

# Common data resources to aid antibiotic drug discovery

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# KEY FACTS ABOUT THE AMR ACCELERATOR

Public-Private collaboration with the shared goal of progressing the development of new medicines to treat or prevent resistant bacterial infections

9  
PROJECTS

13  
ANTIBACTERIAL  
PROGRAMMES

489 M€  
BUDGET

98  
PARTICIPANTS

18  
COUNTRIES

9  
YEARS  
(2019-2028)



[www.amr-accelerator.eu](http://www.amr-accelerator.eu)

# OBJECTIVES OF THE PROJECT

- Foster a wide-ranging series of projects that address many of the scientific challenges in AMR
- Progress a pipeline of potential medicines to treat patients with resistant bacterial infections
  - 10 preclinical candidates
  - 5 Phase II-ready assets
  - Phase II clinical trials



# AMR TOPICS COVERED

## TUBERCULOSIS & NTM



*Accelerating scientific discoveries and advancing the R&D pipeline of new and innovative agents to treat TB and NTM lung disease.*

## GRAM-NEGATIVES



*Advancing the R&D pipeline of new and innovative agents to address AMR in Gram-negative bacteria.*

## CAPABILITY BUILDING

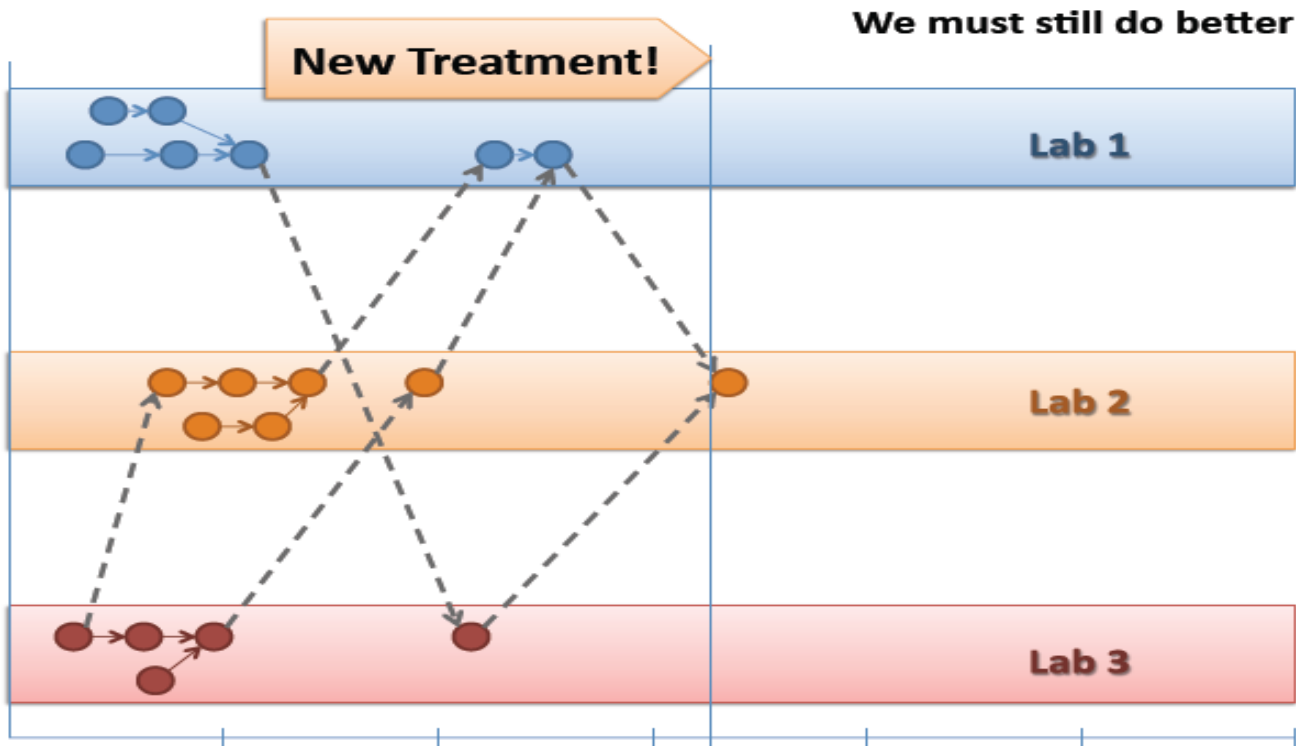


*Accelerating and validating scientific discoveries in AMR. Coordinating and supporting projects across the AMR Accelerator.*



# Guidelines, tools and infrastructure to support data and knowledge management

# WHY WE NEED A GOOD DATA MANAGEMENT?



Flow of information across collaborating yet competing groups with churning membership

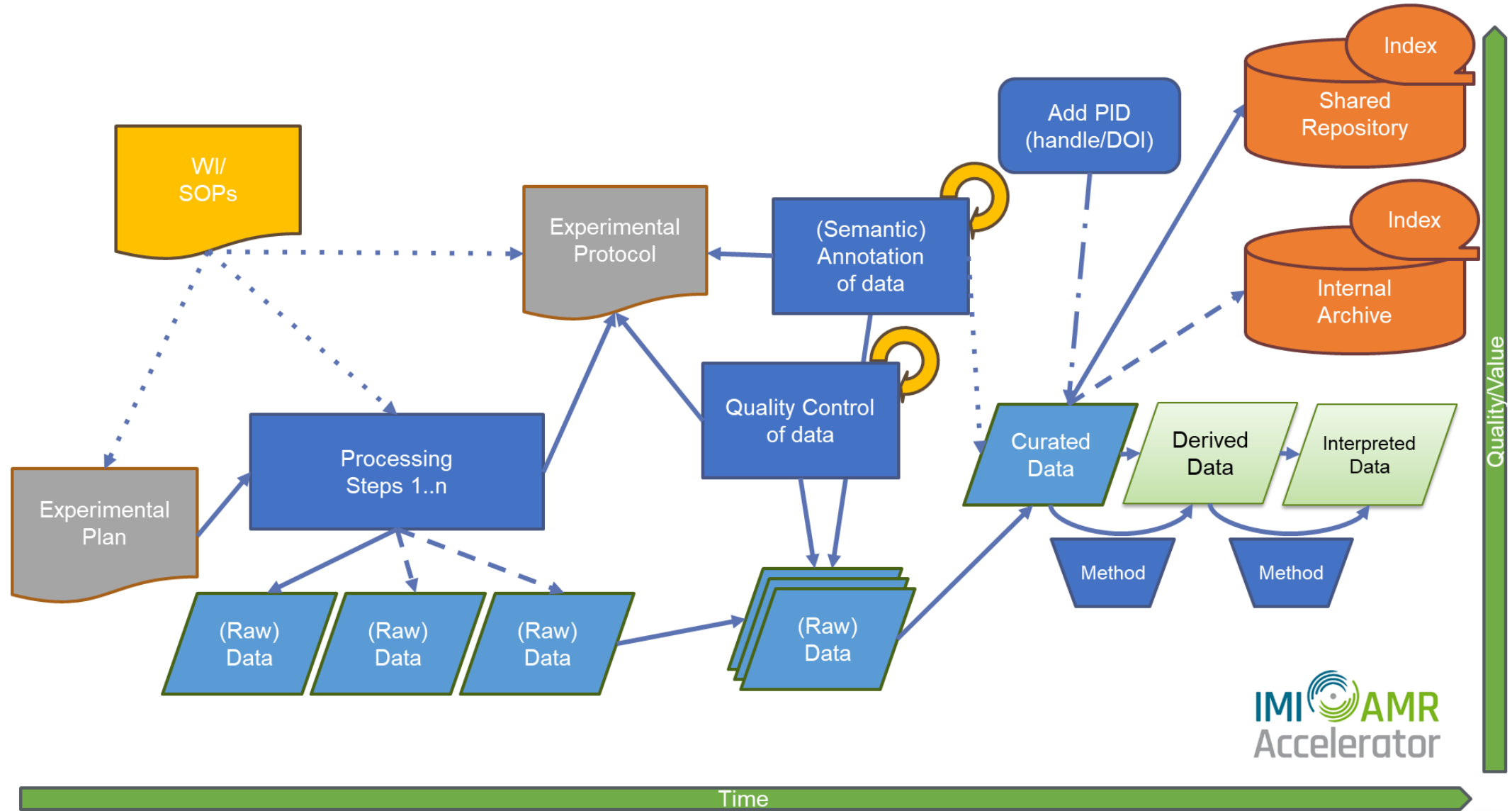
Flow across all social groups *the individual, the lab, the project, the organisation, the community*

Flow across all tech infra  
*platforms, repositories, registries*

Reduce Knowledge Loss

Knowledge Turning, Information Flow  
Josh Sommer, Chordoma Foundation, 2011

# Creation of Value from data and Metadata

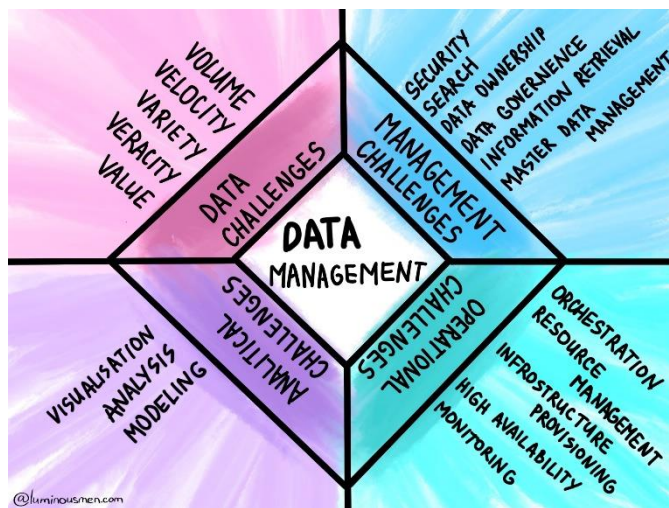


IMI AMR Accelerator

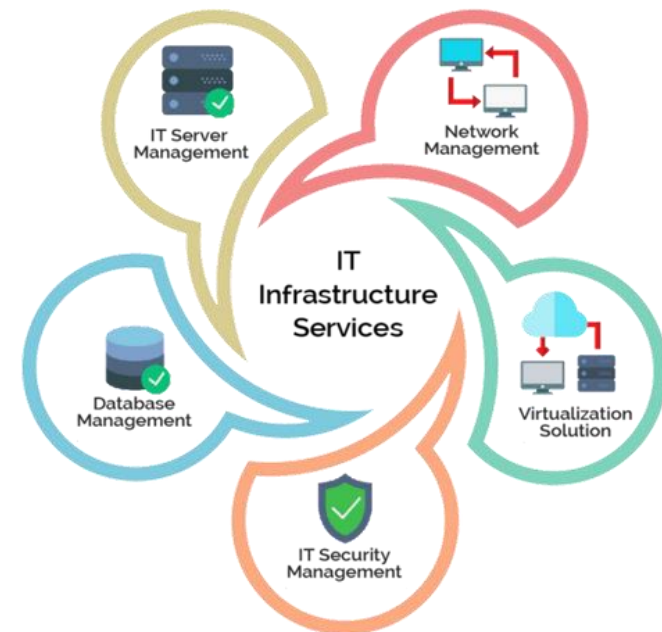
# WHAT DOES DATA MANAGEMENT INCLUDE?



Providing guidelines for FAIR principles



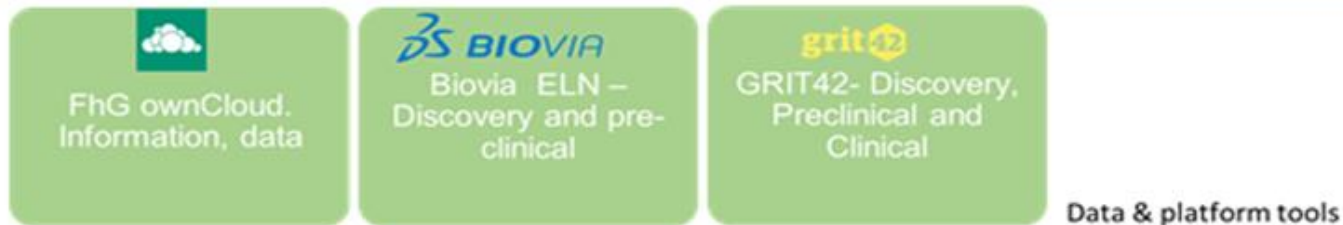
Support data management needs across AMR Accelerator



Establishment of relevant IT infrastructure

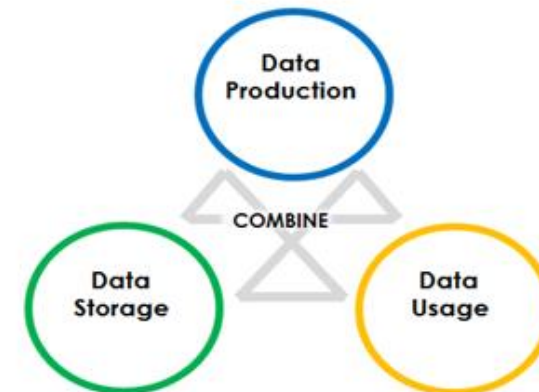


# INFRASTRUCTURE OVERVIEW IN COMBINE



## Expertises

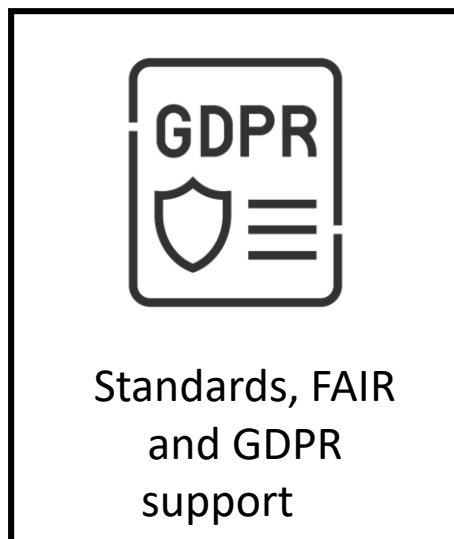
- Standards
- Ontologies
- Data integration
- Access and Analysis
- FAIR
- Implementation
- Software Support



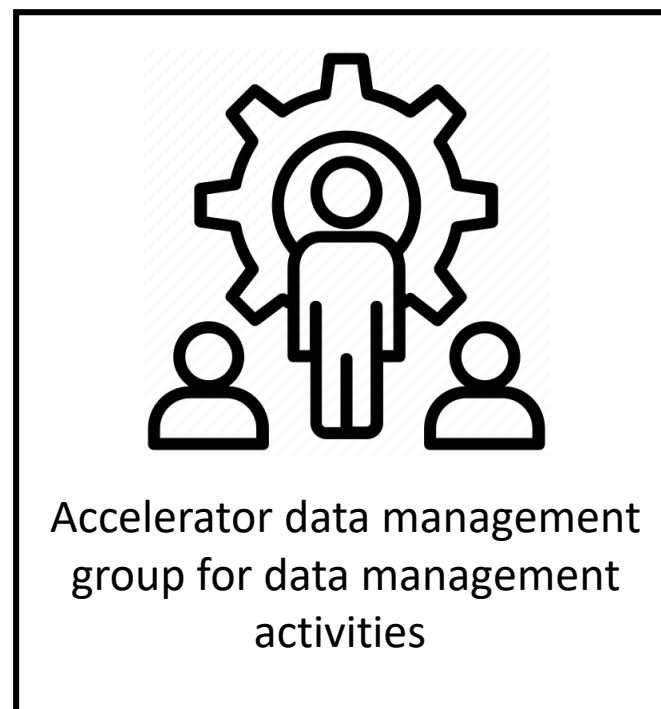
# FAIR Guidelines

Define guidelines for data management across all the Accelerator projects

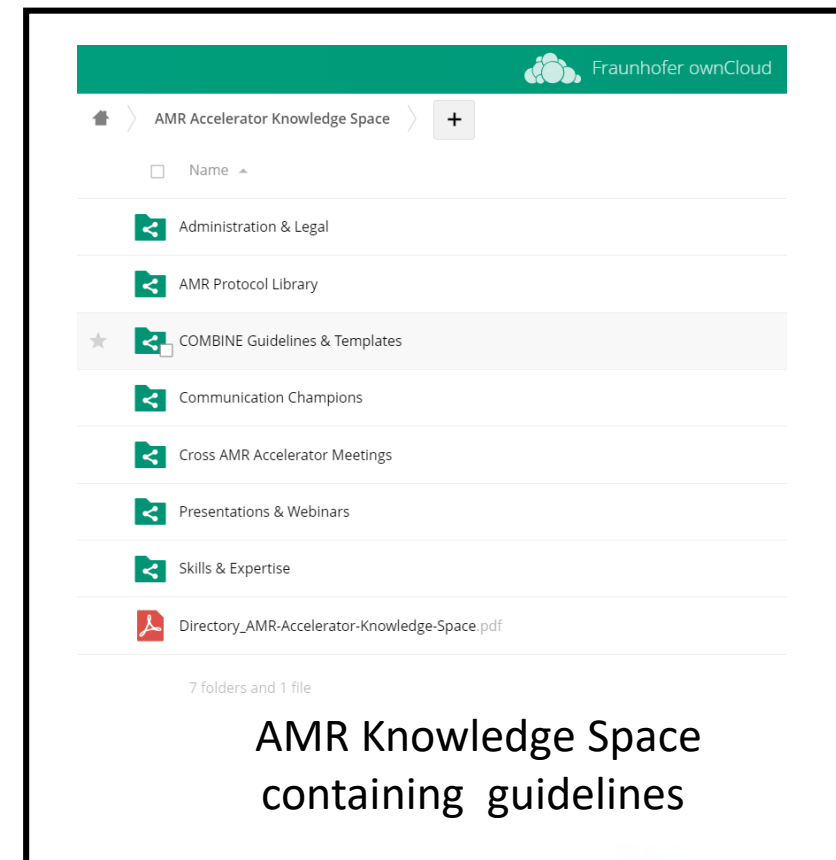
## DATA



## DATA MANAGERS



## DATA STORAGE



# Webinars to communicate and disseminate



## WEBINAR

02 July 2020  
4-5 pm CEST

AMR Accelerator data management, setting up data workflows from electronic lab notebooks to performing cross study analyses



**Philip Gribbon**  
COMBINE WP2 and Fraunhofer IME, Hamburg



**Manfred Kohler**  
COMBINE WP2 and Fraunhofer IME, Hamburg



**Claus Stie Kalleasæ**  
COMBINE WP2 and GRIT42

This webinar will be focused on practical aspects of setting up FAIR data management procedures in AMR accelerator projects. The first part will cover working with FAIR templates using Electronic Lab notebooks. Templates for working with in-vitro data sets will be discussed for MIC and related studies including ADME-tox data. The second part will cover working with in-vivo data sets and the templates which have been established for animal level data sets. The final part will cover data integration in the GRIT42 software and approaches to allow for integrating data from different experiments in the same study, as well as cross study analyses.

For additional information please contact Gesa Witt ([gesa.witt@ime.fraunhofer.de](mailto:gesa.witt@ime.fraunhofer.de)) or Philip Gribbon ([Philip.Gribbon@ime.fraunhofer.de](mailto:Philip.Gribbon@ime.fraunhofer.de)) in order to receive the calendar invite including the dial-in details, please [register here](#).



[www.amr-accelerator.eu](http://www.amr-accelerator.eu)



[www.imi.europa.eu/](http://www.imi.europa.eu/)

These projects have received funding from the Innovative Medicines Initiative 2 Joint Undertaking under grant agreement No 101019715 (IMI2) | 101019715 | 101019715 | 101019715 | 101019715. This Joint Undertaking receives support from the European Union's Horizon 2020 research and innovation programme and EFPIA.



## WEBINAR

28 January 2021  
1-2 pm CET

Tools for working with sensitive and clinical data in the AMR Accelerator: Ethics; templates and software infrastructure



**Philip Gribbon**  
COMBINE WP2 and Fraunhofer IME



**Erik Lottrup Thomsen**  
COMBINE WP2 and GRIT42



**Patrick O'Meara**  
D-Path and COMBINE WP2

### Webinar agenda

- 1) Ethics considerations working with clinical data in the AMR Accelerator (Philip Gribbon)
- 2) Data formats and standards (Patrick O'Meara)
- 3) GRIT42 working with clinical data Demonstration (Erik Lottrup Thomsen)
- 4) How can we support your clinical data analyses - discussion and feedback (All)

The webinar will cover processes for working with aggregated clinical data in the COMBINE consortia and AMR Accelerator. Firstly, the team will outline a set of procedures established for assessing the ethical status of data sets from external organisations. Then, the team will describe data formats and standards for working with clinical data sets uploaded into the GRIT software tool. Finally, the use of the updated GRIT42 software tool will be demonstrated and feedback sought on how it could be applied by potential AMR Accelerator users.

For additional information please contact Philip Gribbon ([Philip.Gribbon@itmp.fraunhofer.de](mailto:Philip.Gribbon@itmp.fraunhofer.de)).



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## WEBINAR

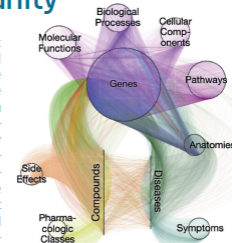
25 May 2021  
3-4 pm CEST

Introduction to tools to help expertise sharing and collaboration in the AMR Accelerator community

This webinar will cover the use of knowledge management tools in the IMI AMR Accelerator and how these can be used to both enhance data analysis workflows and also promote collaborations across projects and teams. To support these efforts the AMR Data Management group have developed a set of database and visualisation tools based on the Knowledge Graph standards. Knowledge Graphs have the capacity to harmonize and link structured and unstructured data, resulting in higher data quality that is ideal for machine learning. In the presentation we demonstrate the utility of the Knowledge Graph, approach including the use of semantic metadata enrichment, taxonomies and ontologies. We will showcase a Knowledge Graph developed to map the expertise of individual scientists across the network of IMI AMR Accelerator projects. This new tool will be deployed to the project teams and will support the identification of and engagement between subject matter experts within our community.

We welcome to this webinar all those who are interested in building co-operations across the AMR Accelerator and those eager to do more with their data and extend their analyses into the area of machine learning.

For additional questions, please contact [philip.gribbon@itmp.fraunhofer.de](mailto:philip.gribbon@itmp.fraunhofer.de)



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# Knowledge Space

Files Fraunhofer ownCloud Witt, Gesa

AMR Accelerator Knowledge Space

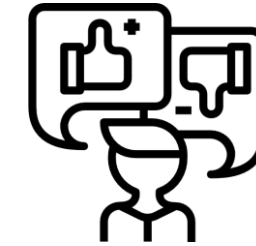
Name	Size	Modified
Administration & Legal	83.2 MB	8 days ago
AMR Protocol Library	3 MB	a year ago
COMBINE Guidelines & Templates	223.4 MB	a day ago
Communication Champions	4.6 MB	2 months ago
★ Cross AMR Accelerator Meetings	96.4 MB	4 months ago
Presentations & Webinars	385.6 MB	23 days ago
Skills & Expertise	0 KB	7 months ago
Directory_AMR-Accelerator-Knowledge-Space.pdf	461 KB	7 months ago

7 folders and 1 file 796.8 MB

# Tools and resources



Upgrades to grit42 for working with *in vivo* and clinical data sets

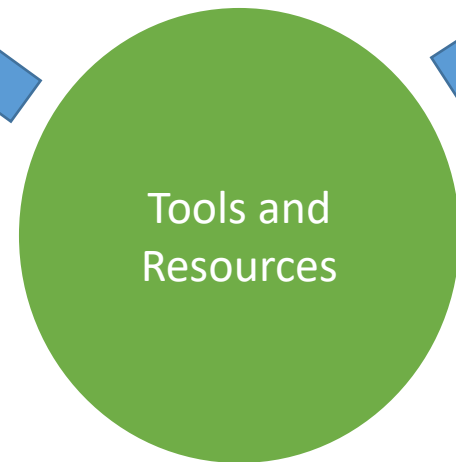


Identification of needs, surveys and feedbacks from data champions

Grouping	Group	Version	Approved	Pre-Treatment Compound	Post-Treatment Compound	Pre-Treatment Assay	Post-Treatment Assay	Pre-Treatment Route of Administration	Post-Treatment Route of Administration	Standardized Name	Unit
Compound	antibiotic group 1	antibiotic number	2019-09-01-01			single dose, intraperitoneal	single dose, intraperitoneal	single dose, intraperitoneal	single dose, intraperitoneal	antibiotic	mg/kg
Grouping	antibiotic	antibiotic	2019-09-01-01			single dose, intraperitoneal	single dose, intraperitoneal	single dose, intraperitoneal	single dose, intraperitoneal	antibiotic	mg/kg
Assay	antibiotic	antibiotic	2019-09-01-01			single dose, intraperitoneal	single dose, intraperitoneal	single dose, intraperitoneal	single dose, intraperitoneal	antibiotic	mg/kg
Route of Administration	antibiotic	antibiotic	2019-09-01-01			single dose, intraperitoneal	single dose, intraperitoneal	single dose, intraperitoneal	single dose, intraperitoneal	antibiotic	mg/kg
Standardized Name	antibiotic	antibiotic	2019-09-01-01			single dose, intraperitoneal	single dose, intraperitoneal	single dose, intraperitoneal	single dose, intraperitoneal	antibiotic	mg/kg
Unit	antibiotic	antibiotic	2019-09-01-01			single dose, intraperitoneal	single dose, intraperitoneal	single dose, intraperitoneal	single dose, intraperitoneal	antibiotic	mg/kg

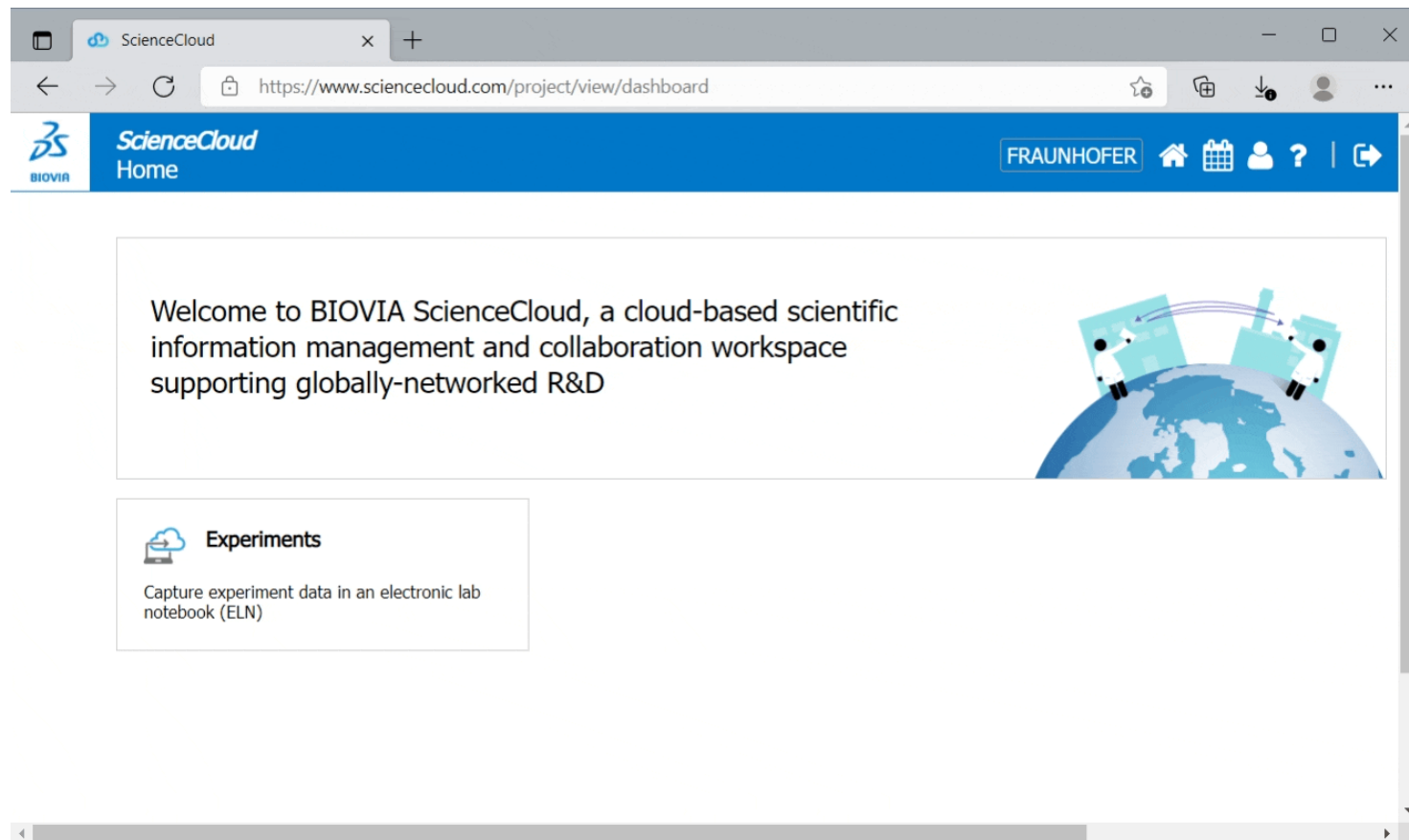
Development of templates for standardized data collection

Electronic lab notebook roll-out for new projects



Review meeting – March 29th 2022

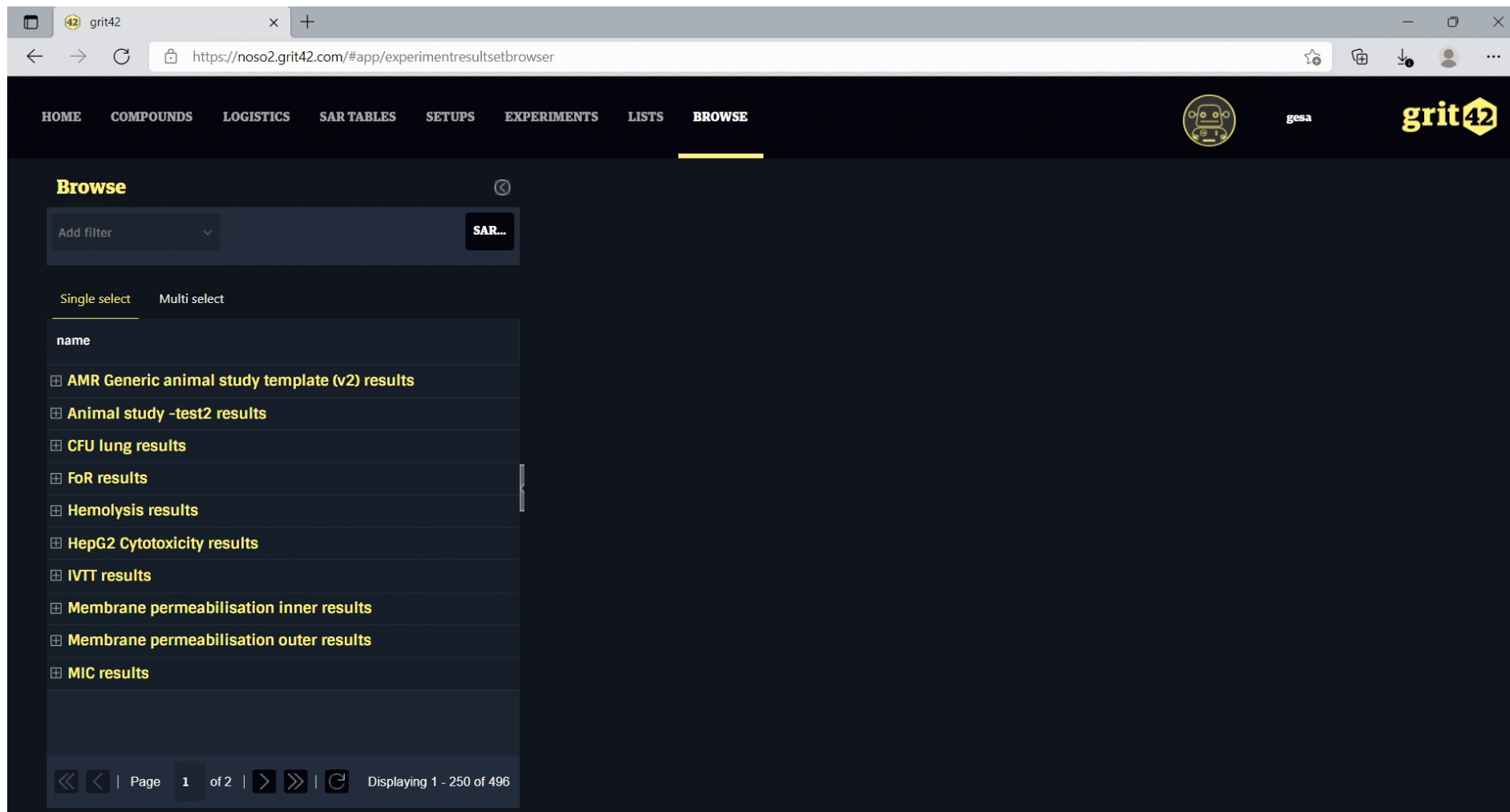
# Electronic laboratory notebooks



- Easy-to-use
  - Access controlled
  - Shared protocols
  - Port data to G42
- Consistent standards
  - In-vitro data templates
  - In-vivo data templates
  - Pre-clinical data templates

# Data storage and analysis infrastructure

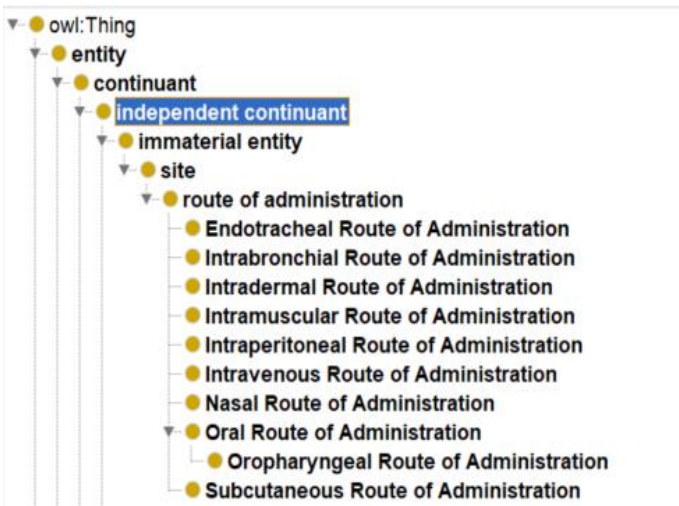
- Enterprise tool
  - Data Schema
  - Storage
  - Query
- Ontologies linked to standards
- Individual animal / patient level analyses



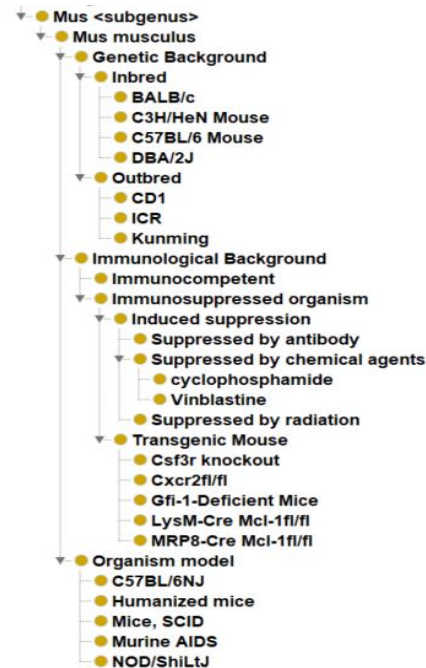
The screenshot displays the Grit42 web application interface. The browser address bar shows the URL <https://noso2.grit42.com/#app/experimentresultsetbrowser>. The navigation menu includes HOME, COMPOUNDS, LOGISTICS, SAR TABLES, SETUPS, EXPERIMENTS, LISTS, and BROWSE. The BROWSE page features a search bar with 'Add filter' and a 'SAR...' button. Below the search bar, there are tabs for 'Single select' and 'Multi select'. A list of results is displayed, including 'AMR Generic animal study template (v2) results', 'Animal study -test2 results', 'CFU lung results', 'FoR results', 'Hemolysis results', 'HepG2 Cytotoxicity results', 'IVTT results', 'Membrane permeabilisation inner results', 'Membrane permeabilisation outer results', and 'MIC results'. The footer of the page shows pagination information: 'Page 1 of 2' and 'Displaying 1 - 250 of 496'.

# Updated Ontology for antibacterial drug discovery

- Abstract number : EA71 Poster by Gadiya et al
- BioAssay Protocol Ontology (BPO) to aid standardization of unstructured protocol data #



Route of administration



Mouse models

merged-2 | Home

Classes | Properties | Individuals | Comments | Changes by Entity | History

Class Hierarchy

- owl:Thing
  - BFO\_0000020
  - BFO\_0000031

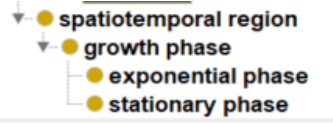
Class: BFO\_0000020

IRI: [http://purl.obolibrary.org/obo/BFO\\_0000020](http://purl.obolibrary.org/obo/BFO_0000020)

Annotations

- rdfs:label: specifically dependent continuant
- IAO\_0000115: b is a specifically dependent continuant = Def. b is a continuant & there is some independent continuant c which is not a spatial region and which is such that b depends on c at every time t during the course of b's existence. (axiom label in BFO2 Reference: [050-003])
- rdfs:isDefinedBy: <http://purl.obolibrary.org/obo/bfo.owl>
- BFO\_0000179: sdc
- BFO\_0000180: SpecificallyDependentContinuant
- IAO\_0000112: of one-sided specifically dependent continuants: the mass of this tomato
- IAO\_0000112: the disposition of this fish to decay
- IAO\_0000112: the pink color of a medium rare piece of grilled filet mignon at its center
- IAO\_0000112: the smell of this portion of mozzarella
- IAO\_0000112: the function of this heart: to pump blood
- IAO\_0000112: the shape of this hole.
- IAO\_0000112: Reciprocal specifically dependent continuants: the function of this key to open this lock and the mutually dependent disposition of this lock: to be opened by this key
- IAO\_0000112: the mutual dependence of proton donors and acceptors in chemical reactions [79]
- IAO\_0000112: the mutual dependence of the role predator and the role prey as played by two organisms in a given interaction
- IAO\_0000112: the role of being a doctor
- IAO\_0000112: of relational dependent continuants (multiple bearers): John's love for Mary, the ownership relation between John and this statue, the relation of authority between John and his subordinates.
- IAO\_0000112: Specifically dependent continuant doesn't have a closure axiom because the

Bacteria growth phase





# AMR Knowledge Graph

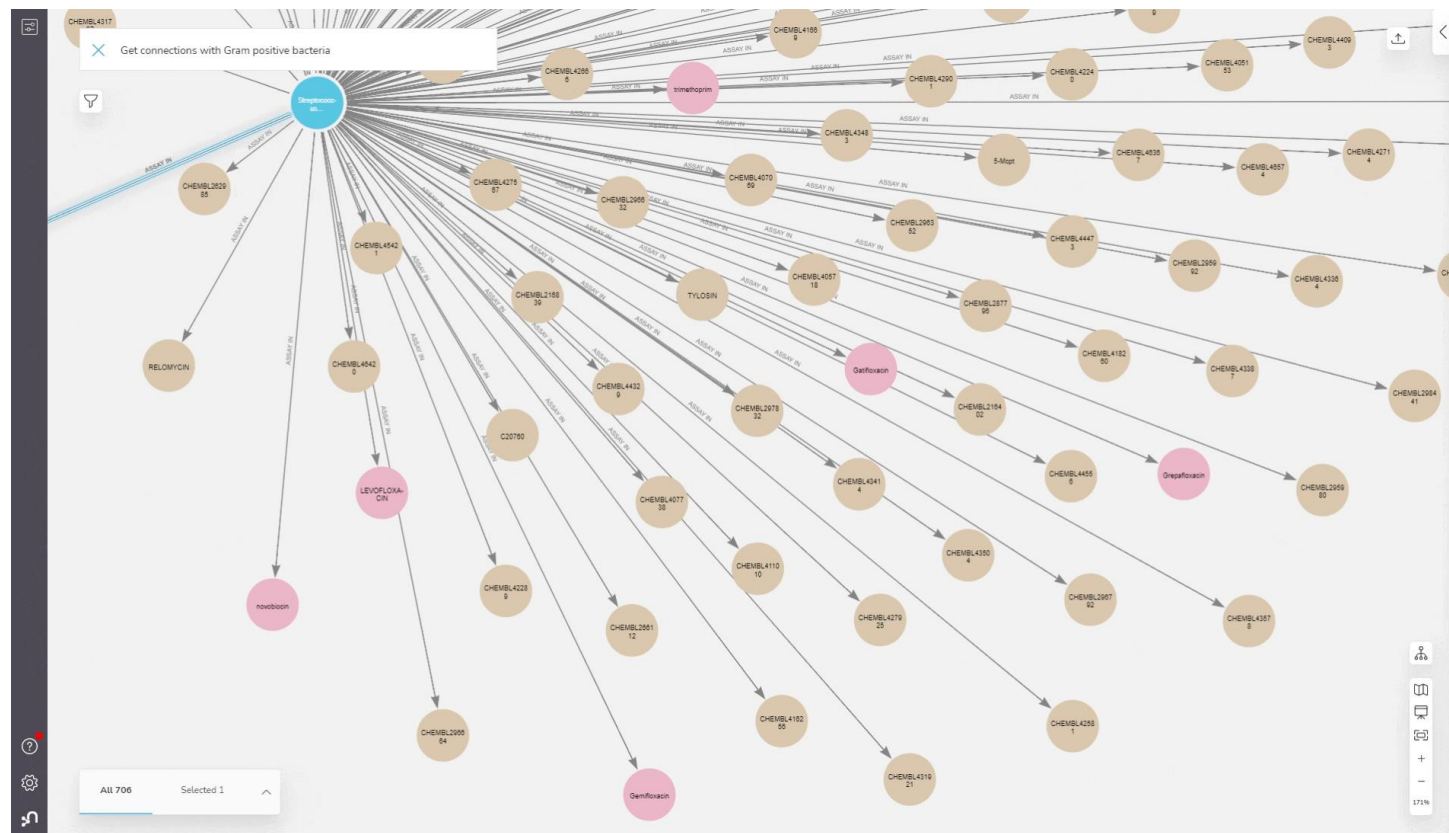
- Data resource is linked with controlled vocabularies aligned with FAIR principles

**ORCID**  
Connecting Research  
and Researchers

**NCBI** National  
Center for  
Biotechnology  
Information

**PubChem**

**ChEMBL**



Information related to *reference pathogens* in AMR-KG

# BE PART OF THE SOLUTION!



Share **expertise**



Support our  
**data quest**



**Combine effort**  
on common  
interests

**BESIDES CONTRIBUTING TO IMPROVING THE SUCCESS OF R&D EFFORTS ACROSS THE AMR COMMUNITY, YOU WILL ALSO:**

Get an early preview  
of the results

Get more out of your  
data by making it  
FAIRifiable

Get involved in the  
analysis

Improve the overall  
data management  
process

Be connected with  
AMR experts from the  
IMI AMR Accelerator

For more information on the  
use of your data:

**CONTACT US**

For more information on data  
protection or to initiate the data  
sharing process:

IMI-COMBINE@pei.de

IMI-COMBINE@pei.de

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The AMR Accelerator projects have received funding from the Innovative Medicines Initiative 2 Joint Undertaking under grant agreement No 853976 | 853967 | 853979 | 853932 | 853903 | 853800 | 853989 | 101007873 | 101034420. The Joint Undertaking receives support from the European Union's Horizon 2020 research and innovation programme and EFPIA. ERA4TB has received additional support from Global Alliance for TB Drug Development, Bill & Melinda Gates Foundation and University of Dundee. UNITE4TB has received funding from the Innovative Medicines Initiative 2 Joint Undertaking under grant agreement No 101007873. The JU receives support from the European Union's Horizon 2020 research and innovation programme and EFPIA, Deutsches Zentrum für Infektionsforschung e. V. (DZIF), and Ludwig-Maximilians-Universität München (LMU). EFPIA/AP contribute to 50% of funding, whereas the contribution of DZIF and the LMU University Hospital Munich has been granted by the German Federal Ministry of Education and Research.

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