NanoSolveIT

Innovative **Nano**informatics models and tools: towards a **Sol**id, **ve**rified and **I**ntegrated Approach to Predictive (eco)**T**oxicology (**NanoSolveIT**)

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

NovaMechanics

NanoSolveIT

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 develop and deliver:

(i) a reliable user friendly knowledge-based infrastructure for data hosting, sharing and exploitation,

(ii) NM fingerprints, sets of nanodescriptors and properties that can be predictively linked to NM functionality, exposure and hazard, thereby supporting NM grouping, safe-by-design (SbD) and regulatory risk assessment (RA),

(iii) innovative methodologies for NMs predictive (eco)toxicology underpinned by artificial intelligence (AI) and state-of-the-art in silico techniques, and,

(iv) integration with currently developing multi-scale modelling, RA and governance frameworks developing in EU H2020 funded projects including caLIBRAte and expected in the newly funded NMBP-13 project(s).

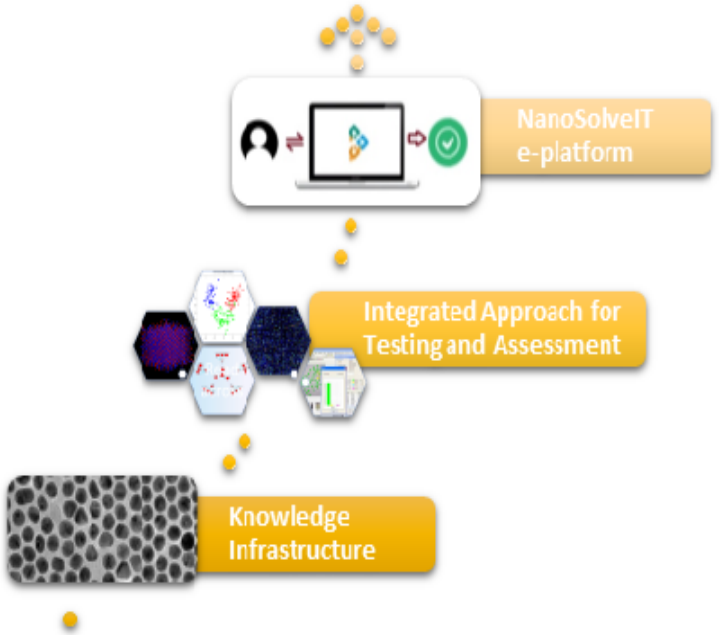
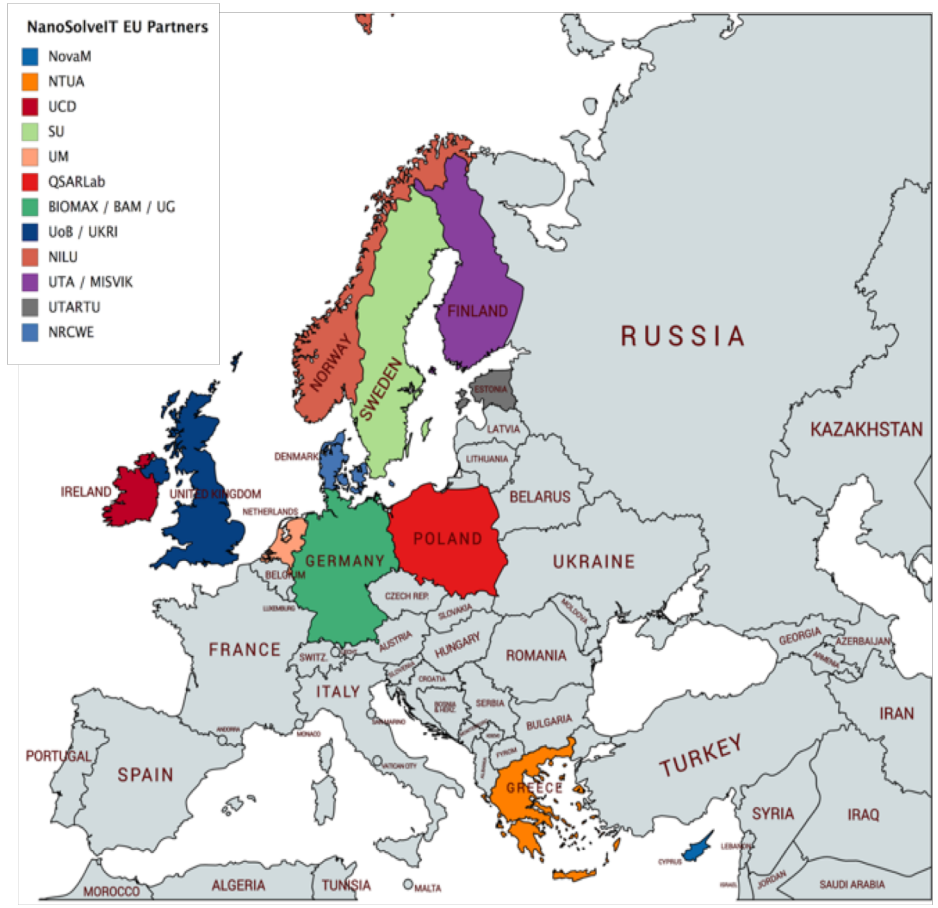


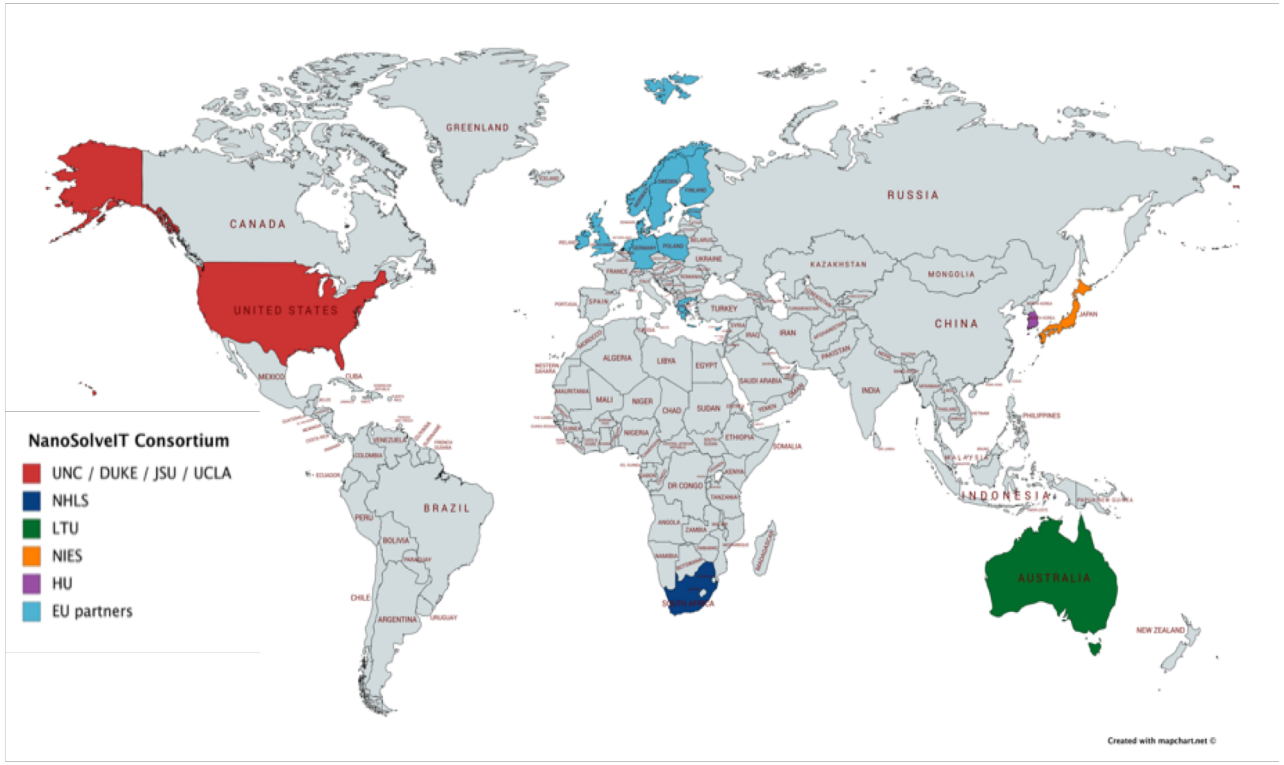
Figure 1. NanoSolveIT key steps

NanoSolveIT will deliver

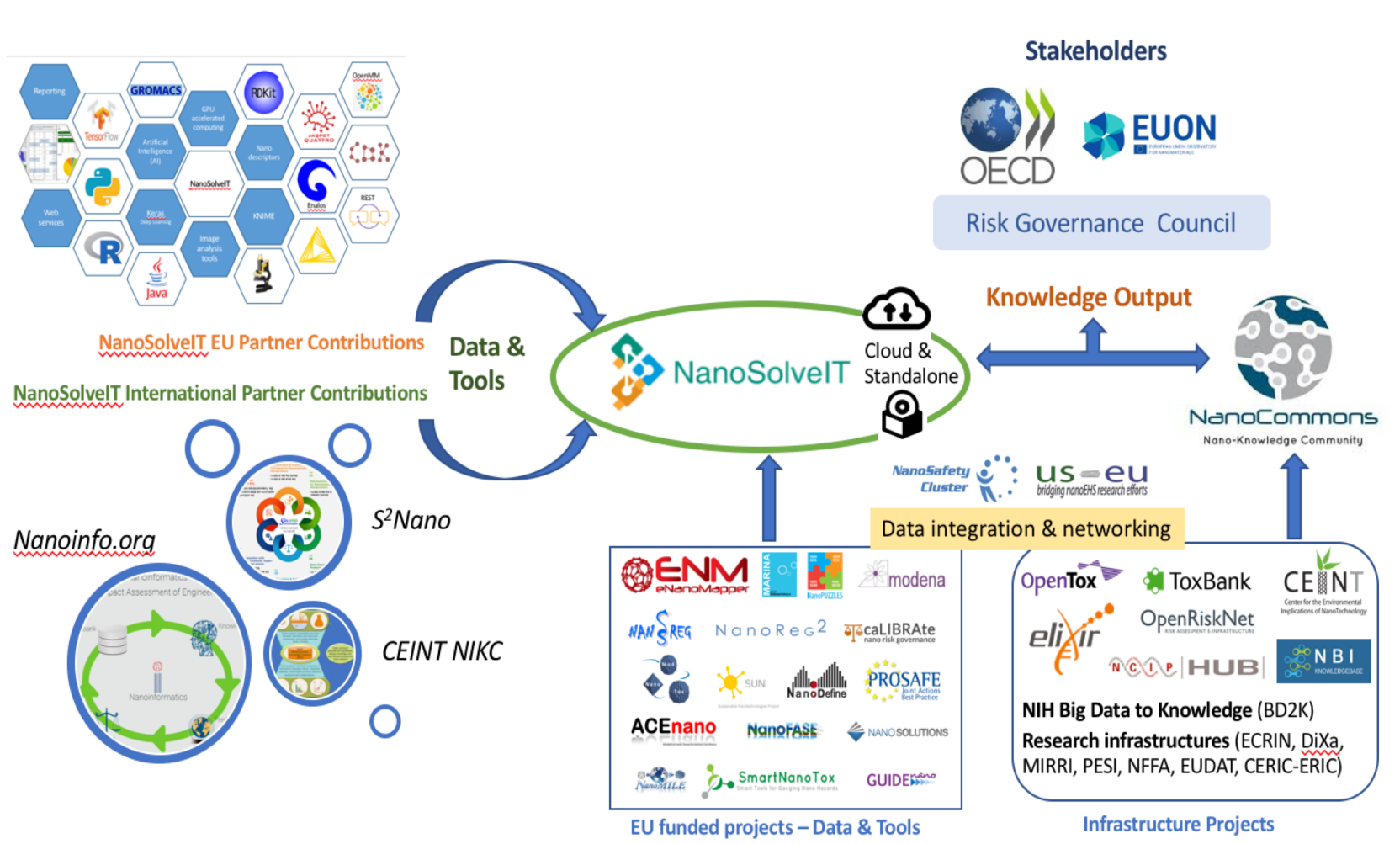
- a validated, sustainable, multi-scale nanoinformatics IATA, tested and demonstrated at TLR6 via OECD-style case studies, to serve the needs of diverse stakeholders at each stage of the NMs value chain, for assessment of potential adverse effects of NM on human health and the environment.

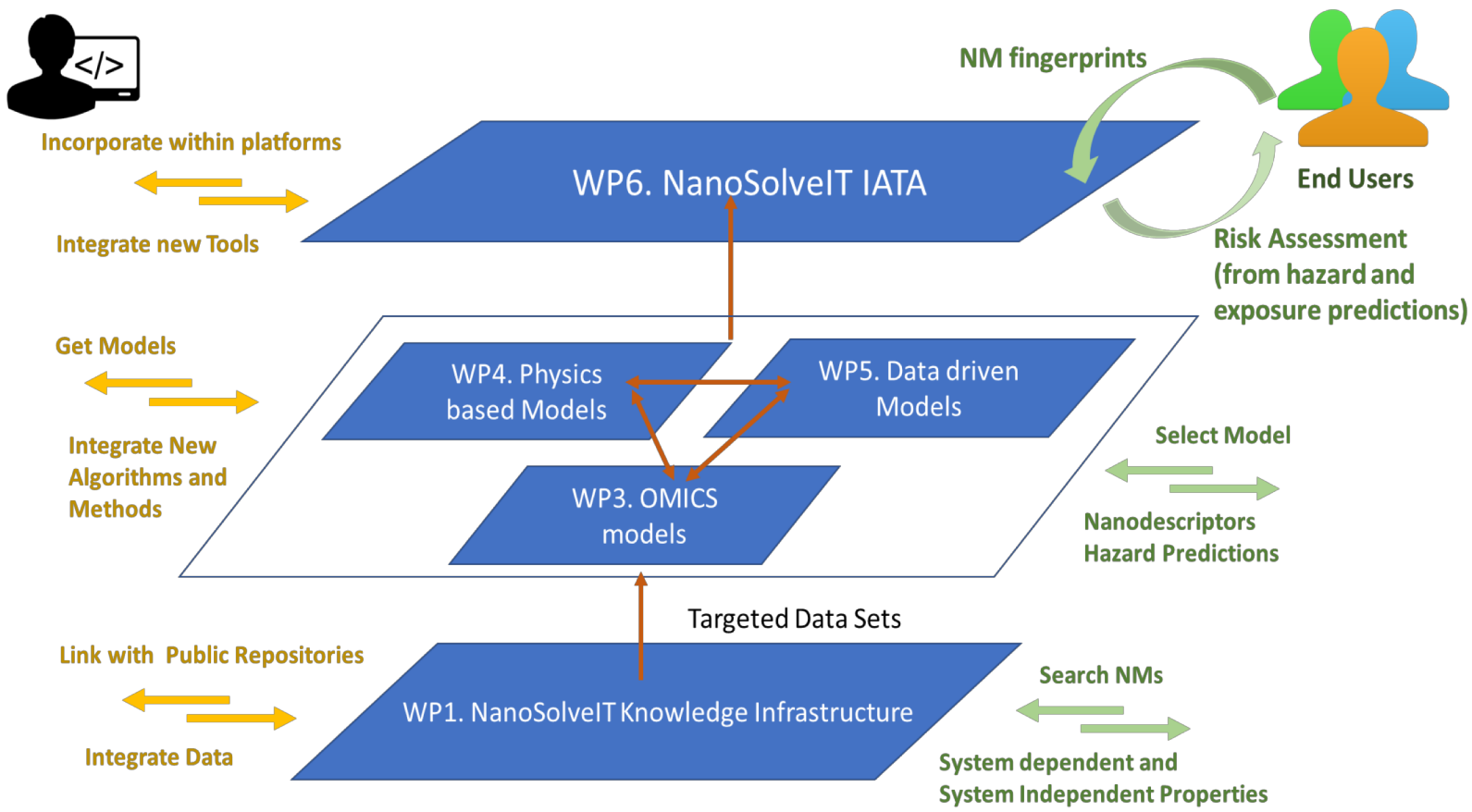
Partners in the NanoSolveIT consortium





NanoSolveIT's positioning and liaison with other initiatives





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

NanoSolveIT WPs

WP No	WP Title	Leader	Lead organisation
1	NanoSolveIT Knowledge Infrastructure	Egon Willighagen	UM
2	Design of Experiments for data gap filling to support in silico models	Eva Valsami - Jones	UoB
3	Predictive toxicogenomics modelling using omics data	Dario Greco	UTA
4	Development of a sustainable multi-scale modelling framework for NMs property prediction	Vladimir Lobaskin	UCD
5	Predictive Nanoinformatics Modeling using AI methodologies	Tomasz Puzyn	QSARLab
6	NanoSolveIT IATA for human and environmental RA	Iseult Lynch	UoB
7	Development of the NanoSolveIT e-Platform	Haralambos Sarimveis	NTUA
8	Dissemination, Knowledge Transfer & Exploitation	Maria Dusinska	NILU
9	Project Coordination & Management	Antreas Afantitis	NovaM

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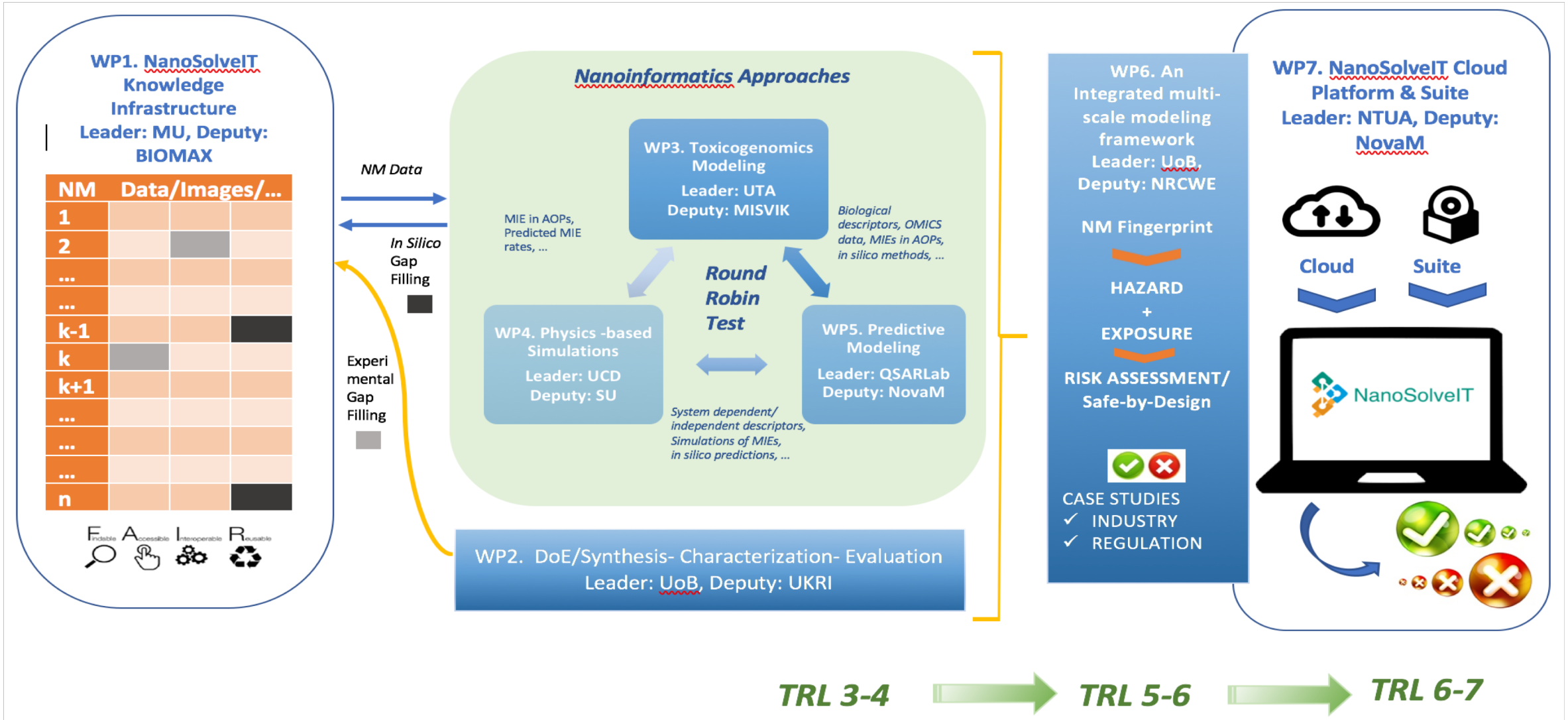
NanoSolveIT Gantt Chart

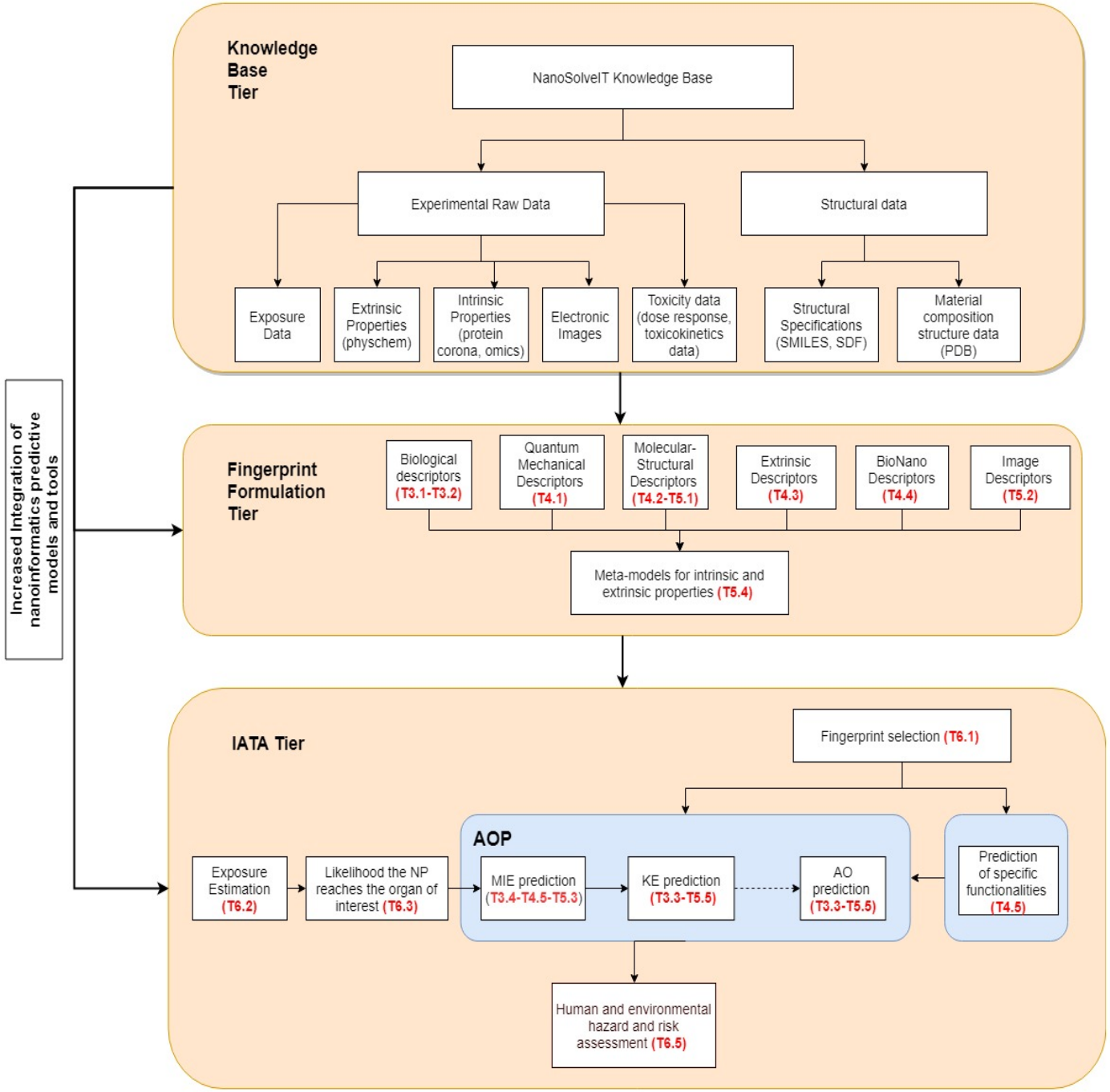
NanoSolveIT Gantt chart showing WP and Task timings

WP	Task	Year	Year 1				Year 2				Year 3				Year 4			
		Quarter	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
1	**NanoSolveIT Knowledge Infrastructure**																	
	1.1 System requirements, Specifications, and Development																	
	1.2 Ontology annotation and Linked Data																	
	1.3 Collection, curation, and operationalization of existing data																	
2	**Design of Experiments for data gap filling to support in silico models**																	
	2.1 Design of Experiments for gap-filling																	
	2.2 NMs Synthesis & Characterisation																	
	2.3 Toxicological assessment																	
	2.4 Ecotoxicological assessment																	
	2.5 Assay kits for data generation to support the IATA																	
3	**Predictive toxicogenomics modelling using omics data**																	
	3.1 Computational analysis of big OMICS data																	
	3.2 Generation of predictive models of ENMs toxicity based on biological descriptors																	
	3.3 Read-across analysis and grouping of ENMs based on biological descriptors																	
	3.4 Exploring pathways of toxicity and Adverse Outcome Pathways (AOPs) of NMs																	
4	**Sustainable multi-scale modelling framework for ENMs property prediction**																	
	4.1 Systematic development of atomistic and coarse-grained (CG) force-fields for NMs																	
	4.2 Calculation of structure descriptors and intrinsic properties of NMs																	
	4.3 Calculation of property descriptors and extrinsic properties of NMs																	
	4.4 Calculation of bionano interaction descriptors for ENMs and relevant biomolecules																	
	4.5 Modelling of ENM functionality																	
5	**Predictive Nanoinformatics Modeling using AI methodologies**																	
	5.1 Developing the system of descriptors related to the structure of ENMs (calculated)																	
	5.2 Developing the system of structure descriptors of ENMs based on electronic images																	
	5.3 Methods for the structural alerts identification in relation to MOA																	
	5.4 Developing the meta-models for intrinsic and extrinsic properties																	
	5.5 Development of the integrated modelling strategy																	
6	**NanoSolveIT IATA for human and environmental RA**																	
	6.1 Development of informative NM fingerprints																	
	6.2 Development of NM exposure models																	
	6.3 Development of toxicokinetics models																	
	6.4 Development of agreed standards / predictive modelling SOPs & benchmarking via RRs																	
	6.5 IATA-Integration/Linking of different types of nanoinformatics models																	
	6.6 IATA Case studies																	
7	**Development of the NanoSolveIT e-Platform**																	
	7.1 Definition of system architecture and specifications																	
	7.2 Packaging of the developed nanoinformatics models and tools as microservices ePlatform																	
	7.3 Development of the NanoSolveIT cloud platform																	
	7.4 Development of the NanoSolveIT standalone application																	
	7.5 Documentation of services and development of training materials																	
8	**Dissemination, Knowledge Transfer & Exploitation**																	
	8.1.Spreading and circulating Information (Dissemination)																	
	8.2 Communication & delivery of information/skills to stakeholders (Knowledge Transfer)																	
	8.3 Making use of and benefiting from created knowledge and resources (Exploitation)																	
	8.4 Long term exploitation of the NanoSolevIT IATA																	
9	**Project Co-ordination & Management**																	
	9.1 Operational management																	
	9.2 Scientific/technical coordination																	
	9.3 Progress control																	

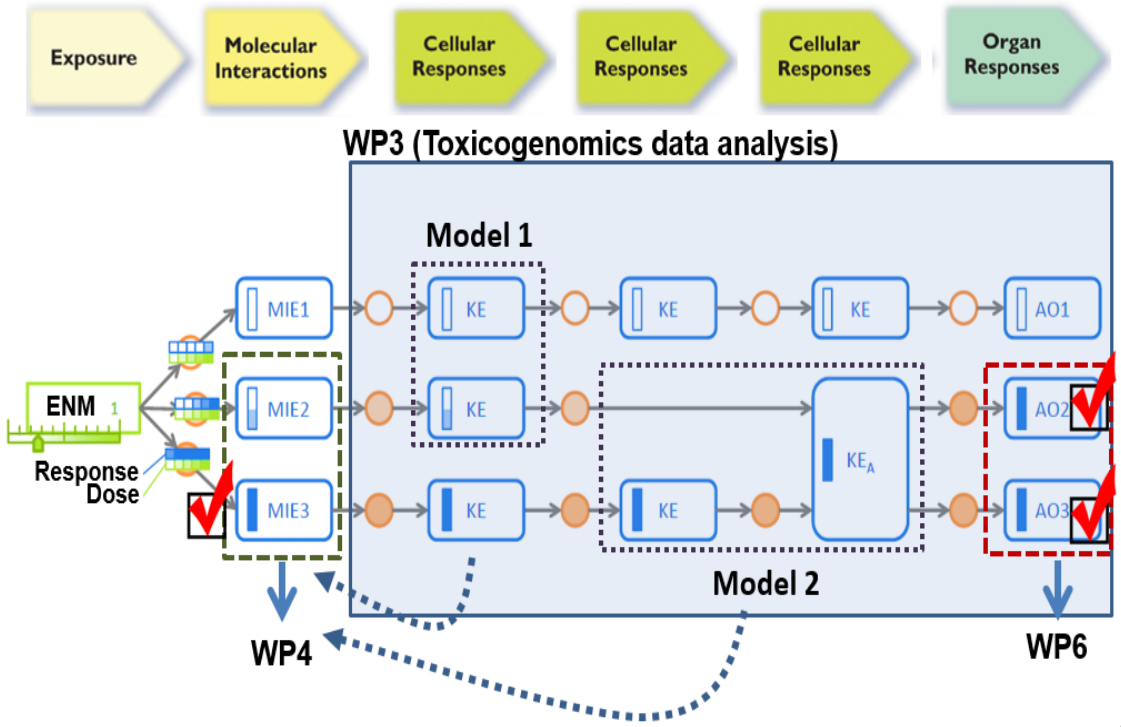
NanoSolveIT Overview WPs Interlinkages



NanoSolveIT overall concept and integration of multi-scale methods and tools



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



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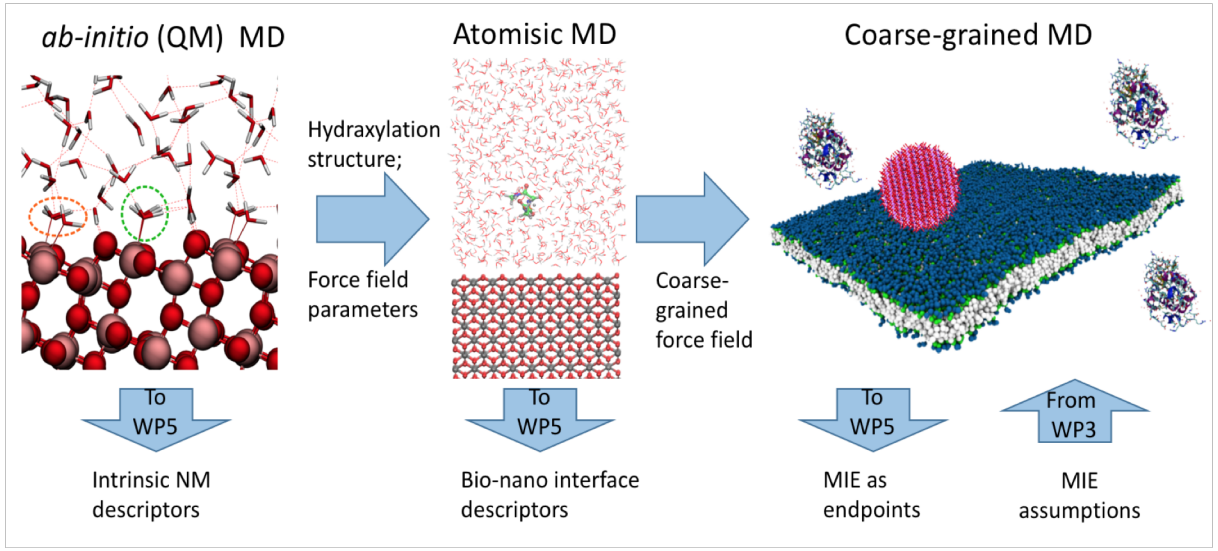

(2)

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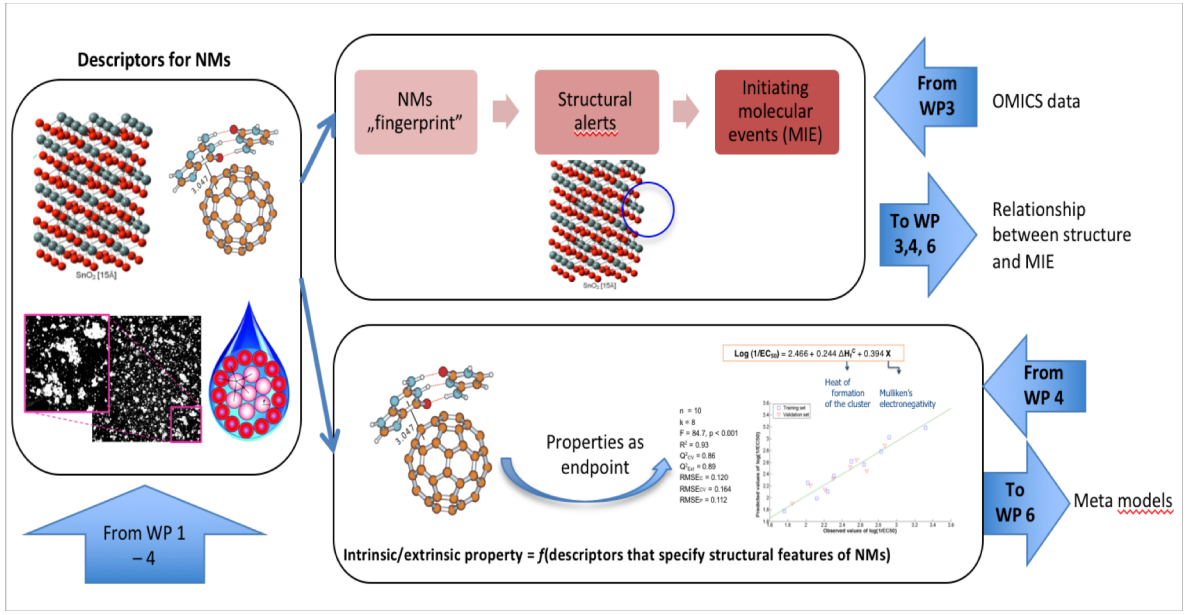
(3) Data-driven artificial intelligence modelling (WP5) and key inputs and outputs
(4) Enalos Cloud Platform & Jaqpot APIs for nanoinformatics software development (WP6)



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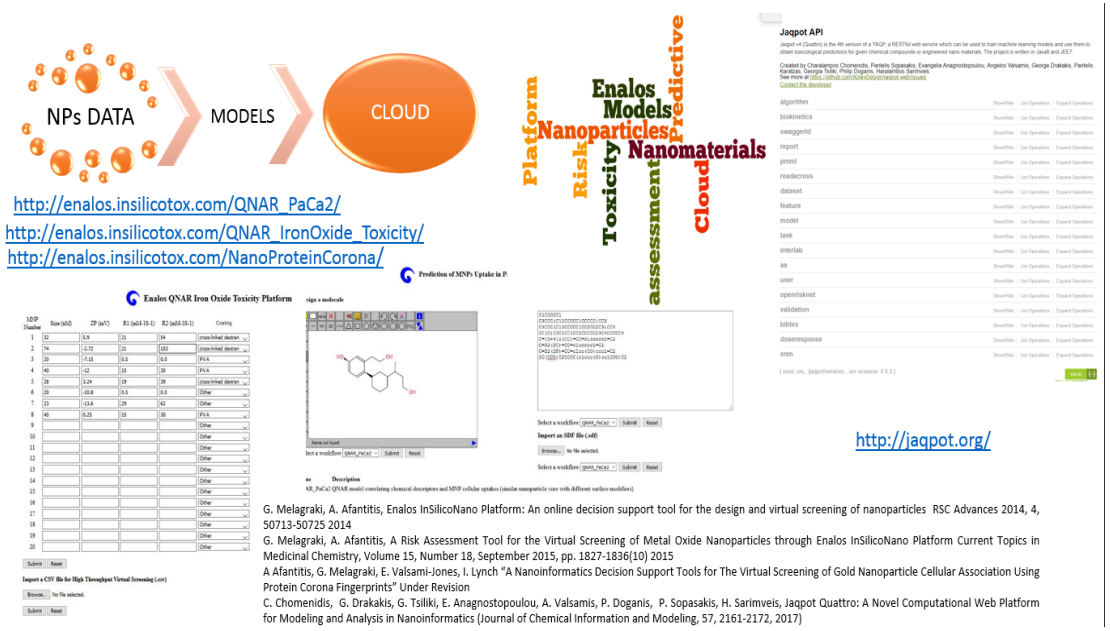

G. Melagraki, A. Afantitis, Enalos InSilicoNano Platform: An online decision support tool for the design and virtual screening of nanoparticles RSC Advances 2014, 4, 50713-50725 2014

G. Melagraki, A. Afantitis, A Risk Assessment Tool for the Virtual Screening of Metal Oxide Nanoparticles through Enalos InSilicoNano Platform Current Topics in Medicinal Chemistry, Volume 15, Number 18, September 2015, pp. 1827-1836(10) 2015

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. Tsiliki, E. Anagnostopoulou, A. Valsamis, P. Doganis, P. Sopasakis, 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)

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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:

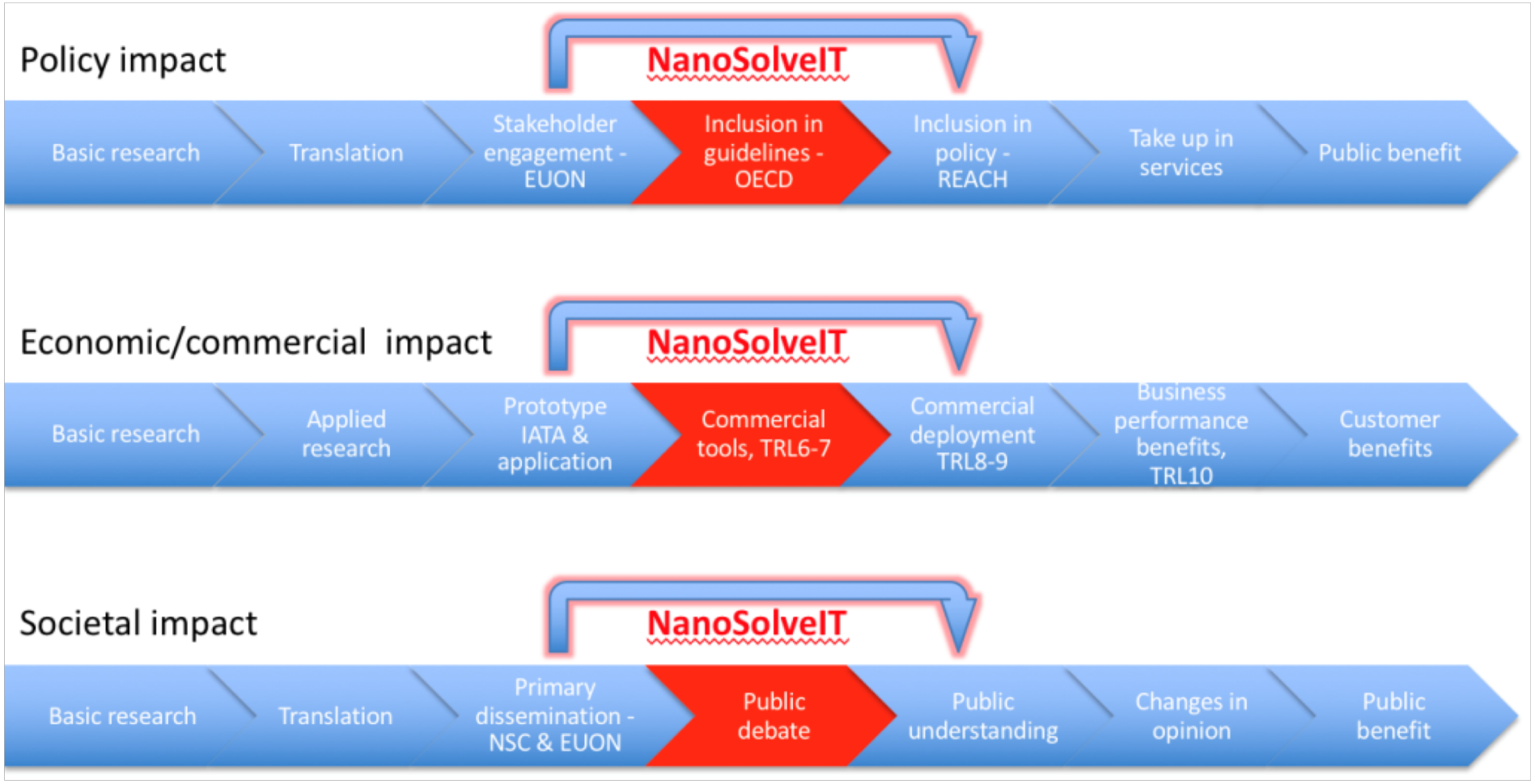
- Cutting-edge research data management approaches (WP1).
- Novel data-gap filling approaches (WP2).
- Development of NanoSolveIT e-platform (WP7).
- Maximize International Synergies (WP8).

Dissemination & Communication Activities

Categories	
Press release	Participation to a Workshop
Non-scientific and non-peer-reviewed publication (popularised publication)	Participation to an Event other than a Conference or a Workshop
Exhibition	Video/Film
Flyer	Brokerage Event
Training	Pitch Event
Social Media	Trade Fair
Website	Participation in activities organized jointly with other H2020 projects
Communication Campaign (e.g. Radio, TV)	Other
Participation to a Conference	

Categories of persons reached
Scientific Community (Higher Education, Research)
Industry
Civil Society
General Public
Policy Makers
Media
Investors
Customers
Other

NanoSolveIT Impact



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