



NanoCommons
Nano-Knowledge Community



Education day
16th November 2020
NanoSafe2020 conference

Session 4: E-tools along data life cycle

Data life cycle – generation processing, evaluation, prediction, curation

Prof. Iseult Lynch,

University of Birmingham

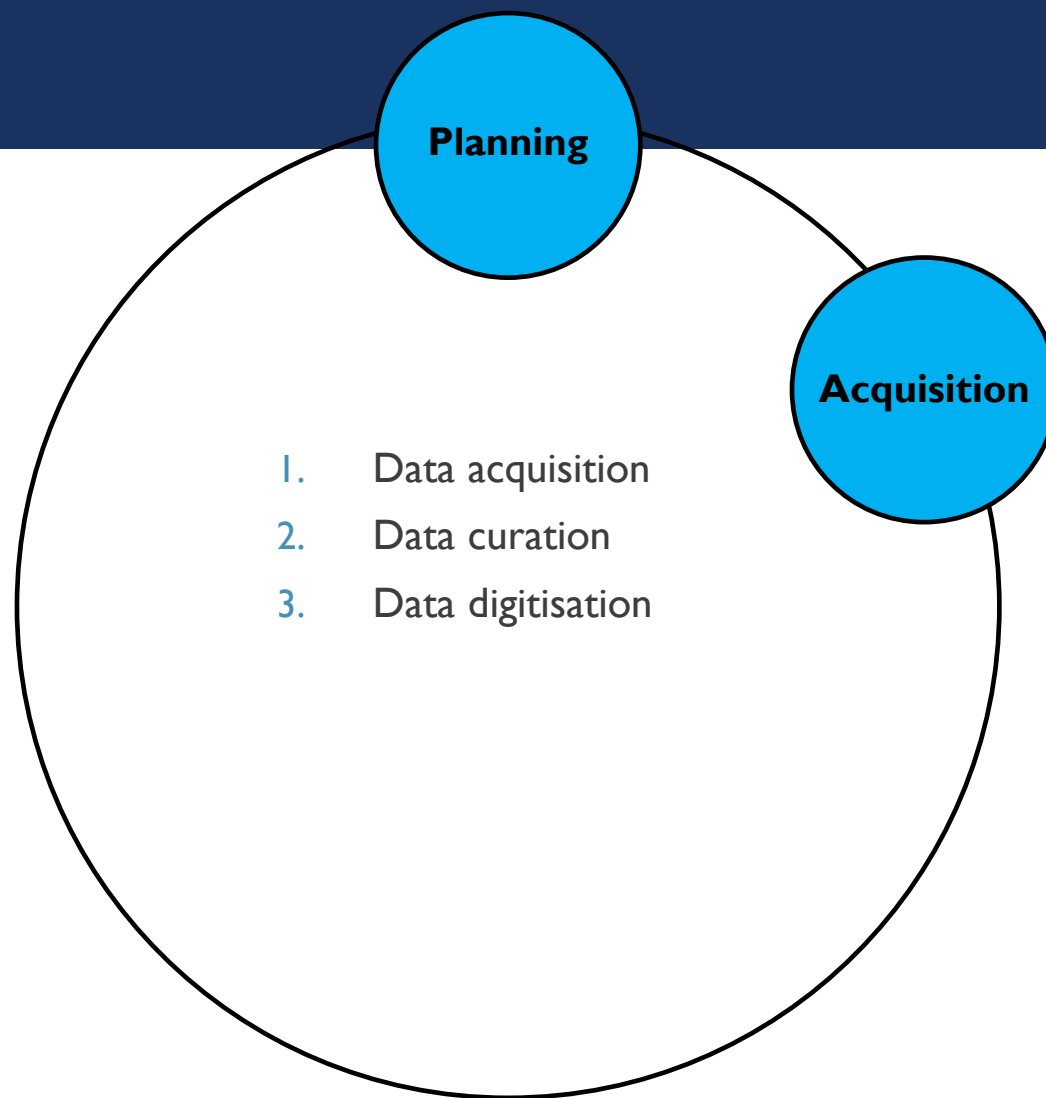
DATA LIFECYCLE

Planning

1. Endpoint identification
2. Experimental design
3. Data management plan
4. Data templates creation



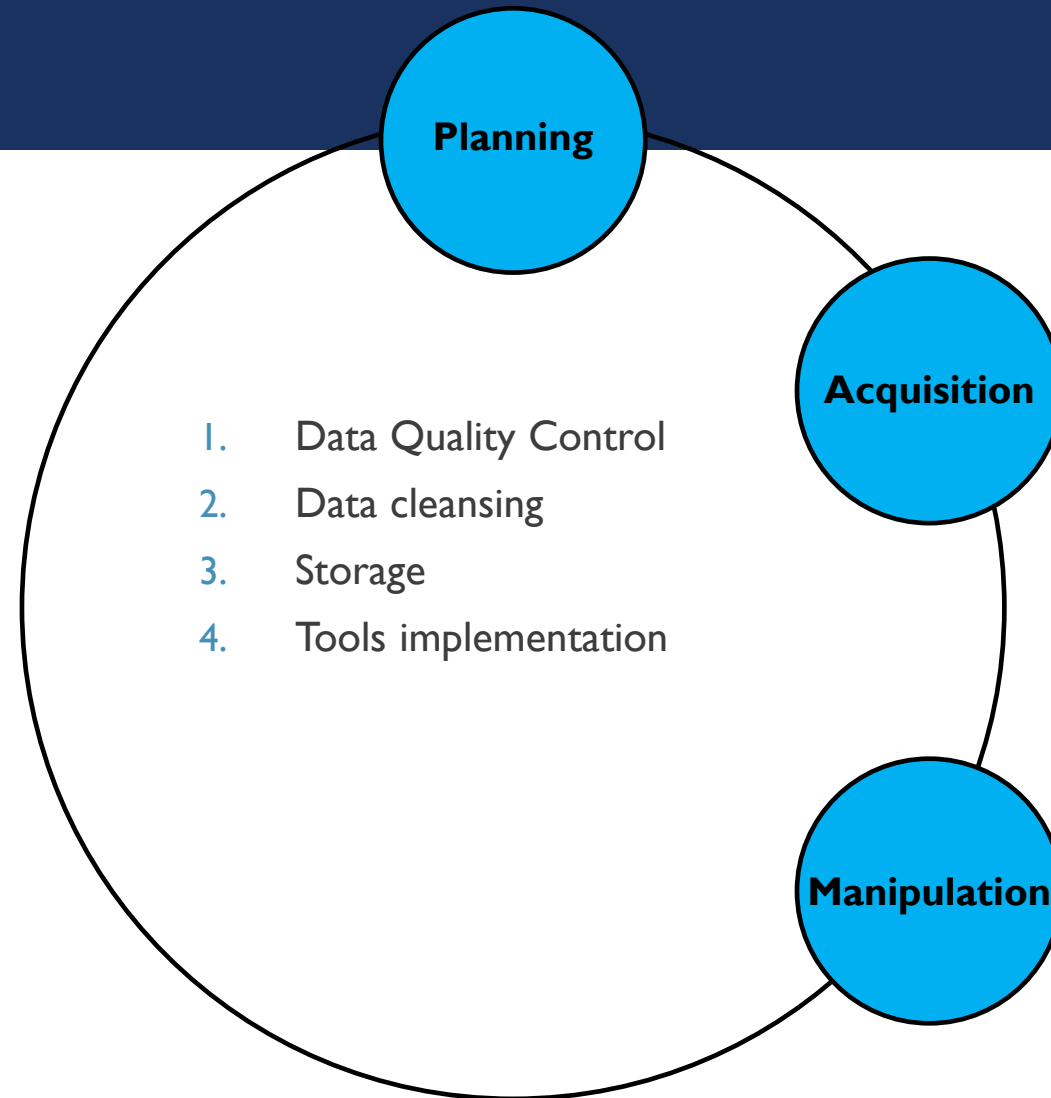
DATA LIFECYCLE



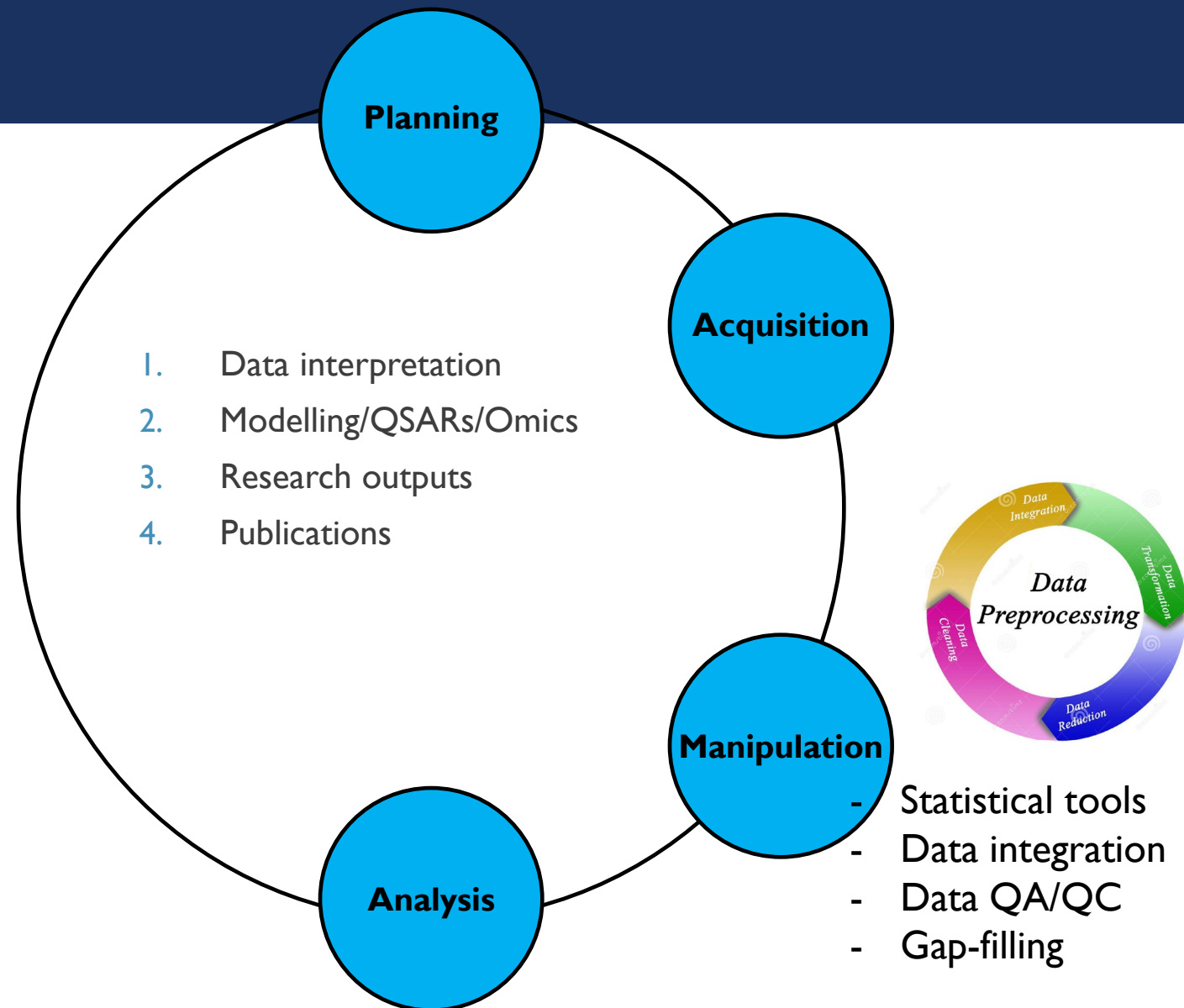
- Electronic lab notebooks
- Automated experimental workflows
- Data capture templates



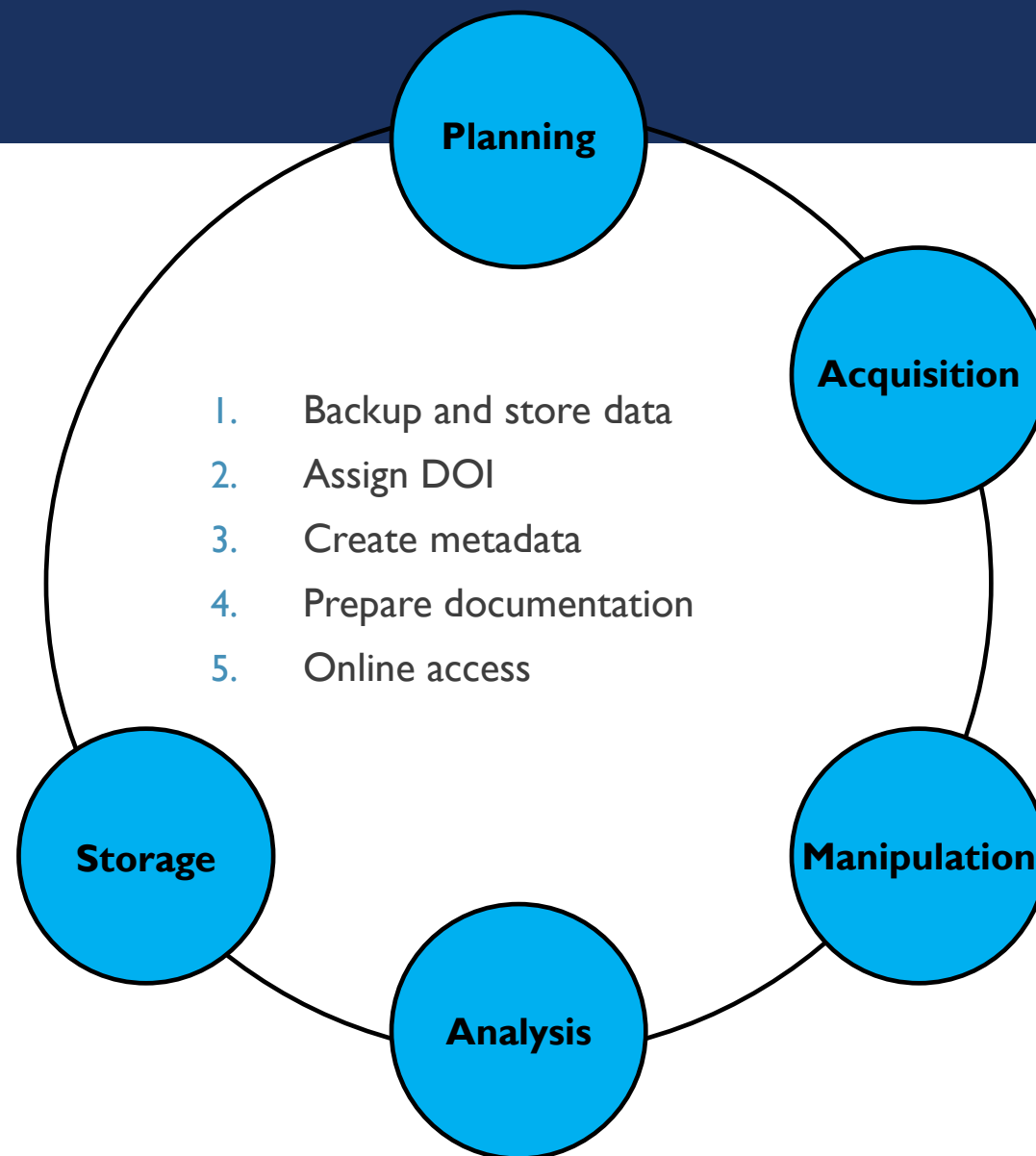
DATA LIFECYCLE



DATA LIFECYCLE

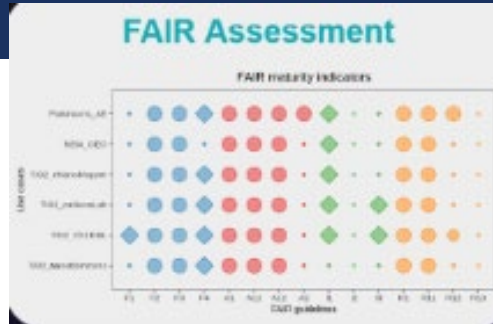


DATA LIFECYCLE

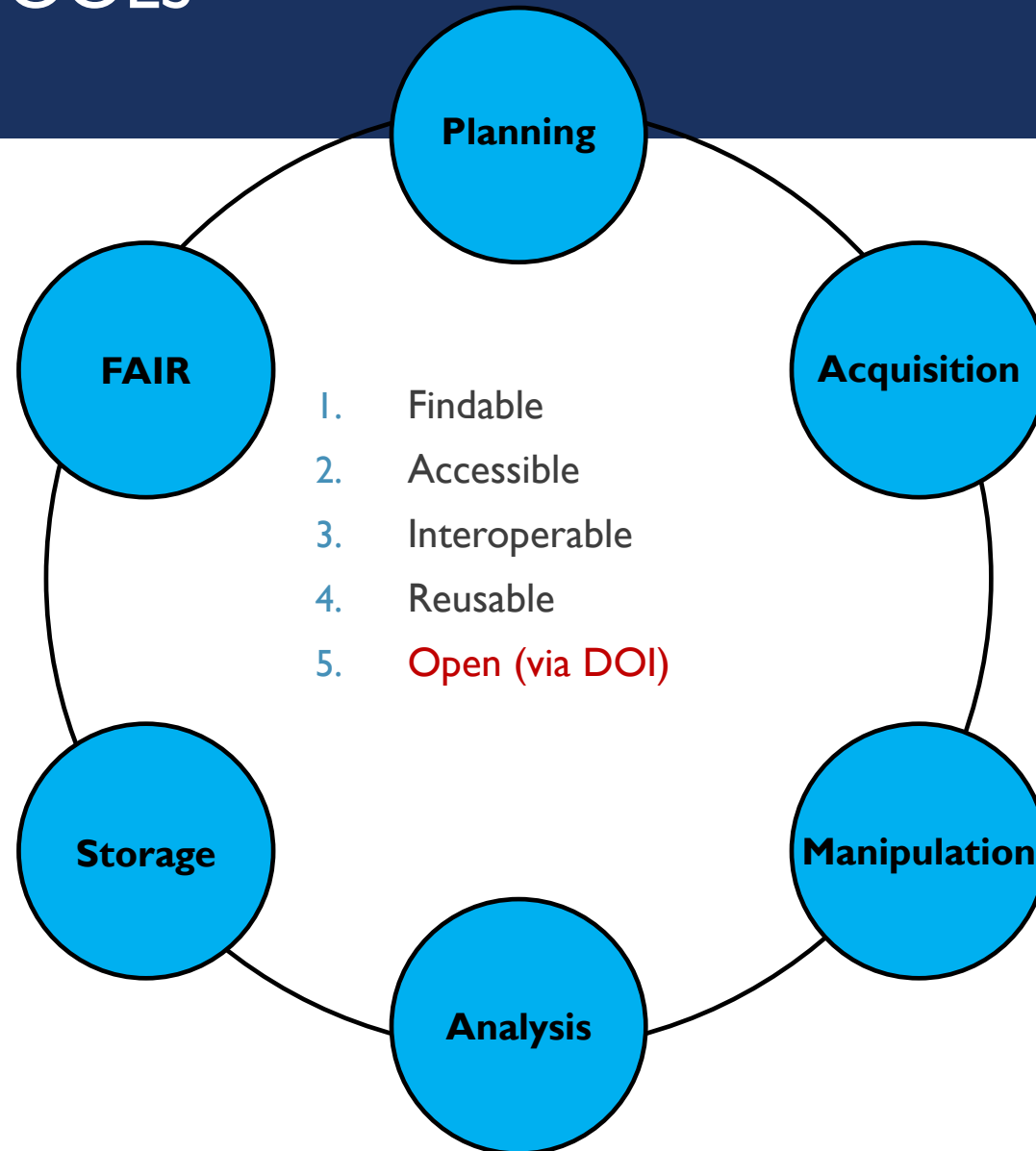


- Data / metadata indexing
- Data / metadata storage
- Dataset interoperability
- Database linking

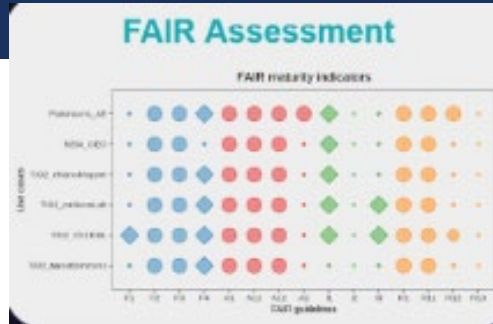
DATA LIFECYCLE TOOLS



- semi-automated FAIR scorecards
- Scientific FAIR principles
- Metadata community consensus



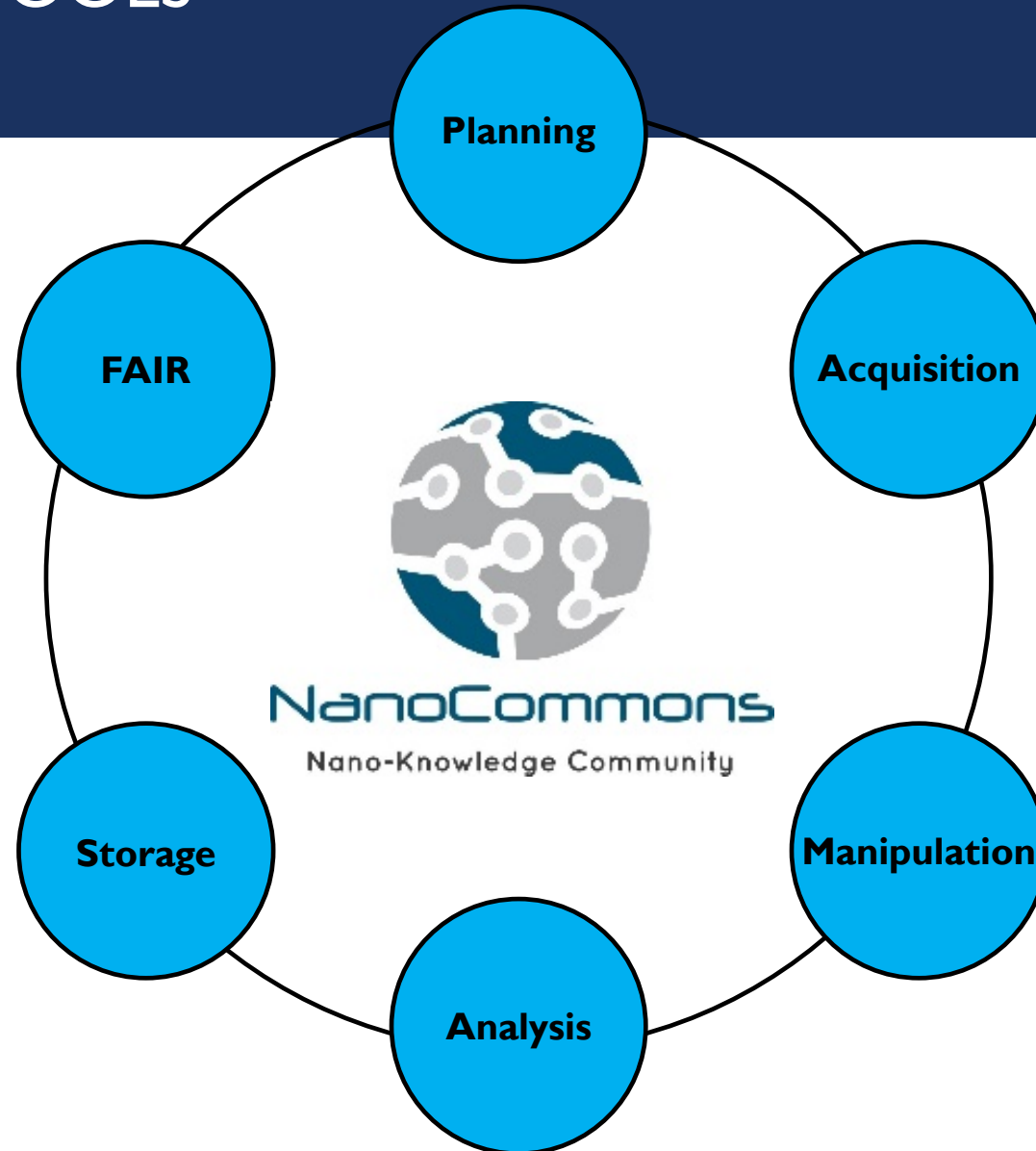
DATA LIFECYCLE TOOLS



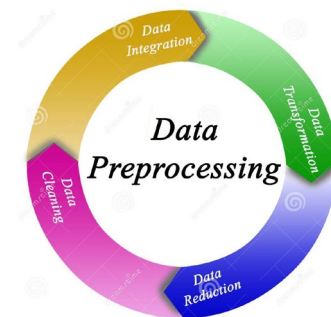
- semi-automated FAIR scorecards
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- Data / metadata indexing
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- Electronic lab notebooks
- Automated experimental workflows
- Data capture templates



- Statistical tools
- Data integration
- Data QA/QC
- Gap-filling (computational)

ACCESS TO ALL TOOLS AVAILABLE VIA NANOCOMONS “TA”



**Experimental Workflows
Design & Implementation**



**Data Processing
& Analysis**



**Data Storage
& Online Accessibility**



**Data Visualisation
& Predictive Toxicity**

Existing tools or custom versions tailored to your needs

Funded access to the expertise needed to implement data life-cycle tools to your workflows

Apply here:

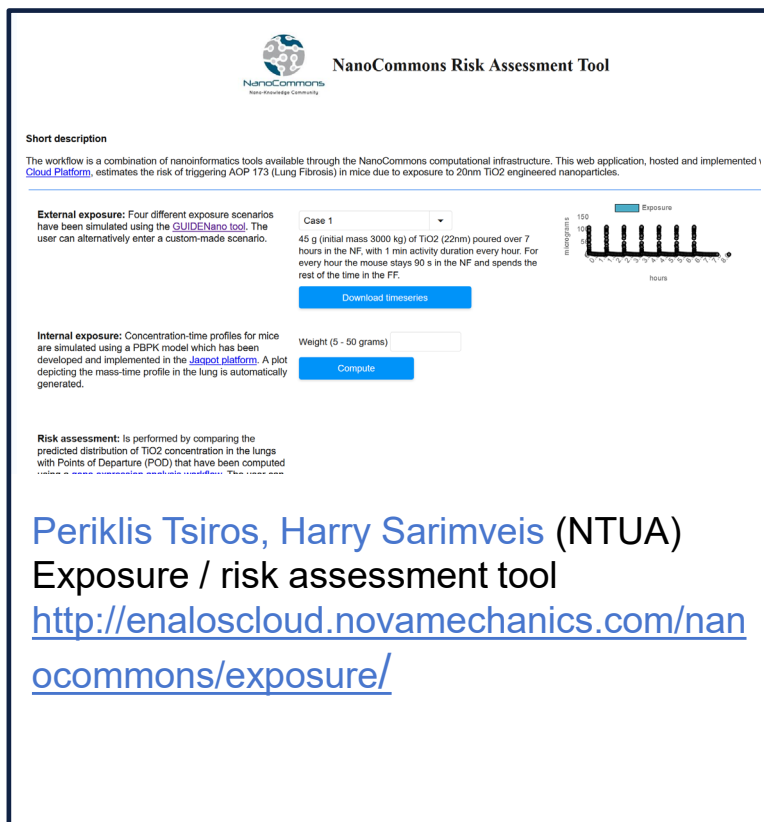
<https://www.nanocommons.eu/apply-for-access/>

Rolling call - next review date: **1st December 2020**

For details contact:

i.lynch@bham.ac.uk or a.Papadiamantis@bham.ac.uk

TOOLS DEMONSTRATED IN THIS SESSION



NanoCommons Risk Assessment Tool

Short description
The workflow is a combination of nanoinformatics tools available through the NanoCommons computational infrastructure. This web application, hosted and implemented in [Cloud Platform](#), estimates the risk of triggering AOP-173 (Lung Fibrosis) in mice due to exposure to 20nm TiO₂ engineered nanoparticles.

External exposure: Four different exposure scenarios have been simulated using the [GUIDENano tool](#). The user can alternatively enter a custom-made scenario.

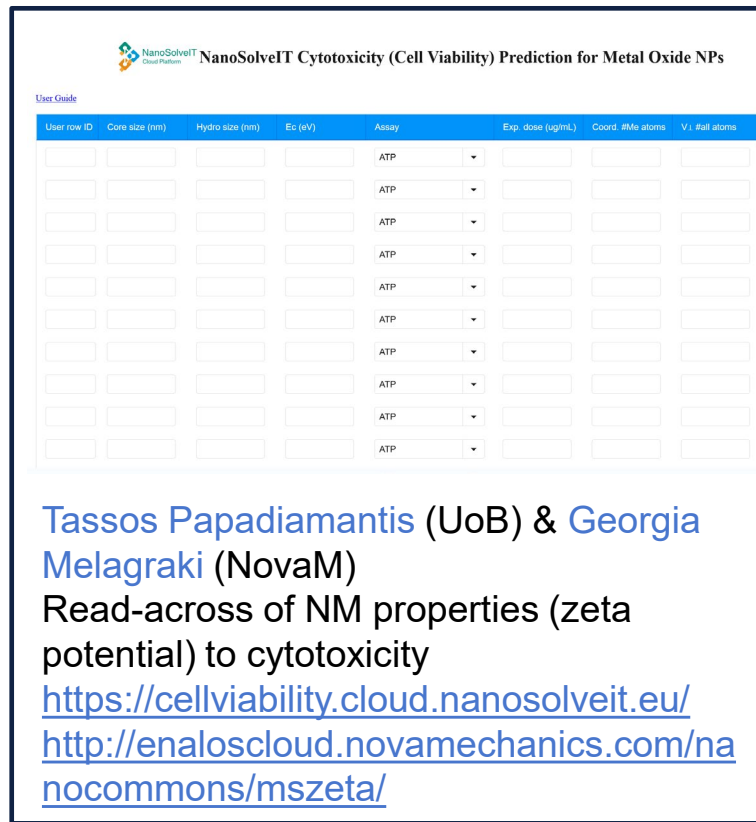
Case 1
45 g (initial mass 3000 kg) of TiO₂ (22nm) poured over 7 hours in the NF, with 1 min activity duration every hour. For every hour the mouse stays 90 s in the NF and spends the rest of the time in the FF.

Internal exposure: Concentration-time profiles for mice are simulated using a PBPK model which has been developed and implemented in the [Jagpot platform](#). A plot depicting the mass-time profile in the lung is automatically generated.

Weight (5 - 50 grams)

Risk assessment: Is performed by comparing the predicted distribution of TiO₂ concentration in the lungs with Points of Departure (POD) that have been computed from [in vivo experimental conditions](#). The user can

Periklis Tsiros, Harry Sarimveis (NTUA)
Exposure / risk assessment tool
<http://enaloscloud.novamechanics.com/nanocommons/exposure/>

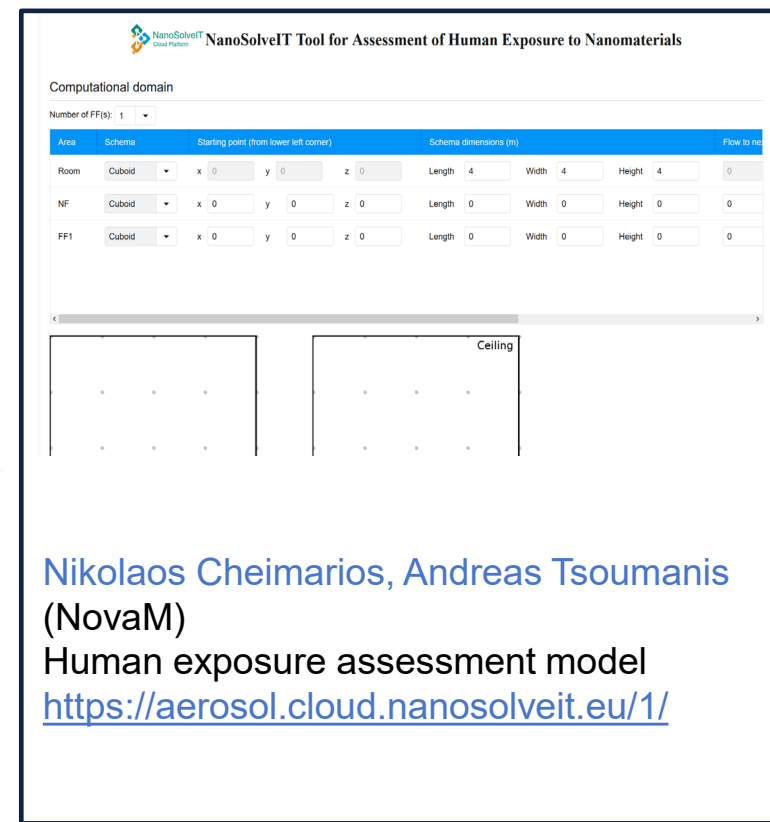


NanoSolveIT Cytotoxicity (Cell Viability) Prediction for Metal Oxide NPs

User Guide

User row ID	Core size (nm)	Hydro size (nm)	Ec (eV)	Assay	Exp. dose (µg/mL)	Coord. #Me atoms	V.L. #all atoms
				ATP			
				ATP			
				ATP			
				ATP			
				ATP			
				ATP			
				ATP			
				ATP			
				ATP			
				ATP			
				ATP			
				ATP			

Tassos Papadimitis (UoB) & Georgia Melagraki (NovaM)
Read-across of NM properties (zeta potential) to cytotoxicity
<https://cellviability.cloud.nanosolveit.eu/>
<http://enaloscloud.novamechanics.com/nanocommons/mszeta/>



NanoSolveIT Tool for Assessment of Human Exposure to Nanomaterials

Computational domain

Number of FF(s): 1

Area	Schema	Starting point (from lower left corner)			Schema dimensions (m)			Flow to net
		x	y	z	Length	Width	Height	
Room	Cuboid	0	0	0	4	4	4	0
NF	Cuboid	0	0	0	0	0	0	0
FF1	Cuboid	0	0	0	0	0	0	0

Nikolaos Cheimarios, Andreas Tsoumanis (NovaM)
Human exposure assessment model
<https://aerosol.cloud.nanosolveit.eu/1/>

Idea, methodology, current state of the NanoinformaTIX platform” by Gianpetro Basei, Greendecision

Call for action on the Gracious Ontology-Wiki” by Thomas Exner, Edelweiss Connect