



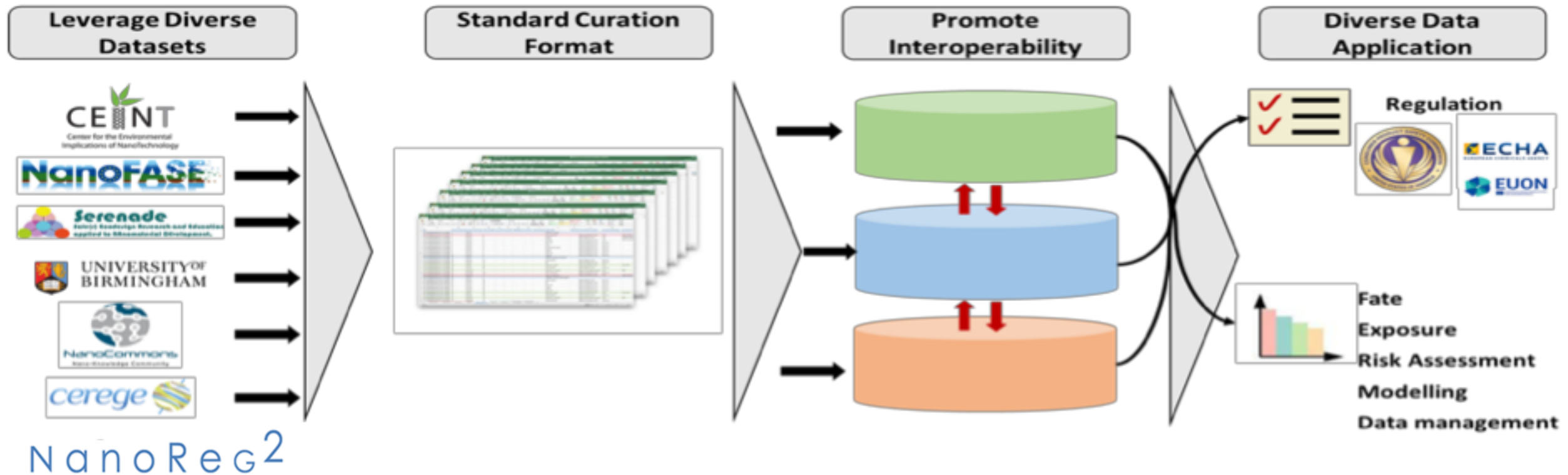
Towards an integrated global platform for nanoinformatics knowledge management and predictive (eco)toxicology modelling: **NanoCommons** and **NanoSolveIT**

Iseult Lynch

University of Birmingham

Coordinator NanoCommons; Deputy Coordinator NanoSolveIT

The European Nanotechnology Community Informatics Platform: Bridging data and disciplinary gaps for industry and regulators



- Bridge different fields by promoting data comparability and project continuity



This project has received funding from the European Union Horizon 2020 Programme (H2020) under grant agreement no. 731032

Data Management

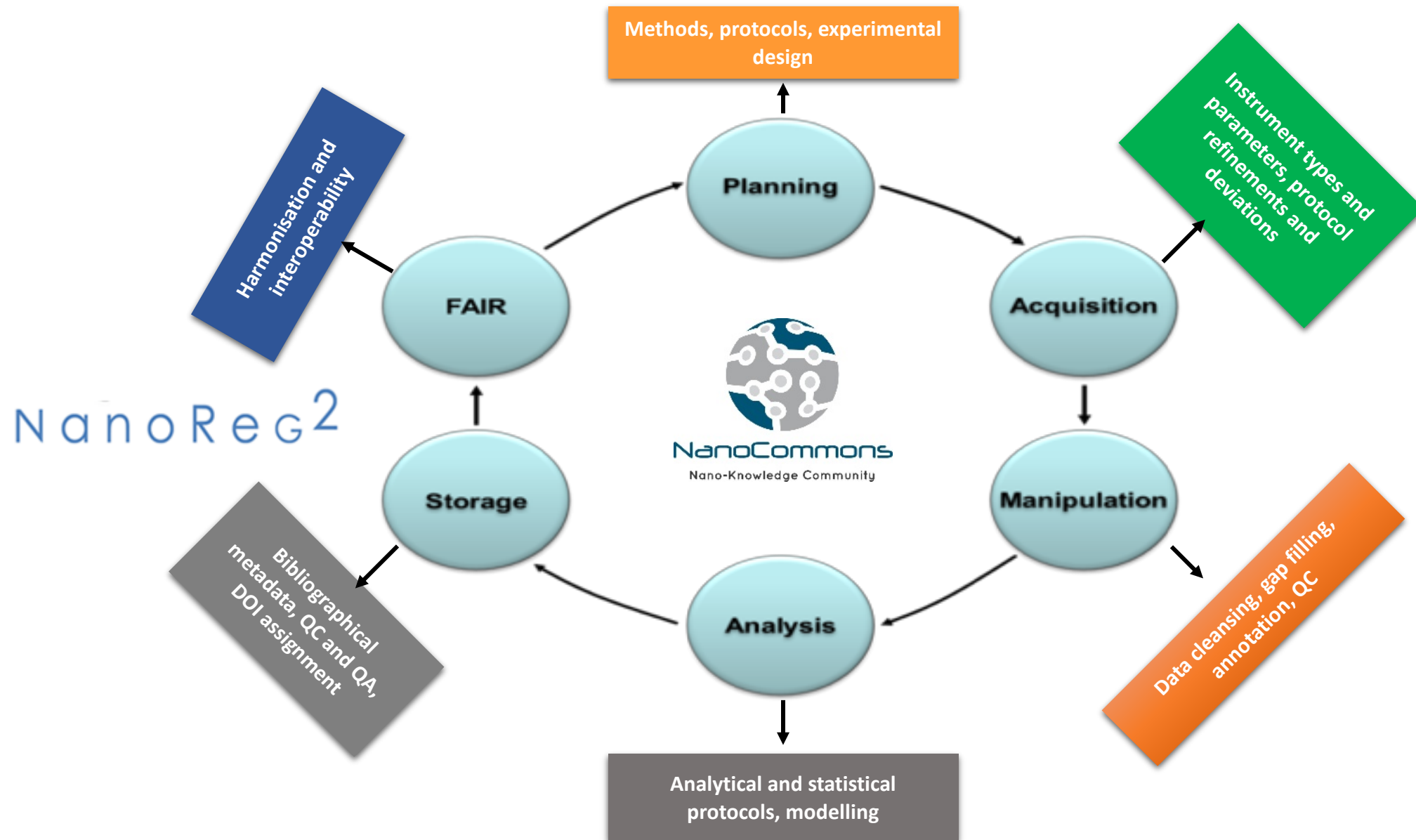
Definition

Data Management is the implementation and application of processes, which allow the acquisition, storage, manipulation and analysis of data during its lifecycle.

Cause & Effect

- Is the most neglected scientific process
- Most labs, at a global scale, are yet to enter the 21st century
- Can lead to significant loss of data and metadata
- Can decrease the quality of data and scientific publications
- Can lead to the loss of significant insights
- Does not allow further data exploitation (e.g. AI, machine learning)

Data management, data lifecycle & metadata



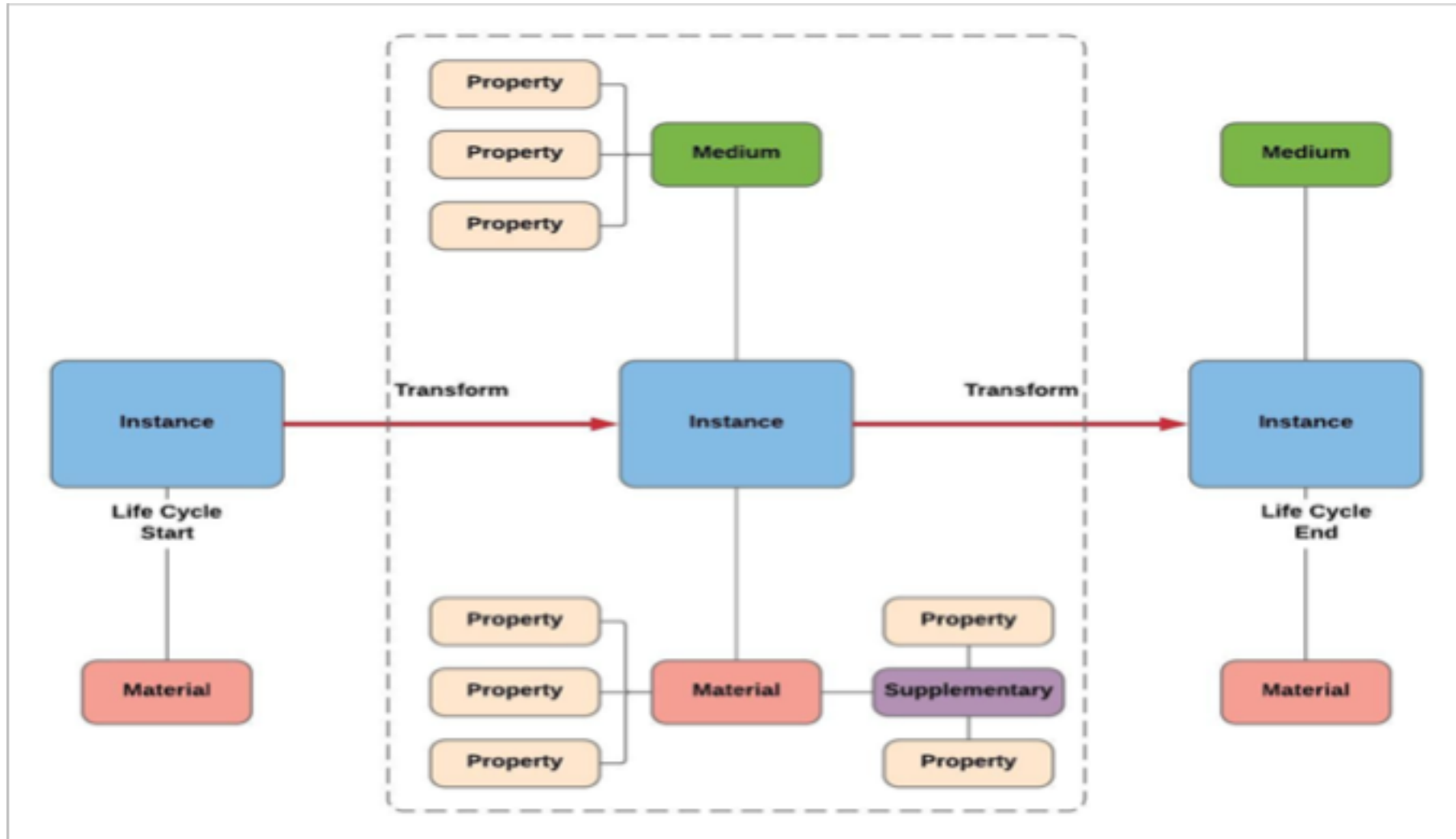
FAIR Data Benefits & Impact

- Knowledge discovery
- Data and knowledge integration
- Data harmonisation, sharing and reusability
- Discipline/field independent, not one fits all model
- Data and metadata are machine readable, promoting interoperability and hidden pattern uncovering
- Maximum data exploitation and impact
- Increased citations and visibility



FAIR ≠ OPEN

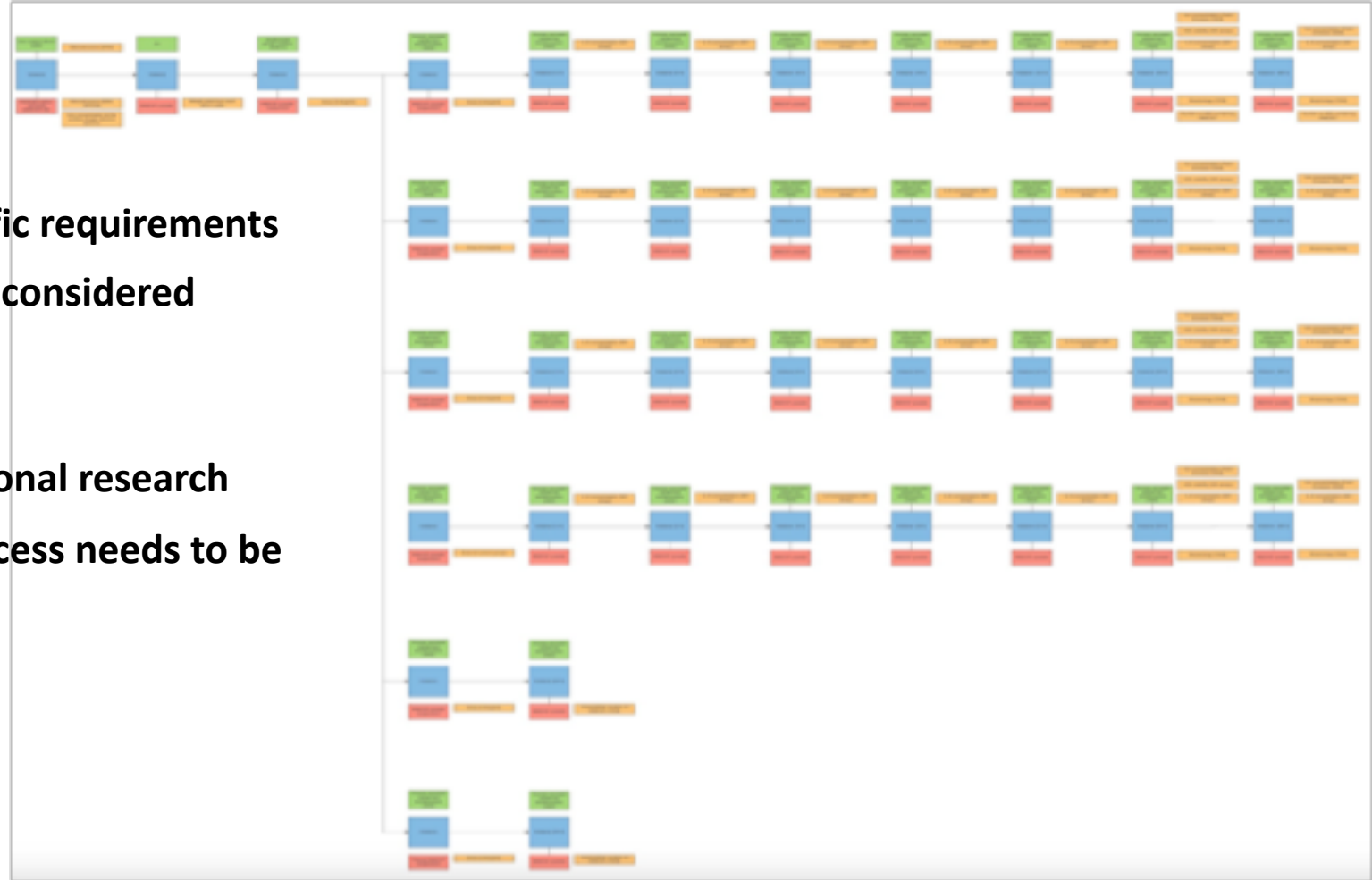
Data Curation – Instance Map



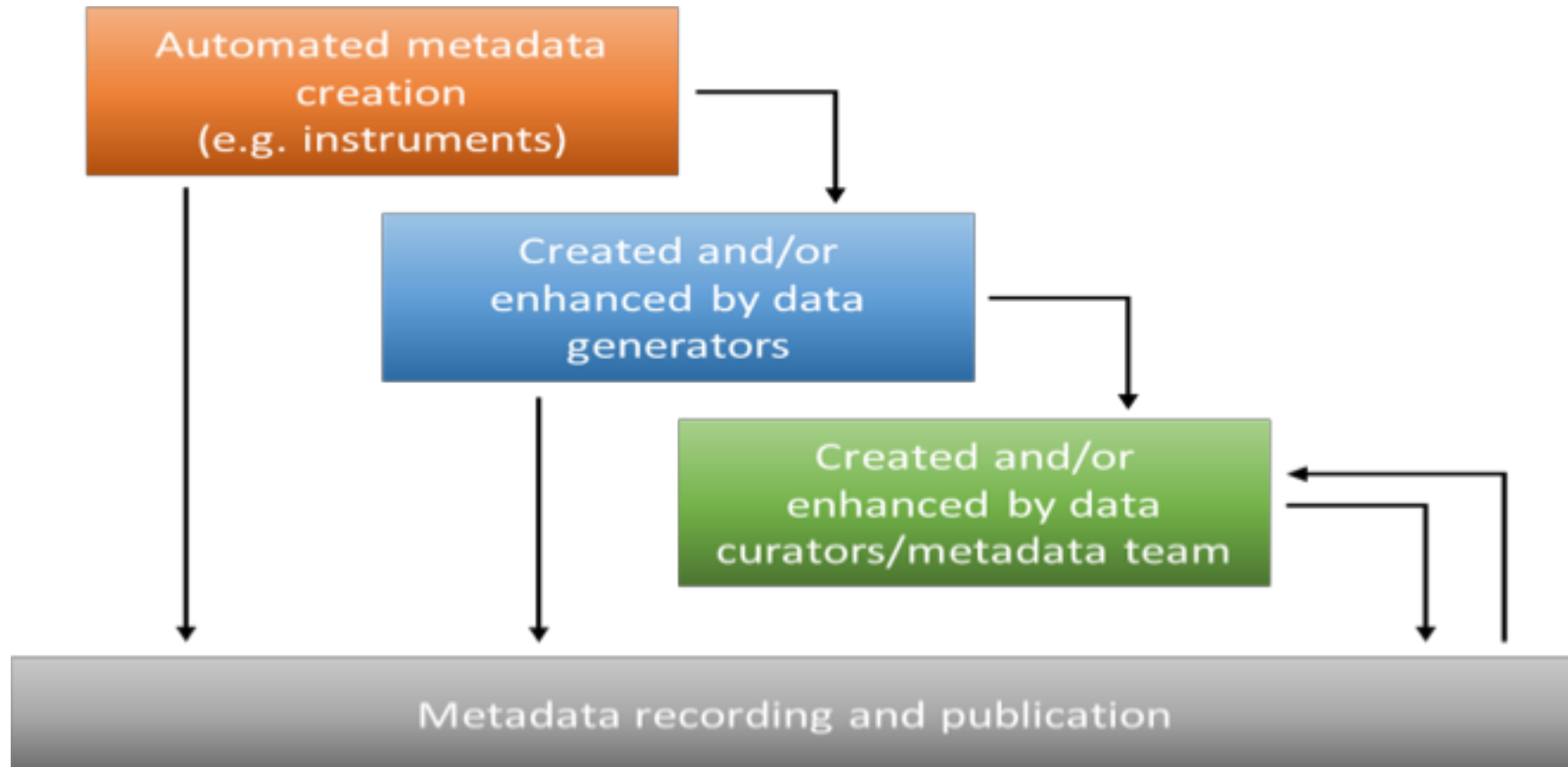
Data Curation: The process of data collection, structuring and organisation

Data Curation & Adaptability

- **Dynamic and versatile templates to fit specific requirements**
- **Experimental protocols and instruments are considered datapoints**
- **Online lab book compatibility**
- **Promoting data harmonisation and translational research**
- **To achieve these goals the data curation process needs to be moved to the data generators**

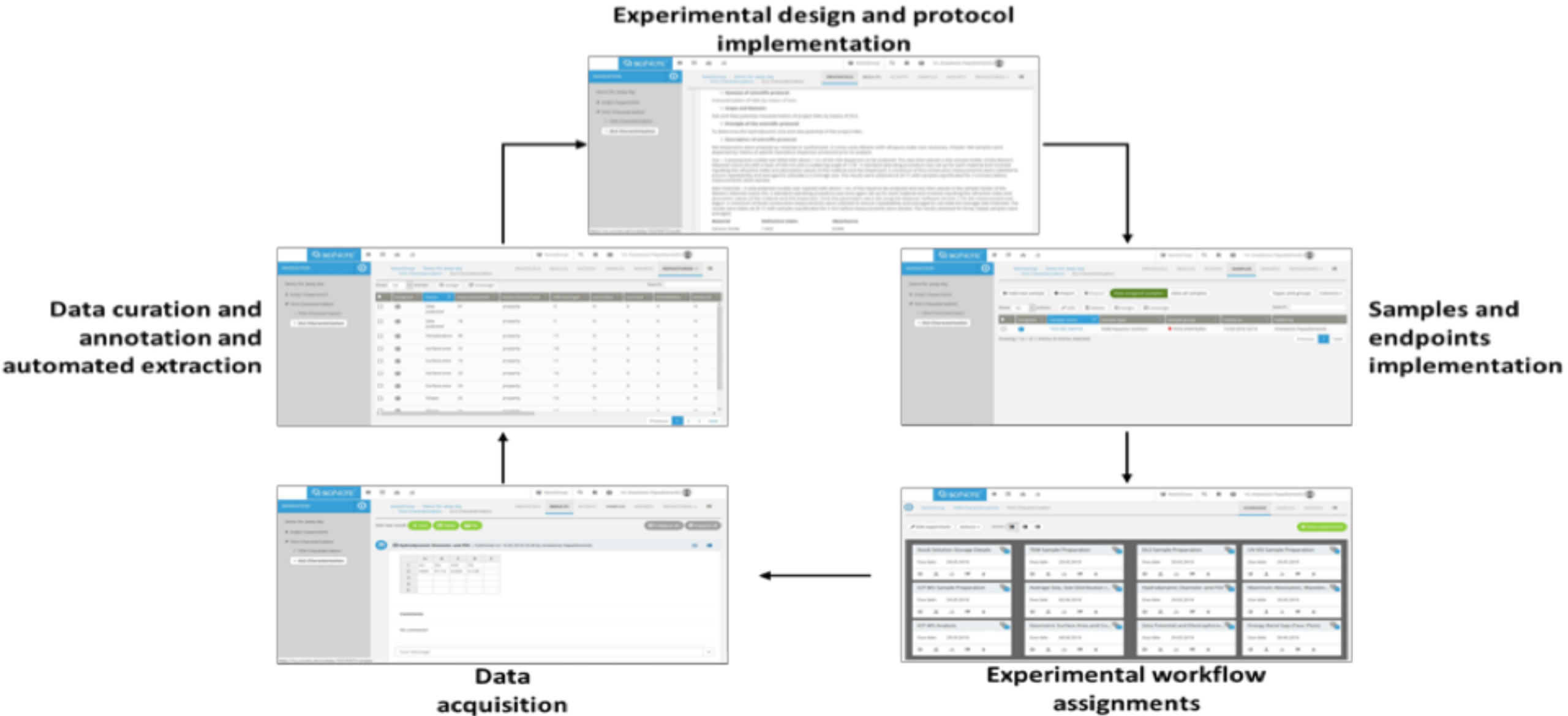


Metadata Implementation

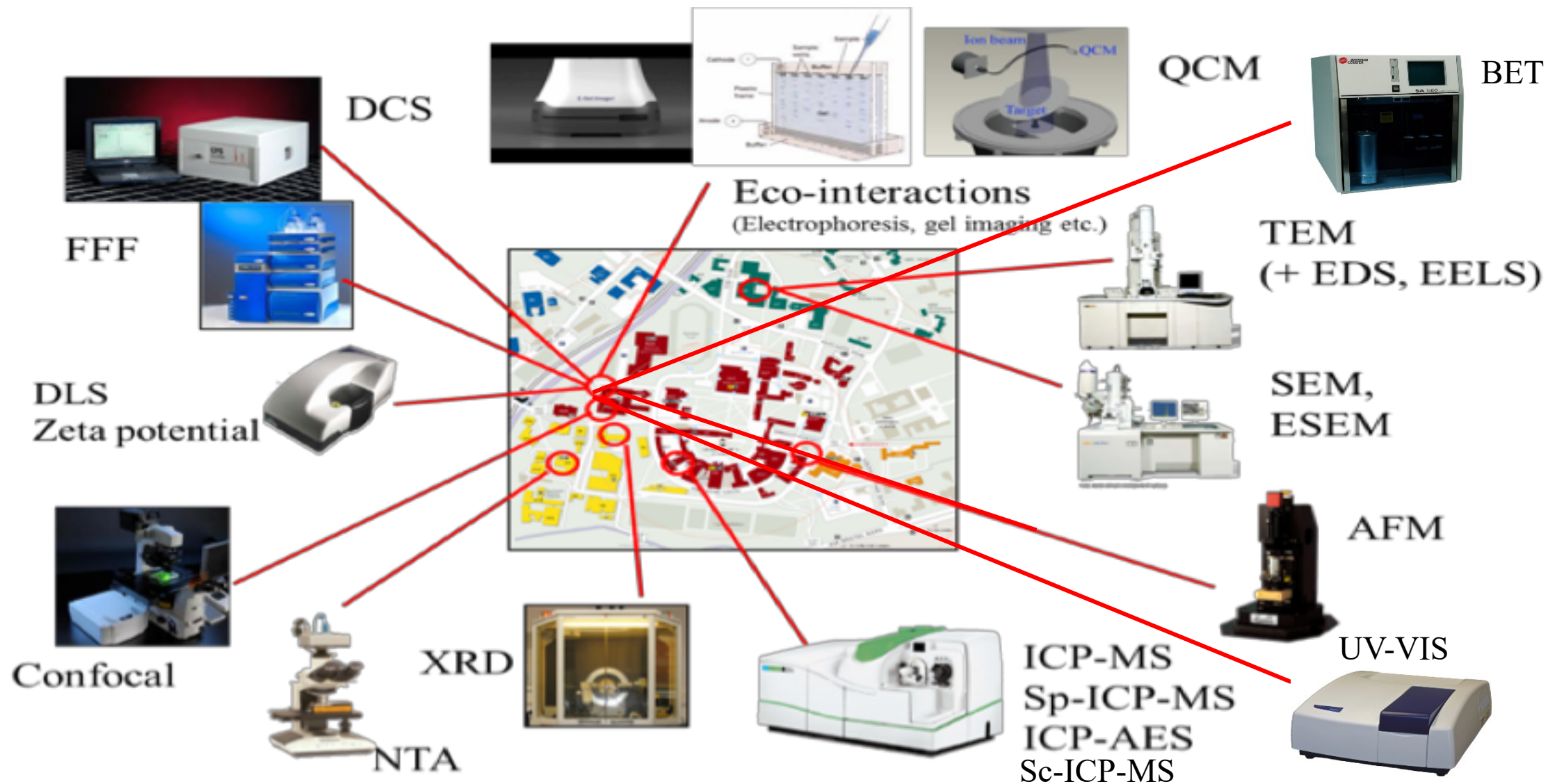


- But we need to **achieve interoperability through data annotation**

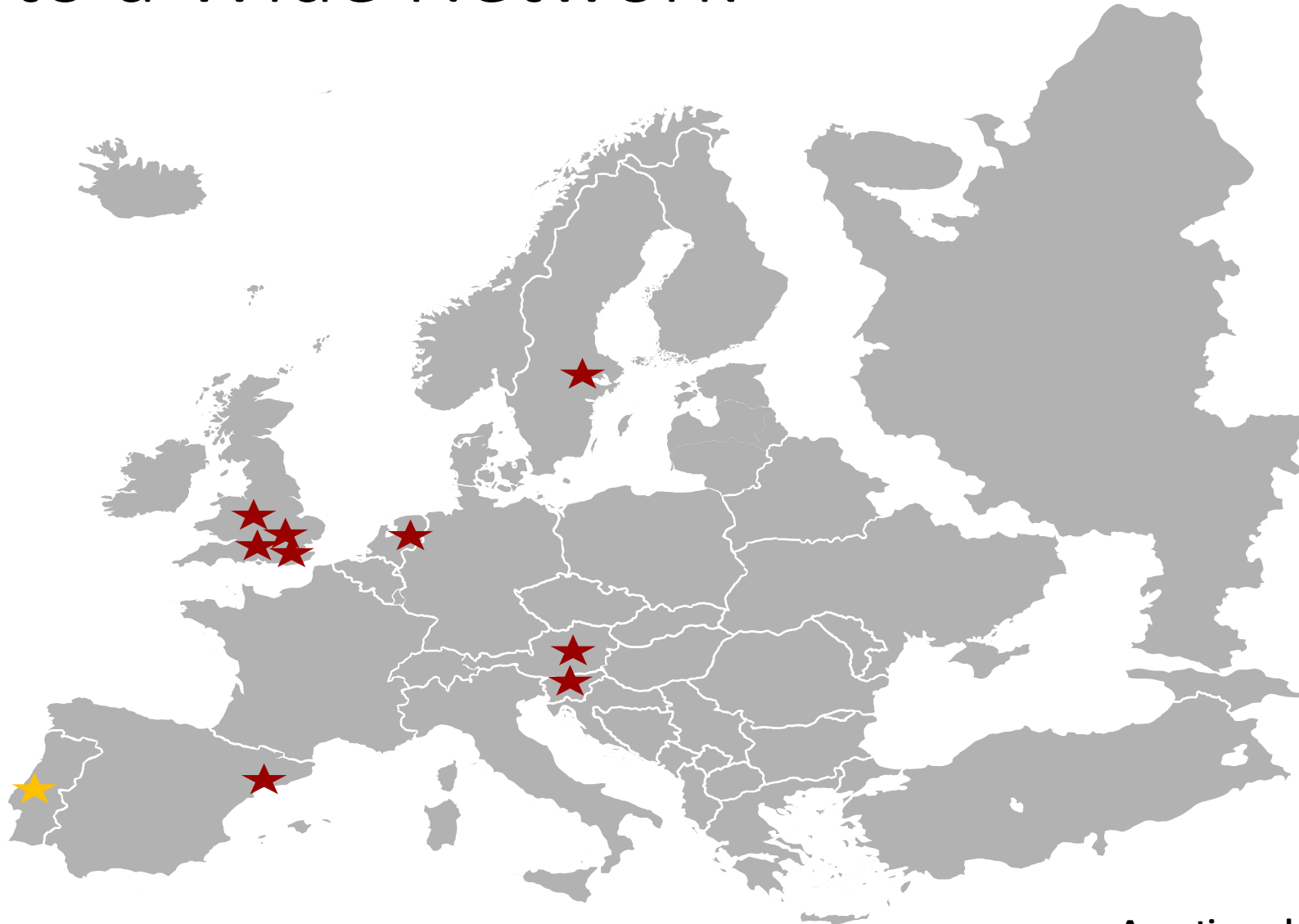
Data Acquisition & Management



From a Local Network...



... to a Wide Network



**Aquatic and terrestrial mesocosm experiment,
7 EU countries and 10 Institutions**

... and Global Network

Support for customised experimental workflows of varying complexity



Transnational Access key aspect

We develop, you access



Experimental Workflows
Design & Implementation

Automated data acquisition, online
lab-books, data curation templates,
nanoinformatics implementation.



Data Processing &
Analysis

From data cleansing, mining and
analysis to modelling and from ISA-
TAB tools to ontologies.



Data Visualisation &
Predictive Toxicity

Omics, QSARs, modelling and risk
assessment tools.



Data Storage & Online
Access

Data repositories, storage, online
access

1st TA call opened **4th February 2019** – users can apply for 1 or more of the data /
informatics services offered

International partnerships possible: Currently implementing similar approach with Brazil, S. Korea & CSN in USA

Innovative **N**anoinformatics models and tools: towards a **S**olid, **v**erified and **I**ntegrated Approach to Predictive (eco)**T**oxicology (**N**ano**S**olve**I**T)

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 814572



NanoSolveIT aspires to introduce a ground-breaking in silico Integrated Approach to Testing and Assessment ([IATA](#)) for the environmental health and safety of Nanomaterials (NM), implemented through a decision support system packaged as both a stand-alone open software and via a Cloud platform.

NanoSolveIT

Duration: 01/01/2019 – 28/02/2023

NanoSolveIT will deliver

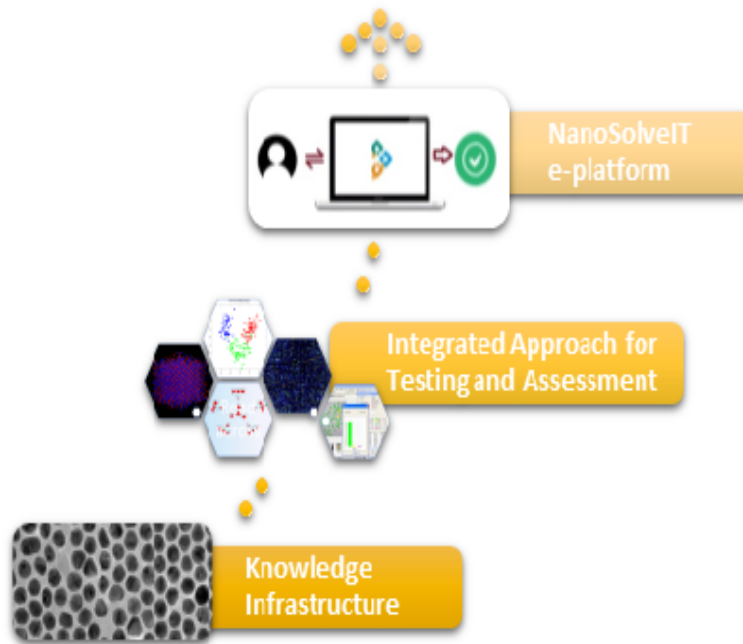
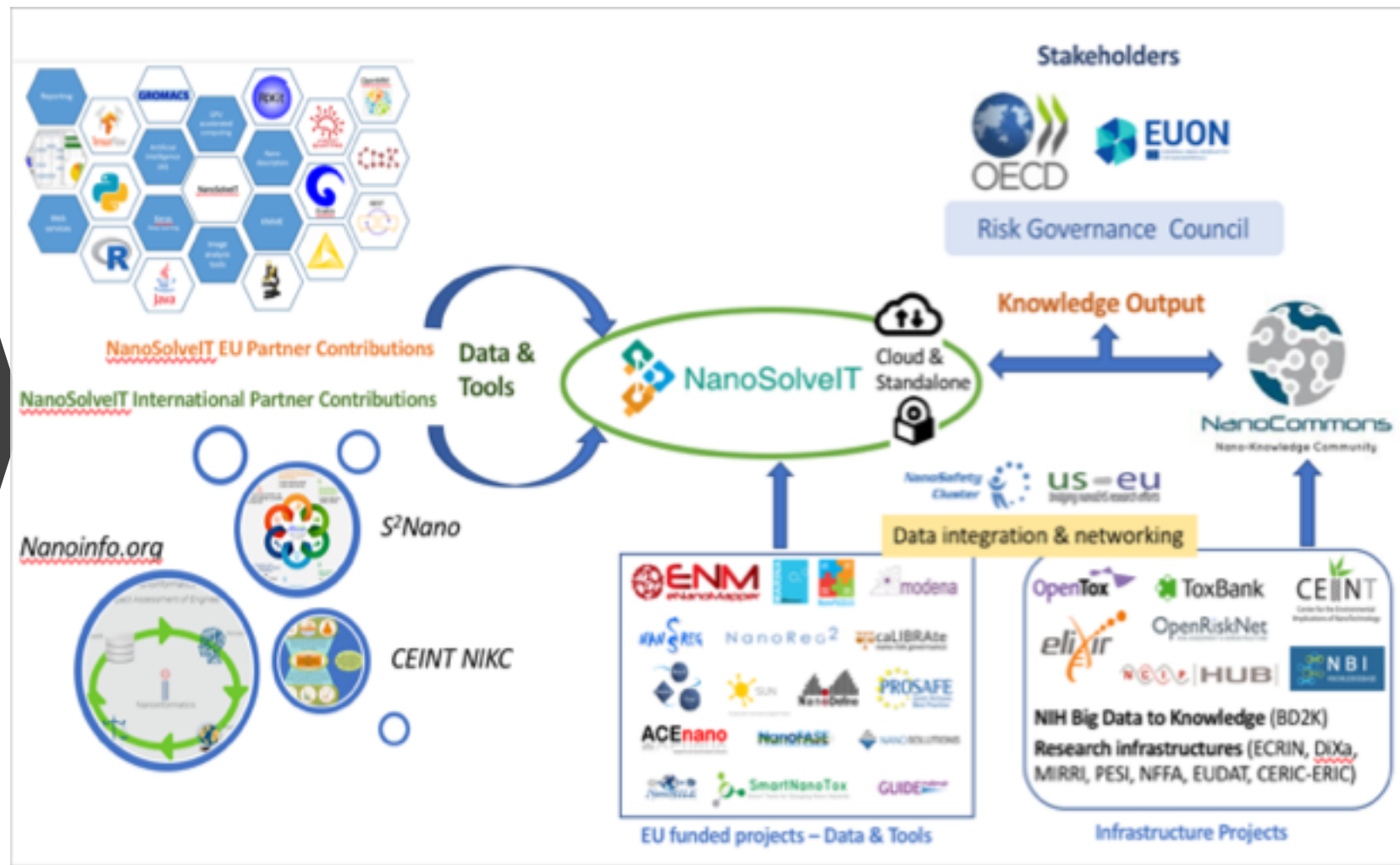
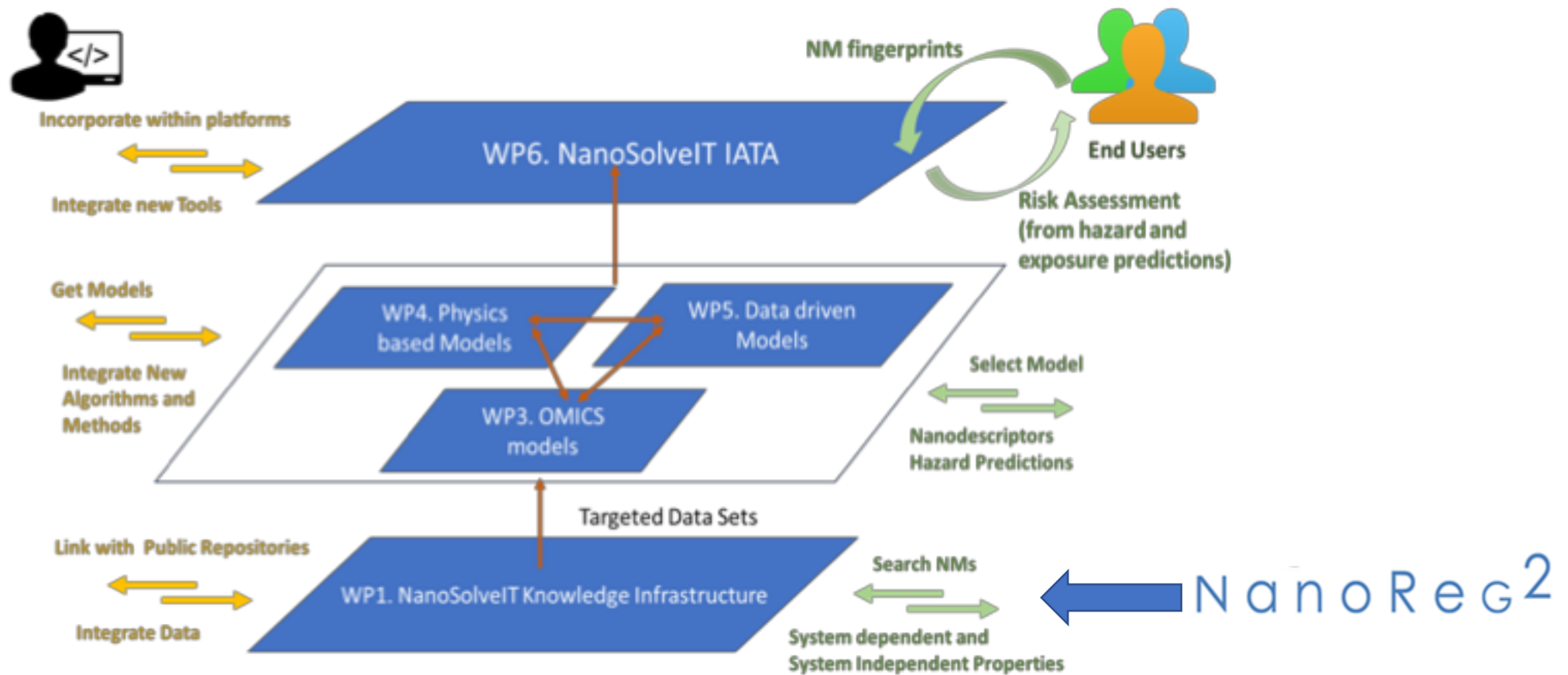


Figure 1. NanoSolveIT key steps

- a validated, sustainable, multi-scale nanoinformatics IATA, tested and demonstrated at TLR6 via OECD-style case studies, to serve the needs of diverse stakeholders at each stage of the NMs value chain, for assessment of potential adverse effects of NM on human health and the environment.

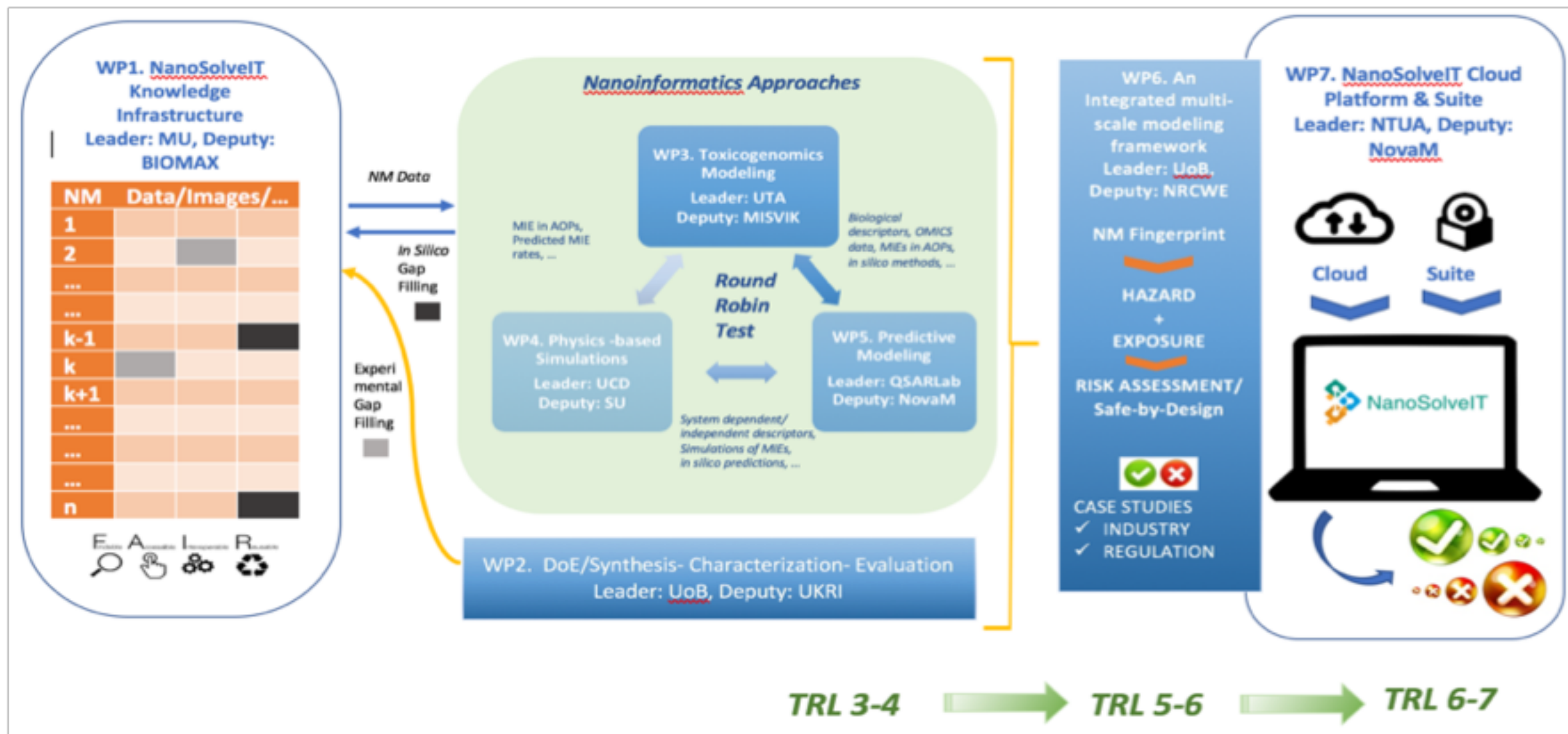
NanoSolveIT's positioning and liaison with other initiatives



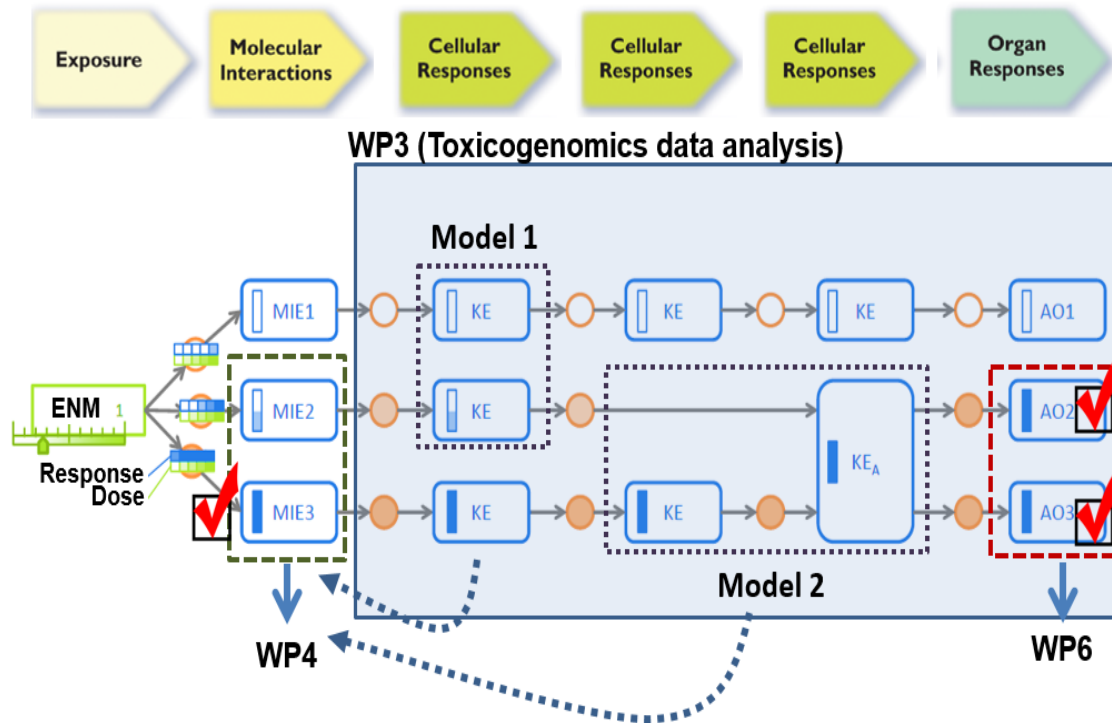


Schematic illustration of the NanoSolveIT nanosafety informatics system components and their interlinkages

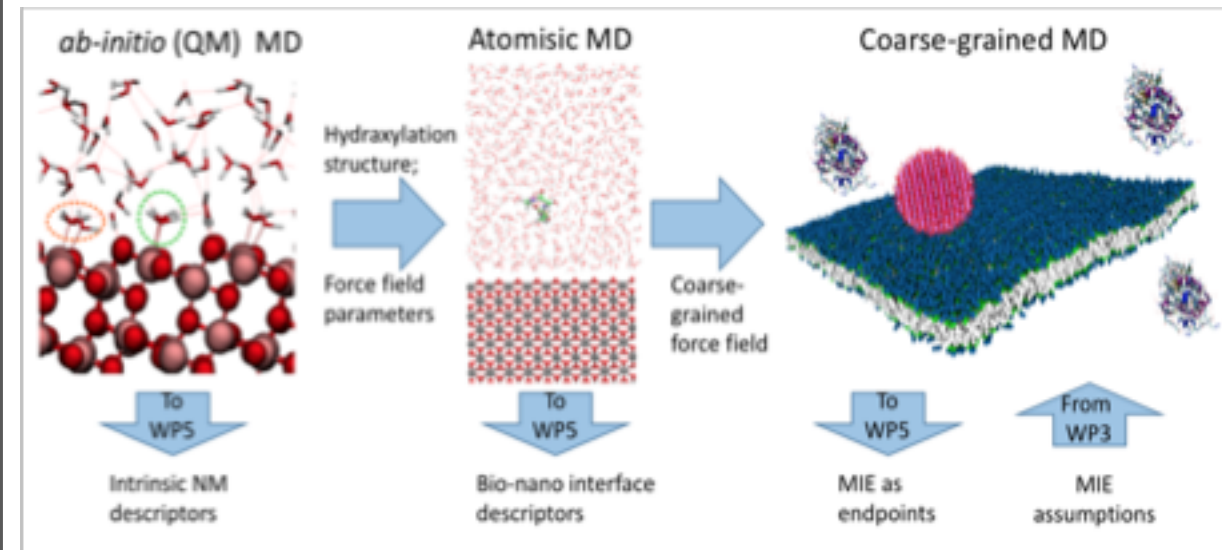
NanoSolveIT Overview WPs Interlinkages



(1) Toxicogenomics data analysis (WP3) and key interactions (2) Multiscale modelling (WP4) and key inputs and outputs



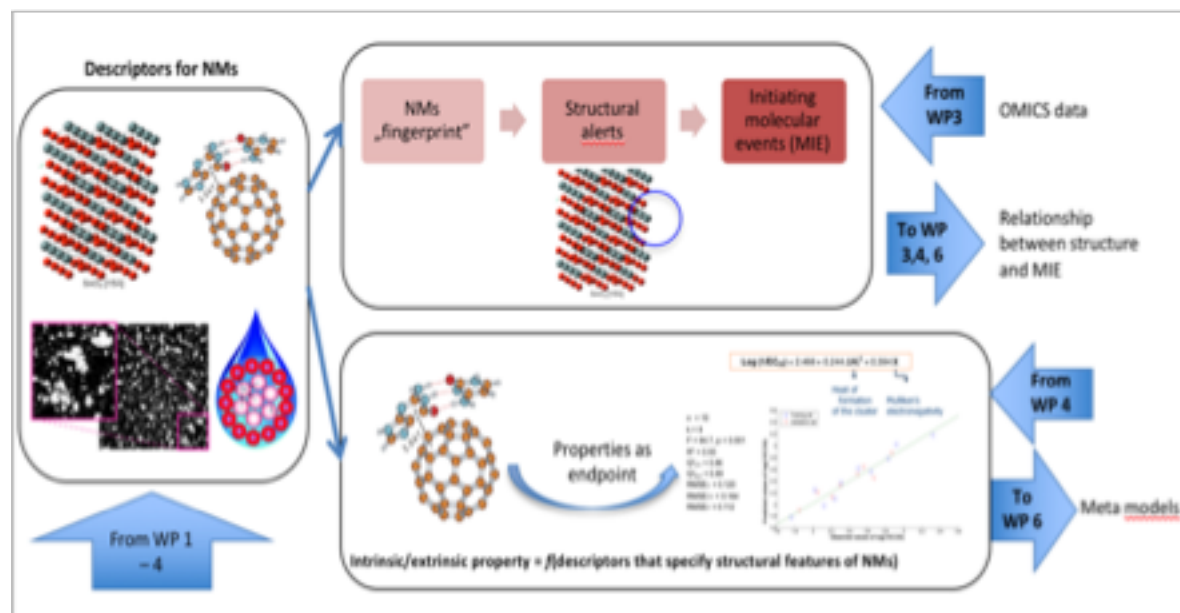
(1)



(2)

(3) Data-driven artificial intelligence modelling (WP5) and key inputs and outputs

(4) Enalos Cloud Platform & Jaqpot APIs for nanoinformatics software development (WP6)



(3)

Enalos QNAR Iron Oxide Toxicity Platform

NP DATA → **MODELS** → **CLOUD**

Platform Nanoparticles Risk Toxicity assessment Cloud

Enalos Models

Jaqpot API

http://enalos.insilicotox.com/QNAR_PaCa2/

http://enalos.insilicotox.com/QNAR_IronOxide_Toxicity/

<http://enalos.insilicotox.com/NanoProteinCorona/>

Enalos QNAR Iron Oxide Toxicity Platform

Table:

Index	Row ID	Q1 (μM)	R1 (μM 10-1)	R2 (μM 10-1)	Coating
1	1	1.0	1.0	1.0	uncoated dextran
2	2	1.0	1.0	1.0	uncoated dextran
3	3	1.0	1.0	1.0	PAA
4	4	1.0	1.0	1.0	PAA
5	5	1.0	1.0	1.0	uncoated dextran
6	6	1.0	1.0	1.0	Other
7	7	1.0	1.0	1.0	Other
8	8	1.0	1.0	1.0	PAA
9	9	1.0	1.0	1.0	Other
10	10	1.0	1.0	1.0	Other
11	11	1.0	1.0	1.0	Other
12	12	1.0	1.0	1.0	Other
13	13	1.0	1.0	1.0	Other
14	14	1.0	1.0	1.0	Other
15	15	1.0	1.0	1.0	Other
16	16	1.0	1.0	1.0	Other
17	17	1.0	1.0	1.0	Other
18	18	1.0	1.0	1.0	Other
19	19	1.0	1.0	1.0	Other
20	20	1.0	1.0	1.0	Other

Chemical structure:

Enalos QNAR Iron Oxide Toxicity Platform

Jaqpot API

<http://jaqpot.org/>

G. Melagraki, A. Afantitis, Enalos InSilicoNano Platform: An online decision support tool for the design and virtual screening of nanoparticles RSC Advances 2014, 4, 50713-50725 2014

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A. Afantitis, G. Melagraki, E. Valsami-Jones, I. Lynch "A Nanoinformatics Decision Support Tools for The Virtual Screening of Gold Nanoparticle Cellular Association Using Protein Corona Fingerprints" Under Revision

C. Chomenidis, G. Drakakis, G. Tsilki, E. Anagnostopoulou, A. Valsamis, P. Daganis, P. Sopaakis, H. Sarimveis, Jaqpot Quattro: A Novel Computational Web Platform for Modeling and Analysis in Nanoinformatics (Journal of Chemical Information and Modeling, 57, 2161-2172, 2017)

(4)

Key Aspects

Advances in individual models to enhance their predictive power:

- Paradigm-breaking omics technologies for predictive toxicology and AOP analysis (WP3).
- A robust multiscale methodology towards material fingerprints (WP4)
- Meta-models development (WP4).
- Innovative *in silico* approaches based on ground-breaking techniques supported by AI (WP5).
- Identification of MIE - a paradigm shift towards integrated physics-based and data-driven models (WP5).
- Beyond control banding to advanced exposure, PBPK and risk assessment modelling tools (WP6):

Key Aspects

Advances in model integration and utility for prediction of NM functional effects, hazard and risk:

- Novel nanodescriptors based on ground-breaking *in silico* techniques developed for NMs (WP6).
- Towards an Alternative Testing Strategy.
- Read-across considering the multi-perspective characterisation of NMs.

Key Aspects

Advances in accessibility of the model platforms and underpinning datasets:

- Cutting-edge research data management approaches (WP1).
- Novel data-gap filling approaches (WP2).
- Development of NanoSolveIT e-platform (WP7).
- Maximize International Synergies (WP8).

Contact Us



@NanoSolveIT



www.nanosolveit.eu



NovaMechanics

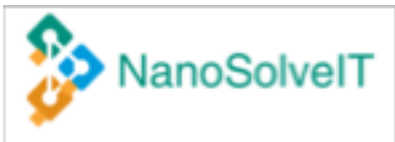
www.novamechanics.com



Project NanoSolveIT



nanosolveit@novamechanics.com



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 814572

