

# PARC approach to ensuring FAIR Chemical Risk Assessment Data”

Partnership for the Assessment of the  
Risks from Chemicals

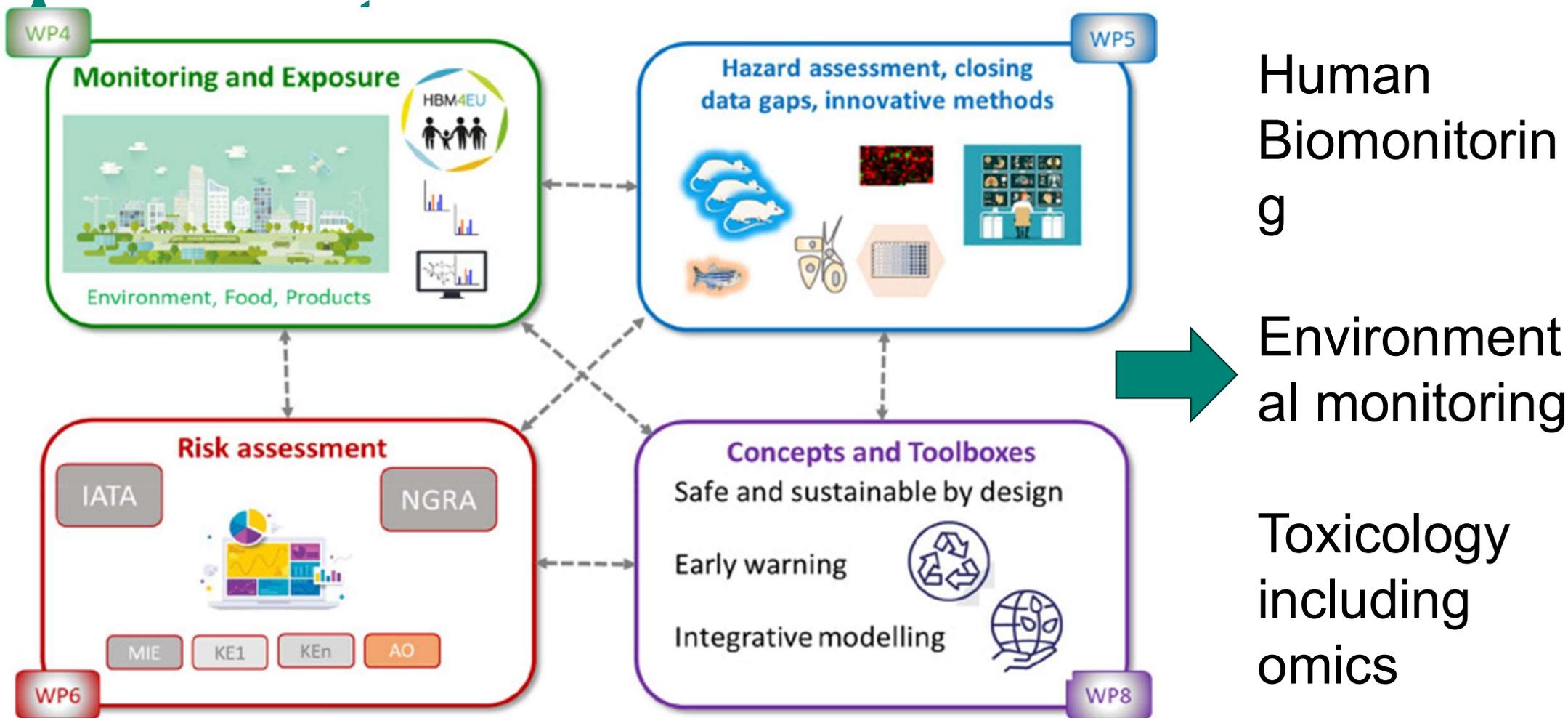
Iseult Lynch, Univeristy of Birmingham, Co-Lead WP7

JRC Webinar - Improving the utility of research data in  
regulatory assessments – 31<sup>st</sup> January 2024

PARC

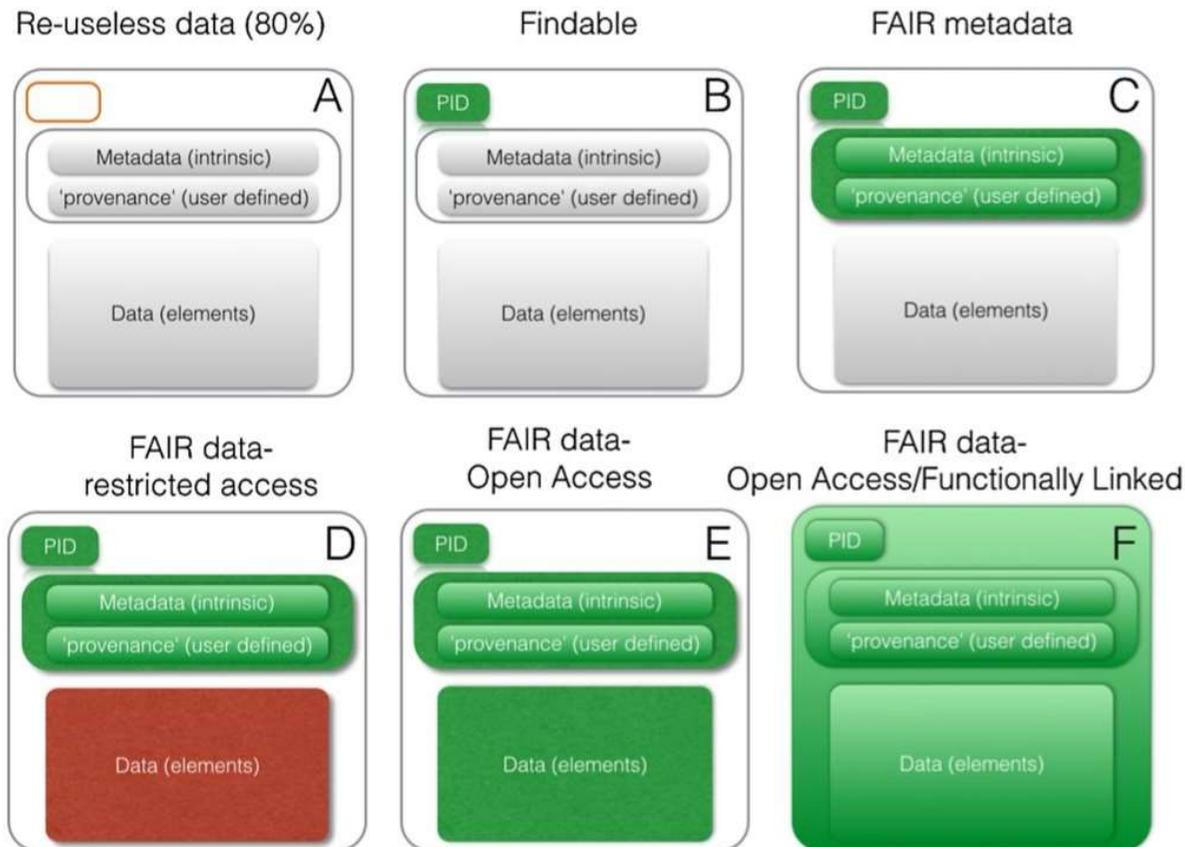


# PARC: Regulatory Research for Chemicals Risk



# PARC's Ambition regarding FAIR and Open Data

Data as increasingly FAIR Digital Objects



## PARC Data Policy

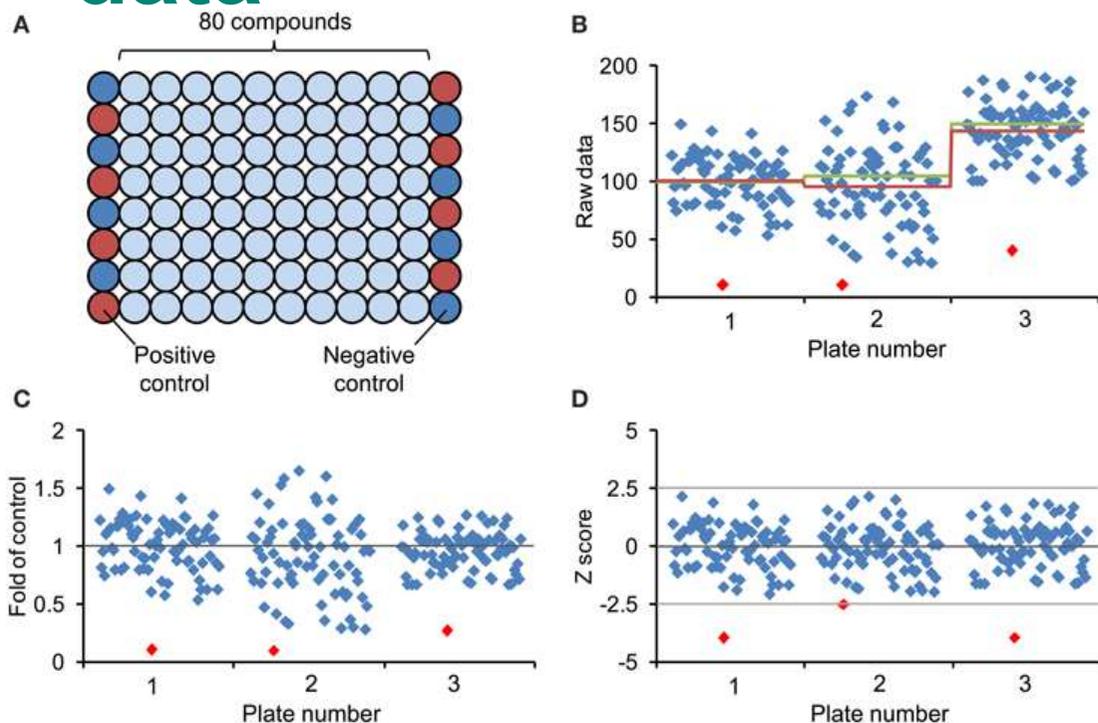
The ambition for PARC is to strive towards FAIR, Open and linked data (Panel F), recognizing that:

1. resources are limited,
2. not every sub-domain within PARC is equally far along the road to FAIRness,
3. not all Participants / Researchers are as experienced in FAIR, and
4. technical constraints may have to be solved.

**PARC will strive for a minimum level of FAIRness for all PARC data and metadata, whether it is Open or Closed, as shown in Panels D and E."**

# What data are we interested in making FAIR?

## Raw data, processed / transformed, summary data



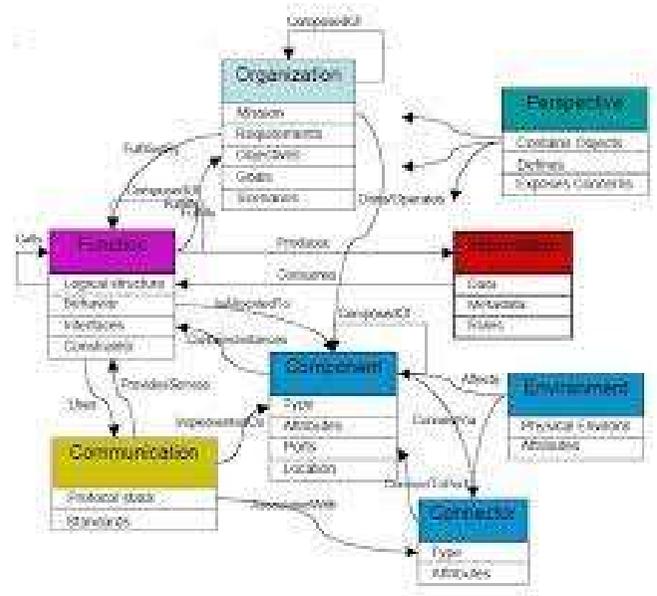
log [antioxidant]	Experiment No.			Mean $\pm$ SD
	1	2	3	
-5.22	39.36%	41.58%	39.04%	40.00 $\pm$ 1.38%
-5.15	45.09%	47.88%	43.19%	45.39 $\pm$ 2.36%
-5.10	49.30%	50.01%	49.99%	49.77 $\pm$ 0.40%
-5.05	54.63%	56.35%	54.35%	55.11 $\pm$ 1.08%
-5.00	56.71%	60.51%	56.17%	57.80 $\pm$ 2.37%
EC <sub>50</sub>	-5.090	-5.097	-5.097	-5.095 $\pm$ 0.004

PARC recommendations for each level of data! Minimum to make the summary data FAIR.

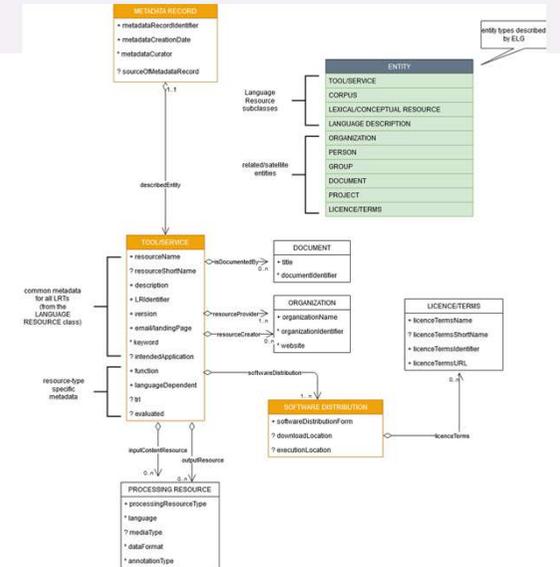
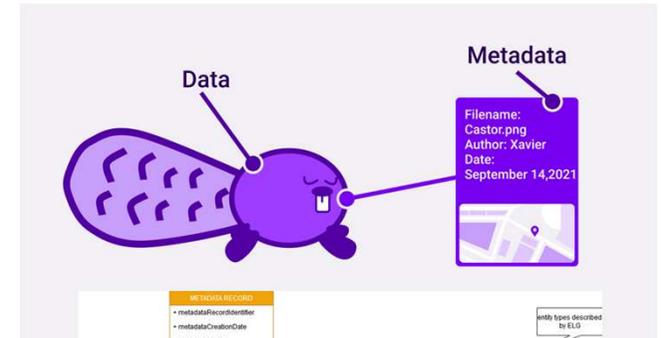
# Key resources being developed in PARC



FAIR Implementation Profiles – per domain / data type



PARC Ontologies  
PARC  
Vocabularies



PARC Metadata  
schema

# Close collaboration with the GO FAIR Foundation

FIP workshops with red and blue experts



Qualified / Certified FAIR Implementation Profile



FAIR principle	
F1	What globally unique, persis
F1	What globally unique, persis
F2	Which metadata schemas d
F3	What is the technology that I
F4	In which search engines are
F4	In which search engines are
A1.1	Which standardized commu
A1.1	Which standardized commu
A1.2	Which authentication & auth
A1.2	Which authentication & auth
A2	Which metadata longevity pl
I1	Which knowledge representi
I1	Which knowledge representi
I2	Which structured vocabulari
I2	Which structured vocabulari
I3	Which models, schema(s) d
I3	Which models, schema(s) d
R1.1	Which usage license do you
R1.1	Which usage license do you
R1.2	Which metadata schemas d
R1.2	Which metadata schemas d

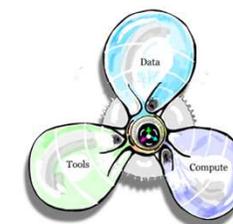
Auto-informed FAIR data management plan (template)



FAIR data management implemented in a project



FAIR data Sharing / visting



FIP2DMP: Linking data management plans with FAIR implementation profiles Cite



Mapping the FIP onto the DMP  
Kristina Hettne, Leiden University Libraries, 2020

<https://github.com/RDA-DMP-Common/hackathon-2020/blob/master/results.md>  
<https://docs.google.com/presentation/d/1h7ITS9gVW8A-bOkSjR3qFNPzaU0NQfGJFR1CHZuC78FY/edit?us>

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**Keywords:** Data Management Plan, FAIR implementation profiles, FAIR enabling resource, metadata standards, machine actionable DMPs  
**DOI:** 10.3233/FC-221515

# All-PARC versus domain-specific community standards

The FIP is a **socio-technical** approach to drive wide-spread FAIR convergence

## FAIR Principles

### To be Findable:

- F1. (meta)data are assigned a globally unique and persistent identifier
- F2. data are described with rich metadata (defined by R1 below)
- F3. metadata clearly and explicitly include the identifier of the data it describes
- F4. (meta)data are registered or indexed in a searchable resource

### To be Accessible:

- A1. (meta)data are retrievable by their identifier using a standardized communications protocol
  - A1.1 the protocol is open, free, and universally implementable
  - A1.2 the protocol allows for an authentication and authorization procedure, where necessary
- A2. metadata are accessible, even when the data are no longer available

### To be Interoperable:

- I1. (meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation.
- I2. (meta)data use vocabularies that follow FAIR principles
- I3. (meta)data include qualified references to other (meta)data

### To be Reusable:

- R1. (meta)data are richly described with a plurality of accurate and relevant attributes
  - R1.1. (meta)data are released with a clear and accessible data usage license
  - R1.2. (meta)data are associated with detailed provenance
  - R1.3. (meta)data meet domain-relevant community standards

### Machine-actionable metadata

Technical infrastructure (accepted generic services) = Technical experts

Social contracts (domain specific agreements) = Domain experts

## FAIR Enabling Resource (FER)

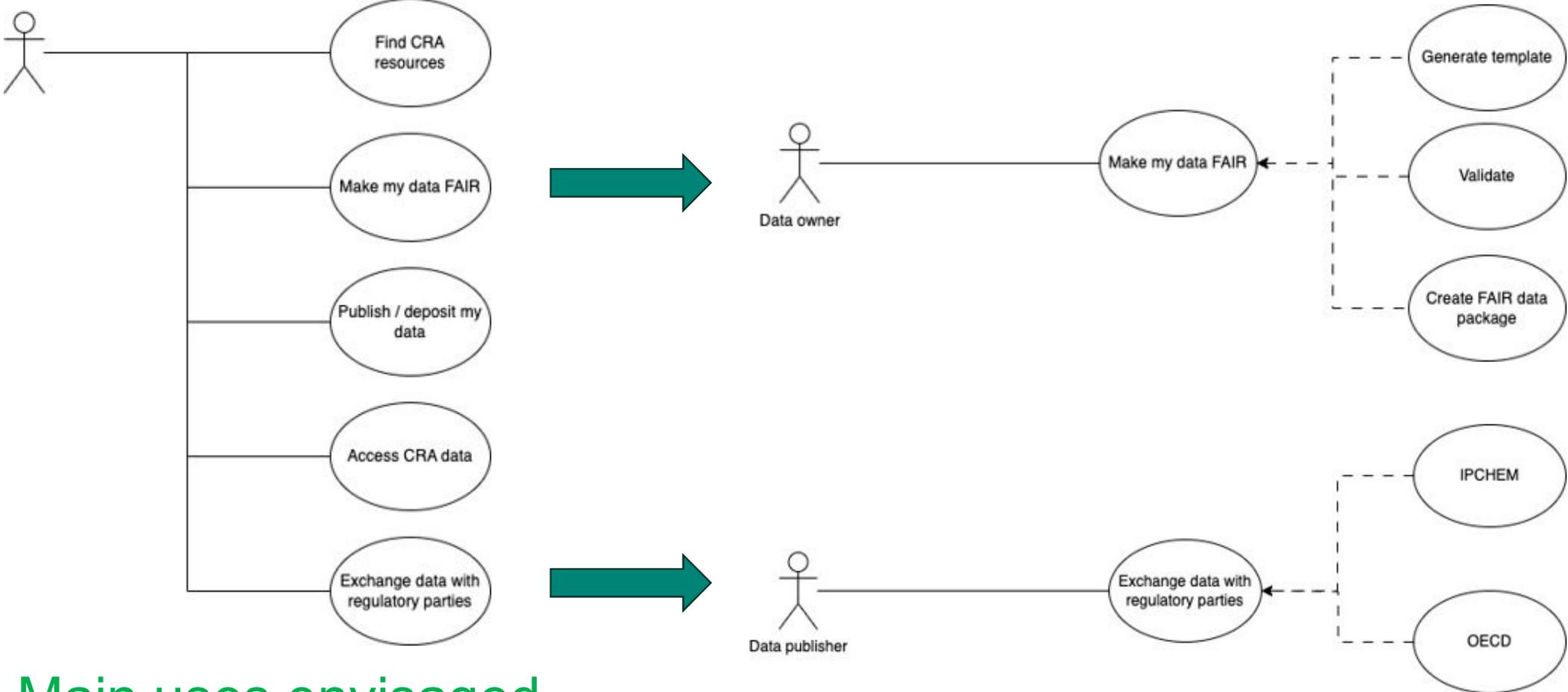


## FAIR Implementation Profile (FIP)

FAIR Implementation Community

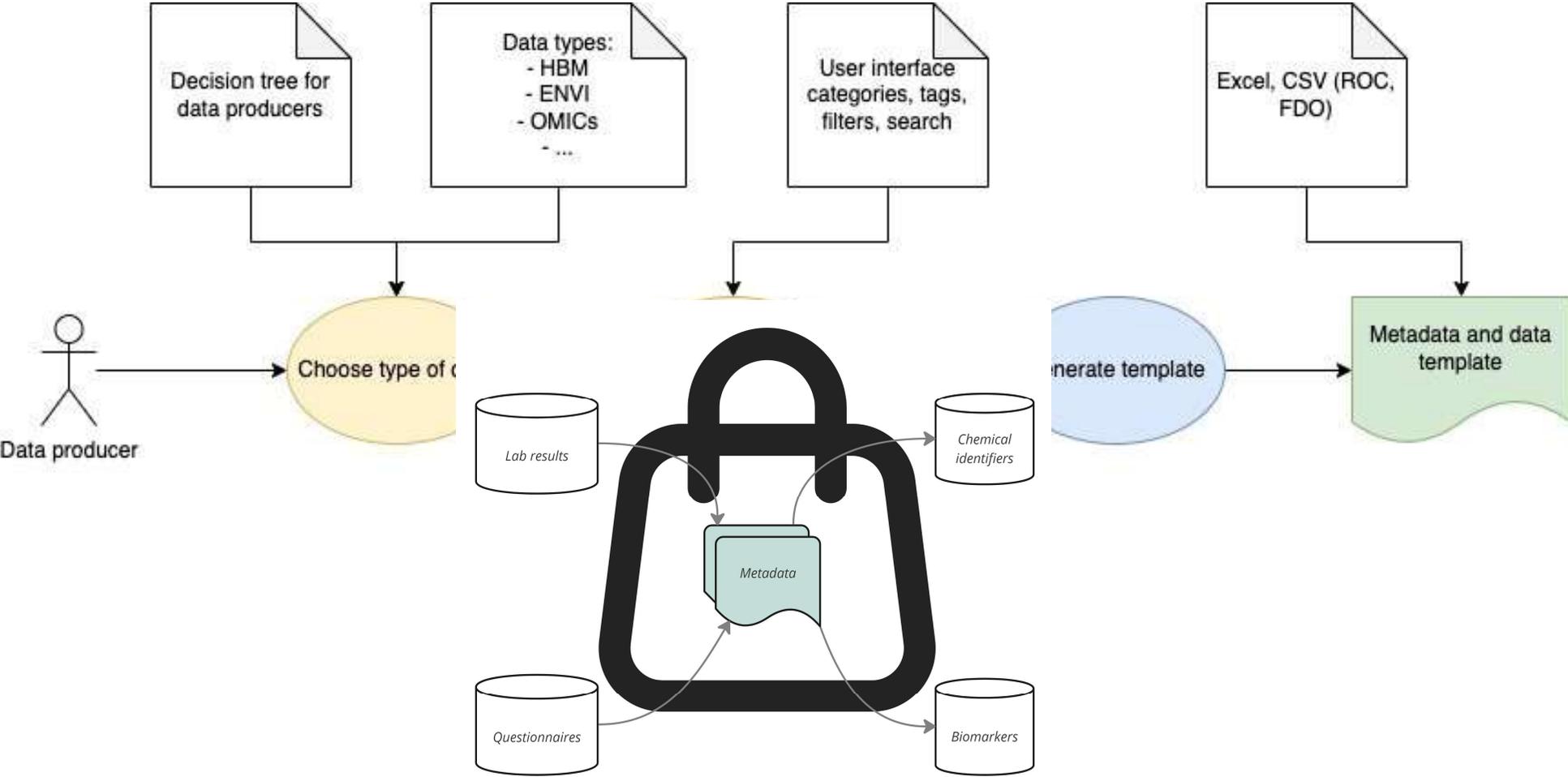


# The PARC Data Hub – an integrating & enabling platform

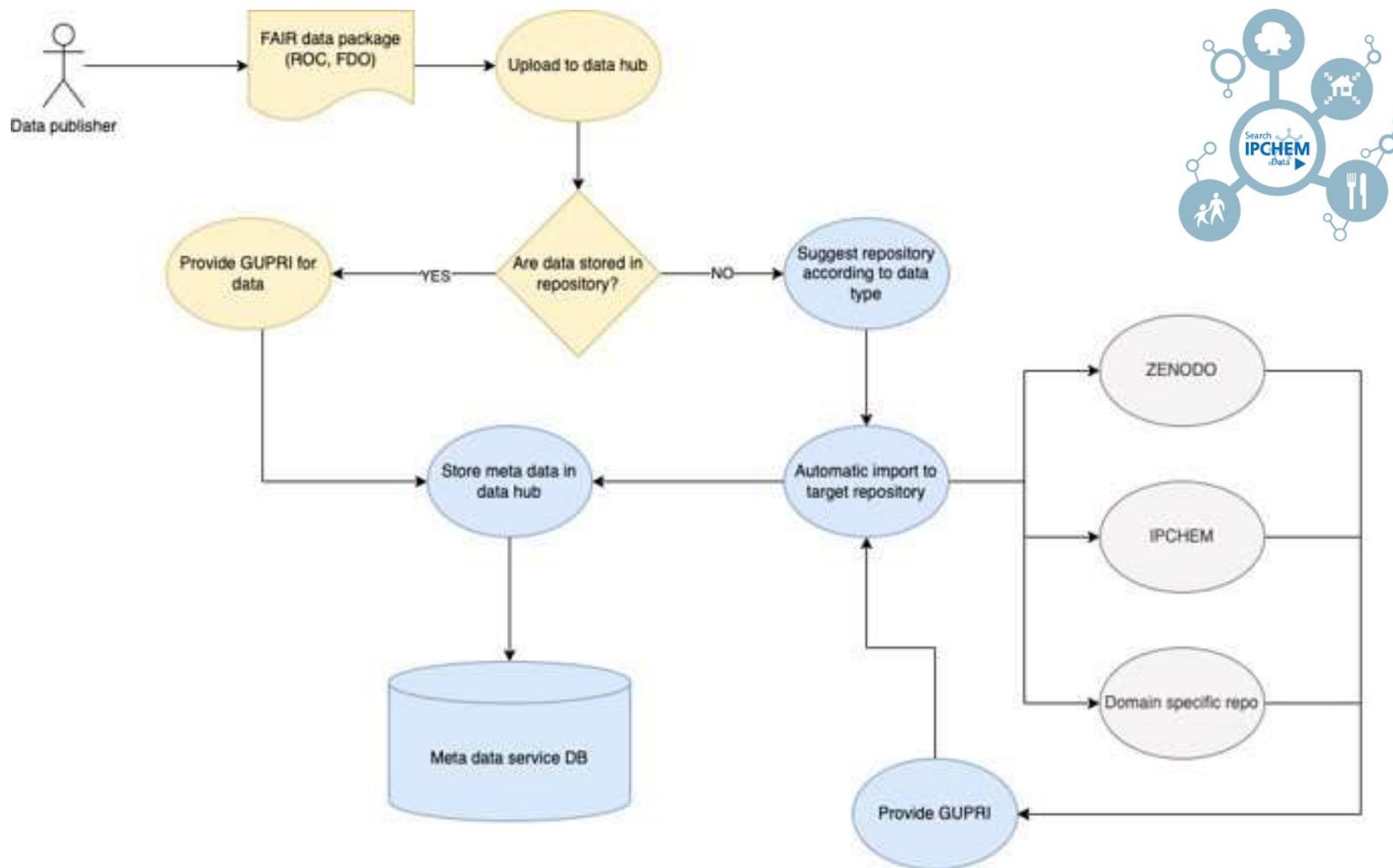


Main uses envisaged

# Example workflow: developing a data / metadata template



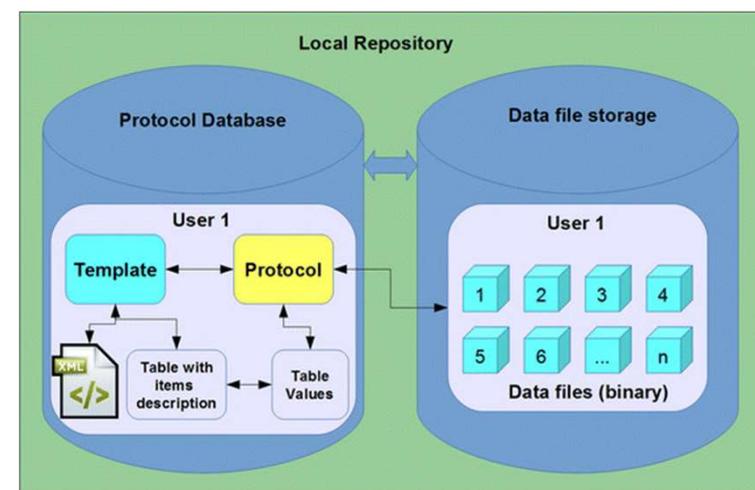
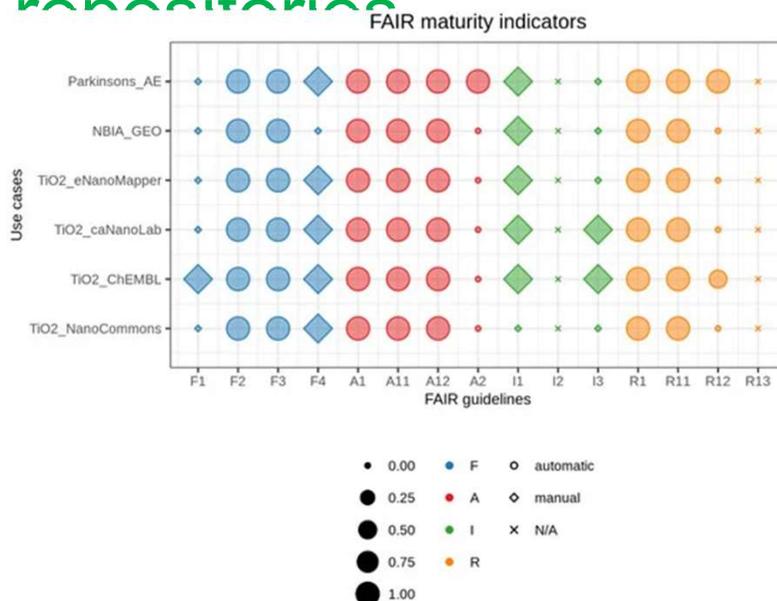
# Example workflow: publishing a FAIR data package



# Other things WP7 will provide for PARC partners



## FAIR maturity indicators for PARC-used repositories



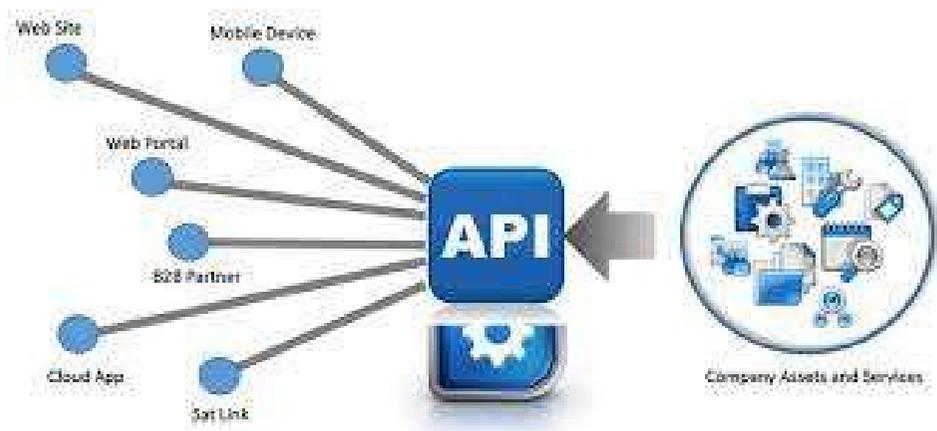
[0.1186/s12938-016-0188-8](https://doi.org/10.1186/s12938-016-0188-8)

## PARC Protocols repository

<https://doi.org/10.3390/nano10102068>

PARC Data "Tools"

# Other things WP7 will provide for PARC partners



Automated visualisation of PARC QA/QC / data completeness criteria. e.g., RToxTool / SciRAP

Automatic data completeness overview  
Based on publications by GRACIOUS, the ToxTool and the NiTox as well as expertise from NanoSolveIT partners we defined use cases such as "Grouping/read-across" and which endpoints and metadata are required to judge data as "complete" i.e. re-usable in the context of the use case.

For each nanomaterial and each use case we defined a list of required endpoints and tested automatically for their availability for any of the available nanomaterials.

Filter results by:

Selected items: 0 Show/Hide Sort by

NM	Chemical Elements	Names	Grouping/read-across	Nanomorph identification	NiTox	QSAR model development	Regulatory	Tox-prediction PhysChem
<input type="checkbox"/> NP00190	Ce	Micron sized control:CeO2 bulk	<div style="width: 13%;"><div style="width: 13%;"></div></div> 13% [1/8]	<div style="width: 25%;"><div style="width: 25%;"></div></div> 25% [1/4]	<div style="width: 33%;"><div style="width: 33%;"></div></div> 33% [2/6]	<div style="width: 25%;"><div style="width: 25%;"></div></div> 25% [2/8]	<div style="width: 0%;"><div style="width: 0%;"></div></div> 0% [0/2]	<div style="width: 17%;"><div style="width: 17%;"></div></div> 17% [1/6]
<input type="checkbox"/> NP00191	Ce	Cerium (IV) Oxide (precipitated, uncoated) NM-211;JRCNM02101a:Ce NM 211	<div style="width: 25%;"><div style="width: 25%;"></div></div> 25% [2/8]	<div style="width: 25%;"><div style="width: 25%;"></div></div> 25% [1/4]	<div style="width: 33%;"><div style="width: 33%;"></div></div> 33% [2/6]	<div style="width: 38%;"><div style="width: 38%;"></div></div> 38% [3/8]	<div style="width: 50%;"><div style="width: 50%;"></div></div> 50% [1/2]	<div style="width: 33%;"><div style="width: 33%;"></div></div> 33% [2/6]
<input type="checkbox"/> NP00192	Ce	Cerium (IV) Oxide (precipitated, uncoated) NM-212;JRCNM02102a:Ce NM 212	<div style="width: 25%;"><div style="width: 25%;"></div></div> 25% [2/8]	<div style="width: 25%;"><div style="width: 25%;"></div></div> 25% [1/4]	<div style="width: 33%;"><div style="width: 33%;"></div></div> 33% [2/6]	<div style="width: 38%;"><div style="width: 38%;"></div></div> 38% [3/8]	<div style="width: 50%;"><div style="width: 50%;"></div></div> 50% [1/2]	<div style="width: 33%;"><div style="width: 33%;"></div></div> 33% [2/6]
<input type="checkbox"/> NP00193	Ce	Cerium(IV) oxide (Undoped):PROM CeO2	<div style="width: 25%;"><div style="width: 25%;"></div></div> 25% [2/8]	<div style="width: 25%;"><div style="width: 25%;"></div></div> 25% [1/4]	<div style="width: 33%;"><div style="width: 33%;"></div></div> 33% [2/6]	<div style="width: 38%;"><div style="width: 38%;"></div></div> 38% [3/8]	<div style="width: 50%;"><div style="width: 50%;"></div></div> 50% [1/2]	<div style="width: 33%;"><div style="width: 33%;"></div></div> 33% [2/6]
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<input type="checkbox"/> NP00195	Zr Ce	Ce0.5Zr0.5O2:PROM CeO2-Zr 020 B:PROM-Zr-CeO2-2	<div style="width: 25%;"><div style="width: 25%;"></div></div> 25% [2/8]	<div style="width: 25%;"><div style="width: 25%;"></div></div> 25% [1/4]	<div style="width: 33%;"><div style="width: 33%;"></div></div> 33% [2/6]	<div style="width: 50%;"><div style="width: 50%;"></div></div> 50% [4/8]	<div style="width: 50%;"><div style="width: 50%;"></div></div> 50% [1/2]	<div style="width: 33%;"><div style="width: 33%;"></div></div> 33% [2/6]
<input type="checkbox"/> NP00196	Zr Ce	Ce0.25Zr0.75O2:PROM CeO2-Zr 021:PROM-Zr-CeO2-3	<div style="width: 25%;"><div style="width: 25%;"></div></div> 25% [2/8]	<div style="width: 25%;"><div style="width: 25%;"></div></div> 25% [1/4]	<div style="width: 33%;"><div style="width: 33%;"></div></div> 33% [2/6]	<div style="width: 50%;"><div style="width: 50%;"></div></div> 50% [4/8]	<div style="width: 50%;"><div style="width: 50%;"></div></div> 50% [1/2]	<div style="width: 33%;"><div style="width: 33%;"></div></div> 33% [2/6]
<input type="checkbox"/> NP00197	Zr	PROM-ZrO2:ZrO2 (Undoped)	<div style="width: 25%;"><div style="width: 25%;"></div></div> 25% [2/8]	<div style="width: 25%;"><div style="width: 25%;"></div></div> 25% [1/4]	<div style="width: 33%;"><div style="width: 33%;"></div></div> 33% [2/6]	<div style="width: 50%;"><div style="width: 50%;"></div></div> 50% [4/8]	<div style="width: 50%;"><div style="width: 50%;"></div></div> 50% [1/2]	<div style="width: 33%;"><div style="width: 33%;"></div></div> 33% [2/6]
<input type="checkbox"/> NP00198	Ce	Cerium (IV) oxide:UoB-CeO2-1	<div style="width: 0%;"><div style="width: 0%;"></div></div> 0% [0/8]	<div style="width: 0%;"><div style="width: 0%;"></div></div> 0% [0/4]	<div style="width: 17%;"><div style="width: 17%;"></div></div> 17% [1/6]	<div style="width: 13%;"><div style="width: 13%;"></div></div> 13% [1/8]	<div style="width: 0%;"><div style="width: 0%;"></div></div> 0% [0/2]	<div style="width: 0%;"><div style="width: 0%;"></div></div> 0% [0/6]
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<input type="checkbox"/> NP00201	Zr Ce	CeO2 - redox ratio 2:Ce0.73Zr0.27O2:PROM CeO2-Zr 024C	<div style="width: 25%;"><div style="width: 25%;"></div></div> 25% [2/8]	<div style="width: 25%;"><div style="width: 25%;"></div></div> 25% [1/4]	<div style="width: 33%;"><div style="width: 33%;"></div></div> 33% [2/6]	<div style="width: 25%;"><div style="width: 25%;"></div></div> 25% [2/8]	<div style="width: 25%;"><div style="width: 25%;"></div></div> 25% [2/8]	<div style="width: 25%;"><div style="width: 25%;"></div></div> 25% [2/8]
<input type="checkbox"/> NP00201	Zr Ce	CeO2 - redox ratio 2:Ce0.73Zr0.27O2:PROM CeO2-Zr 024C	<div style="width: 0%;"><div style="width: 0%;"></div></div> 0% [0/8]	<div style="width: 0%;"><div style="width: 0%;"></div></div> 0% [0/4]	<div style="width: 0%;"><div style="width: 0%;"></div></div> 0% [0/6]	<div style="width: 0%;"><div style="width: 0%;"></div></div> 0% [0/8]	<div style="width: 0%;"><div style="width: 0%;"></div></div> 0% [0/2]	<div style="width: 0%;"><div style="width: 0%;"></div></div> 0% [0/6]

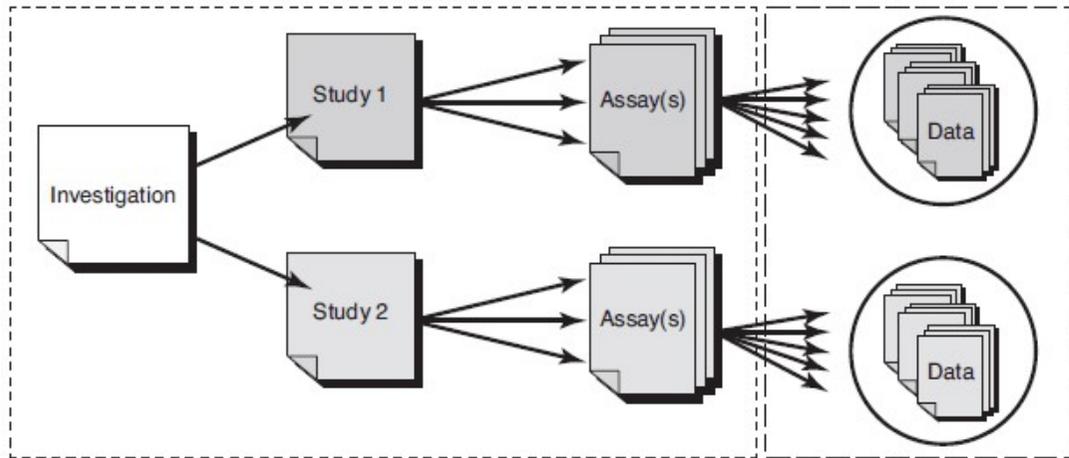


PARC APIs  
PARC interoperability layer  
Link to Modelling tools /  
SSbD

# Key performance indicator: No. & % PARC datasets made FAIR

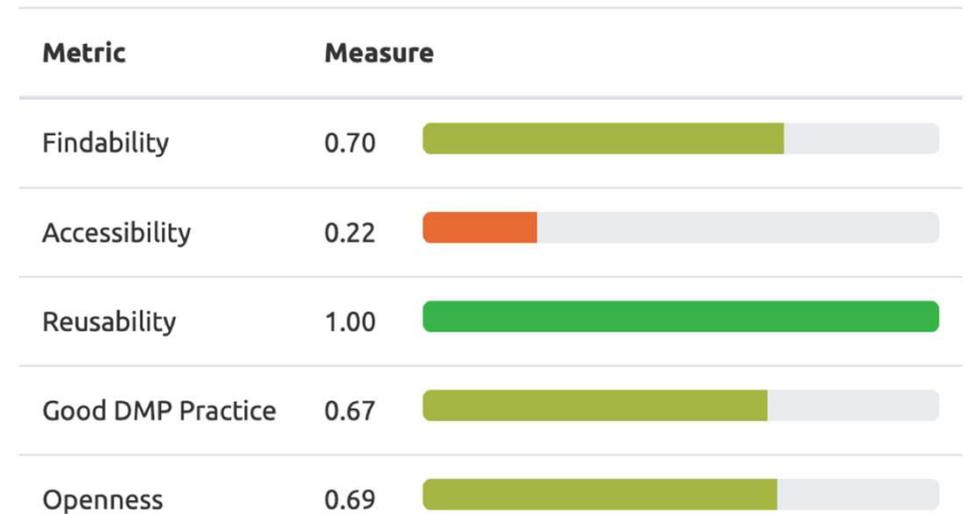
What is the unit of a dataset?

FAIR Scoring approaches?



Investigation (project in PARC) / study / assay

Initially using unit of a publication and its data



DSW has some indicators

FAIR metrics for databases

**Many thanks for listening....**



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