driven antibiotic discovery: From gaps to solutions

Guest speakers: Mark Blaskovich, Matthew Todd & Luiza Galarion
Moderator: Heike Brötz-Oesterhelt
Host: Shirine Derakhshani

27 November 2025

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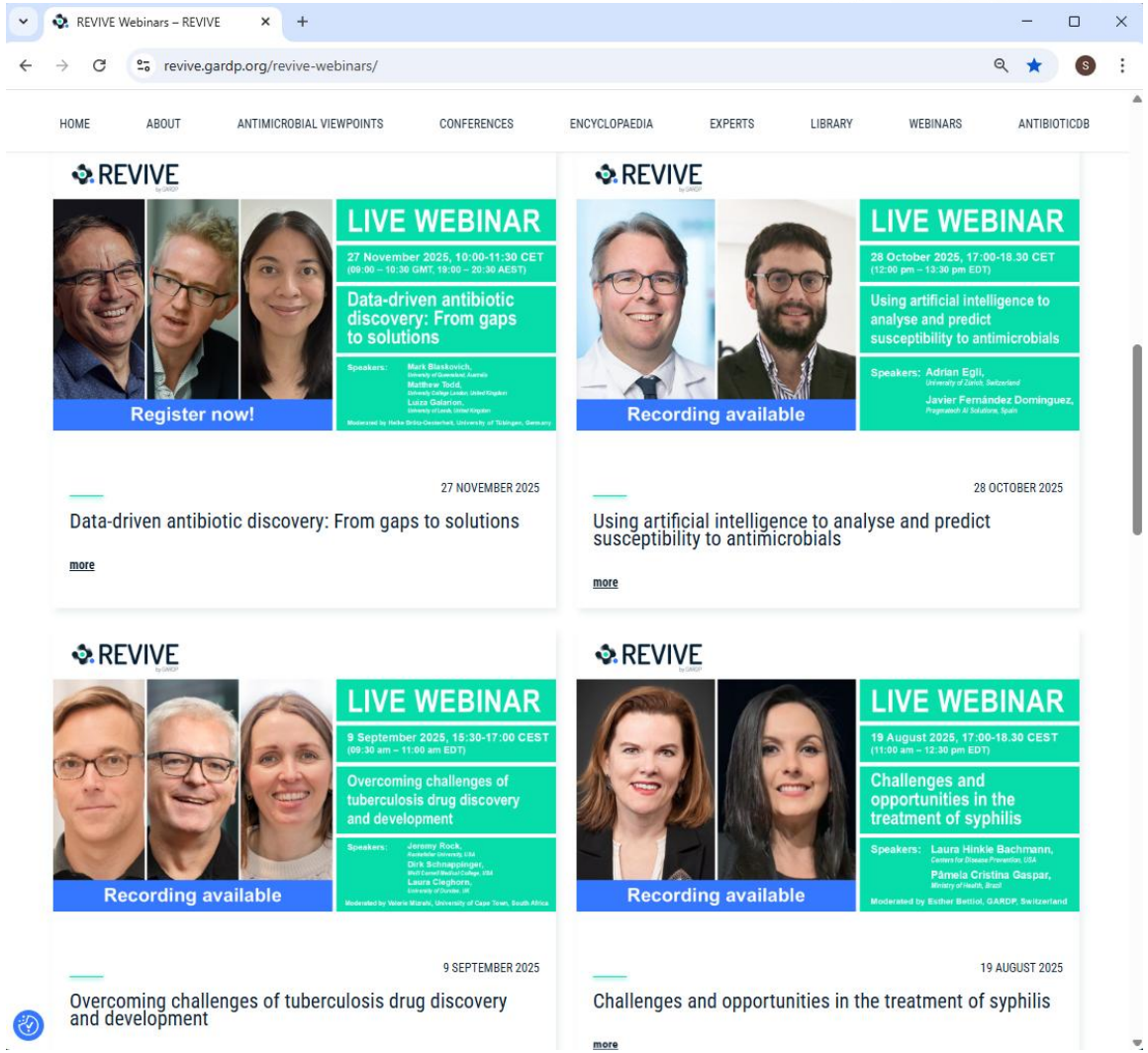

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Antimicrobial Viewpoints

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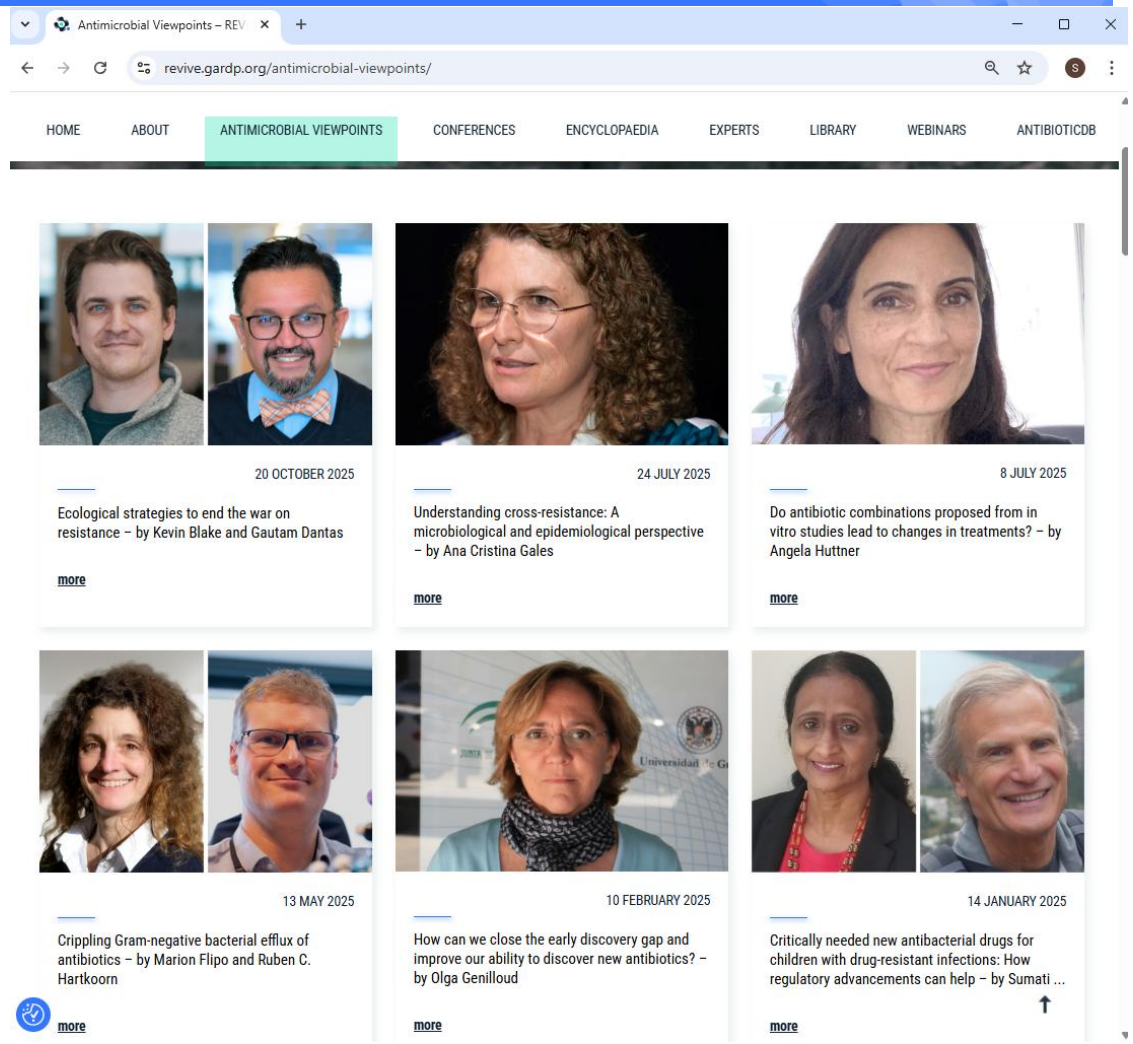

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Antimicrobial Encyclopaedia

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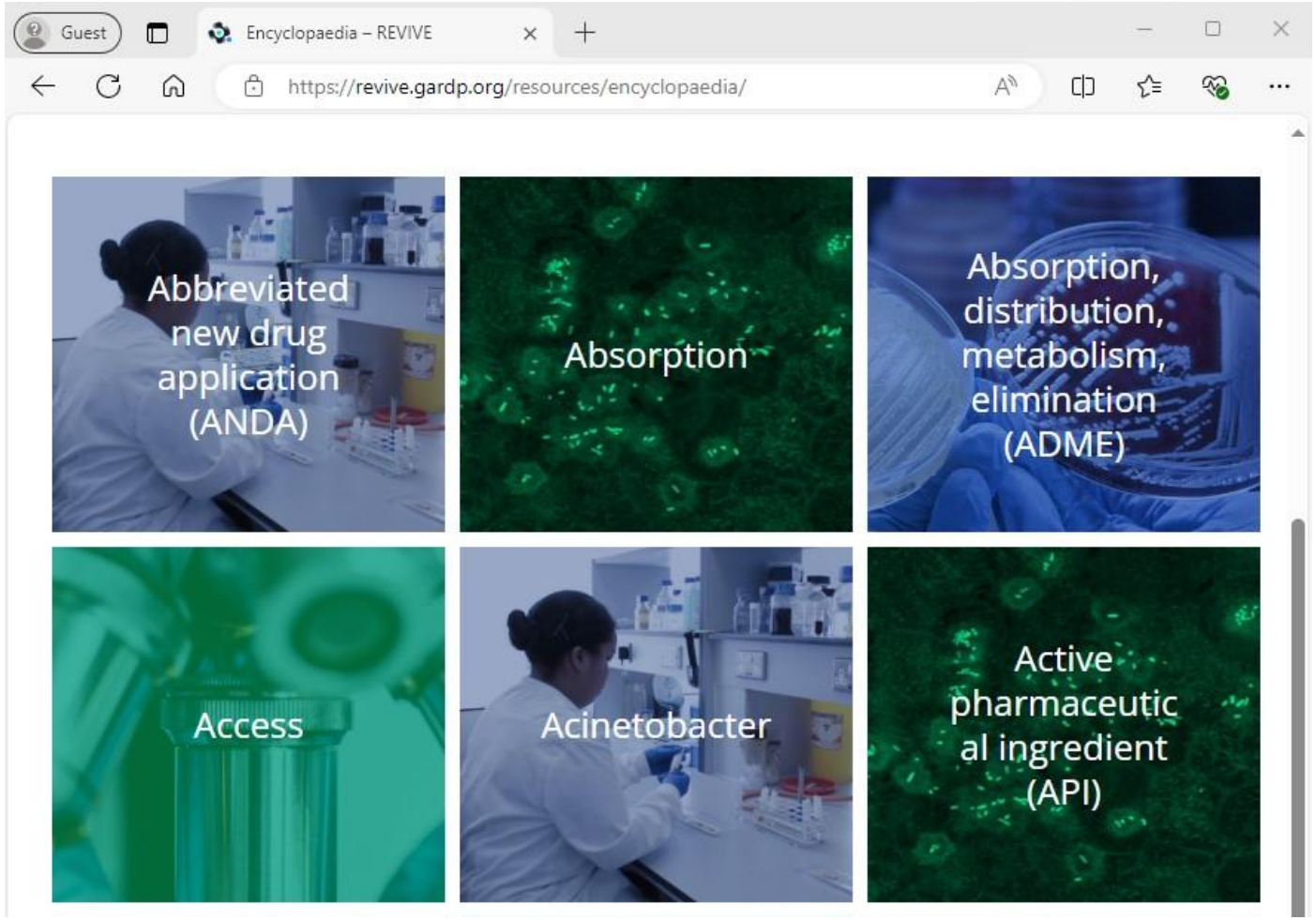
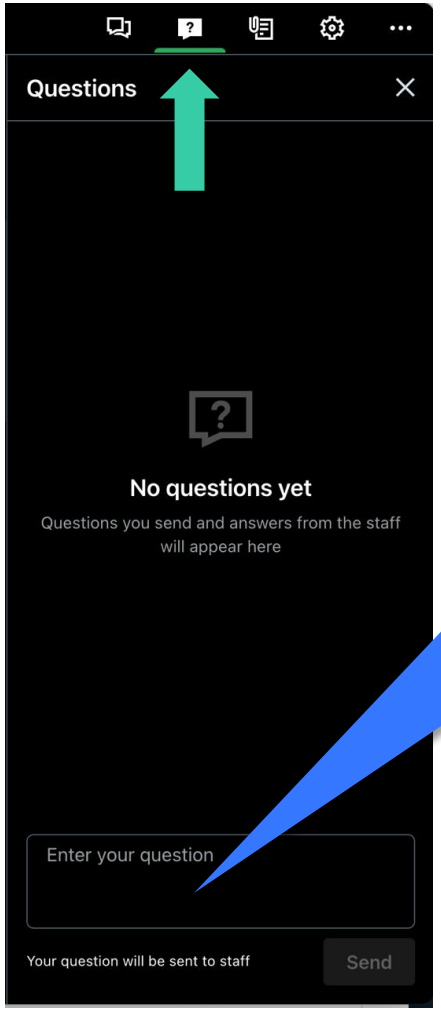


revive.gardp.org/resources/encyclopaedia

How to submit your questions

REVIVE by GARDP

If your question is addressed to a specific speaker, please include their name when submitting the question.



Please submit your questions through the box provided after clicking the ‘questions’ button. We will review all questions and respond to as many as possible after the presentation.

Today’s speakers

REVIVE by GARDP

An introduction to antibiotic research and development (R&D)

Moderator:
Heike Brötz-Oesterhelt
University of Tübingen, Germany

Mark Blaskovich
University of Queensland, Australia

Matthew Todd
University College London, UK

Luiza Galarion
University of Leeds, UK

EBERHARD KARLS
UNIVERSITÄT
TÜBINGEN

Data-driven antibiotic discovery: Why is it important?

Heike Brötz-Oesterhelt
Interfaculty Institute of Microbiology and Infection Medicine, University of Tübingen
Dept. Microbial Bioactive Compounds

Data sharing and FAIR data use are essential because …

… bacteria are tough opponents and challenging to overcome,
especially nowadays with soaring resistance rates.
→ **We need all the help we can get, and community efforts are powerful.**

… we race against the clock to avoid a post-antibiotic era.
→ **We need to minimize the time per learning cycle.**

… most current antibiotic discovery and development is performed
in SMEs and at universities.
→ **We need to preserve knowledge and work along (regionally dispersed) pipelines.**

… most of current antibiotic research is financed by public funds.
→ **We need to spend tax payers‘ money efficiently.**

Data sharing … from gap analysis to solutions

Each analysis provides us with new insights into bottlenecks and how to overcome them.
→ **We will get continuously wiser.**

Each successful joint effort inspires new collaborative efforts.
→ **We will keep getting faster.**

Community efforts allow the sharing of expertise, workload, and responsibility
→ **We can pick our „community brain“ for innovation. And it is fun ☺.**

Antibiotic resistance is a global problem.

Good antibacterial agents are a global, joint, and limited resource.

Let‘s make antibiotic discovery and development a global task !!!

Mark Blaskovich

Mark Blaskovich is an ‘antibiotic hunter’ and Director of Translation for the Institute for Molecular Bioscience at The University of Queensland. He also leads the ARC Industrial Transformation Training Centre CEAStAR (Centre for Environmental and Agricultural Solutions to Antimicrobial Resistance) and the antibiotic crowdsourcing initiative CO-ADD (Community for Open Antimicrobial Drug Discovery). A medicinal chemist with 15 years of industrial drug development experience at three biotech companies, since 2010 he has been developing new antibiotics, antibiotic alternatives, and diagnostics to detect and treat resistant bacterial and fungal infections. His research includes multiple industry collaborations focused on antimicrobial resistance. Blaskovich is a member of the WHO antibiotic pipeline advisory panel and chair of the GARDP REVIVE review panel.

https://imb.uq.edu.au/research-groups/blaskovich

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CREATE CHANGE

GARDP
Global Antibiotic Research & Development Partnership

Scientific Bottlenecks in Antibiotic Discovery

LIVE WEBINAR

27 November 2025, 10:00-11:30 CET
(09:00 – 10:30 GMT, 19:00 – 20:30 AEST)

Data-driven antibiotic discovery: From gaps to solutions

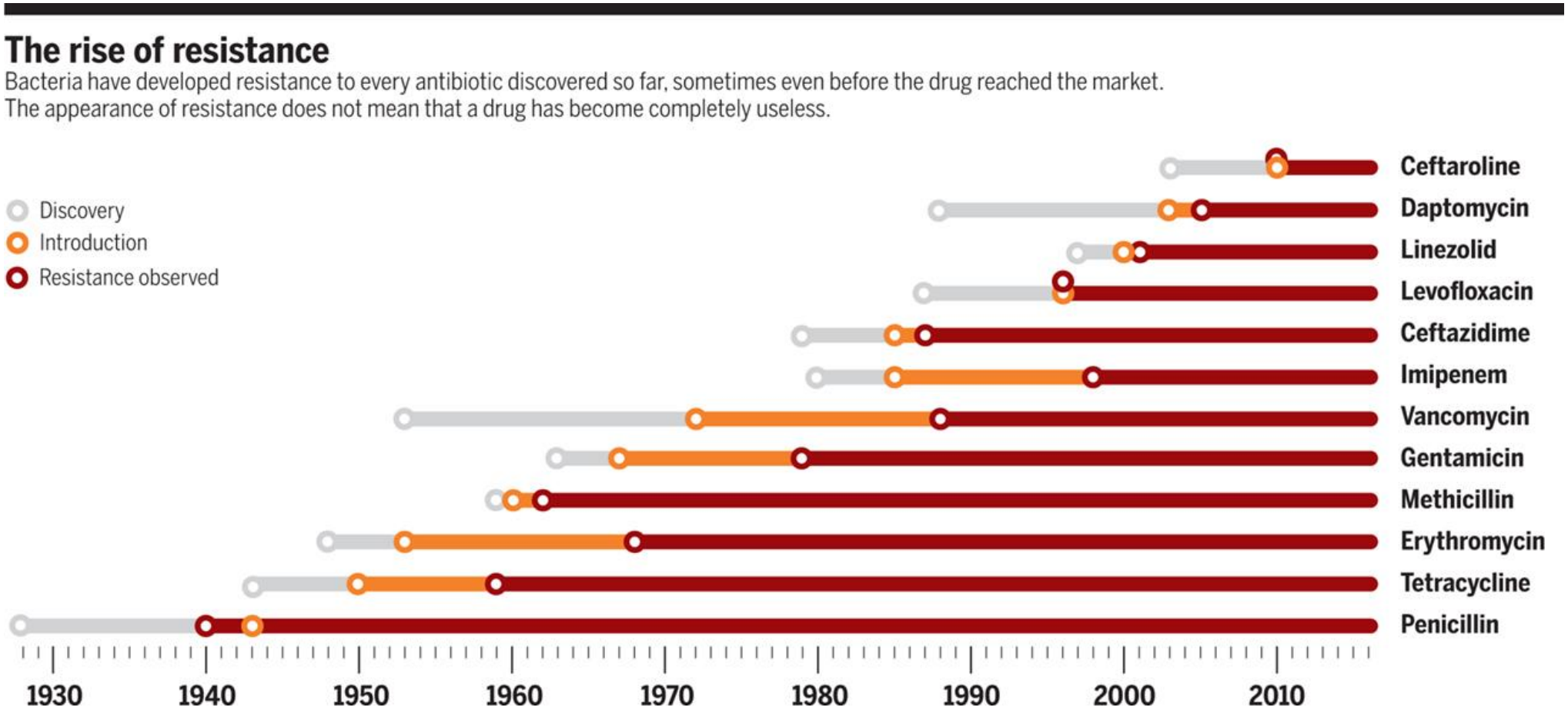
Speakers:
Mark Blaskovich,
University of Queensland, Australia
Matthew Todd,
University College London, United Kingdom
Luiza Galarion,
University of Leeds, United Kingdom

Moderated by Heike Brötz-Oesterhelt, University of Tübingen, Germany

Prof Mark Blaskovich
Centre for Superbug Solutions
Institute for Molecular Bioscience
The University of Queensland

27 November 2025

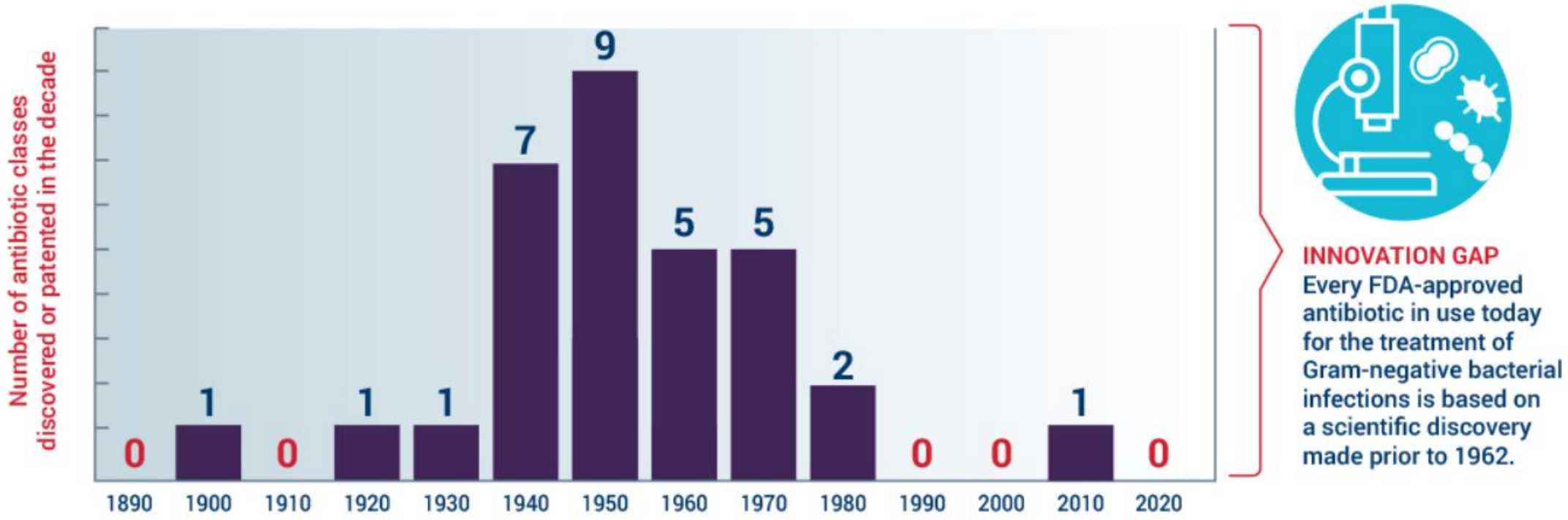
The Problem: Antibiotic Resistance



Kai Kupferschmidt Science 2016;352:758-761

Antibiotic Void

- Discovery of new antibiotics is not keeping pace with development of resistance



* Cefiderocol was approved by FDA in 2019 and EMA in 2020. The FDA-approved label for cefiderocol classifies the drug as a cephalosporin, and therefore not a new class but certainly a new mechanism of action. Some experts consider cefiderocol to be a first-in-class sideromycin. The predecessors to cefiderocol were discovered at Shionogi in the early 1990s. CID 2019;69(7):S538-S543
* This chart excludes bedaquiline, which is the first drug in a new class to treat tuberculosis.
Source: Pew Charitable Trusts; Deak D, Powers JH, Outterson K, Kesselheim AS. Progress in the Fight Against Multidrug Resistant Bacteria?: A Review of FDA Approved Antibiotics 2010-2015. ANNALS OF INTERNAL MED. 2016 MAY 31. DOI: 10.7326/M16-0291.

Figure provided courtesy of CARB-X. Source: Pew Charitable Trust. https://carb-x.org/about/global-threat/

Decline in Antibiotic Approvals

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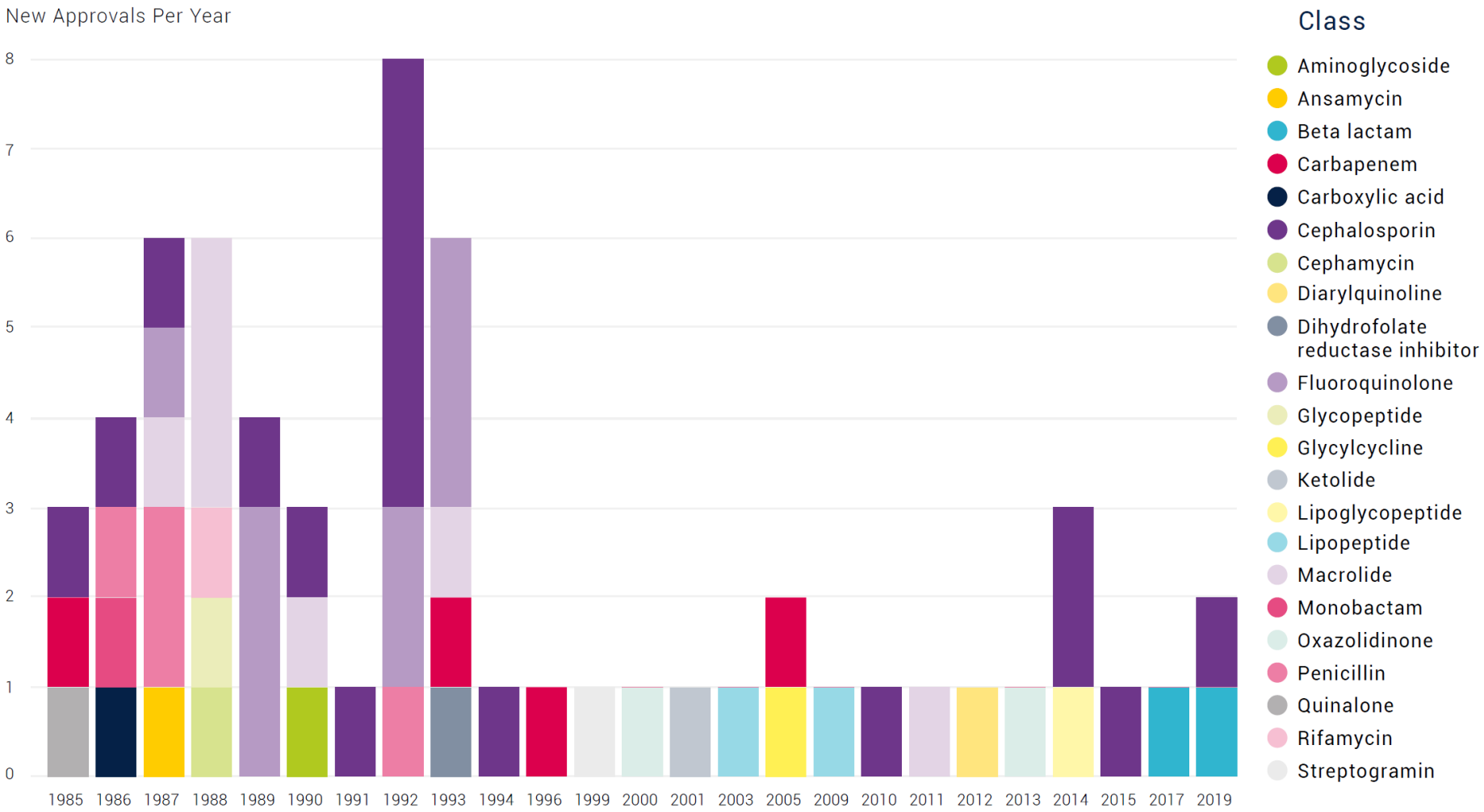
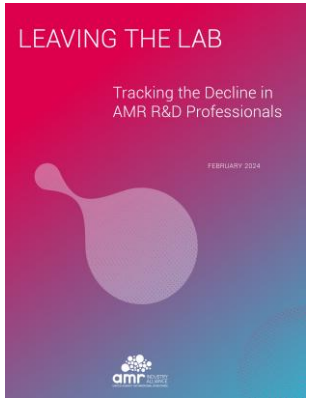
FIGURE 1. ANNUAL FDA APPROVALS OF ANTIBIOTICS HAVE FALLEN FOR DECADES



amr INDUSTRY ALLIANCE
UNITED AGAINST ANTIMICROBIAL RESISTANCE



Bottleneck 1: Loss of Knowledge

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Big Pharma Exit

Bloomberg US Edition

Live Now | Markets | Economics | Industries | Tech | AI | Politics | Wealth | Pursuits | Opinion | Businessweek | Equality | Green

Business Prognosis

Superbugs Win Another Round as Big Pharma Leaves Antibiotics

- Novartis shuts down efforts; Glaxo reviewing some assets
- Public measures to spur research not working for drug giants

As Novartis Exits, Who Will Make New Antibiotics?

July 25, 2018

Pfizer Draws Curtain On Anti-infective Research; Refocuses On Next-gen Vaccines

This article was originally published in PharmAsia News

13 May 2013

NEWS AND OPINIONS – 2018

Despite Industry AMR Declaration commitments Sanofi quits R&D on anti-infectives

AstraZeneca pulls out of antibiotic drug development

BOWHOUSE / 2ND SEPTEMBER 2016 / UNCATEGORISED

Bottleneck 1: Loss of Knowledge - AMR Researchers

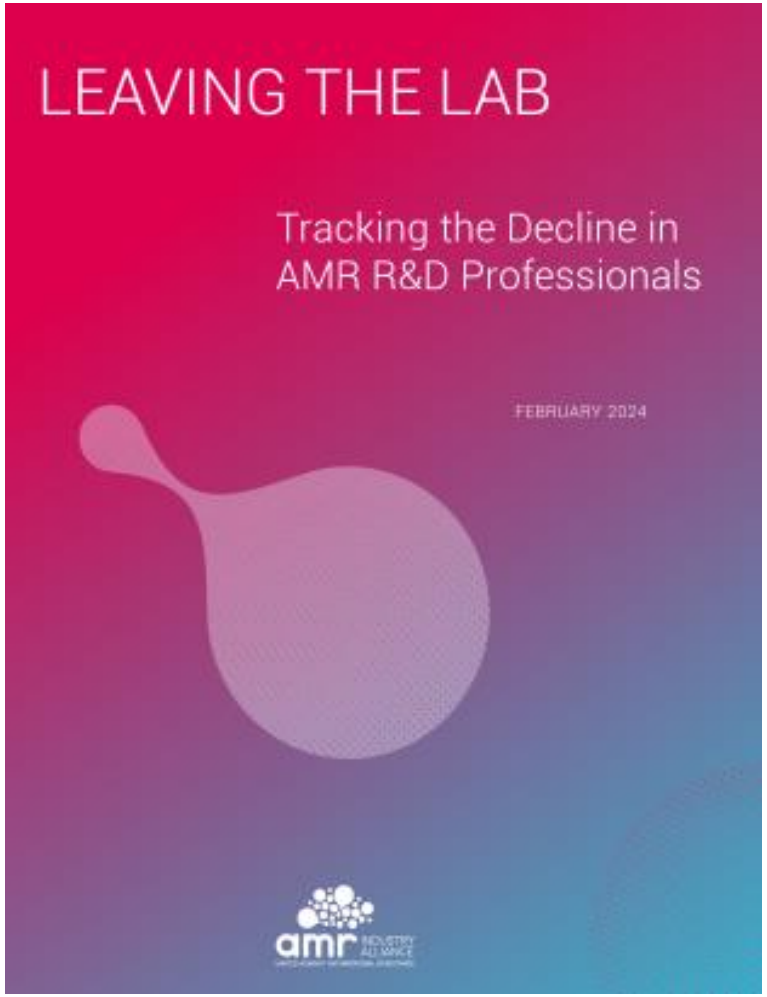


FIGURE 2. AMR PUBLICATIONS HAVE DECLINED FOR 20+ YEARS

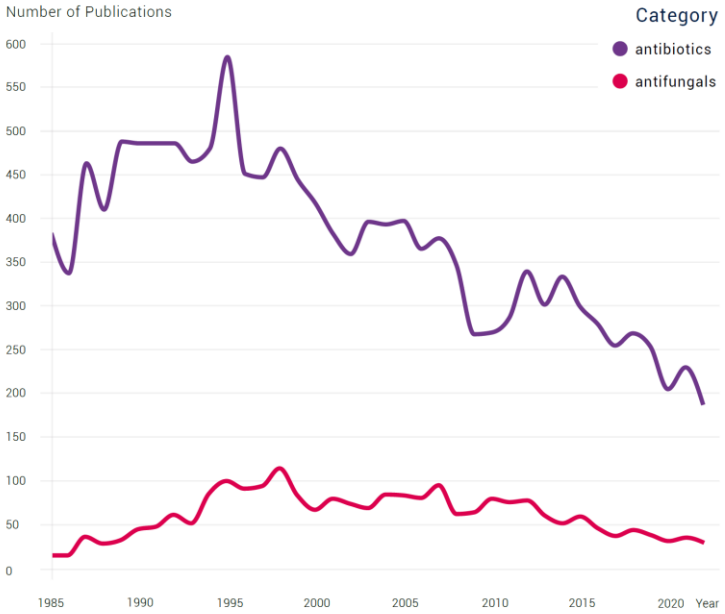


FIGURE 4. PUBLICATIONS ON CANCER AND HIV/AIDS FAR OUTSTRIP AMR TOPICS

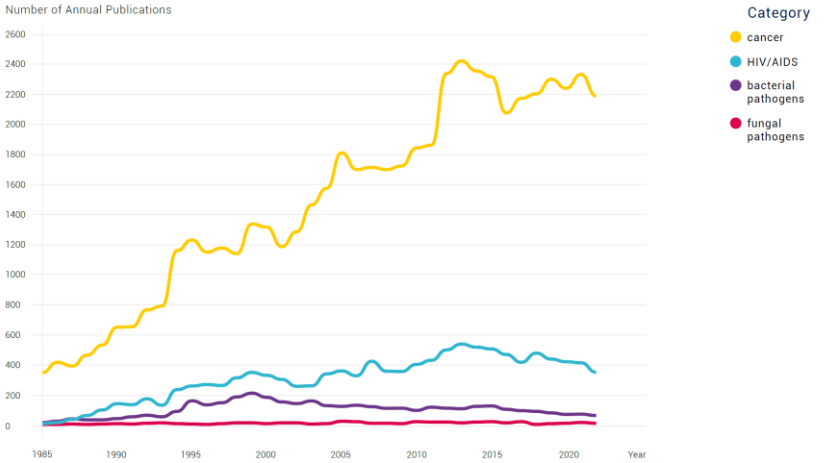
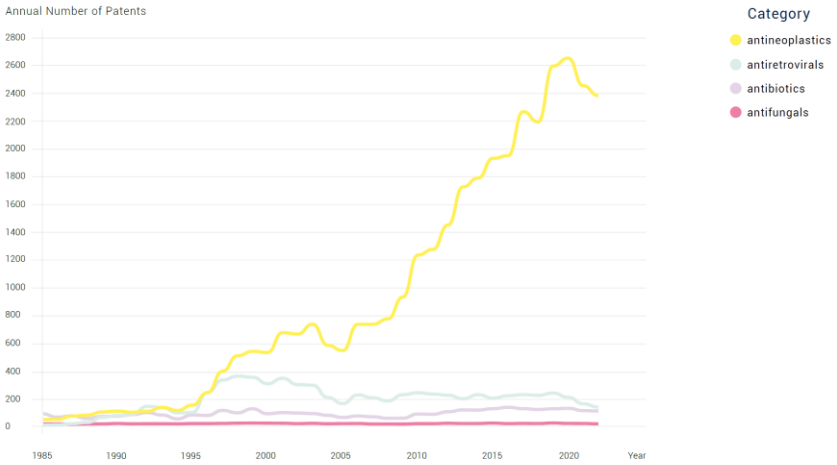


FIGURE 5. PATENTS FOR ANTINEOPLASTICS AND ANTIRETROVIRALS EXCEED ANTIBIOTICS AND ANTIFUNGALS



Bottleneck 1: Loss of Knowledge - AMR Researchers

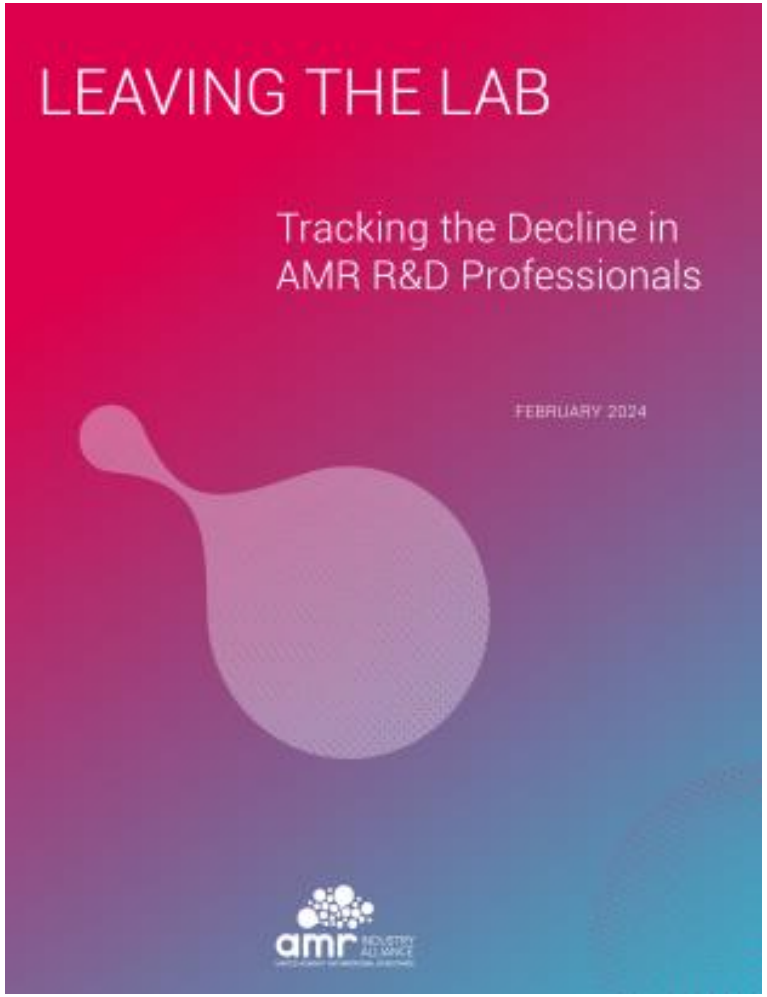
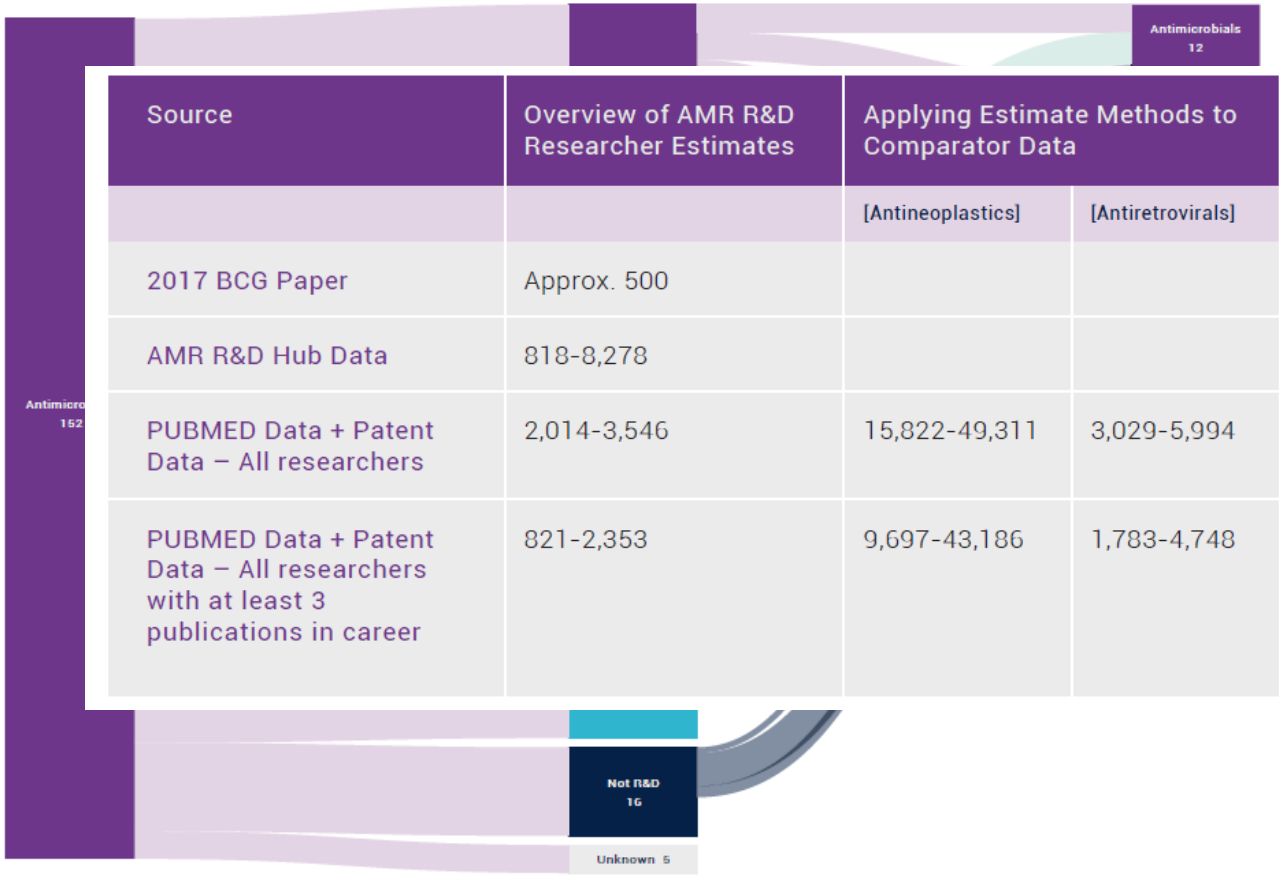


FIGURE 6. CAREER PATHS AT SIX FIRMS WHO ABANDONED AMR-RELATED R&D



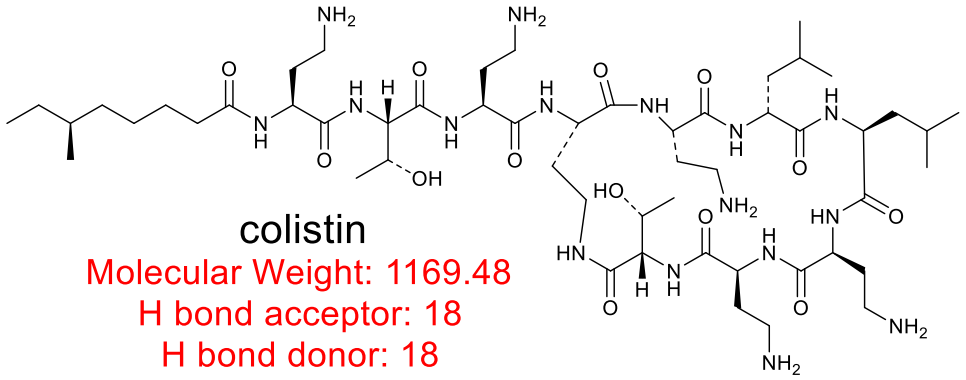
Source	Overview of AMR R&D Researcher Estimates	Applying Estimate Methods to Comparator Data	
		[Antineoplastics]	[Antiretrovirals]
2017 BCG Paper	Approx. 500		
AMR R&D Hub Data	818-8,278		
PUBMED Data + Patent Data – All researchers	2,014-3,546	15,822-49,311	3,029-5,994
PUBMED Data + Patent Data – All researchers with at least 3 publications in career	821-2,353	9,697-43,186	1,783-4,748

Bottleneck 2: New Chemical Diversity

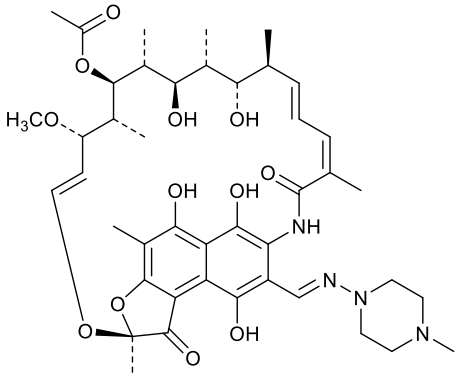
Antibiotics are not ‘drug-like’

Don’t obey the ‘rules’

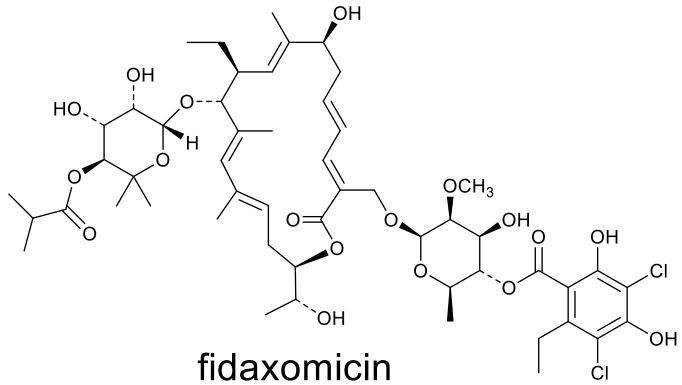
“Rule of Five”
Molecular Weight: <500
H bond acceptor: ≤10
H bond donor: ≤ 5
logP: ≤ 5



colistin
Molecular Weight: 1169.48
H bond acceptor: 18
H bond donor: 18
ALogP: -7.1

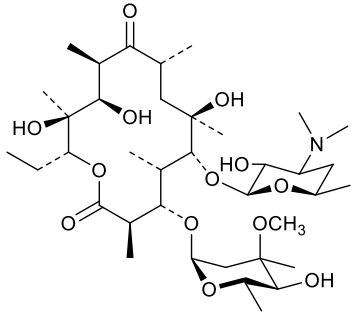


rifampicin
Molecular Weight: 822.95
H bond acceptor: 15
H bond donor: 6
ALogP: 3.3

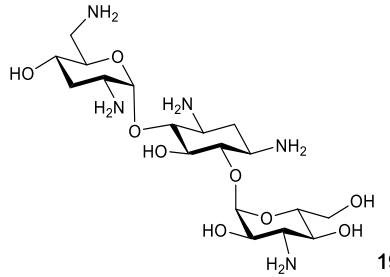


fidaxomicin
Molecular Weight: 1058.05
H bond acceptor: 18
H bond donor: 7
ALogP: 7.8

erythromycin
Molecular Weight: 733.94
H bond acceptor: 18
H bond donor: 7
ALogP: 7.7



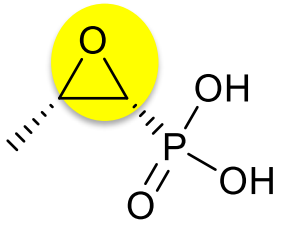
tobramycin
Molecular Weight: 467.52
H bond acceptor: 14
H bond donor: 10
ALogP: -6.9



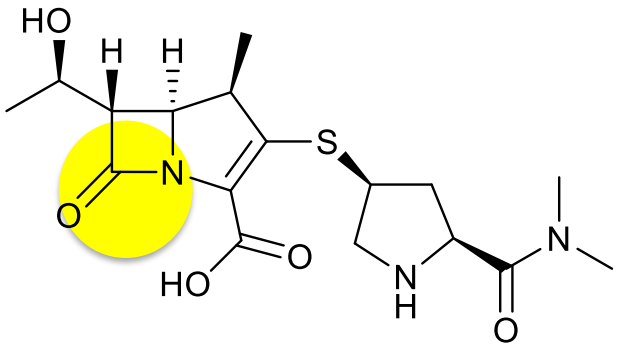
Bottleneck 2: New Chemical Diversity

Antibiotics are not ‘drug-like

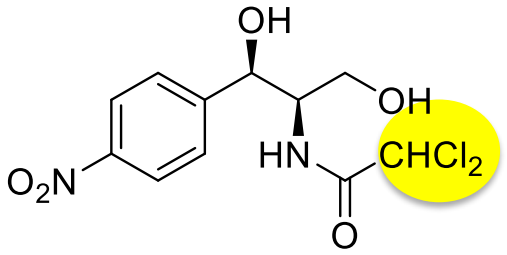
Often reactive



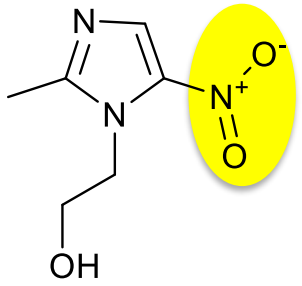
fosfomycin



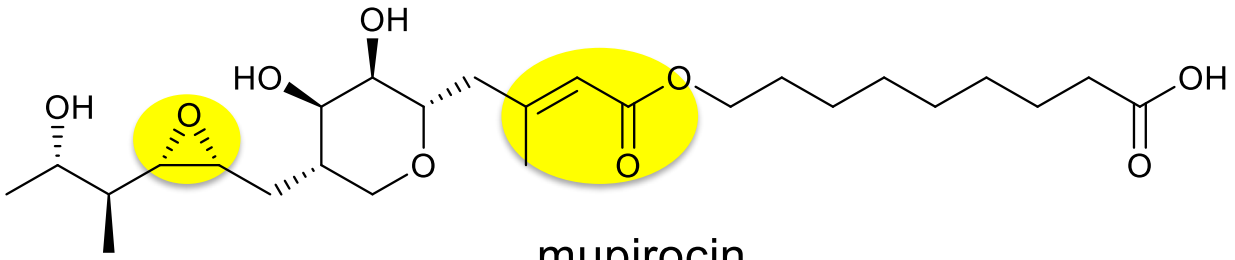
meropenem



chloramphenicol



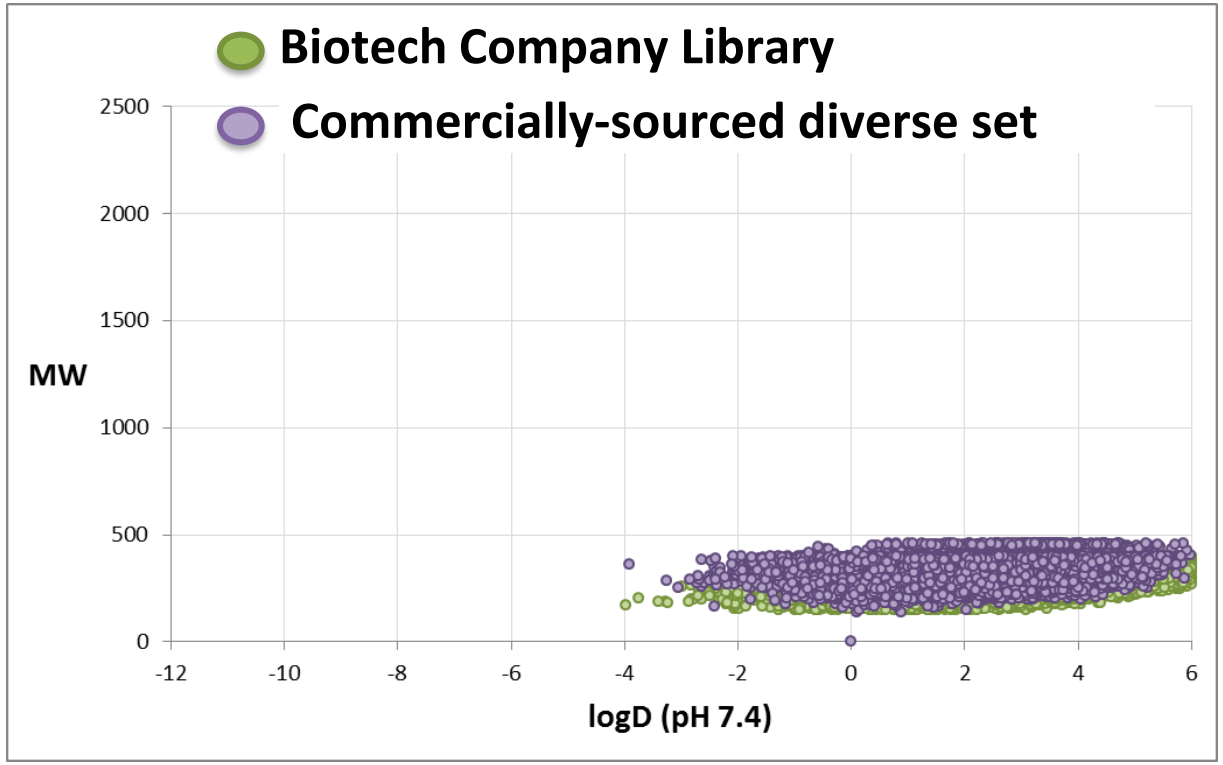
metronidazole



mupirocin

Bottleneck 2: New Chemical Diversity

Pharma vs Academic Compounds

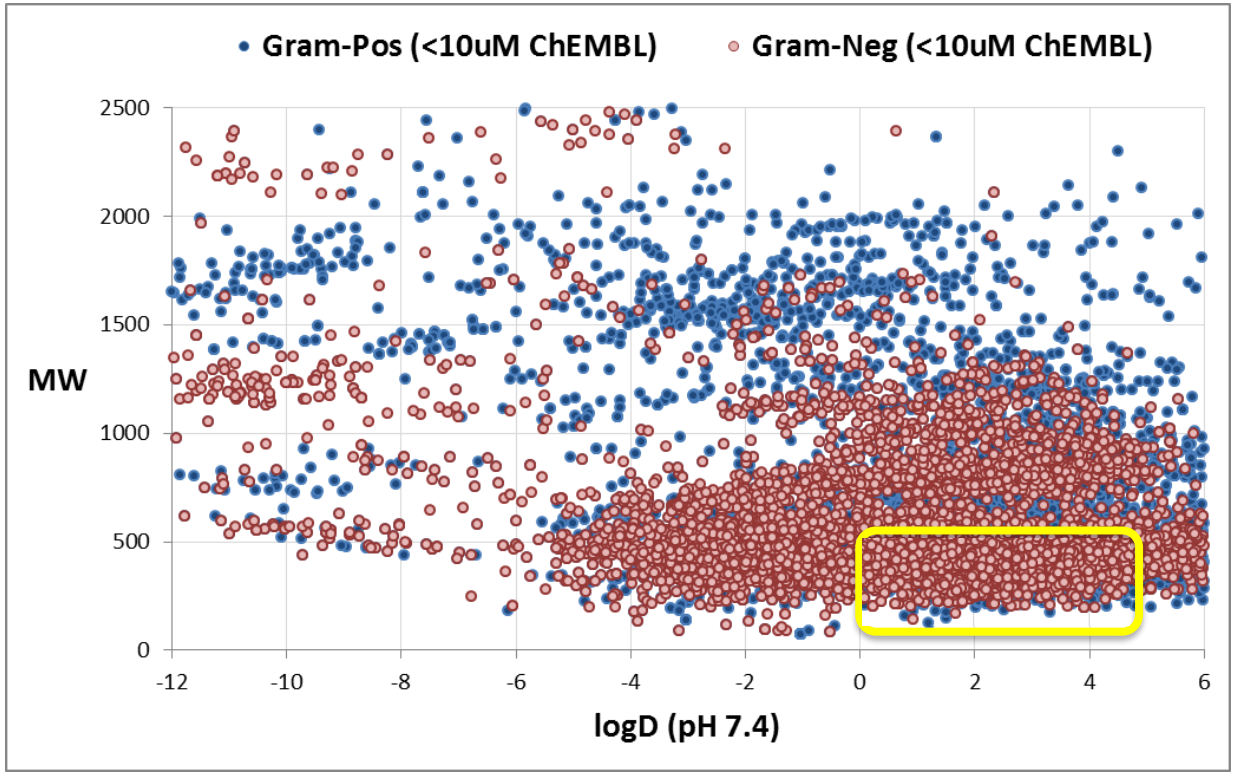


Typical Corporate Library

G-ve hit rate (MIC ≤ 32ug/mL)

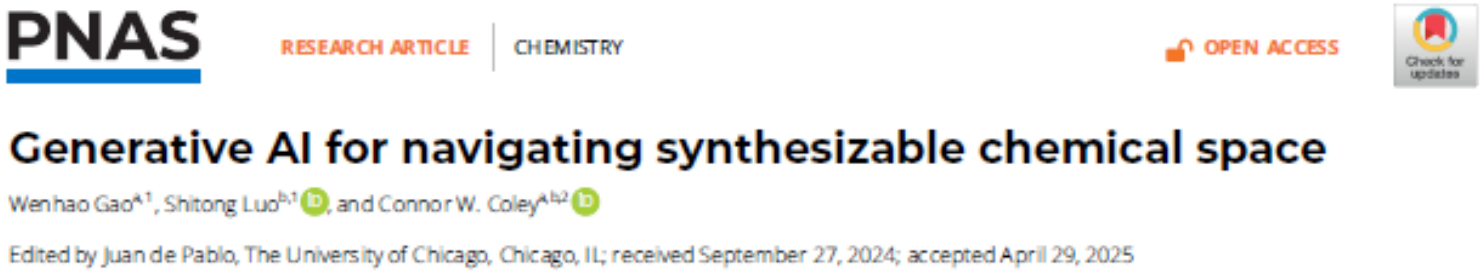
0.008%

Published Academic Antibiotics



Bottleneck 2: New Chemical Diversity

- Lack of novelty in compound libraries
- Reliance on same compound screening libraries from commercial vendors
- Until recently natural product discovery has focused on same species cultured under similar conditions = rediscovery of existing antibiotics
- Generative AI can produce un-synthesizable molecules



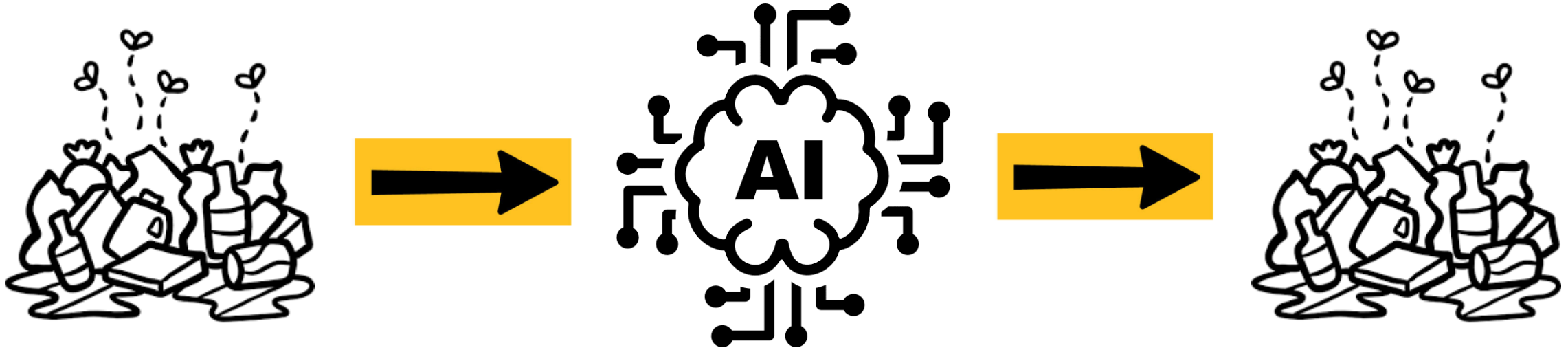
PNAS RESEARCH ARTICLE | CHEMISTRY OPEN ACCESS

Generative AI for navigating synthesizable chemical space

Wenhao Gao[a,1], Shitong Luo[b,1], and Connor W. Coley[a,b,2]

Edited by Juan de Pablo, The University of Chicago, Chicago, IL; received September 27, 2024; accepted April 29, 2025

Bottleneck 3: Standardised Large Data Sets



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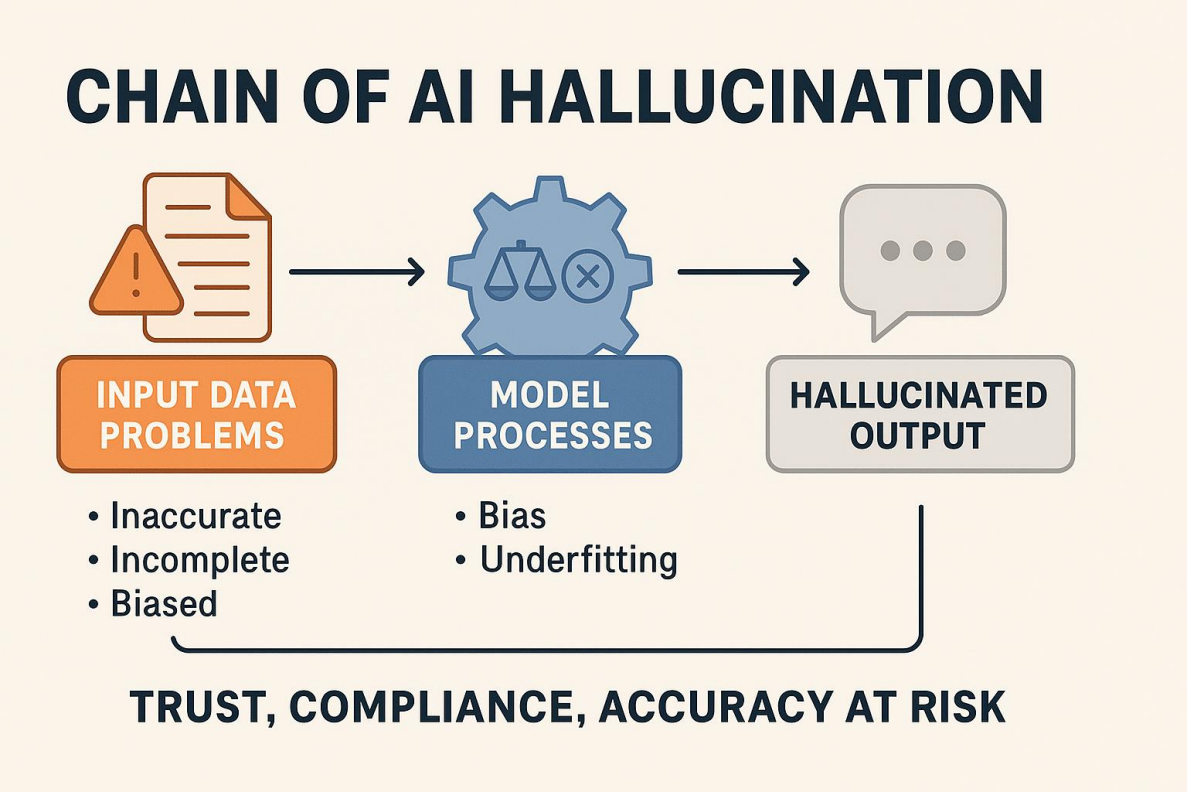
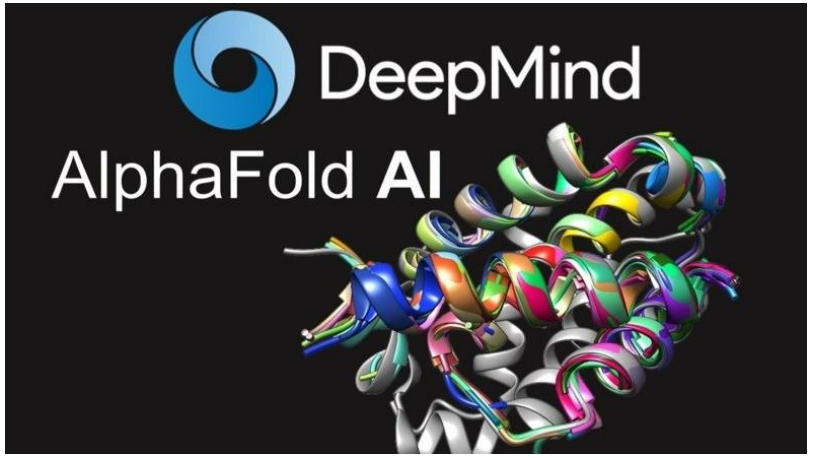
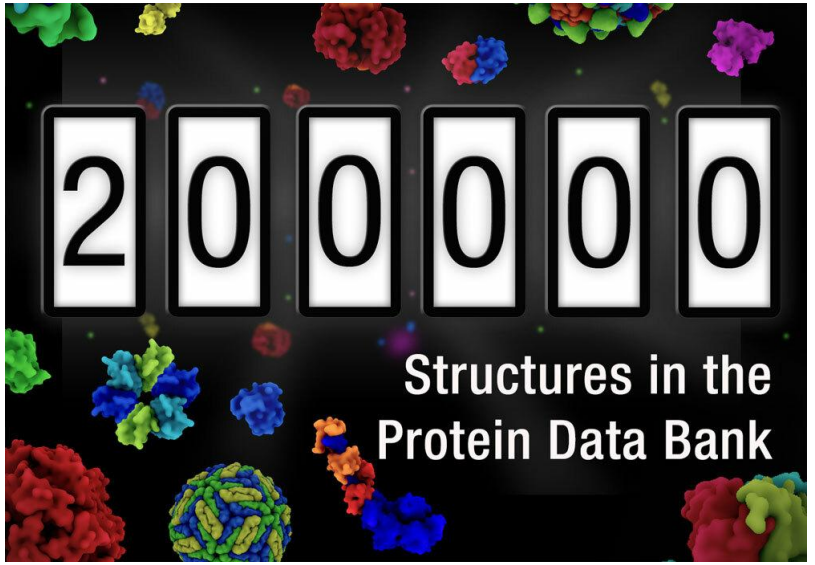






https://shelf.io/blog/garbage-in-garbage-out-ai-implementation/

Bottleneck 3: Standardised Large Data Sets

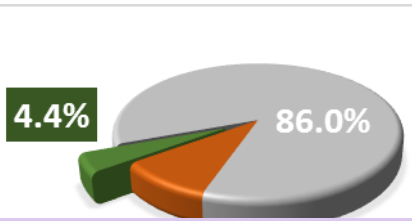
Dr Johannes Zuegg

ChEMBL www.ebi.ac.uk/chembl

ChEMBL Activities 14,675,320
Compounds **1,735,422**

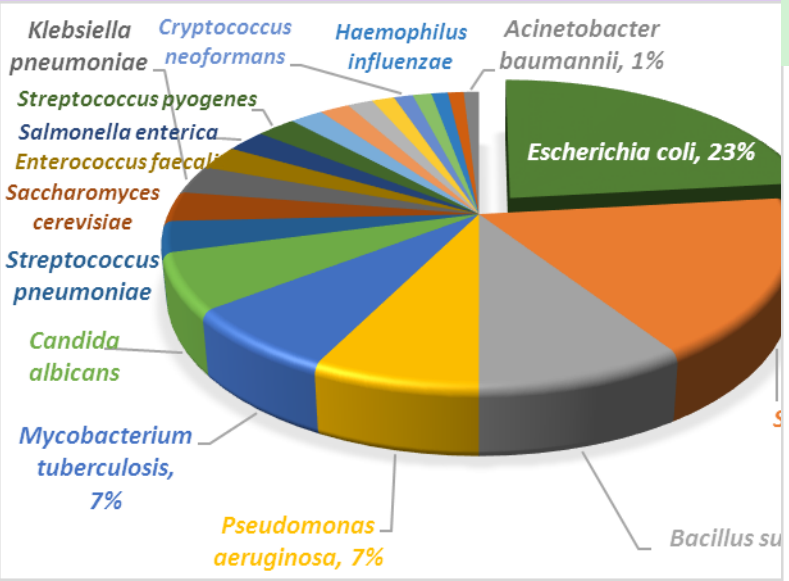
Compounds with **antimicrobial MIC** data (76,876)

Compounds with **antimicr** (243,710)

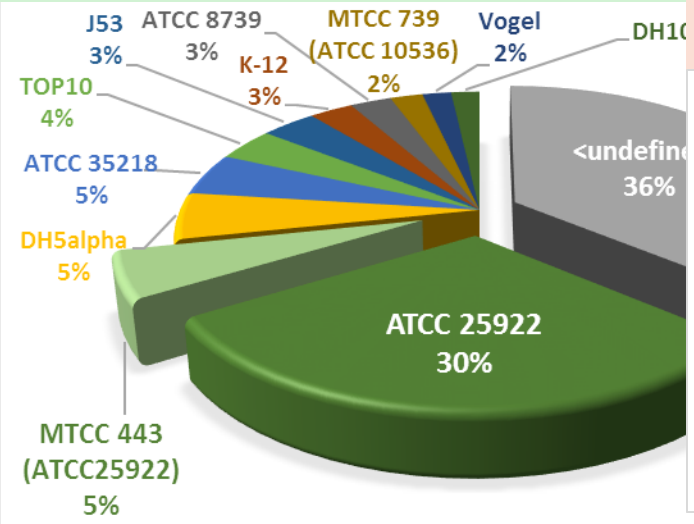


- Model building requires clean data
- ‘negative’ data often absent – never reported

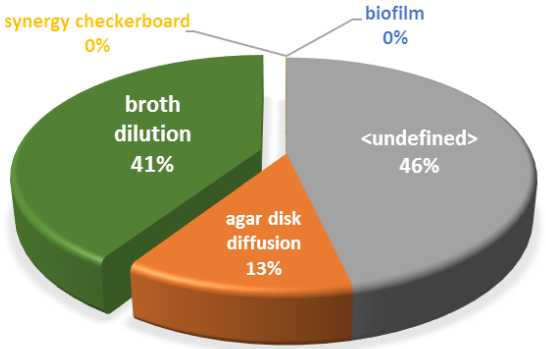
Organisms with MIC



***E. coli* strains**



Assay conditions *E. coli* ATCC



***E. coli* ATCC 25922**
no additives,
broth dilution (CLSI, EUCAST?)

Compounds 8,225

Bottleneck 4: Data Integration

Biological Activity - Antimicrobial

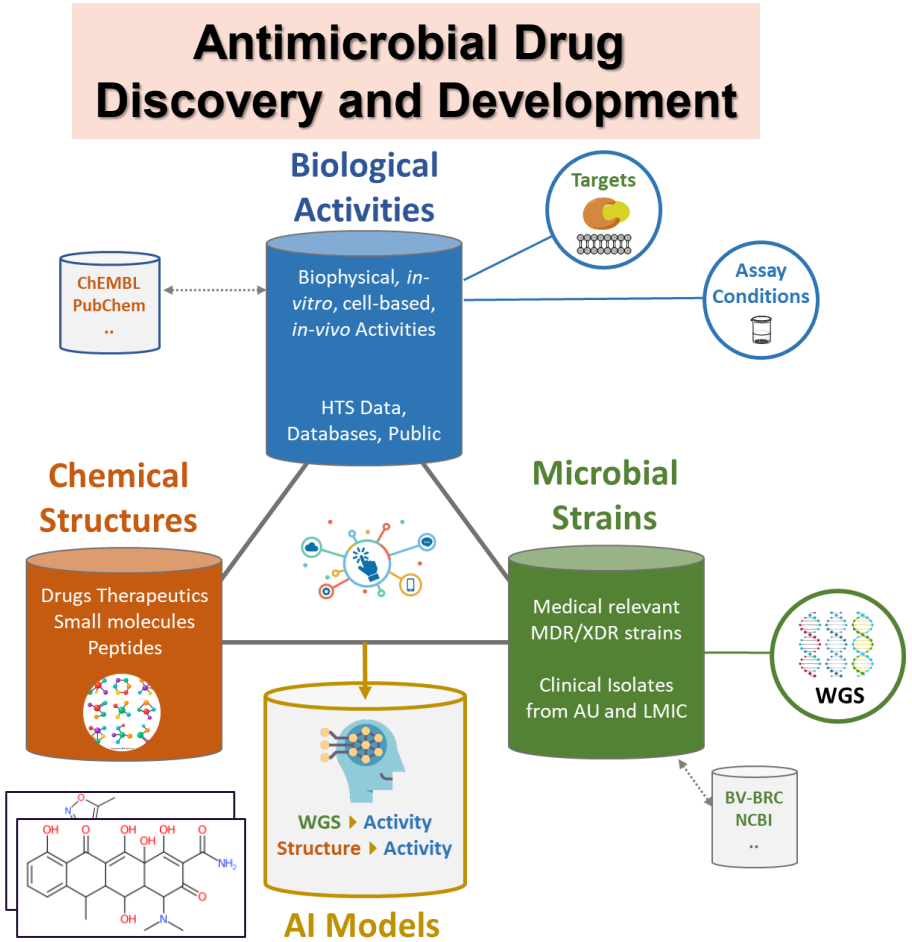
IC_{50} EC_{50} CC_{50}, %Inhibition, MIC, …
biophysical, in vitro, in vivo efficacy

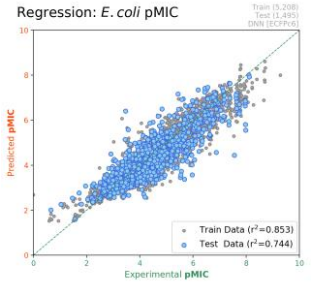
- Standardized results/units
- Standardized assay conditions ontologies
- **Non actives**
- **Combination/Synergies**

Biological Activity - ADMET

in vitro and in vivo toxicity, PK,

- Standardized results/units
- Standardized assay conditions ontologies
- **Non actives**
- **Combination/Synergies**





Chemical Structures

2D SMILES, HELM, BILN, …
3D MOL, SDF …

- Standardized structures protonation, tautomers, salt forms

Isolate/Sequence Data

short-reads Illumina
(**long-reads** ONT)
links to NCBI, PATRIC

- **Phenotype**
- Fast**q**, Fast**a**
- **Genotype:** Res/Vir genes, MLST

AI models

- Predicting Antimicrobial activity
- Genotype to phenotype

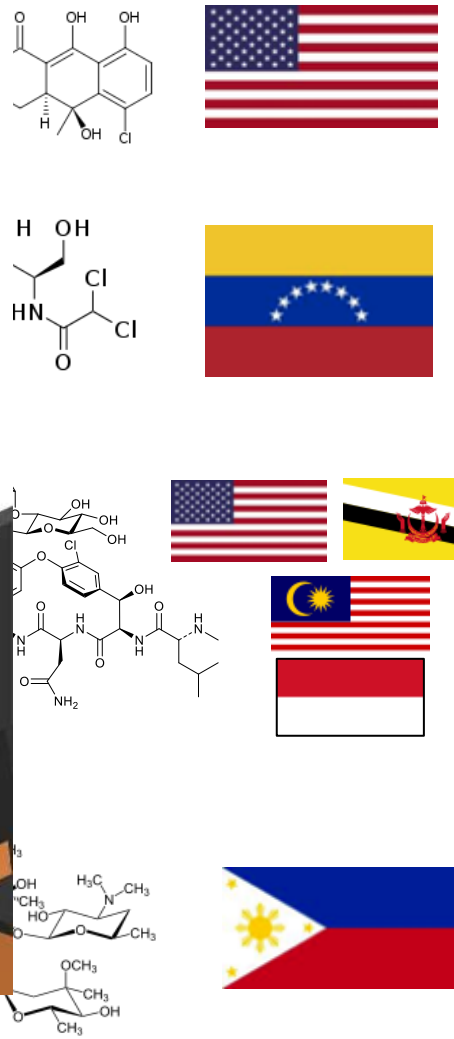
Bottleneck 5: Collaboration

THE UNIVERSITY OF QUEENSLAND AUSTRALIA

Antibiotic R&D Us

MTAs, CDAs, CRAs…

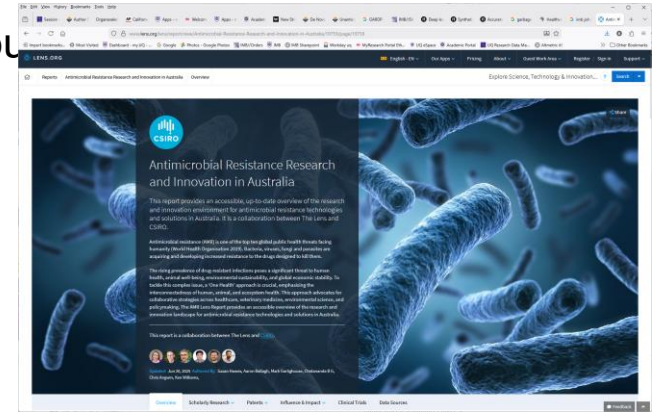
- **1945** tetracycline isolat
  Duggar, a retired botan
  in New York.
- **1947**, chloramphenicol
  Langham, an agricultur
- **1951**, vancomycin isola
  samples collected in Bo
  Conley, E.C. Kornfield
- **1952**, erythromycin isol
  biochemists at Eli Lilly
  the Philippines.



Bottleneck 5: Collaboration

- How do we enable better transparency and collaboration across academia, SMEs, and industry?
- Multiple small datasets held by individual entities
- Multiple entities trying to connect AMR researchers
- Lack of single-point government coordination
  - Department of Health, Disability and Ageing (hospitals, TGA, reimbu
    Australian Centre for Disease Control, NHMRC, MRFF)
  - Department of Industry, Science and Resources
  - Department of Agriculture, Fisheries and Forestry
  - Department of Defence (DMTC, DST, HSAA, SABRE Alliance)
  - Department of Education

AAMRNet
Australian Antimicrobial Resistance Network
Powered by MTP Connect



Our attempt at a solution to some of these issues. …

‘Crowdsourcing’ initiative to discover new antibiotics

CO-ADD Community for Open Antimicrobial Drug Discovery

CO-ADD Outputs

as of October 2024

52 countries

345 research groups

346,916 compounds received

11,576 hits in primary screenings

3227 confirmed hits that are non-cytotoxic

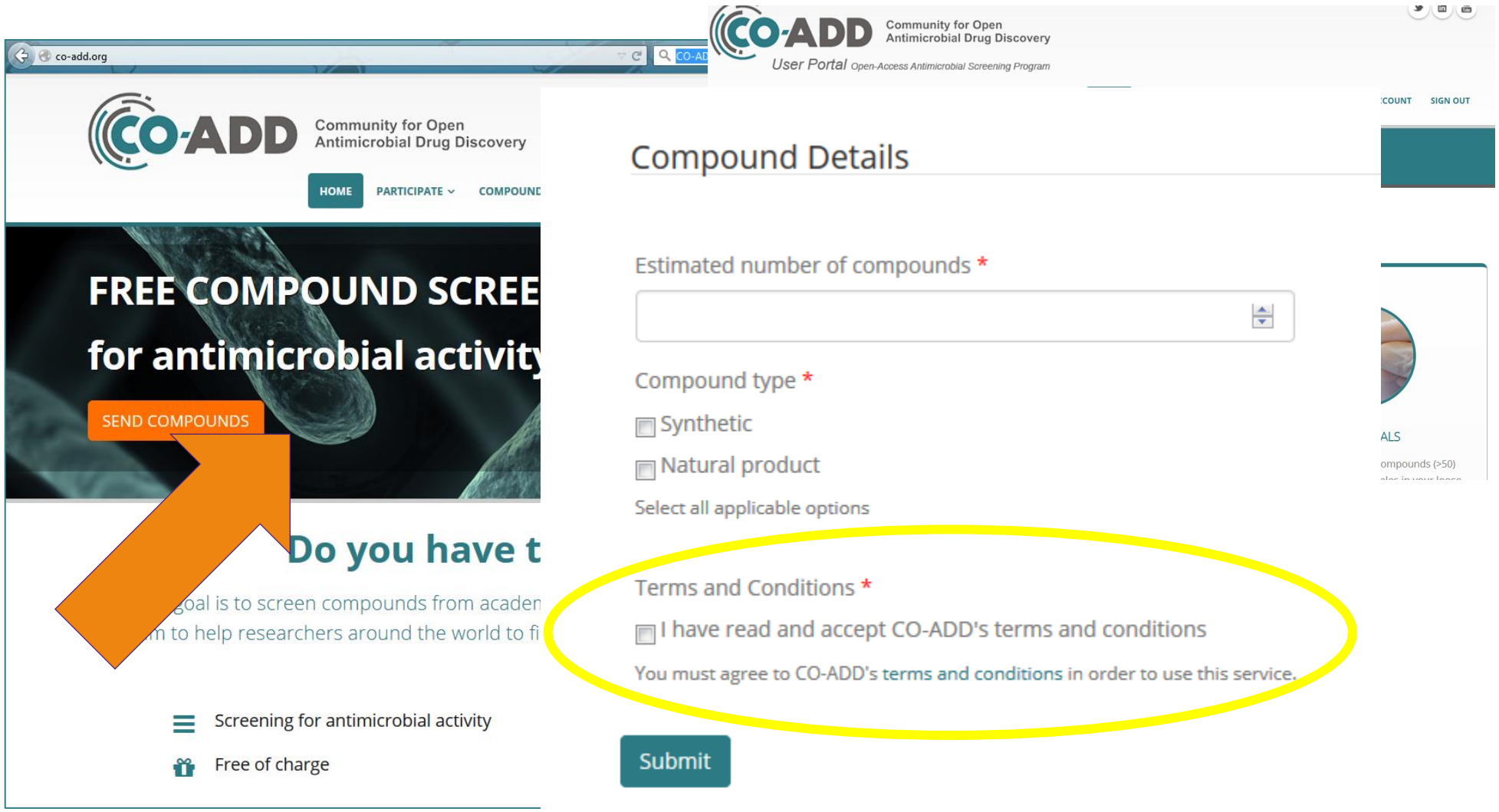
CO-ADD screening activities have helped research groups across the world. To date, collaborators have benefited from free screening of their compounds.

- **>129** research journal articles (+ 10 under review)
- **>40** oral and poster presentations
- **>41** grant applications
- **>16** patent applications

ACS Infect Dis 2020, 6: 1302-1034

www.co-add.org

www.co-add.org



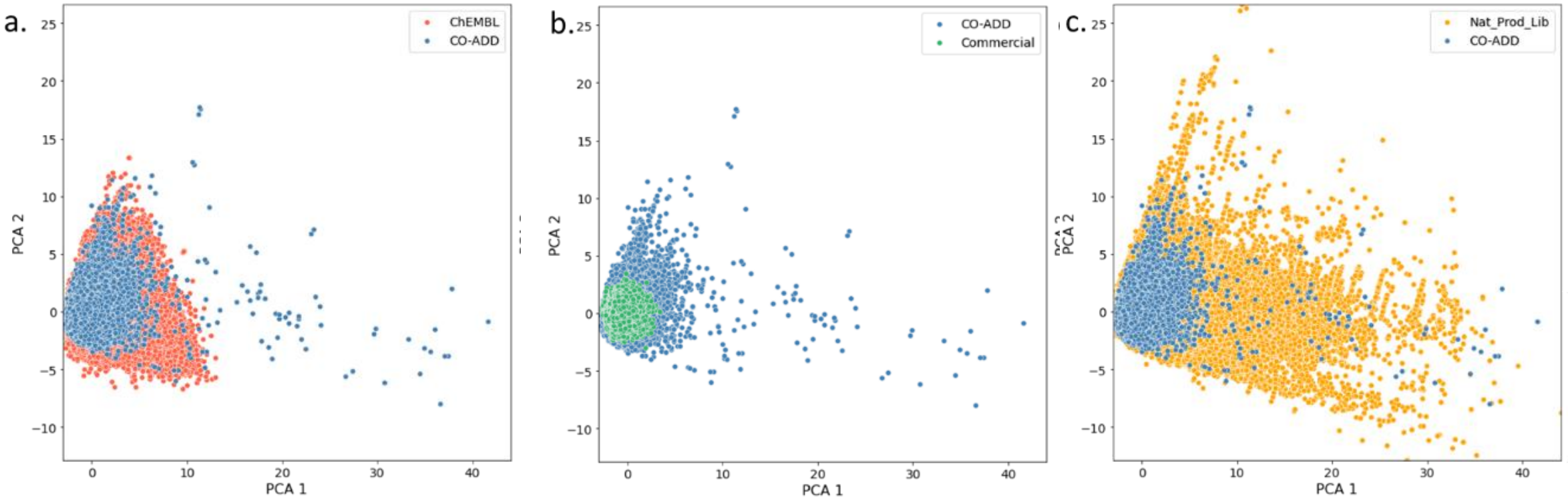
Chemical Diversity?

PCA biplot of major physicochemical properties (logP, RotBonds, MW, HBA and HBD) of CO-ADD library compared with:

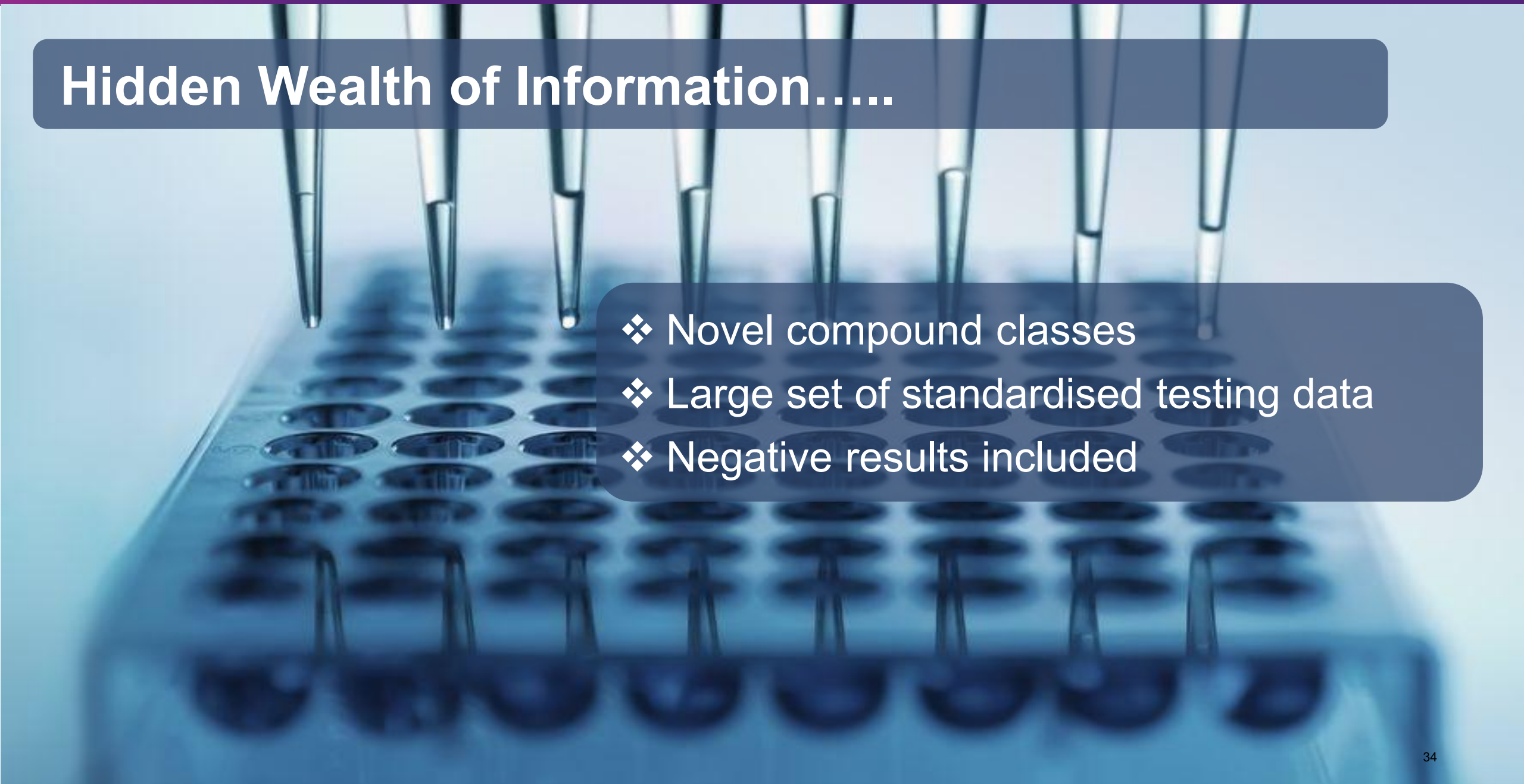
(a) ChEMBL

(b) Commercial library

c) Natural products



Hidden Wealth of Information…..



- Novel compound classes
- Large set of standardised testing data
- Negative results included

"Antimicrobial resistance is outpacing advances in modern medicine, threatening the health of families worldwide"

Dr. Tedros Adhanom Ghebreyesus, WHO Director-General.

AMR is not tomorrow's problem. It is a crisis that we must address today.

Matthew Todd

Matthew Todd is Professor and Chair of Drug Discovery at University College London. He has a significant interest in open science, and how it may be used to accelerate research, with particular emphasis on open source discovery of new medicines. He founded and currently leads several open science consortia such as Open Source Malaria (OSM) and is a founder of a broader Open Source Pharma movement. He leads the Structural Genomics Consortium (SGC) at UCL and leads the SGC's Open Chemistry Networks initiative as part of Target 2035. With Tim Willson of UNC Chapel Hill he led the medicinal chemistry core of the open READDI-AViDD antiviral discovery project.

https://todd-lers.github.io/about/

Leveraging Shared Data to Strengthen Discovery

Prof Matthew H. Todd
Chair of Drug Discovery, University College London
CSO, Structural Genomics Consortium at UCL
@mattoddchem

We're Surrounded by Open Data We Can Leverage

ON THE ANTIBACTERIAL ACTION OF CULTURES OF A PENICILLIUM, WITH SPECIAL REFERENCE TO THEIR USE IN THE ISOLATION OF *B. INFLUENZÆ*.

ALEXANDER FLEMING, F.R.C.S.

From the Laboratories of the Inoculation Department, St Mary's Hospital, London.

Received for publication May 10th, 1929.

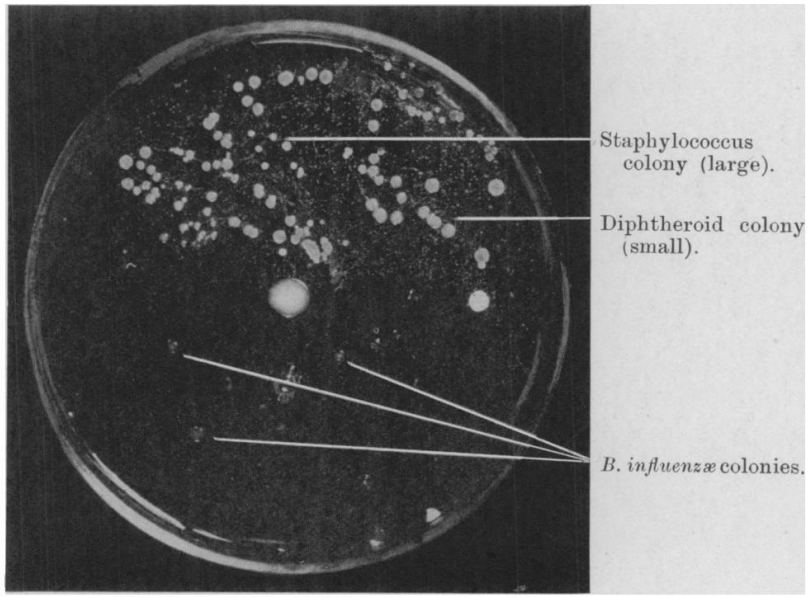


FIG. 4.—Photograph of a culture-plate (Fildes medium) which had been evenly planted with nasal mucus from an individual suffering from a "cold." Six drops of penicillin were spread over the lower half of the plate before incubation. Note profuse growth of staphylococci and diphtheroid bacilli in untreated half, whereas in **treated** half only some three colonies of *B. influenzæ* are seen.

TABLE III.—*Inhibitory Po*

	1/5.	1/10.
Staphylococcus aureus	0	0
„ *epidermidis*	0	0
Pneumococcus	0	0
Streptococcus (hæmolytic)	0	0
„ *viridans* (mouth)	0	0
„ *fæcalis*	++	++
B. anthracis	0	0
B. pseudo-tuberculosis rodentium	+	+
B. pullorum	+	+
B. dysenteriæ	+	++
B. coli	++	++
B. typhosus	++	++
B. pyocyaneus	++	++
B. proteus	++	++
V. choleræ	++	++

B. diphtheriæ (3 strains)	.
Streptococcus pyogenes (13 strains)	.
„ „ (1 „)	.
„ *fæcalis* (11 „)	.

A. Fleming, *Brit. J. Exp. Pathol.* **1929**, *10*, 226-236.

The Various “Open”s

*Open **Access** – to read*

*Open **Data** – to re-use*

*Open **Innovation** – to … what?*

*Open **Science** – something more, like samples, liberal licence*

*Open **Source** – all that, and **full details** and can **participate***

Licences (yawn…) are crucial

this is Wikipedia’s, on every page:

The Power of Open Data: **Re-use**

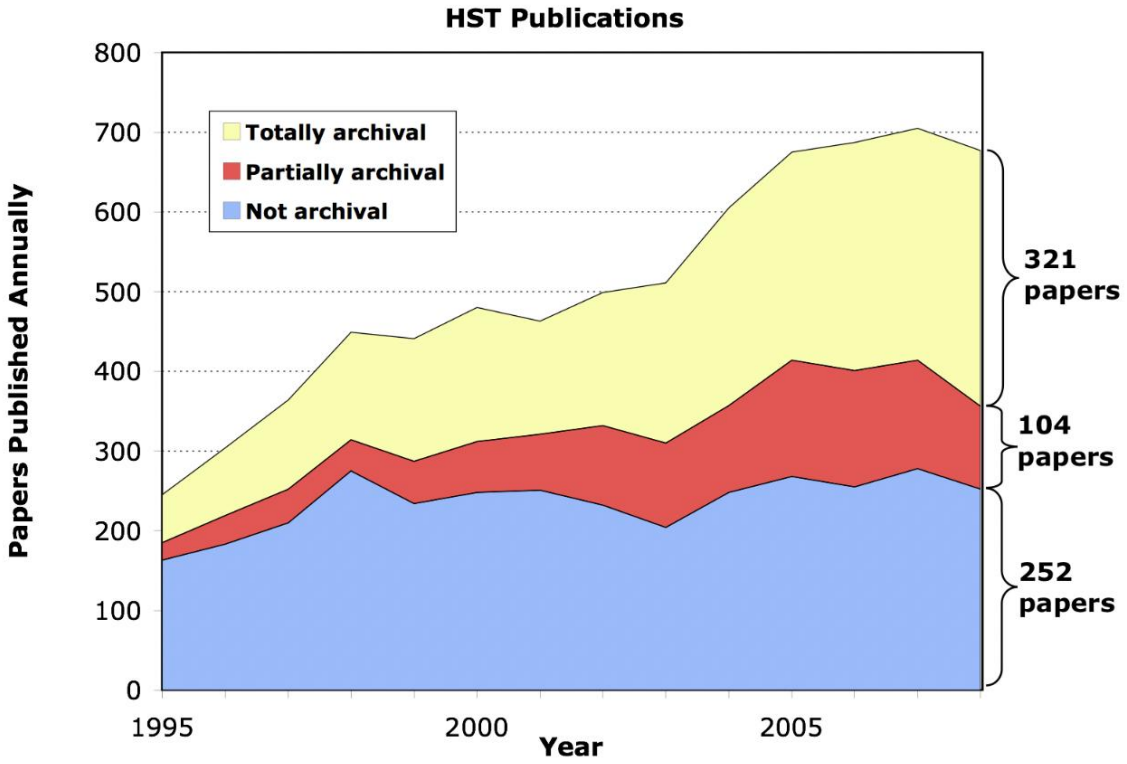


Figure 1: Number of annual publications using Hubble Telescope data. The publications have been divided into non-archival papers written by the original investigators (blue), totally archival publications not involving none of the original proposers (yellow), and papers that include data from multiple proposals with some being archival and some not (red). The number of archival papers has exceeded the number of PI-led papers since 2006.

The High Impact of Astronomical Data Archives

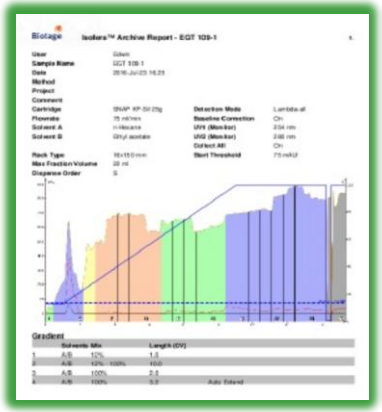
**Richard L. White (MAST/STScI), Alberto Accomazzi (ADS/CfA),
G. Bruce Berriman (IPAC/Caltech), Giuseppina Fabbiano (Chandra/CfA),
Barry F. Madore (IPAC/NED/OCIW), Joseph M. Mazzarella (IPAC/Caltech),
Arnold Rots (Chandra/CfA), Alan P. Smale (HEASARC/GSFC),
Lisa Storrie-Lombardi (SSC/Caltech), Sherry Winkelman (Chandra/CfA)**

What I Mean When I Talk about Open

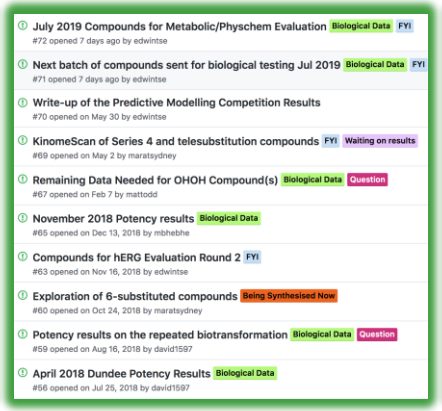
1st Law: All data are open and all ideas are shared
2nd Law: Anyone can take part at any level
3rd Law: There will be no patents
4th Law: Suggestions are the best form of criticism
5th Law: Public discussion is much more valuable than private email
6th Law: An open project is bigger than, and is not owned by, any given lab

Schisto: *Nature Chemistry* **2011**, *3*, 745; *PLoS NTD* **2011**, *5(9): e1260*. ***Malaria***: *Nature Commun.* **2024**, *15*, 937; *ACS Med. Chem. Lett.* **2024**, *15 1645; J. Med. Chem.* **2021**, *64*, 16450; *J. Org. Chem*. **2020**, *85*, 13438; *J. Med. Chem.* **2020**, *63*, 11585; *ACS Cent. Sci.* **2016**, *2*, 687. ***Antibiotics***: *ACS Infect. Dis.* **2023**, *9*, 2423. ***TB***: *J. Med. Chem.* **2018**, *61*, 11327. ***Antifungals***: *PLoS NTD* **2018**, *12(4)*: e0006437; *PLoS NTD* **2022**, *16*, e0010159; *Chem. Biodiversity* **2023**, *20*, e202300151. ***Platform***: *Chem. Sci.* **2015**, *6*, 1614; *Parasitology* **2014**, *141*, 148. ***Laws***: *ChemMedChem,* **2019**, *14,* 1804. ***Translation/Policy***: *PLoS Med.* **2017**, *14(4)*: e1002276; Wellcome Open Res. **2021**, *6*:146.

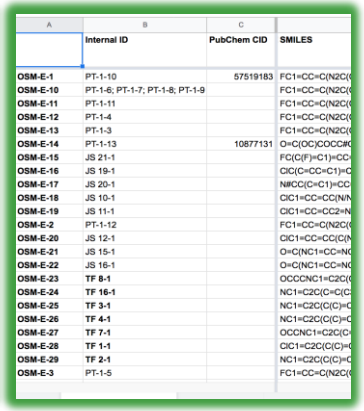
Components



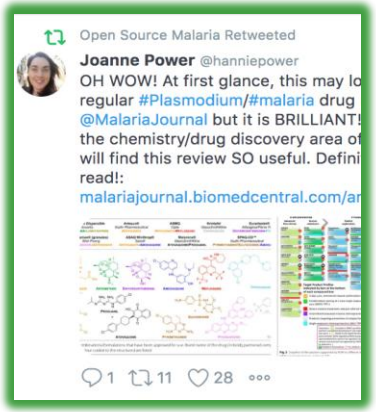
Laboratory Notebooks



Public To Do Lists/Discussion



Open Data



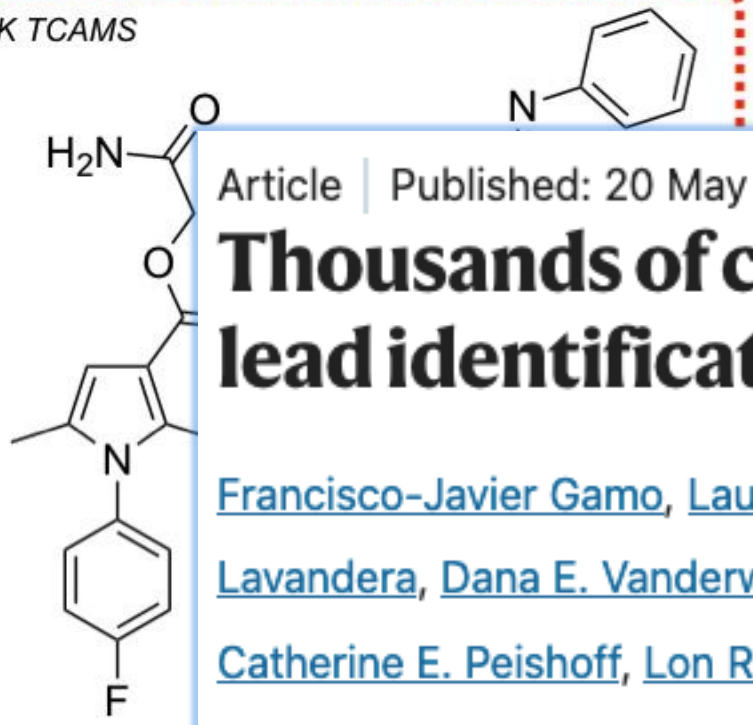
Community

Contributions

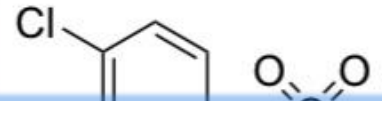
Students → *Pharma*

Open Source Malaria Series

GSK TCAMS



GSK TCAMS



Pfizer

SERIES
Potent
Ester Proble

Novel MoA: ASN Ligase of CA

Article | Published: 20 May 2010

Thousands of chemical starting points for antimalarial lead identification

Francisco-Javier Gamo, Laura M. Sanz, Jaume Vidal, Cristina de Cozar, Emilio Alvarez, Jose-Luis Lavandera, Dana E. Vanderwall, Darren V. S. Green, Vinod Kumar, Samiul Hasan, James R. Brown, Catherine E. Peishoff, Lon R. Cardon & Jose F. Garcia-Bustos

Nature **465**, 305–310 (2010) | Cite this article

Series typically not exhausted - Decision points made to move to another.

Anyone free to employ OSM infrastructure to explore these, or other, series

www.opensourcemalaria.org, @O_S_M

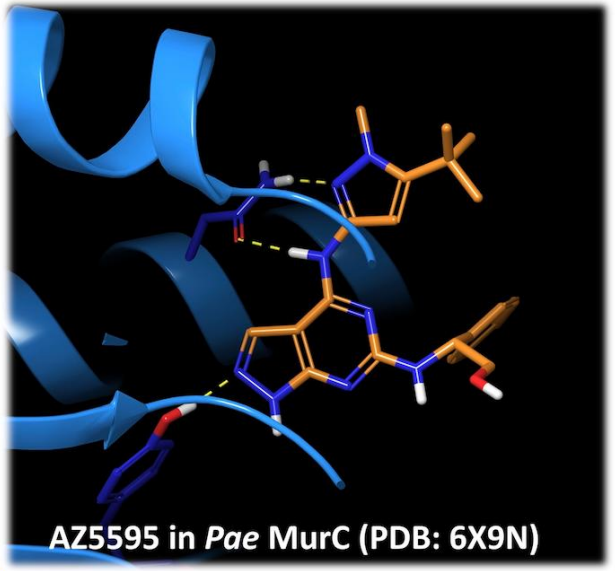
OPEN SOURCE ANTIBIOTICS SERIES 1 – MUR LIGASES

PROJECT DESCRIPTION

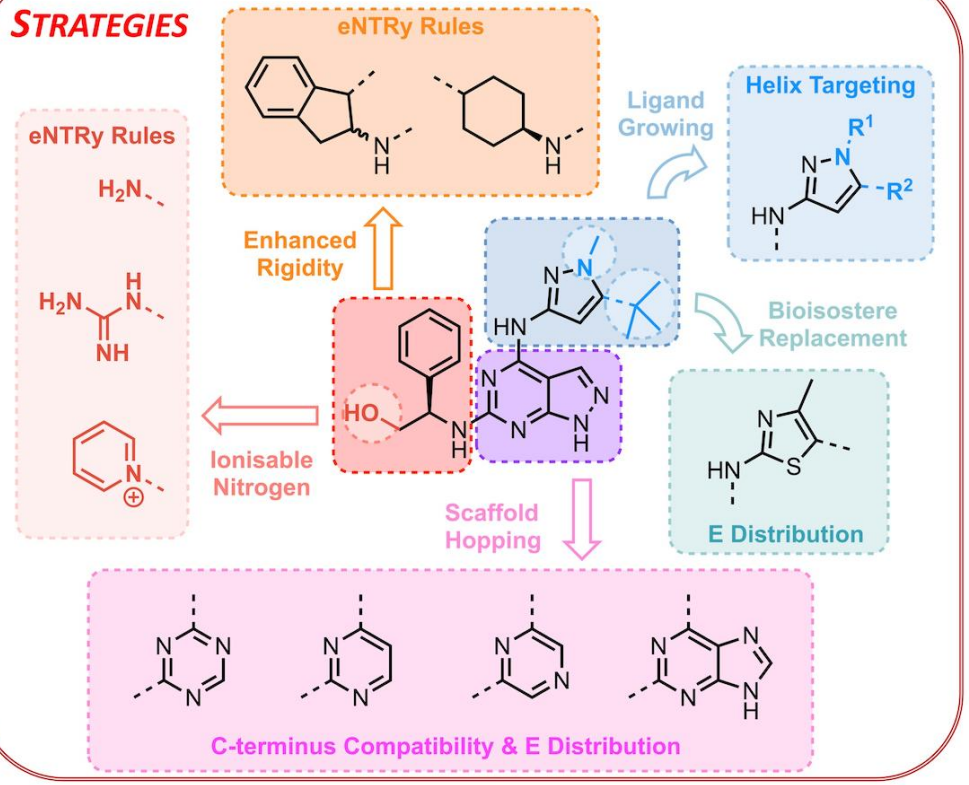
Discovered by **AstraZeneca**, but paused ❌

✅ Potent *in vitro,* ineffective vs Wild Type ❌

New Xstal structure - rational design ✅



STRATEGIES



JOINT EFFORTS

UCL — SYNTHESIS

Antibiotic Research UK — SPONSOR

diamond — CRYSTALS

WARWICK THE UNIVERSITY OF WARWICK — ENZYMOLOGY

AstraZeneca — SAMPLES/EXPERTISE

Northeastern University — EXPERTISE

Seattle Structural Genomics Center for Infectious Disease

Universitatis Kansiensis

CRYSTAL TRIALS

CMC — INFORMATICS

University of Copenhagen — AI/ML

https://github.com/opensourceantibiotics/murligase

ARTICLES | July 18, 2014

Pyrazolopyrimidines Establish MurC as a Vulnerable Target in *Pseudomonas aeruginosa* and *Escherichia coli*

Shahul Hameed P[†], Praveena Manjrekar[†], Murugan Chinnapattu[†], Vaishali Humnabadkar[†], Gajanan Shanbhag[†], Chaitanyakumar Kedari[†], Naina Vinay Mudugal[†],

Data from parked industrial series.

Open Source Antibiotics Series 2 – Diarylimidazoles vs. MRSA

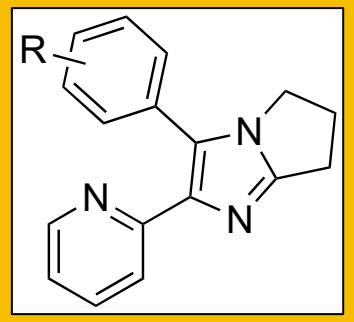
Funding via PharmAlliance

UCL

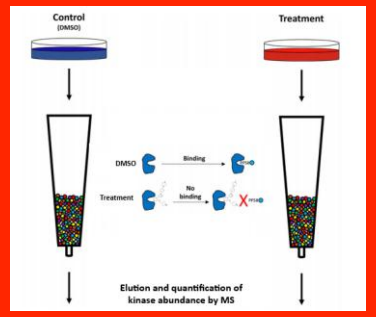
The University of North Carolina at Chapel Hill

Monash University

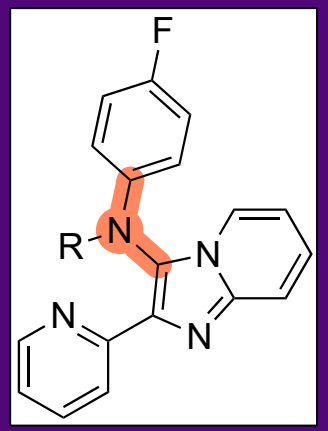
Core SAR



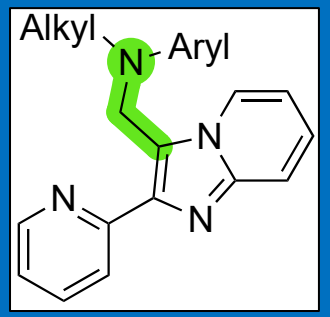
Mechanism



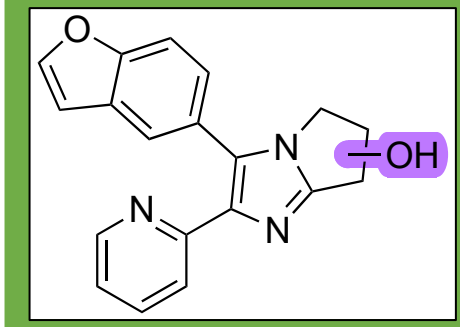
N Linker



Homologation



Metabolites



CO-ADD Community for Open Antimicrobial Drug Discovery

CMC

Citizen science

Northeastern University

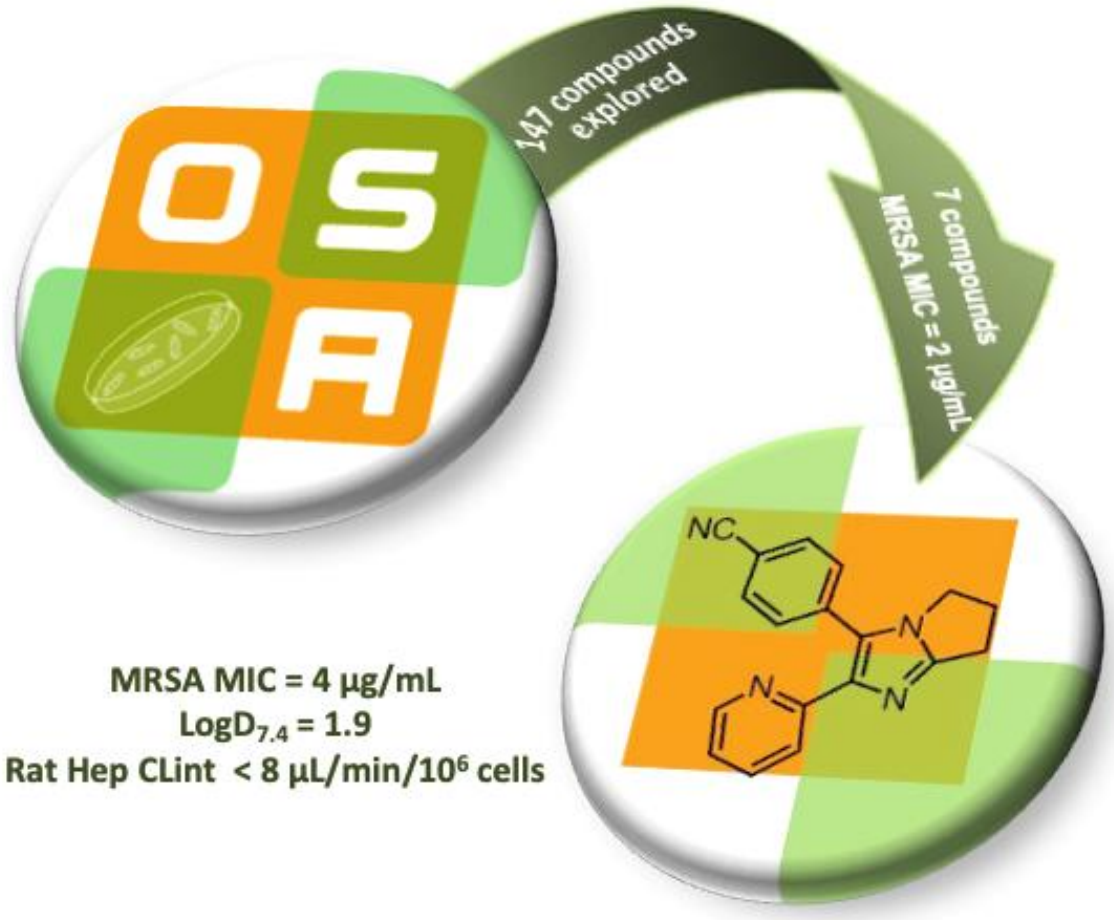
DNDi

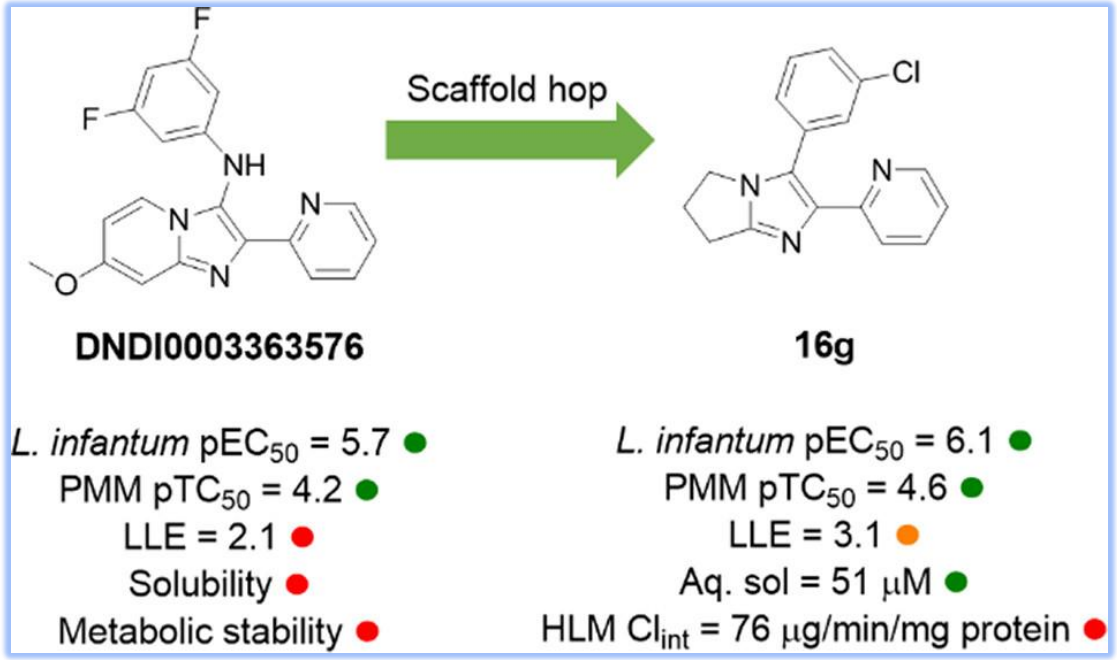
USP Universidade de São Paulo

Discovery Hypha

Additional Contributors Not Grant Funded

OSA2: SHARING COMPOUNDS → NEW PROJECTS





Parent Project: Antibiotics

Open Source Antibiotics - Simple Diarylimidazoles are Potent Against Methicillin Resistant Staphylococcus Aureus, *ACS Infect. Dis.* **2023**, *9*, 2423.

Sister Project: Leishmaniasis

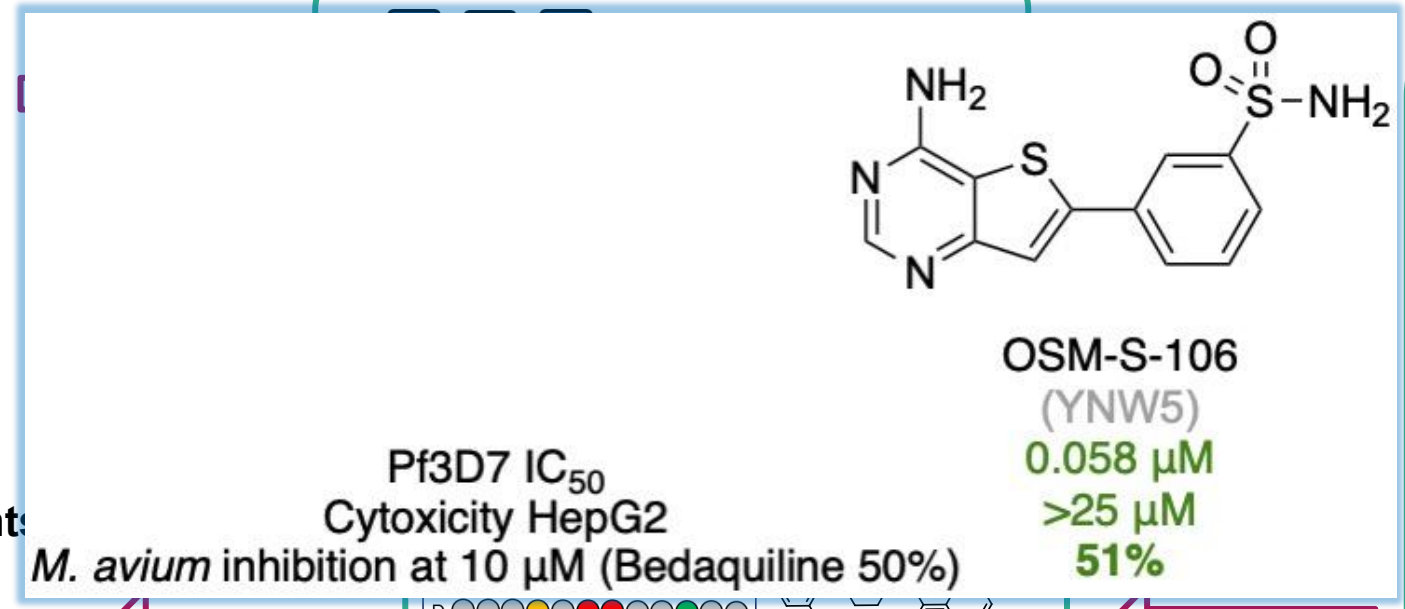
Structure-property Optimization of a Series of Imidazopyridines for Visceral Leishmaniasis, *ACS Infect. Dis.* **2023**, *9*, 1470.

Idler Compounds: Leveraging the Power of the Fridge

Accumulated compounds

Purchased and synthesized

Sharable library



Curate plate – share with UKHSA

Compound nomination

Curate for diversity

Plate preparation

- ✓ New data
- ✓ New starting points
- ✓ Maximize use

Open science

What Kinds of Data Are Missing?

Ideally we'd have a multitude of ways to evaluate compounds (like CO-ADD, UKHSA etc)

A simple submission process to submit data…

…to an open repository…

…that is suitable for machine learning.

An obvious need here: ***Accumulation***

Article | Open access | Published: 17 May 2022

Property space mapping of *Pseudomonas aeruginosa* permeability to small molecules

Inga V. Leus, Jon W. Weeks, Vincent Bonifay, Yue Shen, Liang Yang, Connor J. Cooper, Dinesh Nath, Adam S. Duerfeldt, Jeremy C. Smith, Jerry M. Parks, Valentin V. Rybenkov & Helen I. Zgurskaya

Scientific Reports **12**, Article number: 8220 (2022) | Cite this article

Article | Published: 10 May 2017

Predictive compound accumulation rules yield a broad-spectrum antibiotic

Michelle F. Richter, Bryon S. Drown, Andrew P. Riley, Alfredo Garcia, Tomohiro Shirai, Riley L. Svec & Paul J. Hergenrother

Nature **545**, 299–304 (2017) | Cite this article

SPARK, now part of CO-ADD

ACS Infectious Diseases > Vol 4/Issue 11 > Article

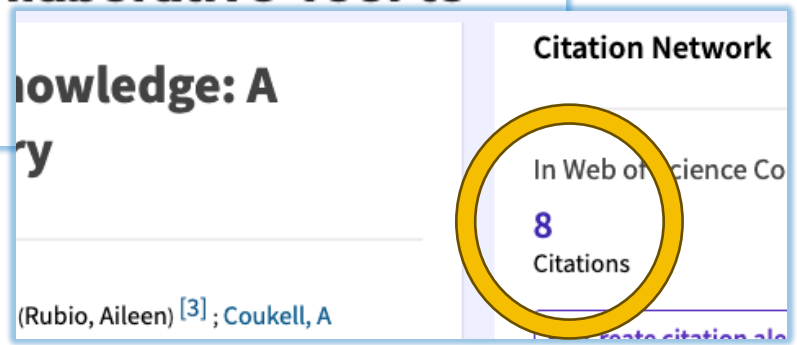
Subscribed

Cite Share Jump to Expand

VIEWPOINT | September 21, 2018

Shared Platform for Antibiotic Research and Knowledge: A Collaborative Tool to SPARK Antibiotic Discovery

Joe Thomas, Marc Navre, Aileen Rubio, and Allan Coukell*



"The *lack of well-described, easily accessible, and open-source datasets* is hindering the rate at which machine-learning and deep-learning tools are built and employed for antibiotic-prediction tasks"

A Brief Guide to Machine Learning for Antibiotic Discovery, G. Liu, J. M. Stokes, Curr Opin Microbiol **2022**, *69*, 102190 (DOI: 10.1016/j.mib.2022.102190)

"Unfortunately, so far, traditional **funding** streams have overlooked the importance of datasets. I anticipate that, in the near future, funding agencies will recognize this gap and start supporting projects with the exclusive aim of developing high-quality datasets."

AI in Infectious Diseases: The Role of Datasets, C. de la Fuente-Nunez, *Drug Resistance Updates* **2024**, *73*, 101067 (DOI: 10.1016/j.drup.2024.101067)

GSK and Fleming Initiative scientists unite to target AMR with advanced AI

by Ryan O'Hare

18 November 2025

An Abundance of Molecules! HTS & Generative AI

Article | Published: 24 October 2025

Deep-learning-based virtual screening of antibacterial compounds

Gabriele Scalia, Steven T. Rutherford, Ziqing Lu, Kerry R. Buchholz, Nicholas Skelton, Kangway Chuang, Nathaniel Diamant, Jan-Christian Hütter, Jerome-Maxim Luescher, Anh Miu, Jeff Blaney, Leo Gendelev, Elizabeth Skippington, Greg Zynda, Nia Dickson, Michał Koziarski, Yoshua Bengio, Aviv Regev, Man-Wah Tan & Tommaso Biancalani

Nature Biotechnology (2025) | Cite this article

Training dataset: experimental HTS (2 million compounds) – Proprietary.
A subset (GNEtolC) has been released.
Test set: 1.4 Bn from Enamine. *Usefully open!*
Code open on Github.

Article | Published: 22 March 2024

Generative AI for designing and validating easily synthesizable and structurally novel antibiotics

Kyle Swanson, Gary Liu, Denise B. Catacutan, Autumn Arnold, James Zou & Jonathan M. Stokes

Nature Machine Intelligence **6**, 338–353 (2024) | Cite this article

14K molecules screened (owned/commercial)
Generative models predicted many
Triaged by synthesisability
Enamine space/molecules used again!

Cell

Go to Cell on ScienceDirect

CellPress

Volume 188, Issue 21, 16 October 2025, Pages 5962-5979.e22

Article

A generative deep learning approach to *de novo* antibiotic design

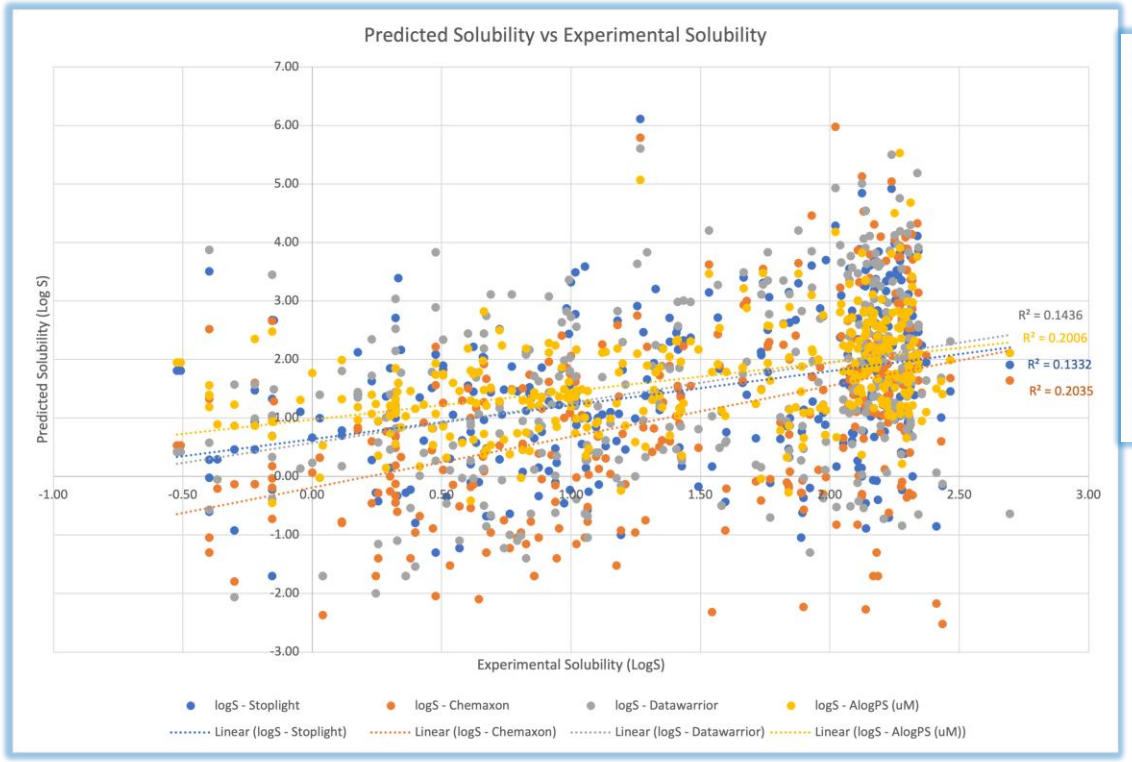
Aarti Krishnan [1 2 3 4 25], Melis N. Anahtar [1 2 4 5 25], Jacqueline A. Valeri [1 2 4 25], Wengong Jin [6 7], Nina M. Donghia [4], Leif Sieben [1 2 4 8], Andreas Luttens [1 2], Yu Zhang [1 2 4], Seyed Majed Modaresi [1 2 4], Andrew Hennes [1 4], Jenna Fromer [9], Parijat Bandyopadhyay [1 2], Jonathan C. Chen [1 2], Danyal Rehman [10], Ronak Desai [1 11 12], Paige Edwards [1 2], Ryan S. Lach [13], Marie-Stéphanie Aschtgen [14], Margaux Gaborieau [14], Massimiliano Gaetani [15 16]... James J. Collins [1 2 4 26 *]

78K screened, generative models trained
→ millions of possibles
Triaged down to 80. 27 attempted syntheses, leading to 2 new.
Also used Enamine/Broad space.

Predicting Solubility is Hard! But This Alone Would be Highly Impactful.

model predictions. Only En-10 and En-23 could be tested for toxicity in mouse models due to insufficient aqueous solubility of the other four generated antibacterial molecules. Indeed,

Swanson *et al, Nat. Machine Intell.* **2024**, *6*, 336 (10.1038/s42256-024-00809-7)



SMILES string · *lengths*	LogD float64	KSOL float64	HLM flo
22 — 88	-2 — 5.2 ø	0 — 325 ø	0
CN(C)CCCOc1ccc2c(c1)c1cc(C(=O)NCCN(C)C)ncc1n2C	null	194	
CNC(=O)COc1ccc2c(c1)c1cc3cnccc3c(C)c1n2C	null	12.5	
COc1ccc2c(c1)c1cc3c(C(=O)NCCN(C)C)nccc3c(C)c1n2C	null	157	
Cc1c2ccncc2cc2c3cc(OCCN4CCCCC4)ccc3n(C)c12	null	140	

OPEN ADMET

https://github.com/StructuralGenomicsConsortium/CNP15-Solubility-Analysis/issues/1

Shared Open Data Using Target-based approaches?

How might we become better at predicting hits vs under- or never-explored bacterial targets, through a large, open shared dataset?

Structural Genomics Consortium (SGC)

About

An international public-private partnership with a mission to accelerate the discovery of new medicines through open science

7 Research Sites

Research labs in Canada, the US, Germany, the UK and Brazil

An International Consortium

Partnerships with pharma and tech companies

Research Focus

Generating open-source protein–ligand data, chemical probes, and benchmarking datasets

20+ Years of Impact

Hundreds of chemical probes, thousands of structures, and widely used open datasets

SGC is leading the next phase of Target 2035

TARGET 2035

An SGC-led global open science initiative to “drug the entire genome”

Mission: To develop pharmacological modulators for every human protein by 2035.

Challenge: Artificial intelligence will enable this mission, but it needs large-scale, open datasets that do not yet exist.

Solution: In the next 5 years, SGC will generate and share protein-ligand datasets, enabling AI and machine learning to expedite the mission of Target 2035 more effectively and efficiently.

In the next 5 years, we will deliver:

- Ultra-large protein–ligand datasets
- FAIR, AI-ready datasets openly shared via the AIRCHECK platform
- Benchmarking challenges with CACHE, CASP & DREAM
- A global open-source machine learning network (MAINFRAME)
- AI & machine learning models validated on open data

- Validated chemical tools & AI-driven pipelines
- A faster and more efficient probe and hit discovery process across the proteome
- A sustainable open-science ecosystem linking academia, industry, and patients.

PARTNERS: PHARMA • AI/TECH • ACADEMIA • FOUNDATIONS • SGC GLOBAL LABS

Academia	Hospitals	Non-Profit	Pharma	Life Sciences	Chemistry	Tech
Goethe Universität, UCL, UNICAMP, EMBL-EBI, VHIO, Vall d'Hebron Institute of Oncology	UHN, SickKids	SGC	Pfizer, AstraZeneca, novo nordisk	abcam, NUVISAN	Vernalis, Enamine, CHEM SPACE	ThermoFisher Scientific, IBM

Learn more at: **https://www.target2035.net/**

TARGET 2035

How to get involved

Target 2035 is structured to support your contributions and amplify your impact

Contribute Proteins

Join the Protein Contribution Network and submit purified, high-quality proteins. These will be screened for ligands using advanced platforms.

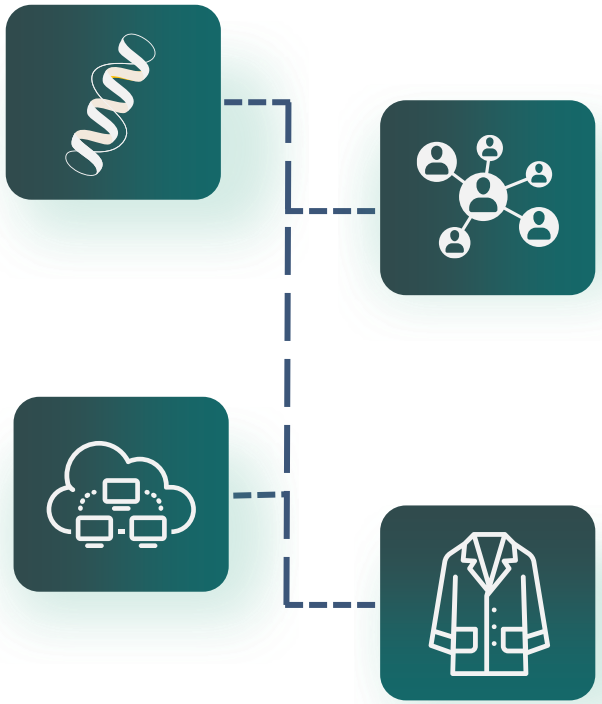
Learn more at:
https://www.thesgc.org/Target2035ProteinContribution

Participate in Open Benchmarking Challenges

Target 2035 provides a unique platform for computational scientists to benchmark hit-finding algorithms in real-world settings, with experimental testing of model predictions.

CACHE CHALLENGE

DREAM CHALLENGES powered by Sage Bionetworks



Join MAINFRAME

A new international network of machine learning researchers, computational chemists, and data scientists, which gives you access to curated datasets to test and benchmark your models.

Learn more at: **https://aircheck.ai/mainframe**

Be Part of the Mission

SGC is actively recruiting trainees to join the Target 2035. We offer opportunities for graduate students and Postdoctoral Fellows in both the experimental and computational arms of the SGC.

Find more on our Careers Page:
https://www.thesgc.org/careers

Join a global open science machine learning network for drug discovery

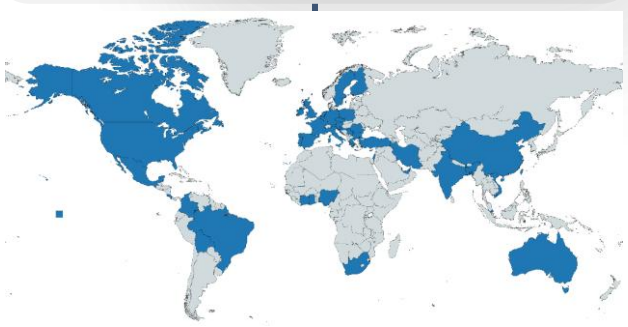
Early Access to Unique Data

Benefit from large-scale, high-quality datasets on protein-small molecule binding for training and improve your machine-learning models.

https://aircheck.ai

AIRCHECK

MAINFRAME



MAINFRAME has recruited over 200 scientists from 42 countries within less than a year since its launch!

Get state-of-the-art experimental validation

Participate in regular prospective or retrospective benchmarking challenges to compare the performance of your machine learning models.

Publications & Networking Opportunities

Engage with global experts and collaborate on impactful scientific papers summarizing challenge results and methods.

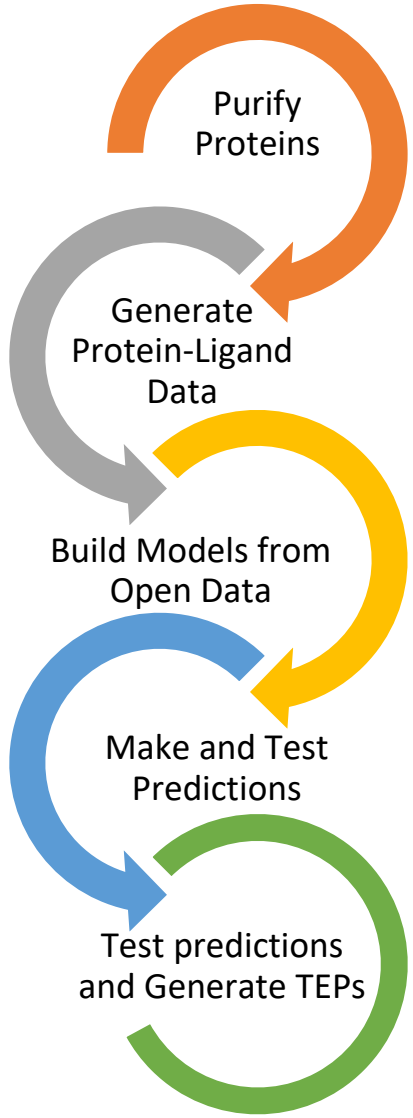
Get involved at

https://aircheck.ai/mainframe

The first MAINFRAME meeting is scheduled to take place in Barcelona in March 2026.

Towards Target 2035: Hit-Finding Roadmap of the Structural Genomics Consortium 2025–2030

A Major International Open Science Project in Artificial Intelligence and Machine Learning for Drug Discovery



- **Screen >2,000 human proteins against DEL (10B) libraries**
- Produce proteins at SGC and **obtain them from the community**

- Generate ligand binding data experimentally at SGC and in Technology Partners
- ASMS and DEL are the initial screening platforms

- Make screening data and metadata available via SGC database (AIRCHECK)
- **Build models and predict hits** in consortium and **through benchmarking challenges**

- Procure compounds and test predictions at SGC hubs and in Technology Partners
- Make hits, data and algorithms available without restriction

Deliverables:

- **Experimentally verified hits for >500 human proteins**
- **Open protein/ligand data for 2,000 proteins**
- **Improved hit-finding algorithms**

SGC

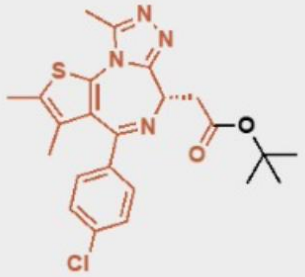
TRANSLATION: MAKING PROBES OPEN SPURS (NOT INHIBITS) DRUG DISCOVERY

SGC Chemical Probes Seed Drug Discovery

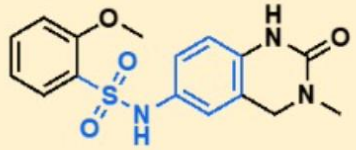
Examples of SGC Chemical Probe-Enabled Clinical Programs (a total of 85)

SGC

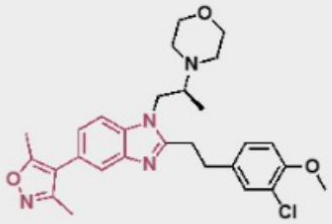
SGC Probe



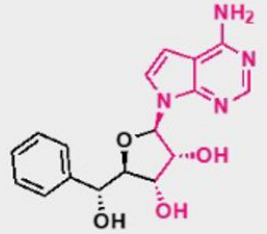
JQ1



PFI-1

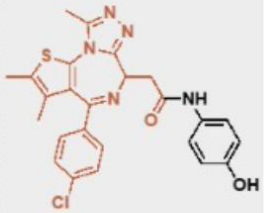


CBP-30



LLY-283

Clinical Candidate

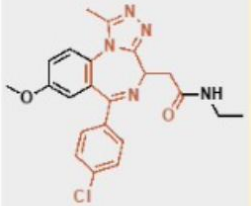


OTX015

Phase 2b

Solid Tumors

MSD/ Mitsubishi Tanabe

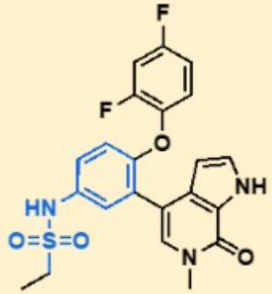


Molibresib

Phase 1

Advanced Lymphoma

GSK

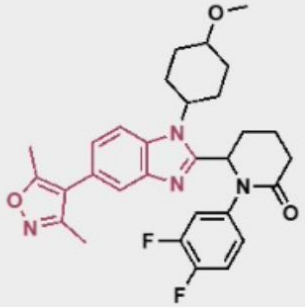


Mivebresib

Phase 1

Advanced Lymphoma

GSK

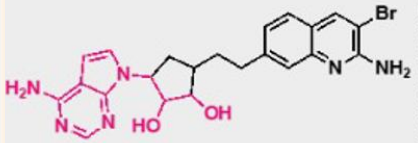


CCS1477

Phase 1/2

Prostate Cancer

CellCentric



JNJ64619178 – Phase 1

Phase 1

Advanced Lymphoma

Solid Tumors

Janssen

Acknowledgements

OSA Series 1 (Mur Ligases)

UCL: Dana Klug, Fahima Idiris, Yuhang Wang, Edwin Tse, Daniel Gedder, Kato Leonard, Giada Sabatino, Dayang Usop, Zige Bu, Brooks Paige, @dehaenw, Paul Stapleton, Alex Vaideanu, Andreas Schatzlein

Warwick: Chris Dowson, Laura Diaz Saez, Becca Steventon, Adrian Lloyd

Northeastern: Lori Ferrins and team

University of Cape Town H3D: Joe Eyermann, Kelly Chibale

Oxford/Diamond: Lizbe Koekemoer, Tobias Krojer, Frank von Delft, Paul Brennan

SSGCID/UCB: Bart Staker, Jan Abendroth, Peter Horanyi

Jan Jensen, Casper Steinman (Uni Copenhagen), Chris Swain (Cambridge MedChem Consulting), Finlay Maclean, Gemma Turon, Tata Consultancy Services, Vandan Revanur, @miquelduranfrigola, @aleixgimeno, @arnaucoma24

OSA Series 2 (Diarylimidazoles)

UCL: Edwin Tse, Dana Klug, Daniel Gedder, Paul Stapleton, Alex Vaideanu, Andreas Schatzlein

Northeastern: Lori Ferrins, Quillon Simpson, Maria Dichiara, Antonio Quotadamo, Bruno Quiroga, Jyoti Chauhan

UNC Chapel Hill: Lee Graves, Tom Gilbert, Laura Herring, Bill Zuercher, Álvaro Lorente-Macías, David Drewry

Monash: Sue Charman

University Sao Paulo: Flavio da Silva Emery

Hypha Discovery Ltd: Julia Shanu-Wilson, Liam Evans

DNDi: Ben Perry and Peter Sjö

Chris Swain (Cambridge MedChem Consulting), Antony Sama (citizen), Huanxu Xie and Yafeng Cao (WuXi)

Yinuo Wang, Yuhang Wang

Antibiotic RESEARCH UK

PharmAlliance

UKRI

wellcome

OSA

Coventry General Charities

Open Source Antibiotics

@OSantibiotics

REVIVE
by GARDP

Luiza Galarion

Luiza Galarion studied at the University of the Philippines, where she later worked in project development, management and part-time senior lecturer. She pursued her PhD in Molecular and Cellular Biology at the University of Leeds under the supervision of Alex O'Neill
She is currently a Research Fellow in Antibiotic Discovery under Prof. O'Neill's supervision and has been involved in projects which focus on antibiotic discovery from non-canonical sources and understanding genetic basis for antibiotic resistance in the important human pathogen, *Staphylococcus aureus*.
In 2023, Luiza joined Alex, a team from The University of Edinburgh, and GARDP in curating and supporting the development of AntibioticDB, an open-access database first introduced in 2017 which captures relevant information on compounds with known or potential antibacterial activity, a project that has been under the support and management of GARDP since 2021.

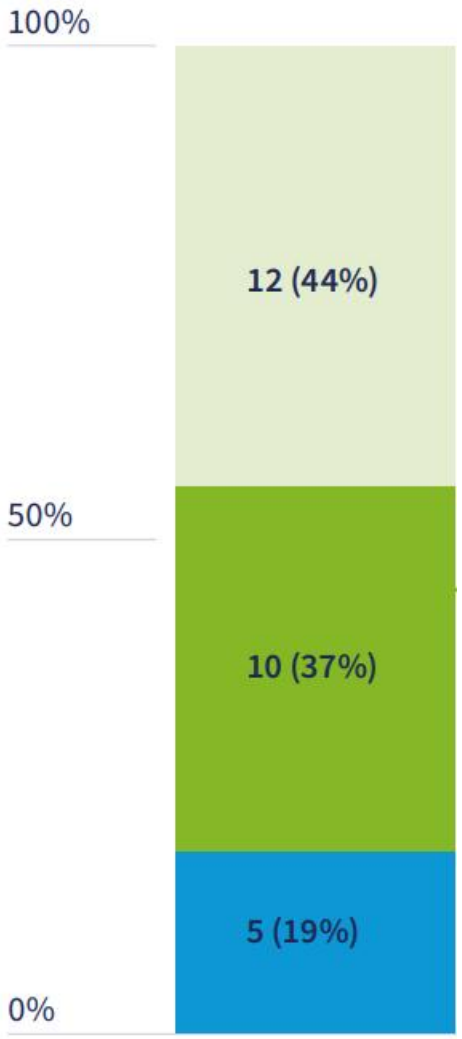
AntibioticDB: A Tool for Smarter Discovery

https://antibioticdb.com

Analysis of antibacterial agents in clinical and preclinical development

Overview and analysis 2025

World Health Organization



- only 5 agents are considered ‘innovative’ by WHO
  - shows no cross resistance

(Figure adapted from https://www.who.int/publications/i/item/9789240113091)

AntibioticDB

https://antibioticdb.com

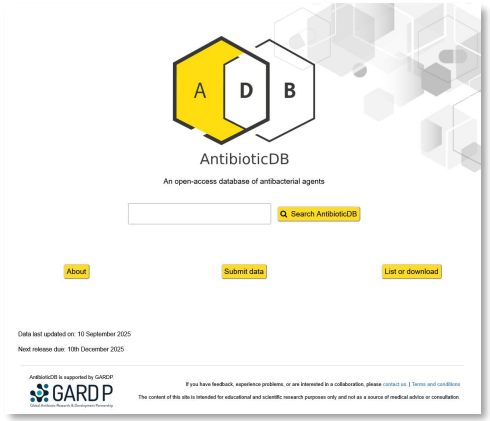
- first, online, freely and globally-accessible database of antibacterial agents

- valuable resource in antibacterial drug discovery for
  - starting compounds
  - revisiting discontinued/undeveloped drug candidates
  - tracking compounds of interest
  - compounds with particular properties/ targets

AntibioticDB created

BRITISH SOCIETY FOR ANTIMICROBIAL CHEMOTHERAPY

GARDP



new website release

2017 — 2018 — 2022 — 2023 — 2024 — 2025

Volume 73, Issue 9
September 2018

UNIVERSITY OF LEEDS

THE UNIVERSITY of EDINBURGH

new improvements

JOURNAL ARTICLE

Revitalizing the drug pipeline: AntibioticDB, an open access database to aid antibacterial research and development FREE

L J Farrell, R Lo, J J Wanford, A Jenkins, A Maxwell, L J V Piddock ✉ Author Notes

Journal of Antimicrobial Chemotherapy, Volume 73, Issue 9, September 2018, Pages 2284–2297,
https://doi.org/10.1093/jac/dky208
Published: 11 June 2018

The Team

managed and supported by:

GARDP

Current:
Alan Hennessy
Astrid Pentz-Murr
Alexandra Santu

Past:
Laura J.V. Piddock (creator, previous curator; formerly GARDP)
Ursula Theuretzbacher (previous curator; consultancy)

curation led by:

UNIVERSITY OF LEEDS

Current:
Alex J. O'Neill
Luiza H. Galarion

database development and integration to Guide to Pharmacology led by:

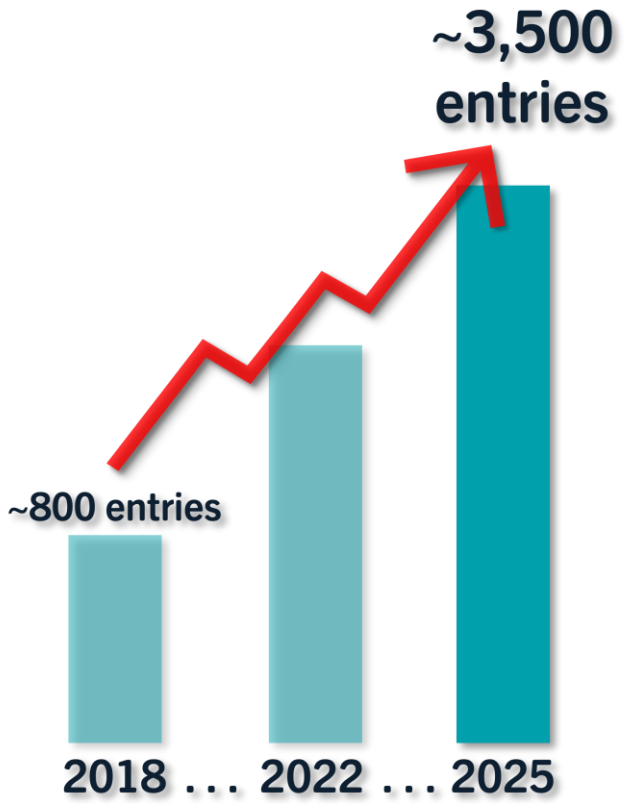
THE UNIVERSITY of EDINBURGH

Current:
Jamie A. Davies
Simon D. Harding
Jane F. Armstrong

Past:
Elena Faccenda (previous developer)
Liangcui Chu (previous developer)

Expanding the database content

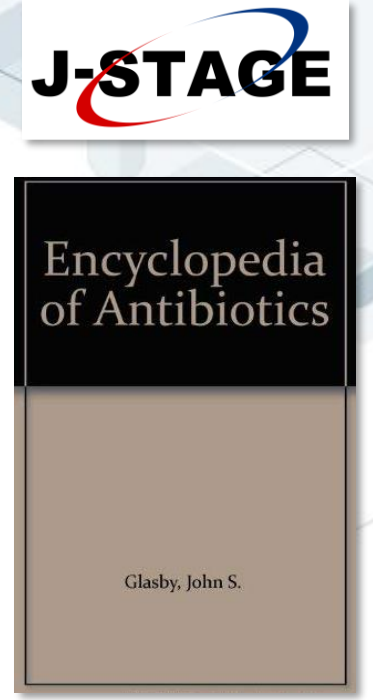
- >3,500 entries, a 4-fold increase over original release in 2018
- now includes historical natural product antibiotics, non-traditional modalities, and antimycobacterial agents



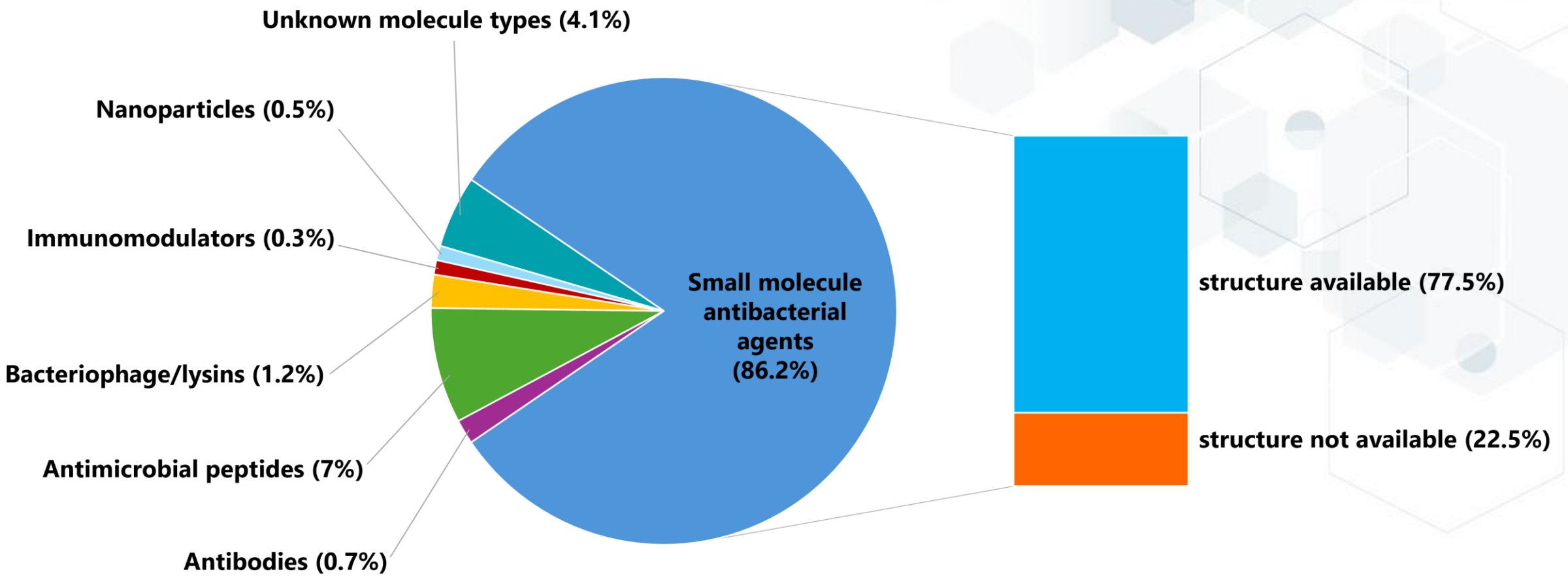
Key sources:

ESCMID
nature
OXFORD ACADEMIC
ACS Publications
Most Trusted. Most Cited. Most Read.
ASM Journals
Antimicrobial Agents and Chemotherapy
The Journal of Antibiotics
Journal of Antimicrobial Chemotherapy
International Society of Antimicrobial Chemotherapy
AMERICAN SOCIETY FOR MICROBIOLOGY
Science
WIPO
WORLD INTELLECTUAL PROPERTY ORGANIZATION
WORKING GROUP ON NEW TB DRUGS
IUPHAR/BPS Guide to PHARMACOLOGY
An expert-curated resource of pharmacological targets and the substances that act on them

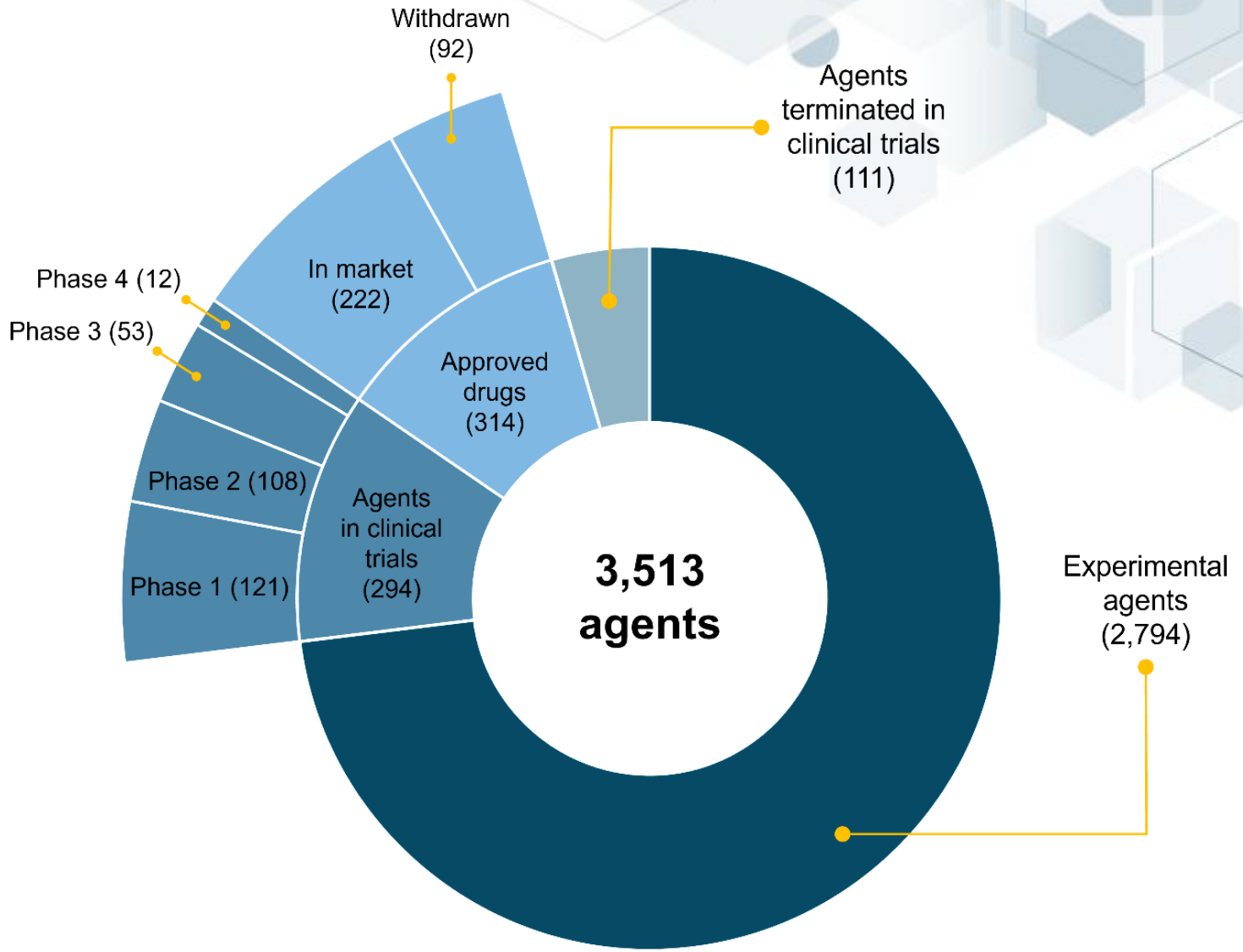
J-STAGE



Composition of AntibioticDB (as of November 2025)

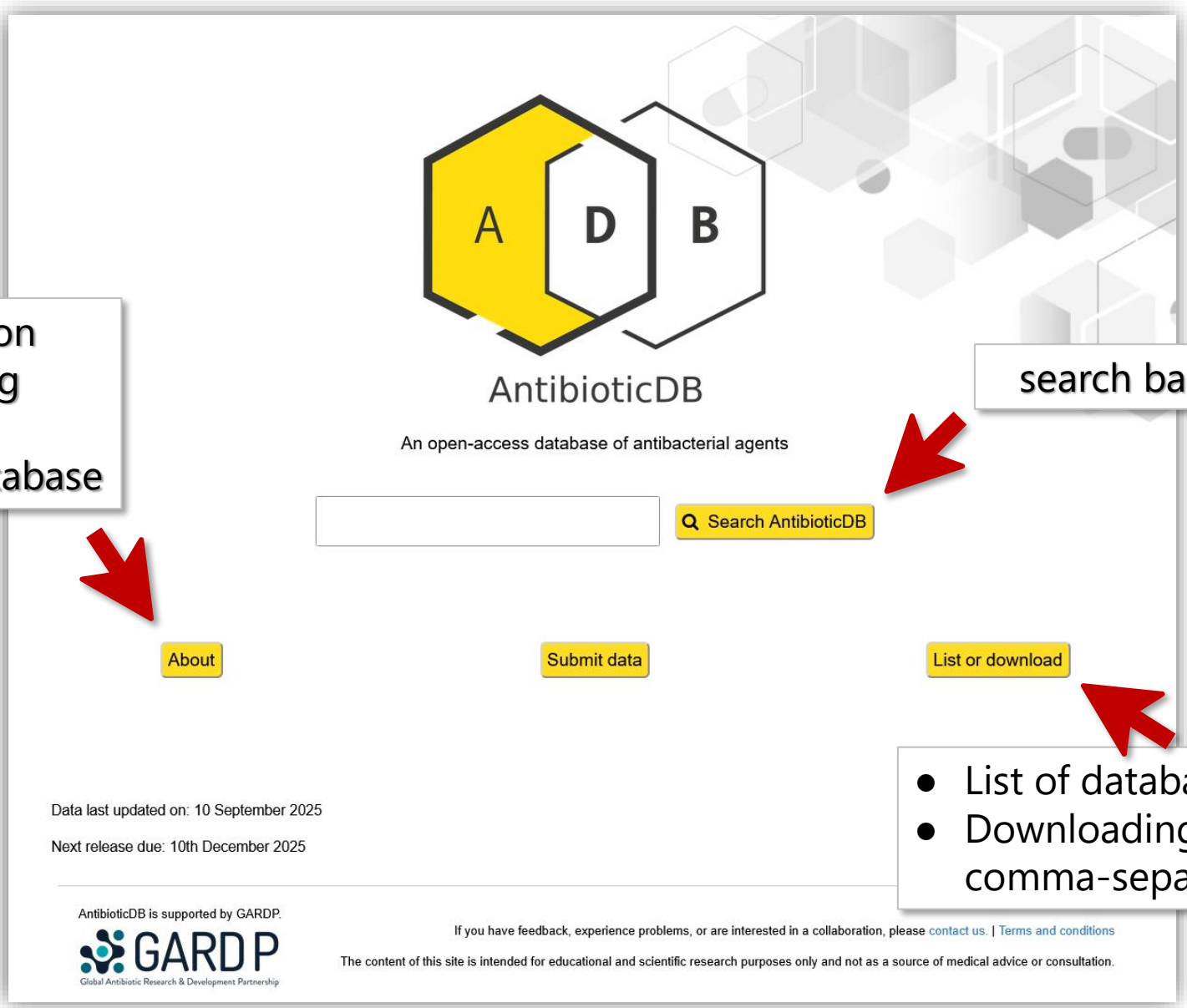


Agents in AntibioticDB and their development status (as of November 2025)



The web portal

- Database description
- 'Wildcard' searching instructions
- How to use the database



search bar

- List of database contents
- Downloading contents as a comma-separated value (.csv)

1. Search page

AntibioticDB

An open-access database of antibacterial agents

zo*

Search AntibioticDB

2. Results page

Search AntibioticDB

Home | About

Filter

Returned 8 results searching for **zo*** (Page 1 of 1)

Order results by: Match Go

*Accept the T&Cs to download.

Download 8 results

Zorbamycin

Description: Natural product from Streptomyces bikiniensis var. **zorbonensis**; protects mice from Escherichia coli when administered subcutaneously

Zorbonomycin

Description: Natural product from Streptomyces bikiniensis var. **zorbonensis**

Zoliflodacin

Zosurabalpin

Fisetin

Institute: **Zoonotic** Infectious Diseases, Key Laboratory for **Zoonosis** Research of the Ministry of Education, College of Veterinary...

3. Entry page

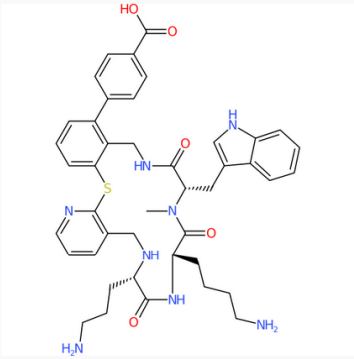
Update compound information

Synonym(s): RG6006

Class: Antimicrobial peptide

Spectrum of activity:	Gram-negative
Details of activity:	Active against carbapenem-resistant *Acinetobacter baumannii*; targets the LptB2FGC complex in the Gram-negative inner membrane blocking lipopolysaccharide transport
Propensity to select resistant mutants:	Yes, at 10^-7 to 10^-9 mutation frequency
Description:	Synthetic compound from the Tranzyme Pharma compound library (RO7075573) which was further modified to produce this second-generation antibiotic; >5-log reduction in neutropenic mouse thigh *Acinetobacter baumannii* infection model; a macrocyclic peptide
Institute where first reported:	Roche Pharma Research and Early Development, Immunology, Infectious Disease and Ophthalmology, Roche Innovation Center Basel, F. Hoffmann-La Roche, Basel, Switzerland
Year first mentioned:	2024
Highest developmental phase:	Phase 1 (NCT05614895)
Development status:	Active (as of 2024)

Chemical structure(s):



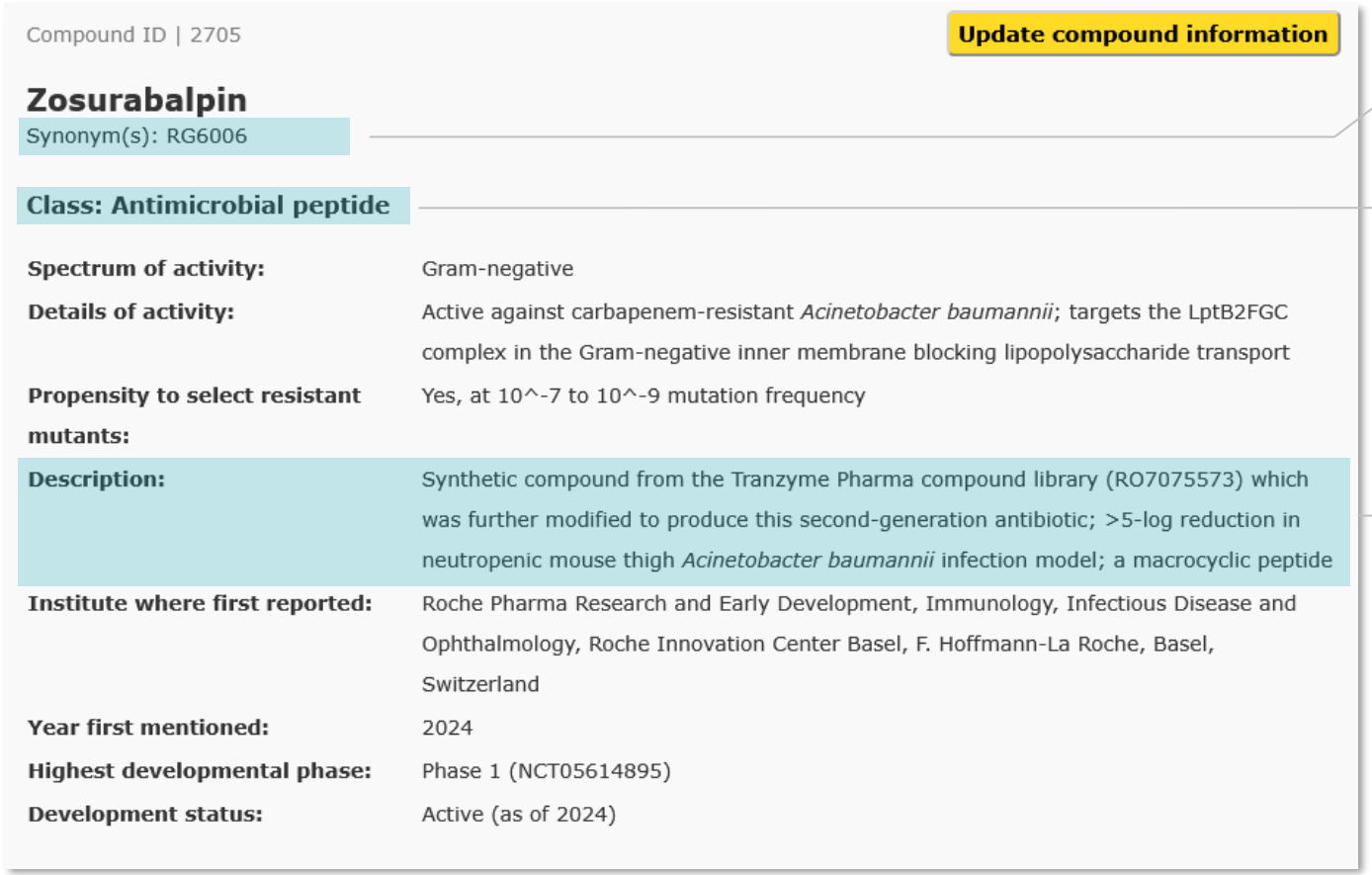
Molecular weight: 790.98

Iso. SMILES:	CN1[C@H](C(=O)NCC2=C(C=CC=C2SC3=C(CN[C@H](C(=O)N[C@H](C1=O)CCCCN)CCCN)C=CC=N3)C4=CC=C(C=C4)C(=O)O)CC5=CNC6=CC=CC=C65
InChI Key:	NJFUXFYUHIHHOJ-FSEITFBQSA-N
Can. SMILES:	CN1[C@@H](CC2=CNC3=C2C=CC=C3)C(=O)NCC4=C(C=CC=C4SC5=NC=CC=C5C N[C@@H](CCCN)C(=O)N[C@@H](CCCCN)C1=O)C6=CC=C(C=C6)C(=O)O
InChI:	InChI=1S/C43H50N8O5S/c1-51-37(23-30-25-47-34-12-3-2-10-32(30)34)40(53)49-26-33-31(27-16-18-28(19-17-27)43(55)56)11-6-15-38(33)57-41-29(9-8-22-46-41)24-48-35(14-7-21-45)39(52)50-36(42(51)54)13-4-5-20-44/h2-3,6,8-12,15-19,22,25,35-37,47-48H,4-5,7,13-14,20-21,23-24,26,44-45H2,1H3,(H,49,53)(H,50,52)(H,55,56)/t35-,36-,37-/m0/s1

External links:

PubChem link:	https://pubchem.ncbi.nlm.nih.gov/compound/148636827
Guide to Pharmacology:	zosurabalpin
Citations:	• https://academic.oup.com/ofid/article/10/Supplement_2/ofad500.1749/7446954 • https://www.nature.com/articles/s41586-023-06873-0
Patent:	US2019321440A1

Improved information capture and harmonisation of terminology



Compound ID | 2705

Update compound information

Zosurabalpin

Synonym(s): RG6006

Class: Antimicrobial peptide

Spectrum of activity:	Gram-negative
Details of activity:	Active against carbapenem-resistant *Acinetobacter baumannii*; targets the LptB2FGC complex in the Gram-negative inner membrane blocking lipopolysaccharide transport
Propensity to select resistant mutants:	Yes, at 10^-7 to 10^-9 mutation frequency
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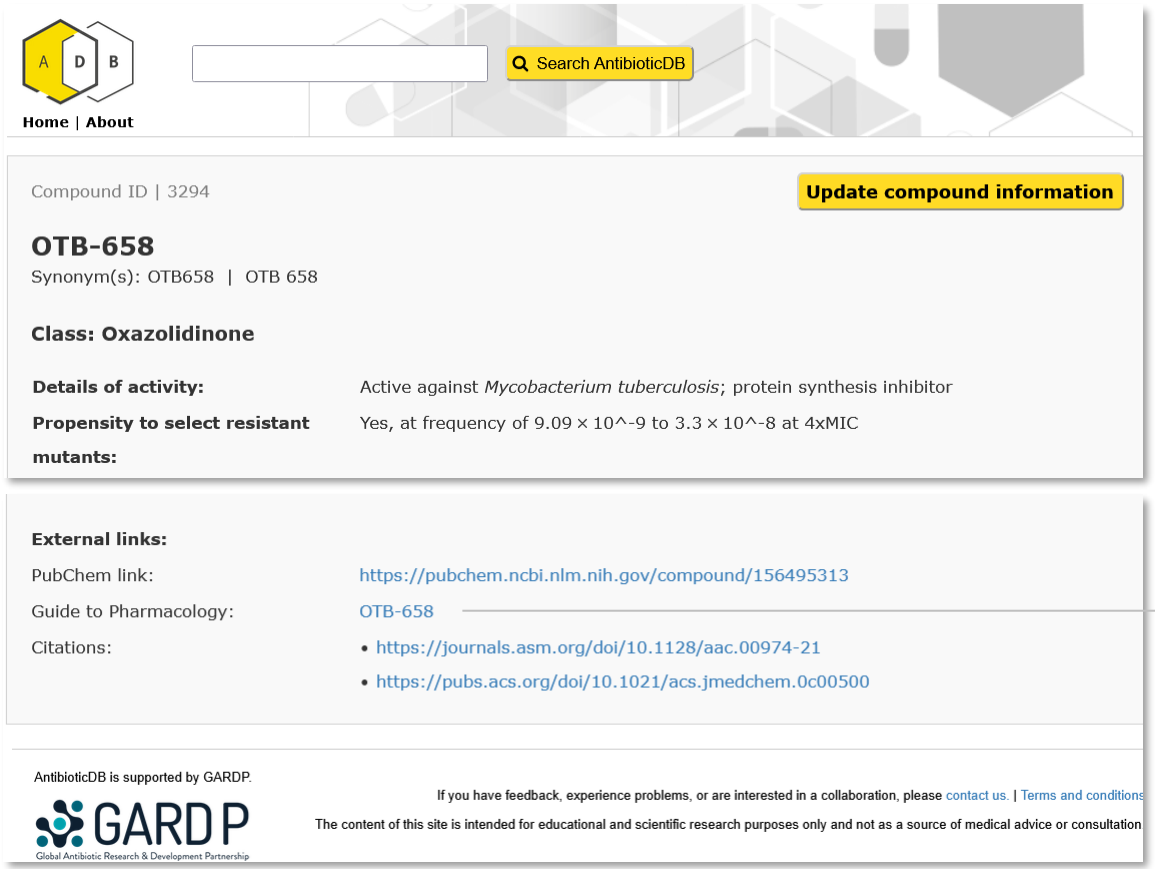
Year first mentioned:	2024
Highest developmental phase:	Phase 1 (NCT05614895)
Development status:	Active (as of 2024)

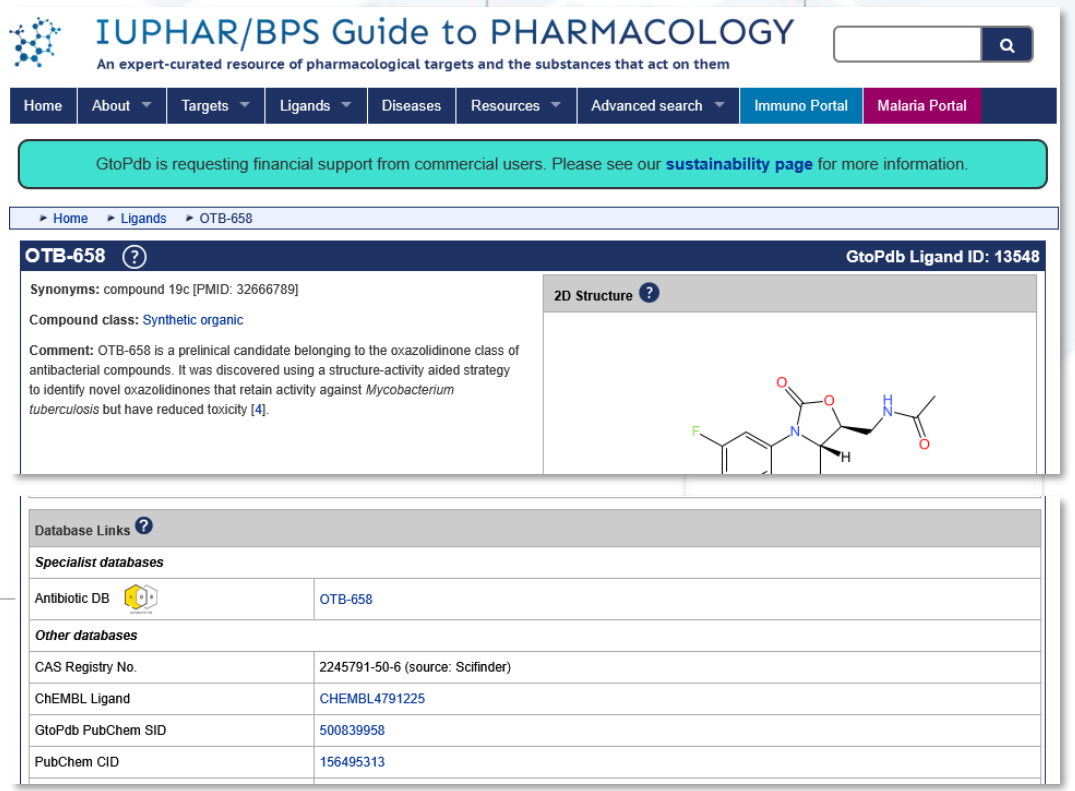
- synonym(s)
- harmonisation of antibacterial class
  - established antibacterial class
  - other recognised groupings (ex: antimicrobial peptide)
  - cellular pathway being inhibited/ specific drug target
  - non-traditional antibacterial modalities
  - nature of compound (ex: small molecule antibacterial agent, natural product antibiotic)
- origin of antibacterial agent (natural product, semi-synthetic, or synthetic)
- therapeutic potential where available

New functionalities: Integration with IUPHAR/BPS Guide to Pharmacology

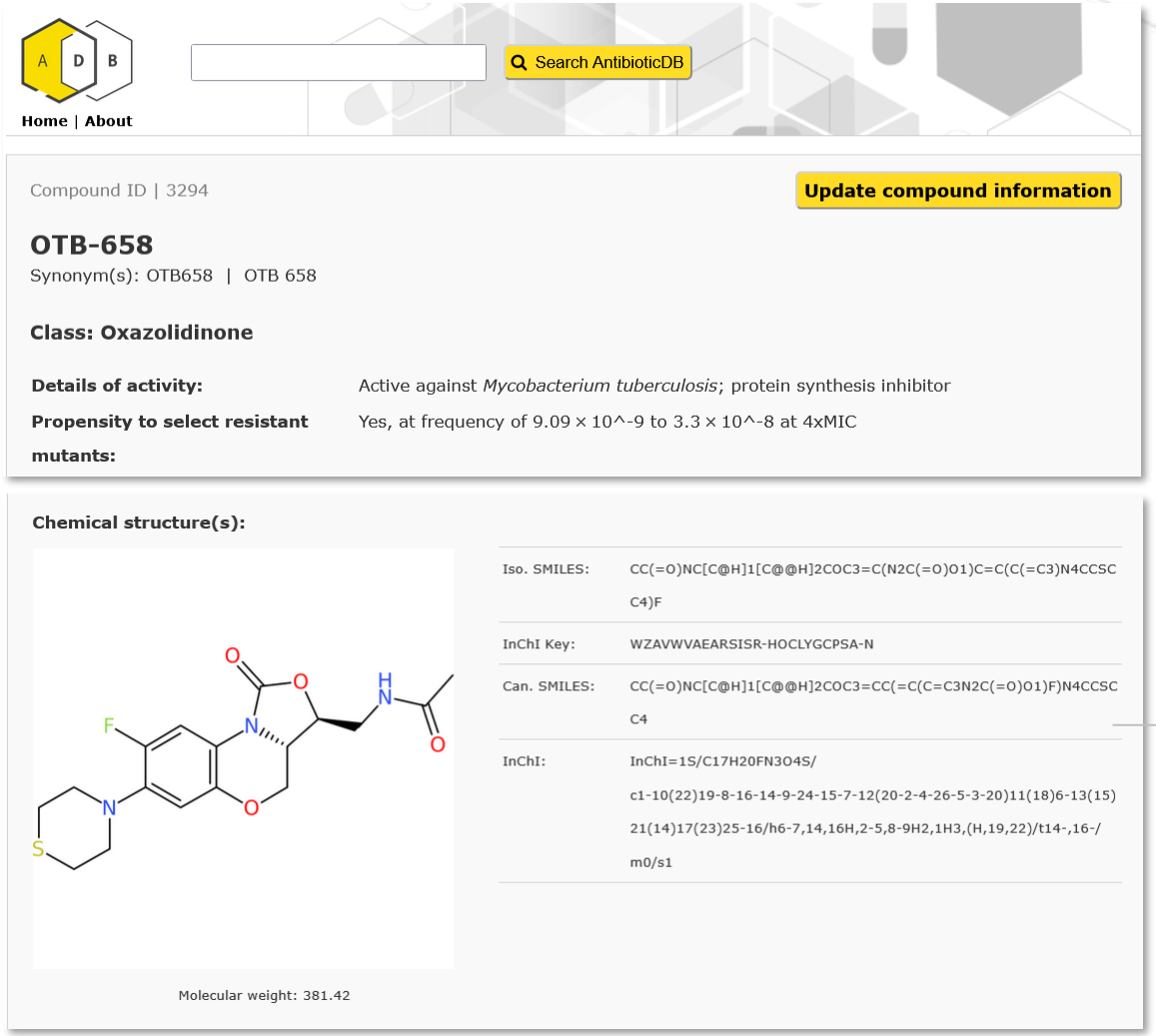
- reciprocal integration of AntibioticDB with IUPHAR/BPS Guide to Pharmacology (GtoPdb) since 2019
- 18% (~632) of AntibioticDB entries have reciprocal links to GtoPdb

https://www.guidetopharmacology.org





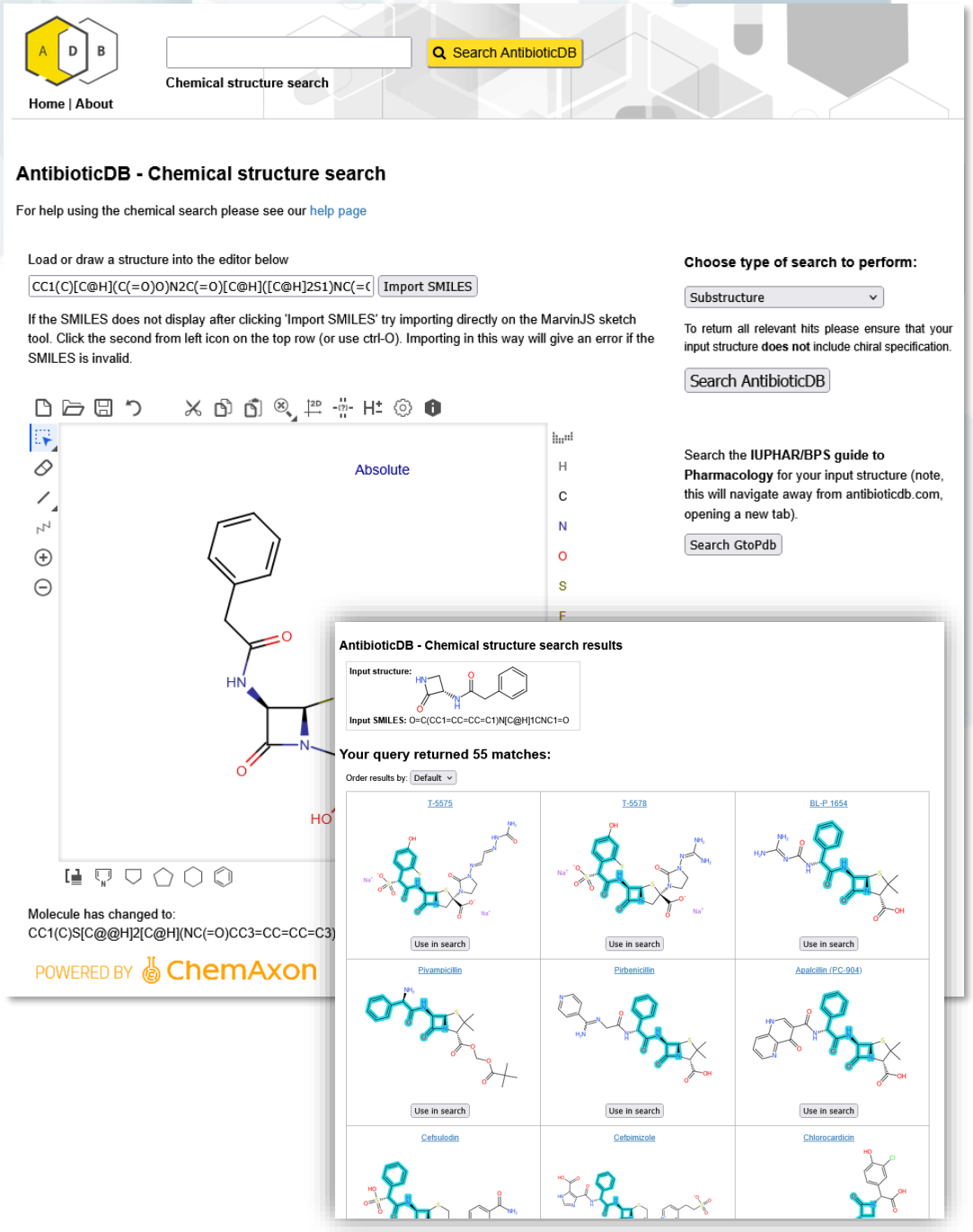
New functionalities: Updated structure information



- ~55% AntibioticDB entries have associated PubChem link
- ~72% of AntibioticDB entries have structural information captured as:
  - 2D structure representation
  - Molecular weight
  - Isomeric SMILES
  - InChI Key
  - Canonical SMILES
  - InChI

Underway...

- structure searching
- improved filtering options for searching:
  - by agent type (natural product, semisynthetic, synthetic)
  - by mechanism of action
  - by activity spectrum
  - direct-acting vs indirect-acting
  - by molecular weight range
- further addition of compounds to grow the database



Submit a compound / provide more information to an entry:

antibioticdb@gardp.org

AntibioticDB https://antibioticdb.com

- valuable reference and source of starting points for future research and (re-) development of antibacterial therapeutics
- >3,500 entries from experimental to preclinical/ clinical candidates, approved and withdrawn/discontinued drugs
- expanded to include both classical direct-acting and diverse non-canonical antibacterial agents (e.g., anti-virulence compounds, antibodies, bacteriophages, immunomodulating agents)
- addition of chemical identifiers and 2D structure representation widens its utility to include medicinal chemists

Submit a compound / provide more information to an entry:

antibioticdb@gardp.org

Acknowledgement

Current:
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Alexandra Santu
Past:
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Ursula Theuretzbacher (previous curator; consultancy)

Current:
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Past:
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Liangcui Chu (previous developer)

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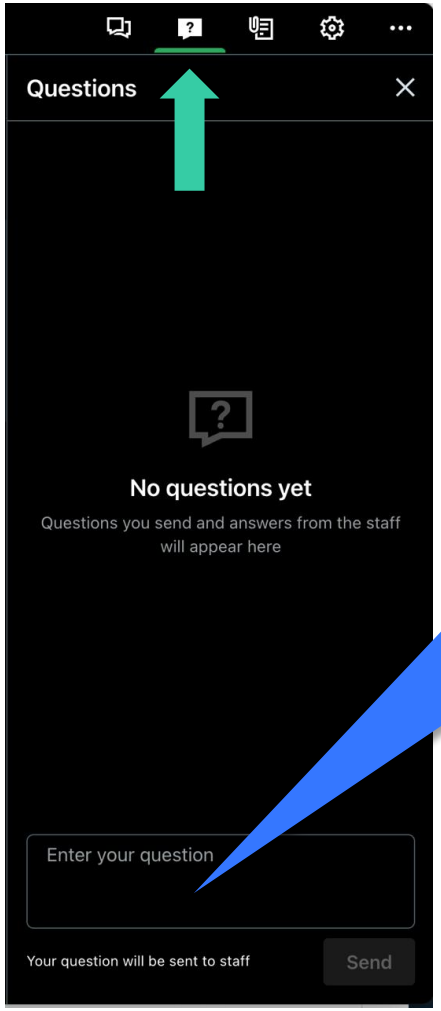
How to submit your questions

REVIVE by GARDP

If your question is addressed to a specific speaker, please include their name when submitting the question.



Please submit your questions through the box provided after clicking the ‘questions’ button. We will review all questions and respond to as many as possible after the presentation.

Survey – participate !

REVIVE by GARDP

OH AMR
European Partnership on One Health Antimicrobial Resistance

Co-funded by the European Union

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement N°101217154.

- Survey to identify gaps in strengthening research capacity in the field of antimicrobial resistance.
- Your insights will help strengthen AMR research capacity within the EU and beyond, by fostering stronger collaboration among AMR researchers and stakeholders from different disciplines and deepening our understanding of how we, the research community and stakeholders, can contribute synergistically.
- Please fill in the survey by 23rd December, 17:00 CET. The survey takes approximately 20 to 25 minutes to complete and can be filled out anonymously. In that case, no personal data will be linked to your answers. Please respond based on your personal experience.

https://forms.office.com/e/9c10cAXyDK

Antimicrobial Chemotherapy Conference ACC2026

REVIVE by GARDP

https://acc-conference.com/

The next REVIVE webinar will be announced soon!

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Thank you for joining us