Easy-MODA

Joint Webinar on Easy-MODA

"Easy-MODA in Action: Case Studies on Nanoparticle Safety Assessment and Protein Adsorption"

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INSIGHT

WorldFAIR

EMMC

What MODA is?

Modelling Data (MODA) reporting guidelines have been proposed by the European Materials Modelling Council (EMMC) as a means to record the metadata related to physics-based models, akin to use of the QSAR model report form (QMRF) for Quantitative Structure-Activity Relationship (QSAR) models to increase industry and regulatory confidence in the models.

Why do we need MODA?

MODA make research software more compliant with the FAIR principles (Findable, Accessible, Interoperable, Reusable)

Despite the incredible advances in computational modelling of materials properties and effects, uptake into regulation has been slow, in part due to concerns regarding lack of interpretability of complex models and to lack of documentation of scientific simulations, which often suffer from complex models, variability in hardware and software, and a lack of standardization in practices.

https://www.oecd.org/en/topics/sub-issues/assessment-of-chemicals/integrated-approaches-to-testing-and-assessment.html

OECD

Topics | Countries & regions | Publications | Data | News & events | About | English

OECD › Topics › Assessment of chemicals › Integrated Approaches to Testing and Assessment (IATA)

Integrated Approaches to Testing and Assessment (IATA)

Integrated Approaches to Testing and Assessment (IATA) combine multiple sources of information to conclude on the toxicity of chemicals. These approaches are developed to address a specific regulatory scenario or decision context.

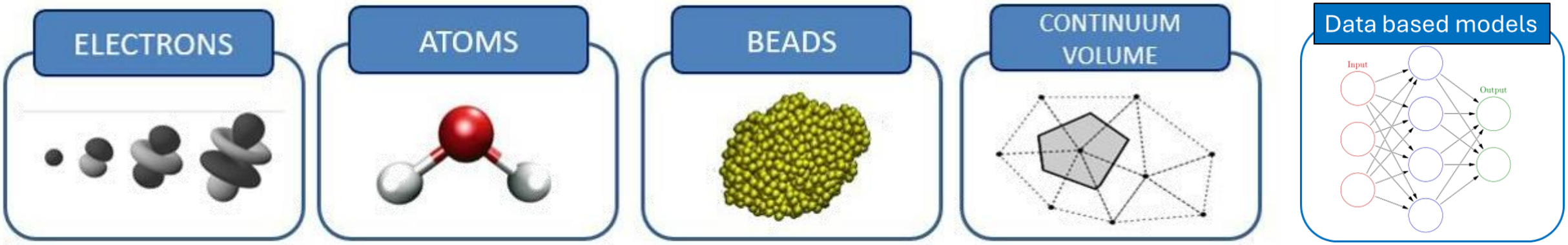
Focus

Key links

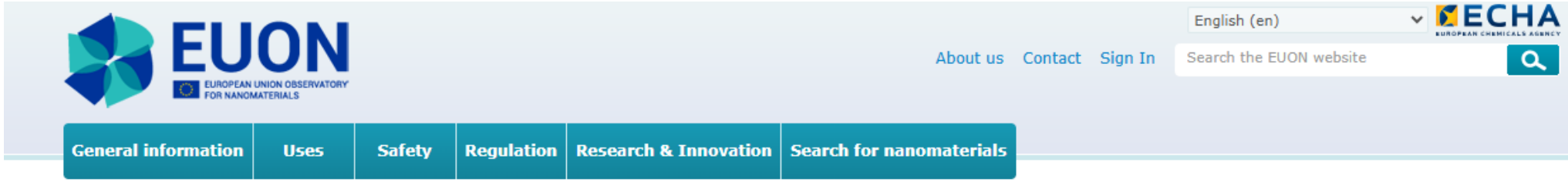
Guiding Principles and Key Elements for Establishing a Weight of Evidence for Chemical Assessment ›

Guidance Document on the Reporting of Defined Approaches to be Used Within IATA ›

Why do we need MODA?



The continuously increasing number of multiscale simulations or physics-based models, and their conjunction with machine learning models (so-called data-driven approaches whereby the models ingest large datasets to identify patterns or connections, with QSAR and machine learning models being examples) demands a standardized way to represent their workflows, which can be merged with other workflows to develop a larger, integrated multi-model workflows.



EASY-MODA: A WEB TOOL TO ENHANCE THE FAIRNESS OF MATERIALS MODELS THROUGH THE REGISTRATION OF SCIENTIFIC SIMULATION WORKFLOWS

by Dr. Panagiotis D. Kolokathis, Dr. Gerhard Goldbeck, Prof. Iseult Lynch and Dr. Antreas Afantitis

From medicine to electronics and environmentally friendly agrichemicals, nanomaterials and advanced materials have opened up boundless possibilities. However, turning a promising idea into a real-world application can be complicated. Researchers and companies need to combine many types of computational models—like physics-based simulations at different time and length scales and data-driven models—to predict how materials behave and assess their safety and sustainability as early in the development cycle as possible. Given the complexity of models being developed and integrated as part of materials design and safety assessment, and the push for explainable artificial intelligence (AI) there is a need for clear documentation of the modelling workflows. This is where Easy-MODA comes in. Easy-MODA is a free-to-use web tool that facilitates and harmonises the registration of scientific simulation workflows. This registration assures the reproducibility of the workflow and allows for the reuse of whole or parts of the registered workflows by other users where relevant. Easy-MODA guides researchers through the creation of clear, reproducible and harmonised documentation of their computer simulations, from start to finish. Developed under ongoing European research efforts (including the WorldFAIR and INSIGHT projects), it is now part of the Enalos Cloud Platform. Easy-MODA is based on a CEN Workshop Agreement called "**MODA**" (Modelling Data), which sets out a standard way to report details of materials modelling. It helps ensure that models are documented in a consistent, transparent manner, allowing anyone to find, replicate or combine them with other models. Below we explore why Easy-MODA matters for the nanosciences, how it streamlines computational experiments, and how you can integrate it into your own research or product development, —especially if you're adopting the **Safe and Sustainable by Design (SSbD)** principles.

https://euon.echa.europa.eu/nanopinion/-/blogs/easy-moda-a-web-tool-to-enhance-the-fairness-of-materials-models-through-the-registration-of-scientific-simulation-workflows

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journal homepage: www.elsevier.com/locate/csbj

Software/web server article

Easy-MODA: Simplifying standardised registration of scientific simulation workflows through MODA template guidelines powered by the Enalos Cloud Platform

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https://doi.org/10.1016/j.csbj.2024.10.018

Is there something similar for experiments?

Characterization Data (CHADA) reporting is to experiments what MODA is for computational workflows .

Why has Easy-MODA been developed?

To simplify the development of MODA documents which is a very complicated process and to provide guidelines to the users on how to make the document.

In addition, **the models developed by Easy-MODA are registered to a database and are easily accessible**

Why is MODA documentation difficult to be written?

We will see it in practice that special treatment is needed to develop the document

MODA DOCUMENTATION

Please fill in the boxes and delete all explanatory text in italics

MODA for <*user-case*>
***Simulated* in project <acronym>**

OVERVIEW of the SIMULATION			
1	USER CASE		*General description of the User Case.* *Please give the properties and behaviour of the particular material, manufacturing process and/or in-service-behaviour to be simulated. No information on the modelling should appear here. The idea is that this user-case can also be simulated by others with other models and that the results can then be compared.*
2	CHAIN OF MODELS	MODEL 1	*Please identify the first model. Note these are assumed to be physics-based models unless it is specified differently.* *Most modelling projects consist of a chain of models, (workflow). Here only the Physics Equations should be given and only names appearing in the content list of the Review of Materials Modelling VI should be entered. This review is available on http://ec.europa.eu/research/industrial_technologies/e-library.cfm).All models should be identified as electronic, atomistic, mesoscopic or continuum.*
		MODEL 2	*Please identify the second model.*
		DATA-BASED MODEL	*If data-based models are used, please specify.*
3	PUBLICATION PEER-REVIEWING THE DATA		*Please give the publication which documents the data of this ONE simulation.* *This article should ensure the quality of this data set (and not only the quality of the models).*
4	ACCESS CONDITIONS		*Please list whether the model and/or data are free, commercial or open source. Please list the owner and the name of the software or database (include a web link if available).*
5	WORKFLOW AND ITS RATIONALE		*Please give a textual rationale of why you as a modeller have chosen these models and this workflow, knowing other modellers would simulate the same end-user case differently.* *This should include the reason why a particular aspect of the user case is to be simulated with a particular model.*

MODA

Physics-based Model

MODEL 1
<Please name the single materials model in the chain you will now document in 4 chapters>

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	*Describe the aspects of the User Case textually.* *No modelling information should appear in this box. This case could also be simulated by other models in a benchmarking operation!* *The information in this chapter can be end-user information, measured data, library data etc. It will appear in the pink circle of your workflow picture.* *Simulated input which is calculated by another model should not be included (but this input is listed in chapter 2.4)* *Also the result of pre-processing necessary to translate the user case specifications to values for the physics variables of the entities can be documented here.*
1.2	MATERIAL	*Chemical composition, …*
1.3	GEOMETRY	*Size, form, picture of the system (if applicable)* *Note that computational choices like simulation boxes are to be documented in chapter 3.*
1.4	TIME LAPSE	*Duration of the User Case to be simulated.* *This is the duration of the situation to be simulated. This is not the same as the computational times to be given in chapter 3.*
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	*If relevant, please list the conditions to be simulated (if applicable).* *E.g. heated walls, external pressures and bending forces.* *Please note that these might appear as terms in the PE or as boundary and initial conditions, and this will be documented in the relevant chapters.*
1.6	PUBLICATION ON THIS DATA	*Publication documenting the simulation with this single model and its data (if available and if not already included in the overall publication).*

https://emmc.eu/moda/

MODA DOCUMENTATION

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	*Model type and name **chosen from RoMM content list** (the PE).* *This PE and only this will appear in the blue circle of your workflow picture. Please do not insert any other text although an indication of the MR is allowed.*	
2.1	MODEL ENTITY	*The entity in this materials model is <finite volumes, grains, atoms, or electrons>*	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE	**Equation**	*Name, description and mathematical form of the PE* *In case of tightly coupled PEs set up as one matrix which is solved in one go, more than one PE can appear.*
		Physical quantities	*Please name the physics quantities in the PE, these are parameters (constants, matrices) and variables that appear in the PE, like wave function, Hamiltonian, spin, velocity, external force.*
2.3	MATERIALS RELATIONS	**Relation**	*Please, give the name of the Material Relation and which PE it completes.*
		Physical quantities/ descriptors for each MR	*Please give the name of the physics quantities, parameters (constants, matrices) and variables that appear in the MR(s)*
2.4	SIMULATED INPUT	*Please document the simulated input and with which model it is calculated.* *This box documents the interoperability of the models in case of sequential or iterative model workflows. Simulated output of the one model is input for the next model. Thus what you enter here in 2.4 will also appear in 4.1 of the model that calculated this input.* *If you do simulations in isolation, then this box will remain empty.* *Note that all measured input is documented in chapter 1 "User Case".*	

3	SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS		
3.1	NUMERICAL SOLVER	*Please give name and type of the solver.* *E.g. Monte Carlo, SPH, FE, …iterative, multi-grid, adaptive,…*	
3.2	SOFTWARE TOOL	*Please give the name of the code and if this is your own code, please specify if it can be shared with an eventual link to a website/publication.*	
3.3	TIME STEP	*If applicable, please give the time step used in the solving operations. This is the numerical time step and this is not the same as the time lapse of the case to be simulated (see 1.4)*	
3.4	COMPUTATIONAL REPRESENTATIO N	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL	*Computational representation of the Physics Equation, Materials Relation and material.* *There is no need to repeat User Case info.* *"Computational" means that this only needs to be filled in when your computational solver represents the material, properties, equation variables, in a specific way.*
3.5	COMPUTATIONAL BOUNDARY CONDITIONS	*If applicable.* *Please note that these can be translations of the physical boundary conditions set in the User Case or they can be pure computational like e.g. a unit cell with mirror b.c. to simulate an infinite domain.*	
3.6	ADDITIONAL SOLVER PARAMETERS	*Please specify pure internal numerical solver details (if applicable), like* • *specific tolerances,* • *cut-off, convergence criteria* • *integrator options*	

https://emmc.eu/moda/

MODA DOCUMENTATION

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT	*Please specify the output obtained by the post processing.* *If applicable then specify the entity in the next model in the chain for which this output is calculated: electrons, atoms, grains, larger/smaller finite volumes.* *In case of homogenisation, please specify the averaging volumes.* *Output can be calculated values for parameters, new MR and descriptor rules (data-based models).*
4.2	METHODOLOGIES	*Please describe the mathematics and/or physics used in this post-processing calculation.* *In homogenisation this is volume averaging. But also physics equations can be used to derive e.g. thermodynamics quantities or optical quantities from Quantum Mechanics raw output.*
4.3	MARGIN OF ERROR	*Please specify the margin of error (accuracy in percentages) of the property calculated and explain the reasons to an industrial end-user.*

https://emmc.eu/moda/

MODA DOCUMENTATION

MODA
Data-based Model

MODEL X

1	USER CASE:	
1.1	ASPECT OF THE USER CASE TO BE CALCULATED	
1.2	MATERIAL	
1.3	GEOMETRY	
1.4	TIME LAPSE	
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	
1.6	PUBLICATION ON THIS ONE DATAMINING OPERATION	

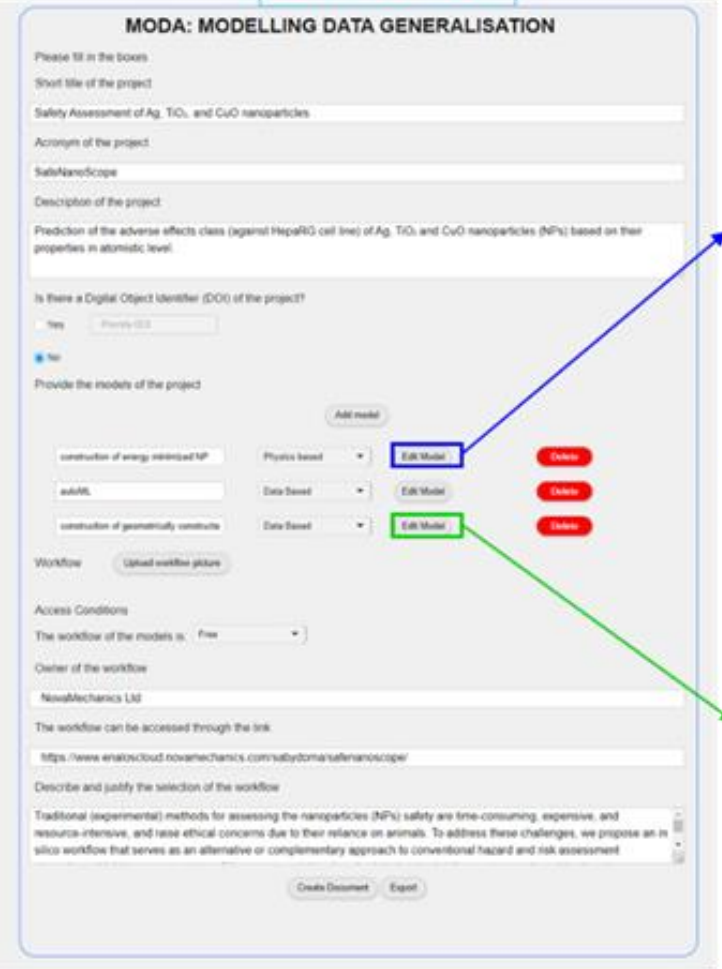
2	THE DATA-BASED MODEL		
2.0	EQUATION TYPE AND NAME	*e.g. energy minimizer*	
2.1	DATABASE AND TYPE	*e.g. thermodynamic database CALPHAD* *e.g. simulated data with DFT model and experimental data from AFM*	
2.2	EQUATION	HYPOTHESIS	*The hypothetical relation assumed*
		PHYSICAL QUANTITIES	

3	COMPUTATIONAL DETAIL OF DATAMINING OPERATION	
3.1	NUMERICAL OPERATIONS	
3.2	SOFTWARE TOOL	
3.3	MARGIN OF ERROR	

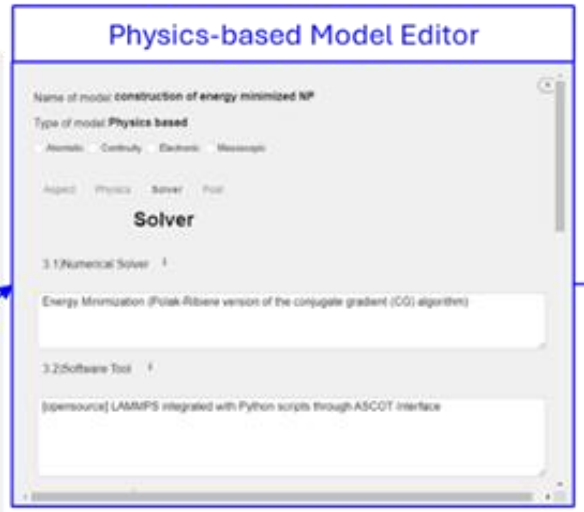
https://emmc.eu/moda/

MODA DOCUMENTATION

Easy-MODA GUI



Physics-based Model Editor



Data-based Model Editor

Easy-MODA Output Document

Moda powered by Enalos Cloud Platform

MODA for

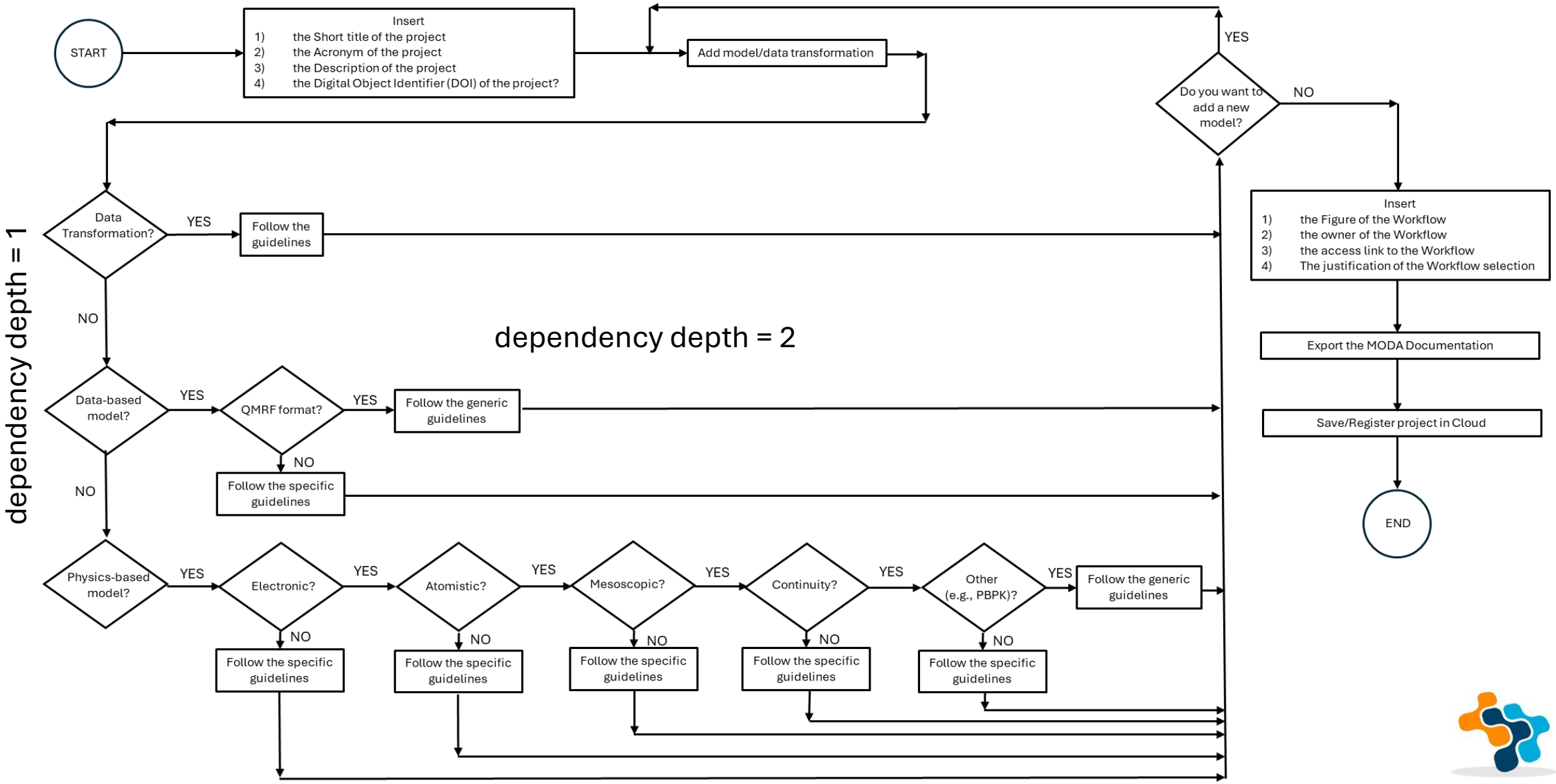
Safety Assessment of Ag, TiO_2, and CuO nanoparticles

Simulated in project:

SafeNanoScope

OVERVIEW of the SIMULATION			
1	**USER CASE**	Safety Assessment of Ag, TiO_2, and CuO nanoparticles	
2	**CHAIN OF MODELS**	**Model 1**	construction of energy minimized NP Physics based
		Model 2	autoML Data Based
		Model 3	construction of geometrically constructed NP Data Based
3	**PUBLICATION PEER - REVIEWING THE DATA**	DOI provided: **No**	
4	**ACCESS CONDITIONS**	Access type: **Free** Owner of workflow: **NovaMechanics Ltd** Workflow access link: https://www.enaloscloud.novamechanics.com/sabydoma/safenanoscope/	
5	**WORKFLOW AND ITS RATIONALE**	Traditional (experimental) methods for assessing the nanoparticles (NPs) safety are time-consuming, expensive, and resource-intensive, and raise ethical concerns due to their reliance on animals. To address these challenges, we propose an in silico workflow that serves as an alternative or complementary approach to conventional hazard and risk assessment strategies, which incorporates state-of-the-art computational methodologies. In detail, an automated machine learning (autoML) scheme is developed employing dose-response toxicity data for silver (Ag), titanium dioxide (TiO_2), and copper oxide (CuO) NPs. This model is further enriched with atomistic descriptors using the ASCOT tool to capture the NPs' underlying structural properties. To overcome the issue of limited data availability, synthetic data generation techniques are used. These techniques help in broadening the dataset, thus improving the representation of different NP classes.	

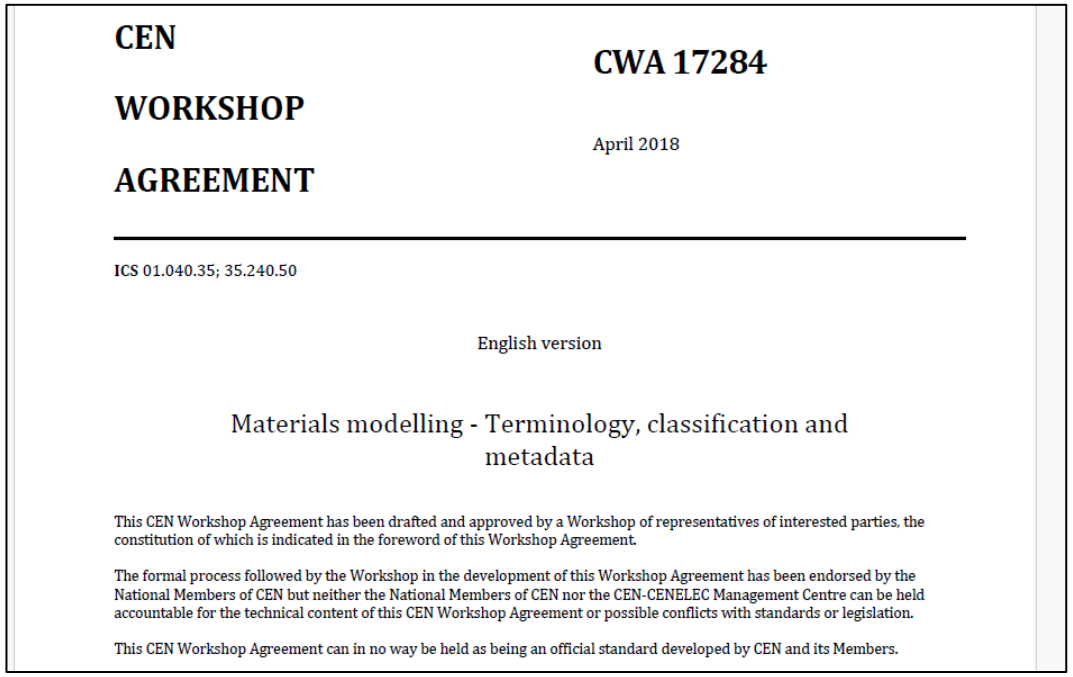
Easy-MODA Outline



How can I have access to MODA guidelines?

Through documents provided by the European Materials Modelling Council (EMMC)
(see the link https://emmc.eu/moda/)

CEN Workshop Agreement (CWA 17284 “Materials modelling - terminology, classification and metadata”)



CEN

WORKSHOP

AGREEMENT

CWA 17284

April 2018

ICS 01.040.35; 35.240.50

English version

Materials modelling - Terminology, classification and metadata

This CEN Workshop Agreement has been drafted and approved by a Workshop of representatives of interested parties, the constitution of which is indicated in the foreword of this Workshop Agreement.

The formal process followed by the Workshop in the development of this Workshop Agreement has been endorsed by the National Members of CEN but neither the National Members of CEN nor the CEN-CENELEC Management Centre can be held accountable for the technical content of this CEN Workshop Agreement or possible conflicts with standards or legislation.

This CEN Workshop Agreement can in no way be held as being an official standard developed by CEN and its Members.

How can I have access to MODA guidelines?

Through documents provided by the European Materials Modelling Council (EMMC)
(see the link https://emmc.eu/moda/)

CEN Workshop Agreement

On the basis of the RoMM, a CEN Workshop Agreement, CWA 17284 "Materials modelling - terminology, classification and metadata" provides clear term definitions and a template for the documentation of simulations, the so-called MODA (Modelling Data).

The MODA comprises a text template and a graphical workflow template which should be used to document materials modelling workflows for EU projects, but they may also find use in organisations' documentations or in supplementary documents of scientific publications.

Has MODA already been used ?

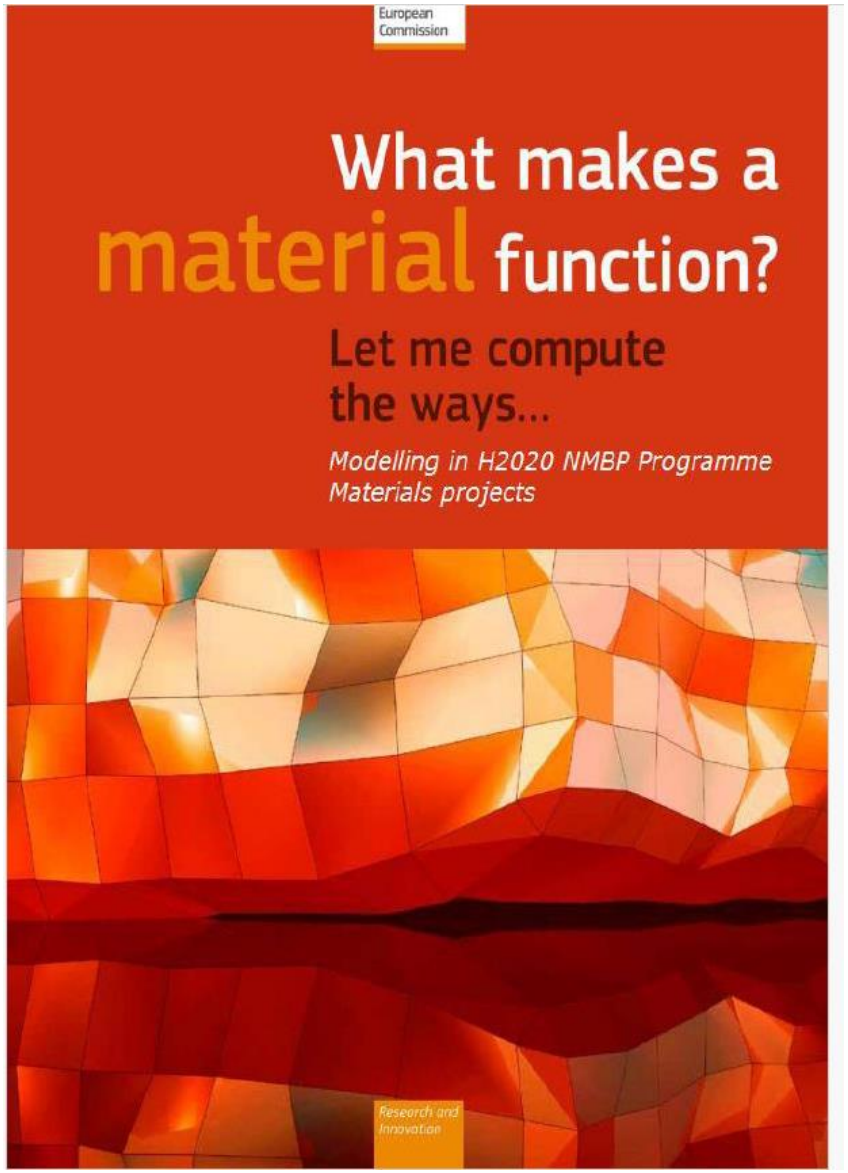
RoMM

The foundation is a compendium of over 100 projects and classification/terminology of materials modelling, the so-called RoMM (Review of Materials Modelling).

Search

Project	Project Link	Document Type	Model	Workflow	Year	Document
ALLIANCE	https://cordis.europa.eu/project/id/723893	MODA	continuum	Tightly Coupled	2016	Members only
ALMA	https://cordis.europa.eu/project/id/645776	MODA	electronic, mesoscopic	Consecutive	2016	Members only
ALMA	https://cordis.europa.eu/project/id/645776	graphical workflow	electronic, mesoscopic	Consecutive	2016	Members only
ARCIGS-M	https://cordis.europa.eu/project/id/720887	MODA	electronic, continuum	Consecutive	2016	Members only
CORNET	https://cordis.europa.eu/project/id/760949	MODA	electronic	Consecutive	2018	Members only

Has MODA already been used ?



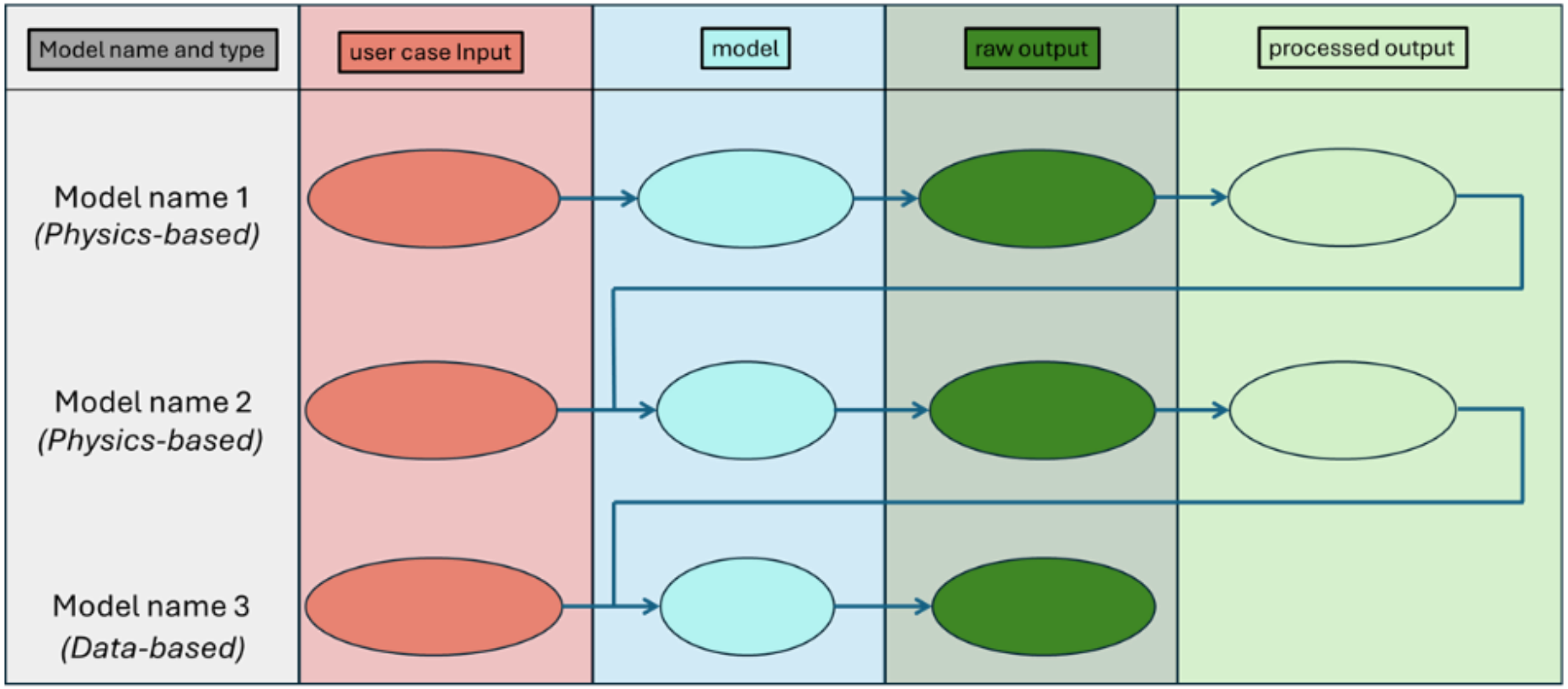
ALLIANCE:	Crash-worthiness of car wheel-house
ALMA:	Heat in an electronic device
AMPHIBIAN:	Magnets for a flywheel
ARCIGS COO:	Optical and electrical behaviour of solar cell
CRITCAT:	Catalist performance of ultra-small metal alloys
DEEPEN:	Behaviour of LED structures
EENSULATE:	Sorption and permeation for windows with insulating material
EIROS:	Materials for extreme environments
EXTMOS:	New models for organic electronics
FASTGRID:	Superconducting fault current limiters
FEMTOSPIN:	Spin dynamics for storage of information
GOFAST:	Correlated materials in insulators and superconductors
ICMEG:	Elastic properties of polycrystalline polypropylenes
	High Throughput Discovery of Single Crystal Ferroelectrics Film
INNOVIP:	Insulation and dynamic behaviour of buildings
IN-POWER:	Mirror support design for thermoelectric plant
INSPIRED:	Reactor design for functionalised nanomaterials
LOCOMATECH:	Forming process for aluminium production
LORCENIS:	Reinforced concrete
MODCOMP:	Ectrical and thermal properties of fiber-based materials
MODENA:	Behaviour of polyurethane foams
MOSTOPHOS:	Stability of organic light emitting diodes
N2B-patch:	Drug delivery fot multiple sclerosis
NANODOME:	Gas-Phasesynthesis of complex nanomaterial structures.
NANOPACK:	Migration into food
NEOHIRE COO:	Permanent Magnets for Wind Energy Application
NEWSOL:	Thermal energy storage
NEXTOWER:	Solar towers
NOVAMAG:	Intermetallic compounds for permanent magnets
PARTIAL-PGMs:	Nanostructured materials for automotive after-treatment systems
POROUS4APP:	Nano-porous carbon fabrication
PRODIA:	Heat flow in an adsorber
PROTECT:	Piezo electric transducer emitting ultrasounds in liquid
SIMPHONY:	Flow in a micro or nano channel
SINTBAT:	Deformation and stresses within the battery anode
STARCELL:	Materials for photovoltaic cells
WALL IN ONE:	Heat and moisture transport in insulation products for buidlings

https://bookshop.europa.eu/en/what-makes-a-material-function--pbKI0616197/

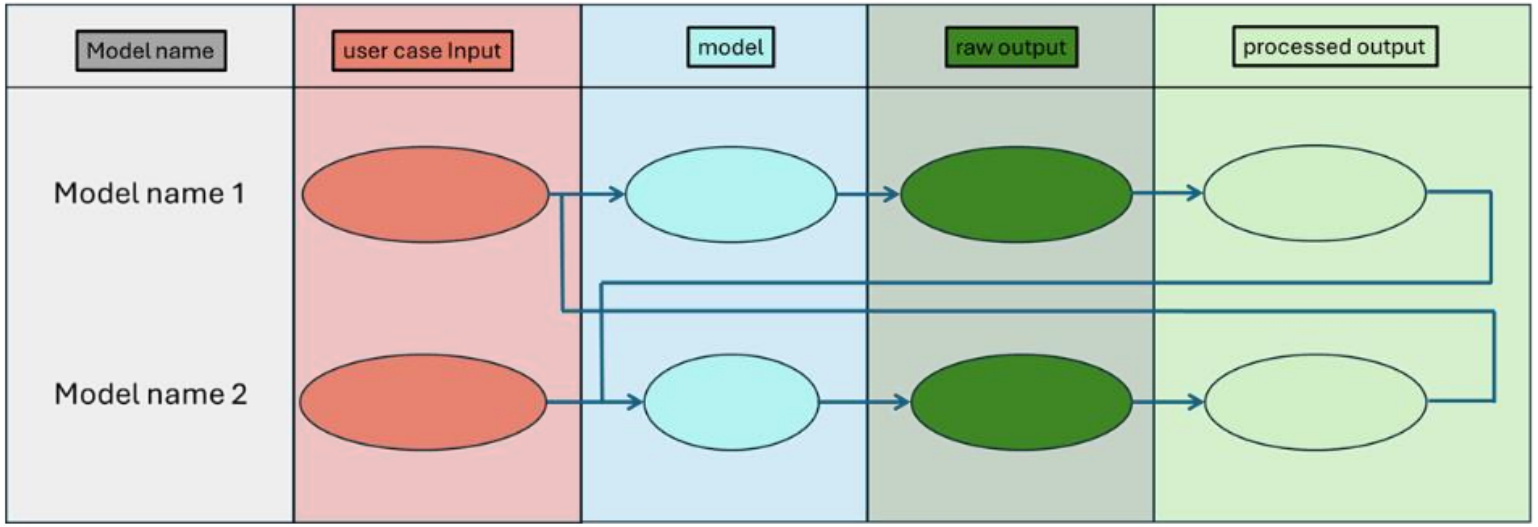
Easy-MODA

Workflows can consist of a) standalone models, b) linked models where the models are run consecutively, iteratively or in parallel c) loosely coupled models (i.e., coupling is due to the input of every model being the output of the rest models by creating a vicious cycle which stops through a tolerance criterion), and d) tightly coupled models which can be considered as one model (i.e., more two or more physical equations are coupled because they share the same variables and they are solved simultaneously through the same solver).

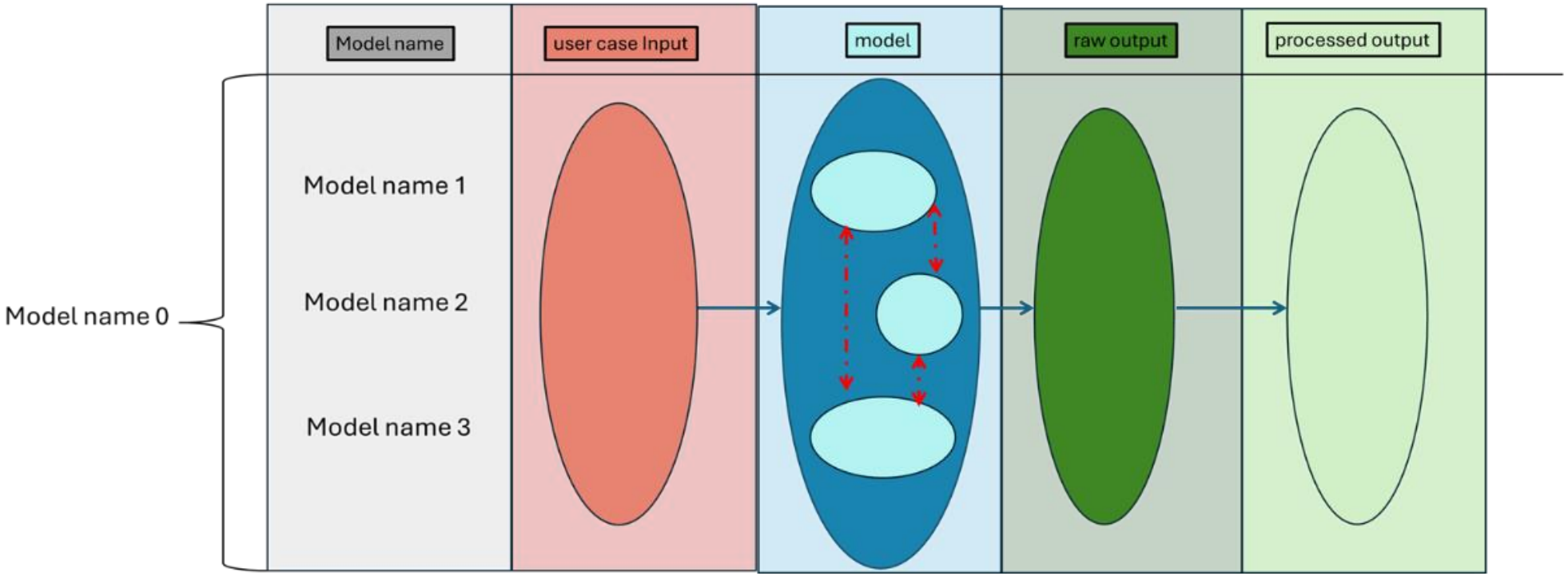
a) Consecutive Workflow



b) Iterative Workflow



c) Tightly Coupled Models Workflow



Easy-MODA

Easy-MODA web application is powered by Enalos Cloud Platform and is accessible through the link https://www.enaloscloud.novamechanics.com/insight/moda/

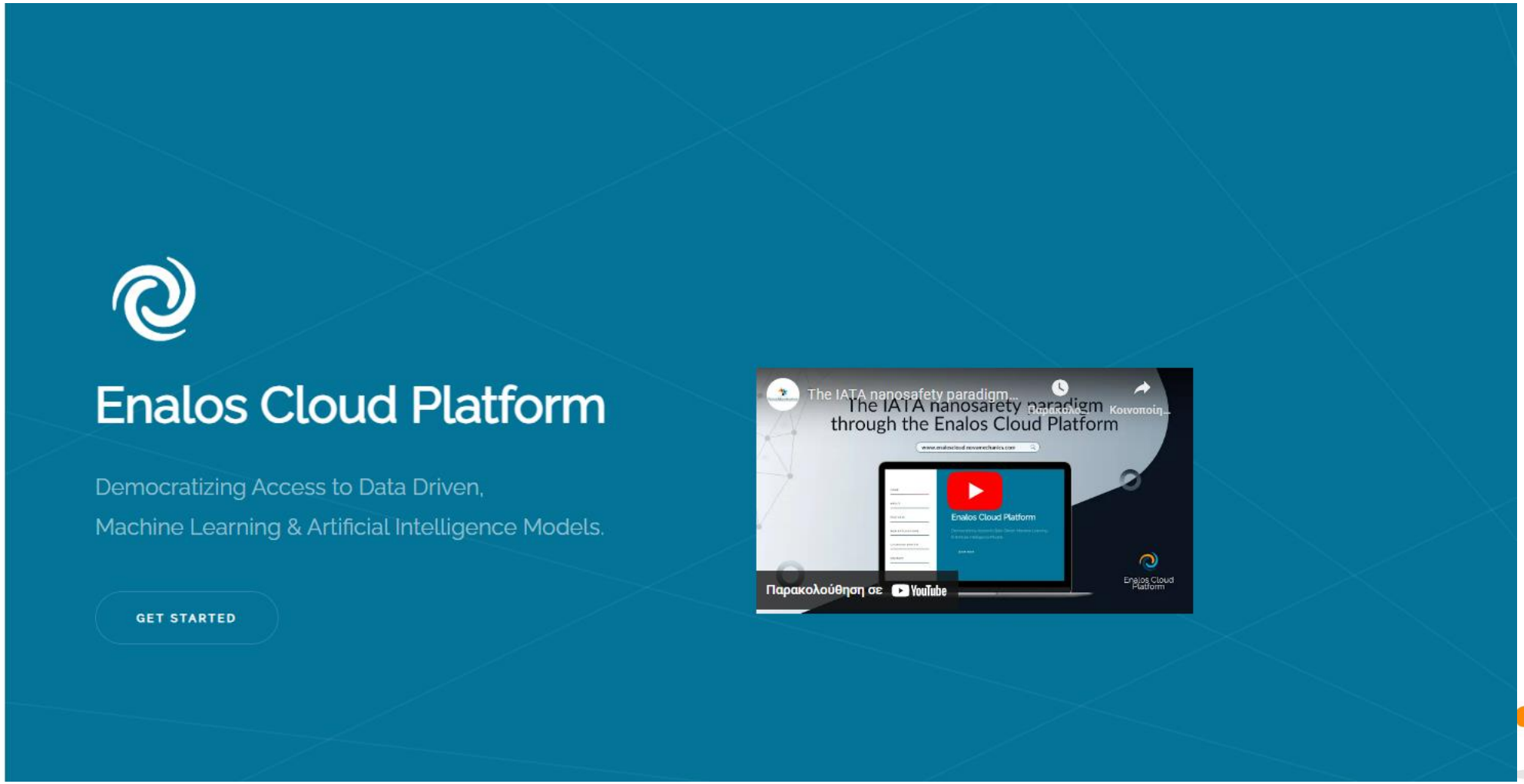
Easy-MODA web application aspires to facilitate the Modelling Data (MODA) registration according to the guidelines that have been proposed by the European Materials Modelling Council (EMMC) and are available in the following links:

a) https://emmc.info/moda-workflow-templates/

b) https://emmc.eu/wp-content/uploads/2021/05/EMMC IntWorkshop Vienna2017 MODA Talk.pdf

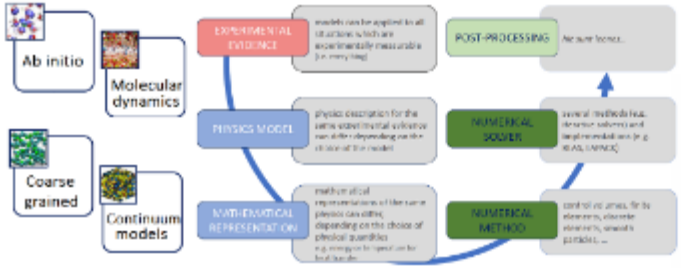
Easy-MODA

https://www.enaloscloud.novamechanics.com/



Easy-MODA

Easy-MODA

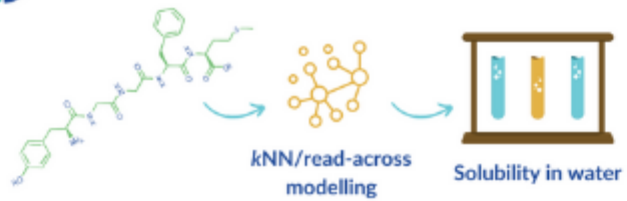


This tool provides an assisted generation of MODA standardised reports for the FAIR and harmonized documentation of materials modelling workflows for EU projects, as proposed by the EMMC.

Visit service Publication Documentation

Read-across model for the prediction of the molecules' water solubility property (logS)

SCENARIOS

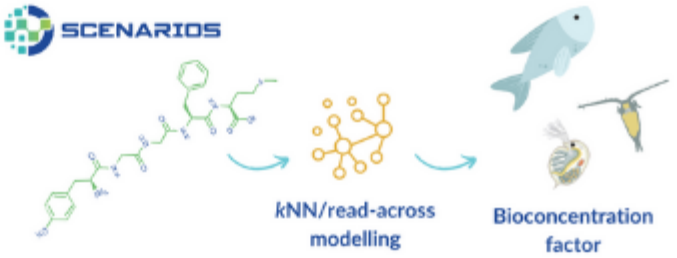


This web-tool permits users to predict the compounds' (log-transformed) water solubility value based on their molecular structure.

Visit service API

Read-across model for the prediction of molecules' bioconcentraiton factor (LogBCF)

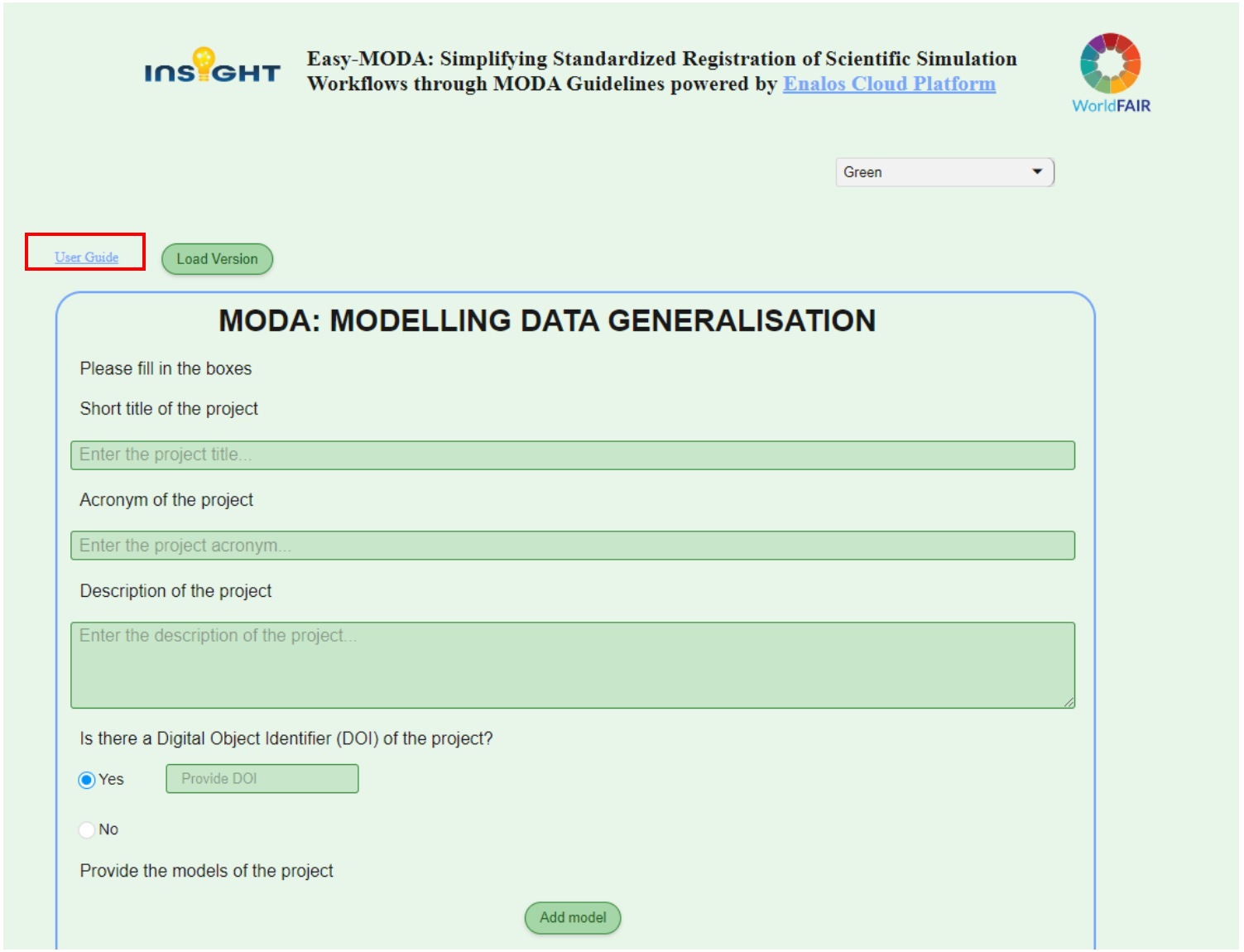
SCENARIOS



This web-tool permits users to predict the molecules BCF value, a measure of the potential of a chemical to accumulate in the tissues of living organisms (particularly fish and other aquatic organisms).

Visit service API

https://www.enaloscloud.novamechanics.com/insight/moda/


INSIGHT
Easy-MODA: Simplifying Standardized Registration of Scientific Simulation Workflows through MODA Guidelines powered by Enalos Cloud Platform
WorldFAIR
Green
User Guide
Load Version
MODA: MODELLING DATA GENERALISATION
Please fill in the boxes
Short title of the project
Enter the project title...
Acronym of the project
Enter the project acronym...
Description of the project
Enter the description of the project...
Is there a Digital Object Identifier (DOI) of the project?
Yes
Provide DOI
No
Provide the models of the project
Add model

Easy-MODA

"Simplifying Standardized Registration of Scientific Simulation Workflows through MODA Template Guidelines"

User Manual

email: info@novamechanics.com

*Easy-MODA web application is powered by Enalos Cloud Platform and is accessible through the link https://www.enaloscloud.novamechanics.com/insight/moda/

**Easy-MODA web application aspires to facilitate the Modelling Data (MODA) registration according to the guidelines that have been proposed by the European Materials Modelling Council (EMMC) and are available in the following links: a) https://emmc.info/moda-workflow-templates/ and b) https://emmc.eu/wp-content/uploads/2021/05/EMMC IntWorkshop Vienna2017 MODA Talk.pdf

The user can access **Easy-MODA** through the link https://www.enaloscloud.novamechanics.com/insight/moda/ or by visiting the Enalos Cloud Platform and searching for the tool.

By clicking the above link, the Graphical User Interface (GUI) of **Easy-MODA** will appear (see the Figure on the right).

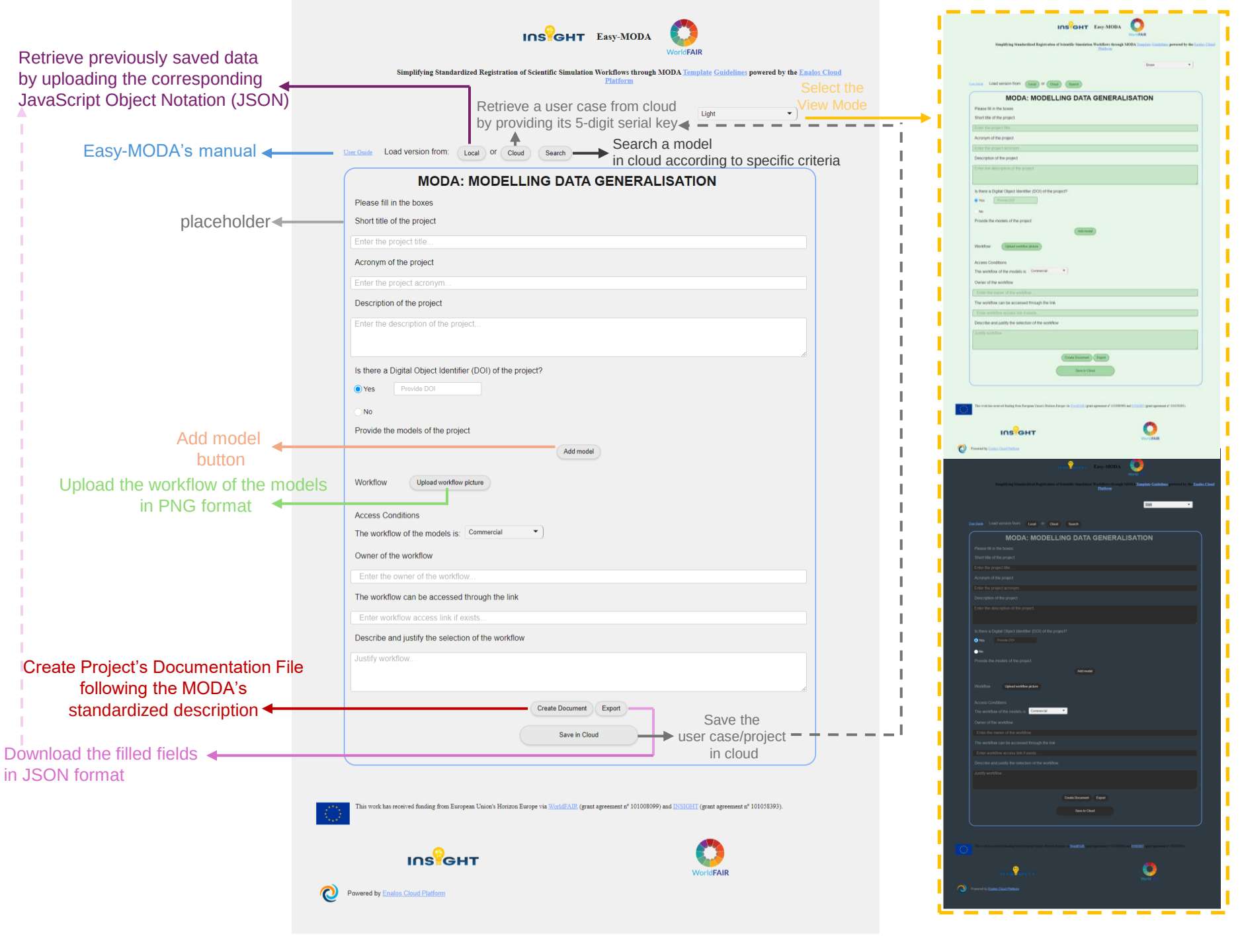
The user can select among three view modes (light, green and dark).

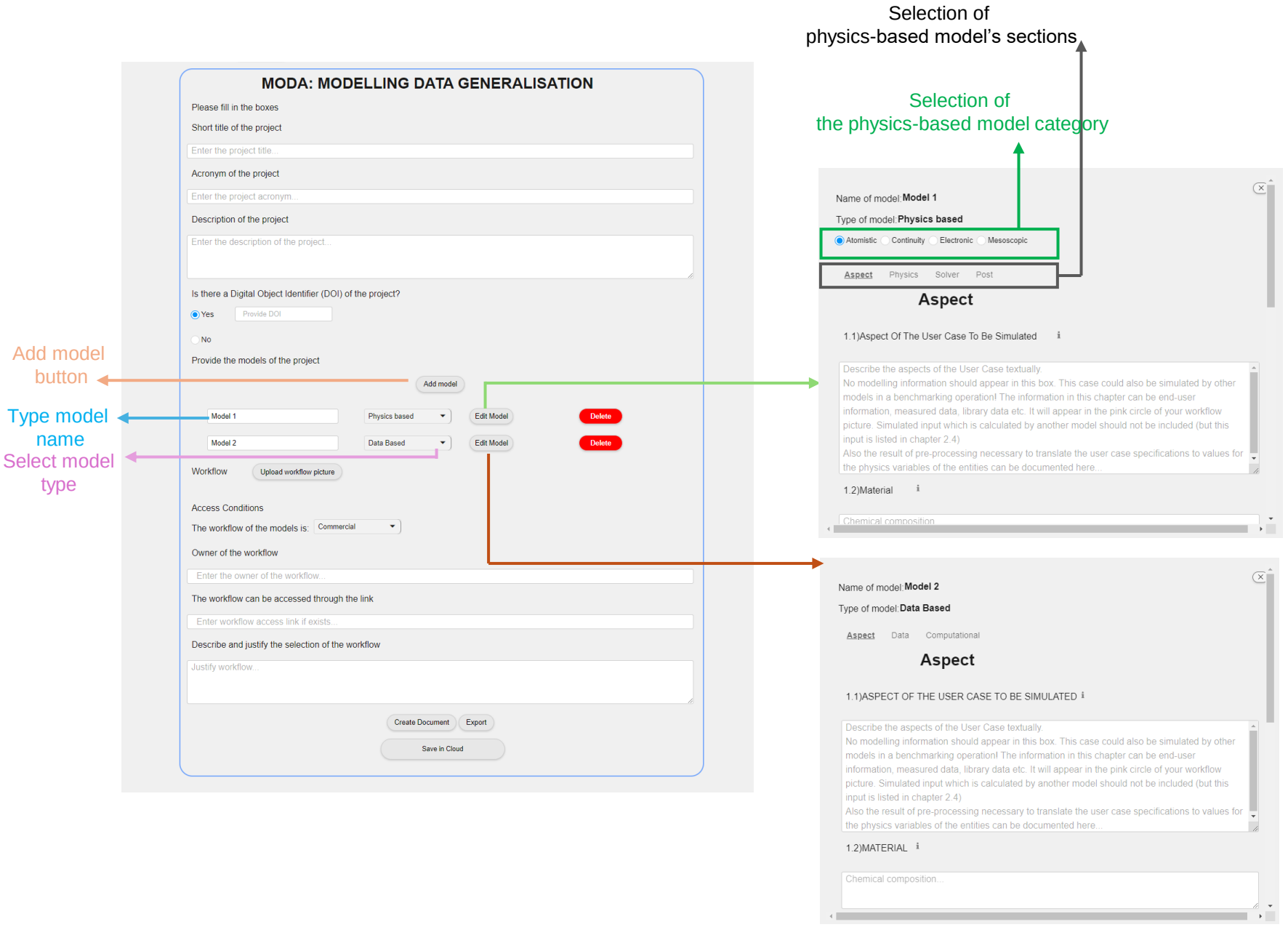
There are placeholders that guide the user through the information that is required to be typed into the GUI.

The user can add a model by clicking the **"Add Model"** button (see next slide for more details) and insert a workflow picture (see later slides).

Next, the project's manual document is downloaded by clicking on the **"Create Document"** button.

Finally, the user can save the inserted data to continue later by clicking on the **"Export"** button, and upload it later by clicking on the **"Load Version"** button.





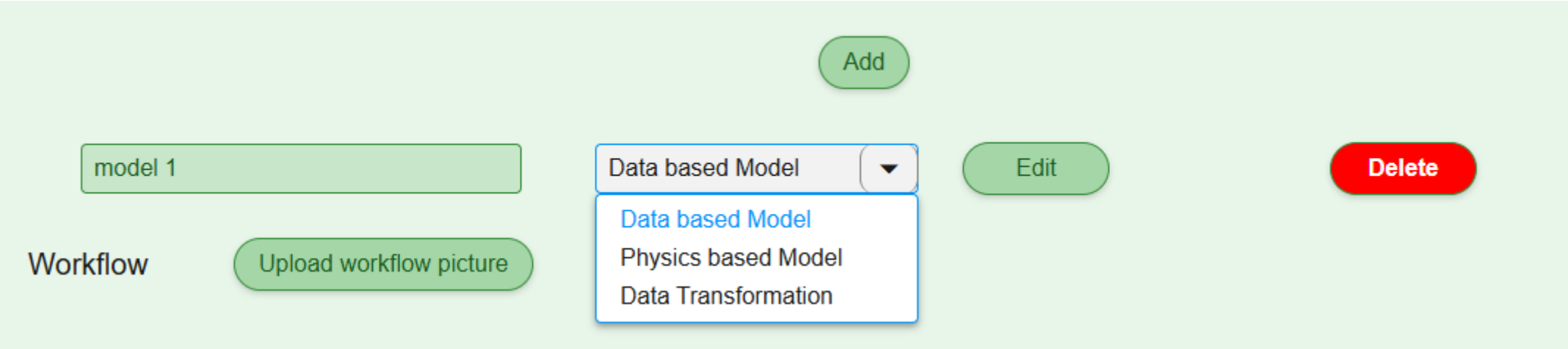
By clicking on the **"Add Model"** button (see the Figure on the left), a new line is created in the Graphical User Interface, where the user types the name of the model, select the model's type (i.e., physics-based or data-driven) and clicks on the "Edit Model" button so that another windows opens where the user can fill in the details of the model.

The user shall select the category of the physics-based model (i.e., Atomistic, Continuity, Electronic, Mesoscopic) which leads to an automated filling of the rest of the fields of the window.

The physics-based models template consists of four sections (i.e., Aspect, Physics, Solver, Post) that need to be filled to follow the MODA guidelines.

The data-based models template consists of only three sections (i.e., Aspect, Data, Computational).

We elaborate more on how to fill the fields in these windows in the next slides.

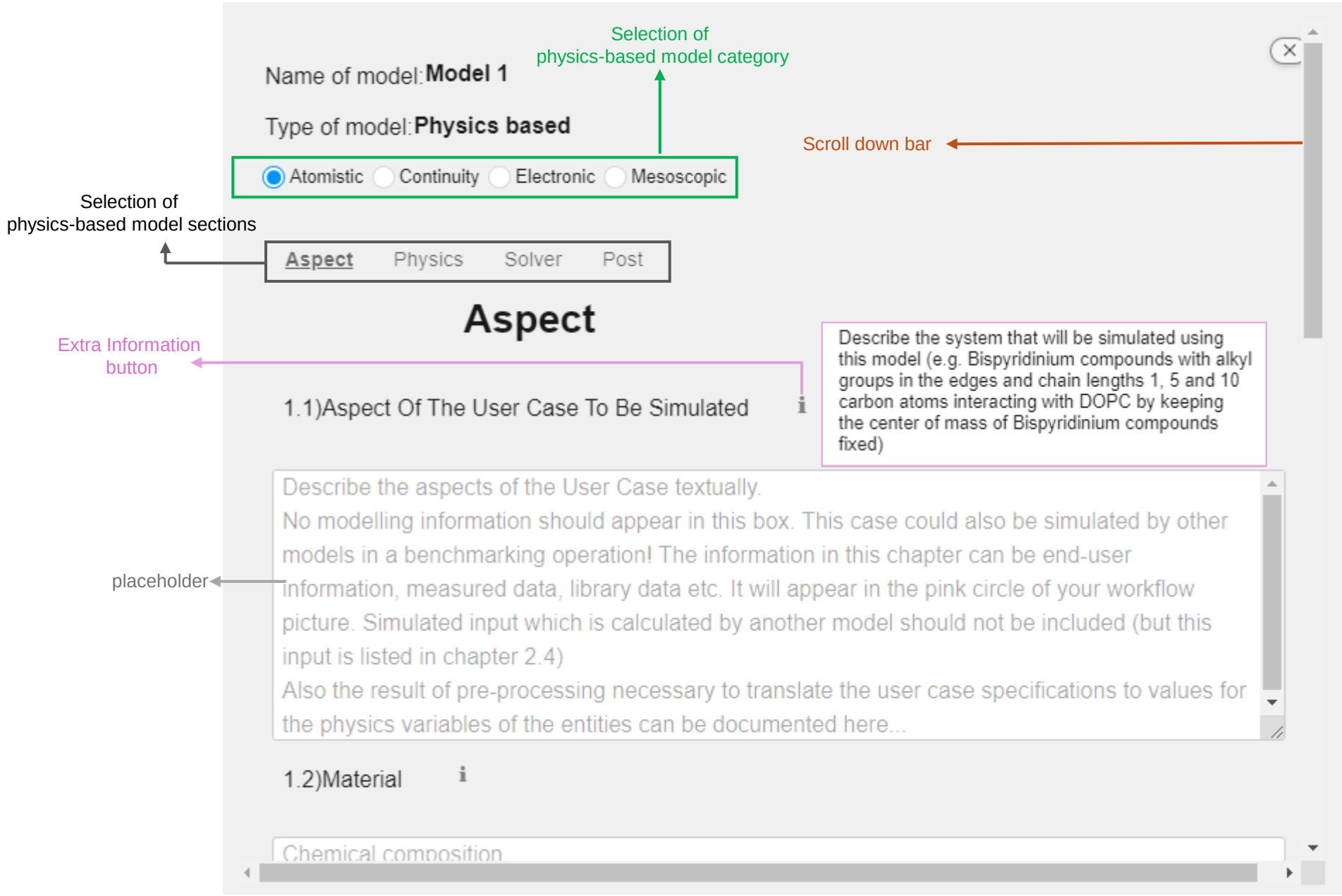

Add
model 1
Data based Model
Edit
Delete
Data based Model
Physics based Model
Data Transformation
Workflow
Upload workflow picture

The user can get more information about how the fields have been filled for models developed in other projects by moving the mouse cursor over the **“i”** button.

If the user later selects another physics-based model category the information that has already been inserted into the fields is erased to assure that that the typed information is compatible with the selected model category.

The user can click on the tabs **“Aspect”**, **“Physics”**, **“Solver”** and **“Post”** to fill in all of the fields needed to describe the model and enhance its re-usability by others.

The **“Scroll down”** bar can be used to access each field of the tab.



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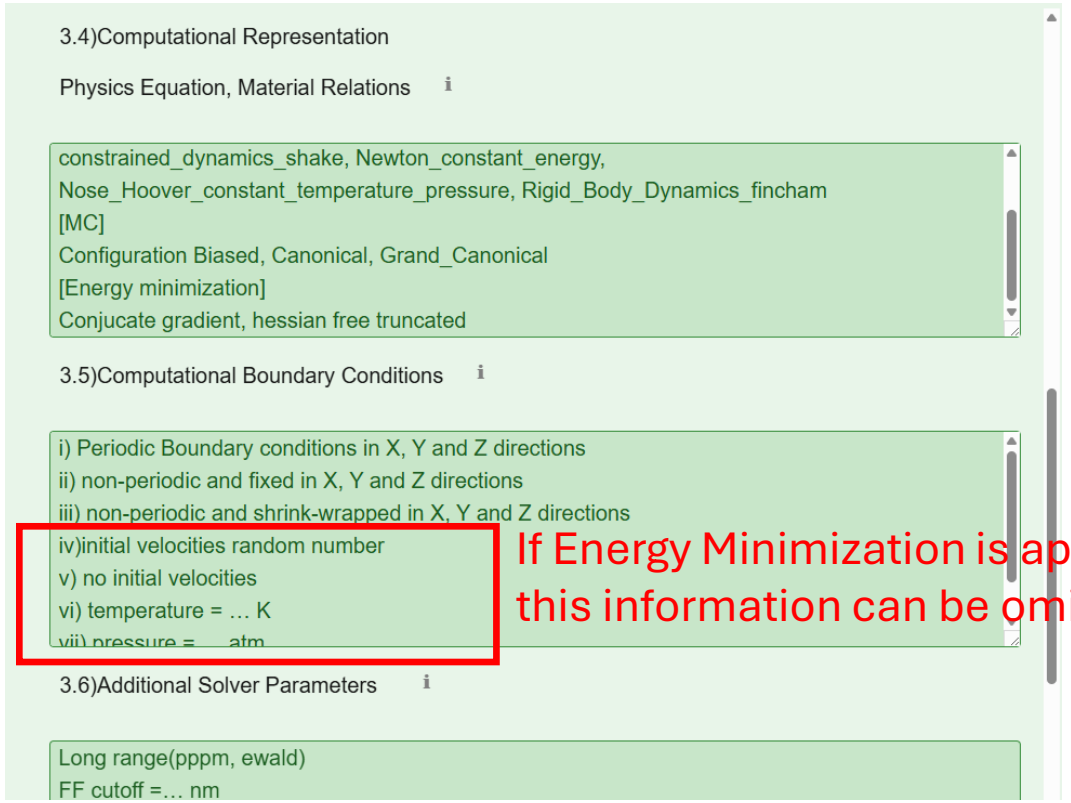
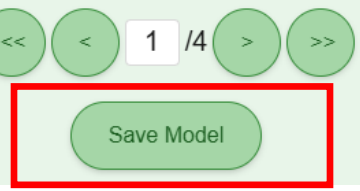


Energy Minimization
Molecular Dynamics
Monte Carlo

If Energy Minimization is applied, this information can be omitted



Before change tab, Save button should be clicked to save the model

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Model Equations/ Algorithms

Energy Minimization

Conjugate gradient
Hessian free truncated

Molecular Dynamics

Langevin
Nose Chain constant temperature thermostat
Nose Hoover constant pressure barostat
Nose Hoover constant temperature thermostat
Constrained dynamics rattle
Constrained dynamics shake
Newton constant energy
Nose Hoover constant temperature pressure thermostat-barostat
Rigid Body Dynamics/Fincham

Monte Carlo

Configuration Biased
Canonical
Grand Canonical

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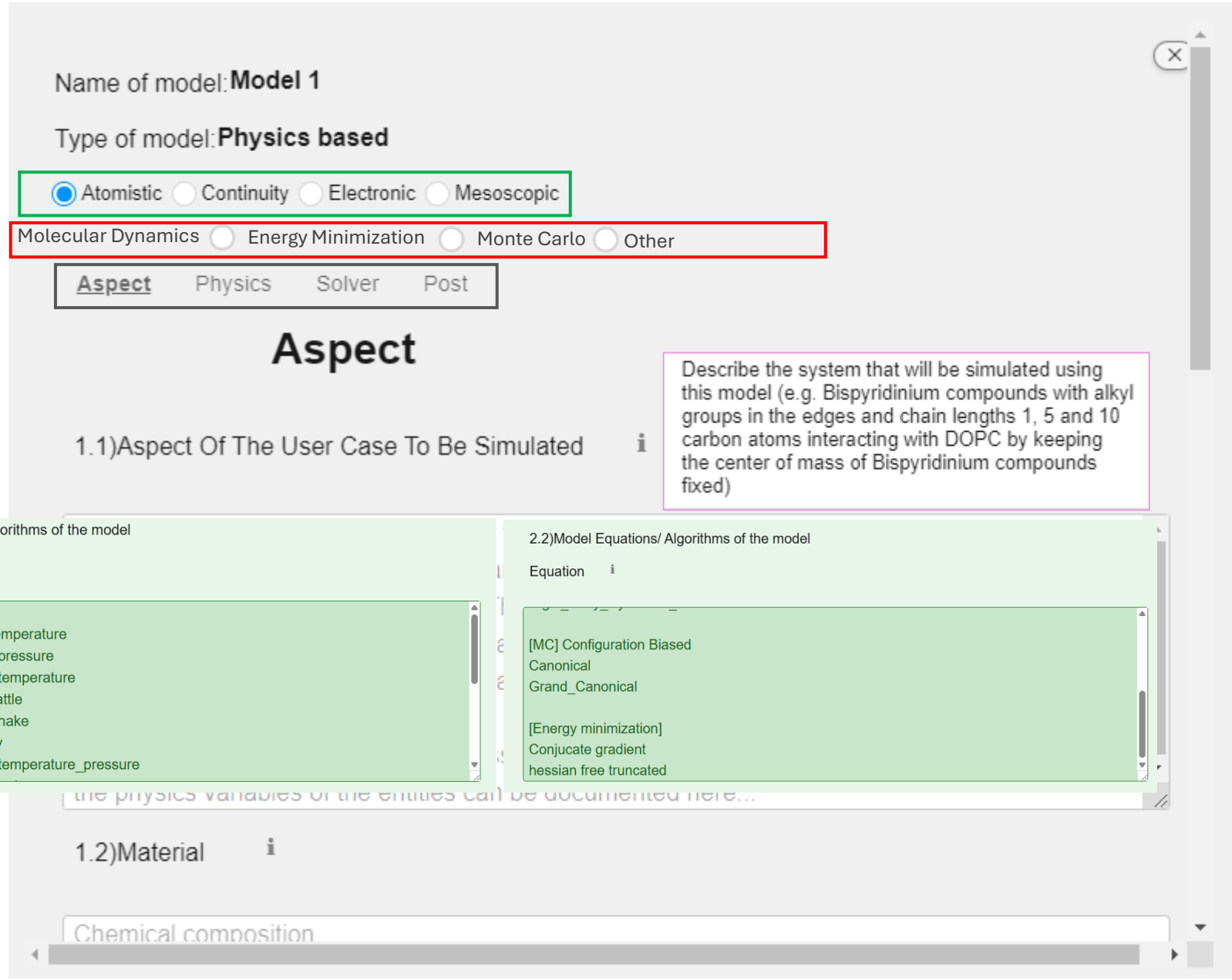

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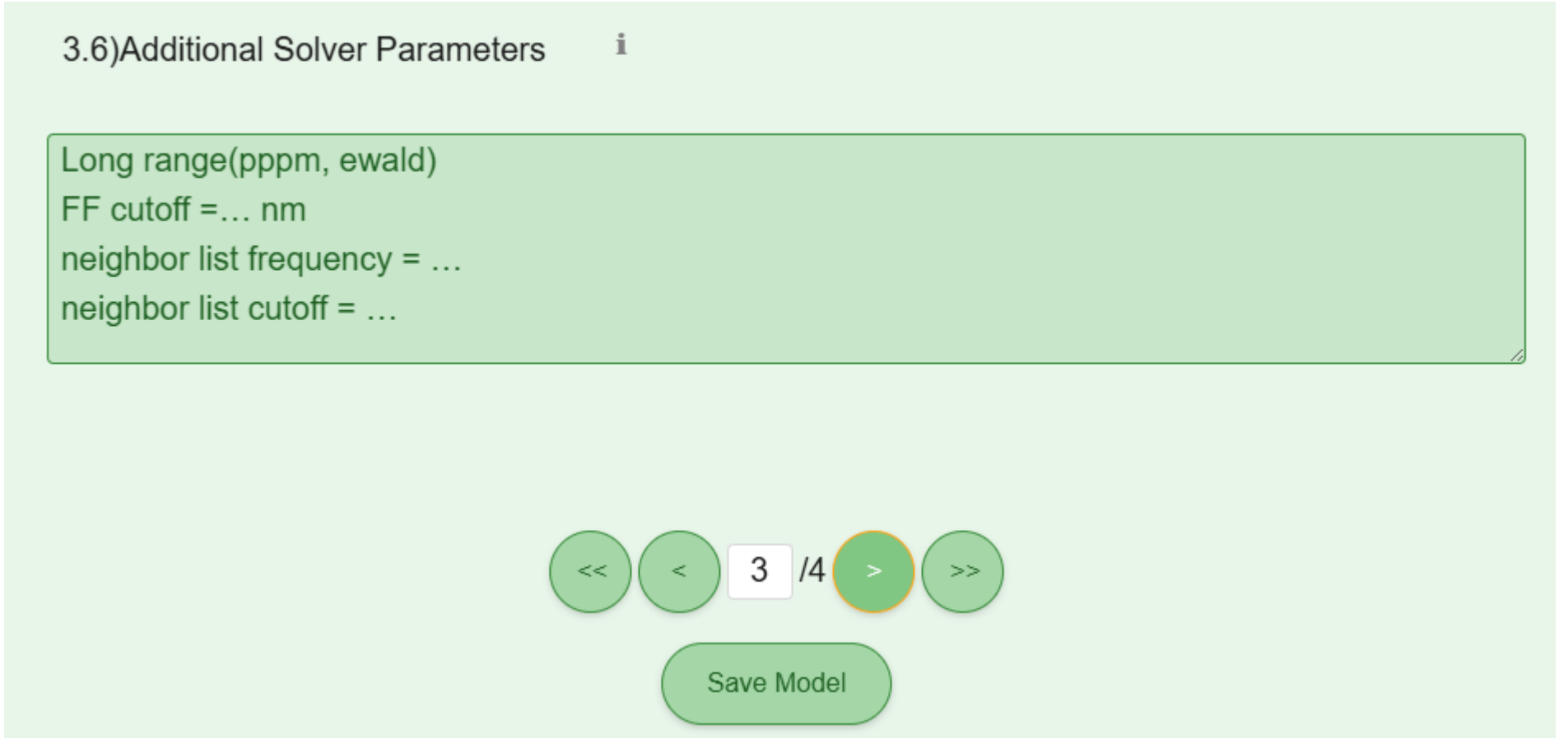
Materials Relations

CHARMM, COMB3, COMPASS, trained with Density Functional Theory, DREIDING, EAM, MEAM, OPLS, ReaxFF, TRAPPE

Physical quantities for each Material Relation

interatomic distances, bonds, angles, dihedrals



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Materials Relations

CHARMM, COMB3, COMPASS, trained with Density Functional Theory, DREIDING, EAM, MEAM, OPLS, ReaxFF, TRAPPE

Physical quantities for each Material Relation

interatomic distances, bonds, angles, dihedrals

4.1)The Processed Output

density, diffusion equation, enthalpy, heat capacity, pressure, radial distribution, temperature, thermal conductivity, viscosity

4.2)Methodologies

Average, Meansquared Displacement, velocity autocorrelation, Virial theorem, Fluctuations, Green Kubo

4.3)Margin Of Error

Standard deviation = …

The user can get more information about how the fields have been filled for models developed in other projects by moving the mouse cursor over the **“i”** button.

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Materials Relations

CHARMM, COMB3, COMPASS, trained with Density Functional Theory, DREIDING, EAM, MEAM, OPLS, ReaxFF, TRAPPE

Physical quantities for each Material Relation

interatomic distances, bonds, angles, dihedrals

3.1)Numerical Solver

Verlet, Leapfrog, Monte Carlo, Energy Minimization (Newton method), Gear predictor corrector, RESPA multiple timesteps

3.2)Software Tool

[commercial] Macromodel, Material_Studio
[inhouse] ….
[opensource] amber, cp2k, dl_poly, gromacs, lammps, namd, Cassandra, RASPA

3.3)Time Step

i)Timestep = … fs
ii)no timestep

Name of model: **model 1**

Type of model: **Physics**

Atomistic Continuity

Aspect Physics

Confirmation

Are you sure you want to fill with automated values?
Any values already filled in will be deleted.

OK Cancel

1.3)Geometry

Provide link of the .cad file

Extra Dependences

Electromagnetism
Fluid Mechanics
Ordinary Differential Equations (Simple Box approximation)
Solid Mechanics

3.6)Additional Solver Parameters

grid_size = …
grid type
grid thickness
provide the grid file

Name of model: **model 1**

Type of model: **Physics based Model**

○ Atomistic ○ Continuity ○ Electronic ○ Mesoscopic ◉ Other

Aspect **Physics** Solver Post

2.2)Model Equations/ Algorithms of the model

Equation ℹ

$$\frac{\mathrm{d}P_i}{\mathrm{d}t} = -\sum_j k_{i\to j} P_i + \sum_j k_{j\to i} P_j .$$

From the PBK Model Reporting template: [D. Model Characterisation / step 2 Model Conceptualisation (model structure. mathematical representation],

Physical quantities ℹ

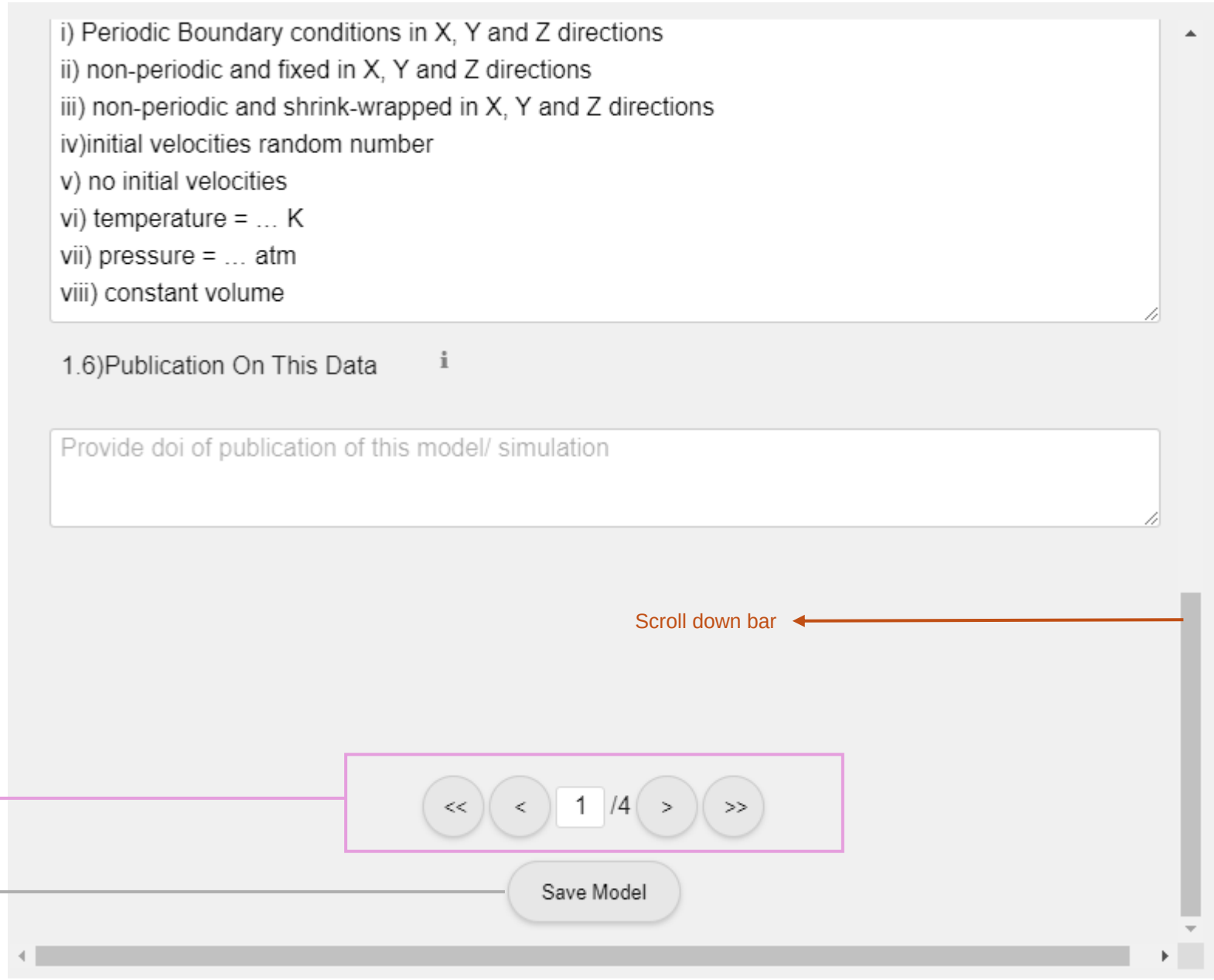
blood flow, incoming arterial blood concentration, the tissue over blood partition coefficient and the volume of compartment.

OECD

Table 3.1 PBK Model Reporting Template

PBK Model Reporting Template sections	Brief description of information to report for each section
A. Name of model	Provide a title of the model. The same should be reported in the checklist.
B. Model developer and contact details	Contact details of model developer.
C. Summary of model characterisation, development, validation, and regulatory applicability	Please capture main points in a brief summary regarding the development, validation and regulatory application.
D. Model characterisation (modelling workflow) Step 1 – Scope and purpose of the model (problem formulation) Step 2 – Model conceptualisation (model structure, mathematical representation) Step 3 – Model parameterisation (parameter estimation and analysis) Step 4 – Computer implementation (solving the equations) Step 5 – Model Performance Step 6 – Model Documentation	Follow the 6 steps of the modelling workflow chapter two. Report in detail the model structure, model biologically plausibility, and parameters with assumptions and limitations, tables can be placed under section H. parameter tables. Under model performance report information on sensitivity analysis, predictive performance. Strategy on how the model validation was performed, e.g. using analogues or other sources or approaches should be reported in detail.
E. Identification of uncertainties model structure input parameters model output other uncertainties (e.g. model developed for different substance and/or purpose)	For each step of the modelling workflow uncertainties should be reported. Use the information provided in the guidance to report and assess (e.g. table in figure 3.3. to capture information on sensitivity and uncertainty for input parameters).
F. Model implementation details software (version no) availability of code software verification / qualification	Information on the model equation solver/software to run the equation should be reported here.
G. Peer engagement (input/review)	Report the extent of peer engagement and review in development of the model.
H. Parameter tables	All information relevant to model parameterisation should be included here: physiological anatomical, physicochemical and biochemical. Report values and units and the source of the parameters (e.g. in case of *in vitro* studies detailed experimental conditions and motivation for choice of experimental conditions in case of non-guideline studies, in case of *in silico* studies add information on models).
References and background information publications links to other resources	Main reference and publications linked to development and description of the model

https://www.doi.org/10.1787/d0de241f-en



The user can also change tabs by selecting the arrow buttons at the bottom of the model's window.

If the user wants to save the entries (e.g., to complete further sections at a later time), then the **"Save Model"** button shall be used, otherwise the information will get lost if the user closes the window.

The user should also click on the **Export Data** button on the main GUI (see slide 1) to download the inserted information for the project and its models in order to save its entries and to be able to reload it.

QMRF and MODA

(Q)SAR model reporting format (QMRF)

	Element	Explanation
1.	**QSAR identifier**	
1.1.	QSAR identifier (title)	SafeNanoScope: Ag-TiO_2-CuO safety assessment powered by Enalos SABYDOMA Cloud Platform
1.2	Other related models	Not applicable
1.3.	Software coding the model	https://www.enaloscloud.novamechanics.com/sabydoma/safenanoscope/
2.	**General information**	
2.0	Abstract	A nanoQSAR-type model for the prediction of the toxicity class of Ag, TiO_2 and CuO nanoparticles (NPs) based on their properties in atomistic level. More information can be found in the respective publication: Varsou *et al.* In Silico Assessment of Nanoparticle Toxicity Powered by the Enalos Cloud Platform: Integrating Automated Machine Learning and Synthetic Data for Enhanced Nanosafety Evaluation, *Computational and Structural Biotechnology Journal*, 2024.
2.1.	Date of QMRF	06 February 2024
2.2.	QMRF author(s) and contact details	Dimitra-Danai Varsou – varsou@novamechanics.com Antreas Afantitis – afantitis@novamechanics.com
2.3.	Date of QMRF update(s)	Not applicable
2.4.	QMRF update(s)	Not applicable
2.5.	Model developer(s) and contact details	Dimitra-Danai Varsou – varsou@novamechanics.com
2.6.	Date of model development and/or publication	Date of model publication: February 2024.
2.7.	Reference(s) to main scientific papers and/or software package	Varsou *et al.* In Silico Assessment of Nanoparticle Toxicity Powered by the Enalos Cloud Platform: Integrating Automated Machine Learning and Synthetic Data for Enhanced Nanosafety Evaluation, *Computational and Structural Biotechnology Journal*, 2024.

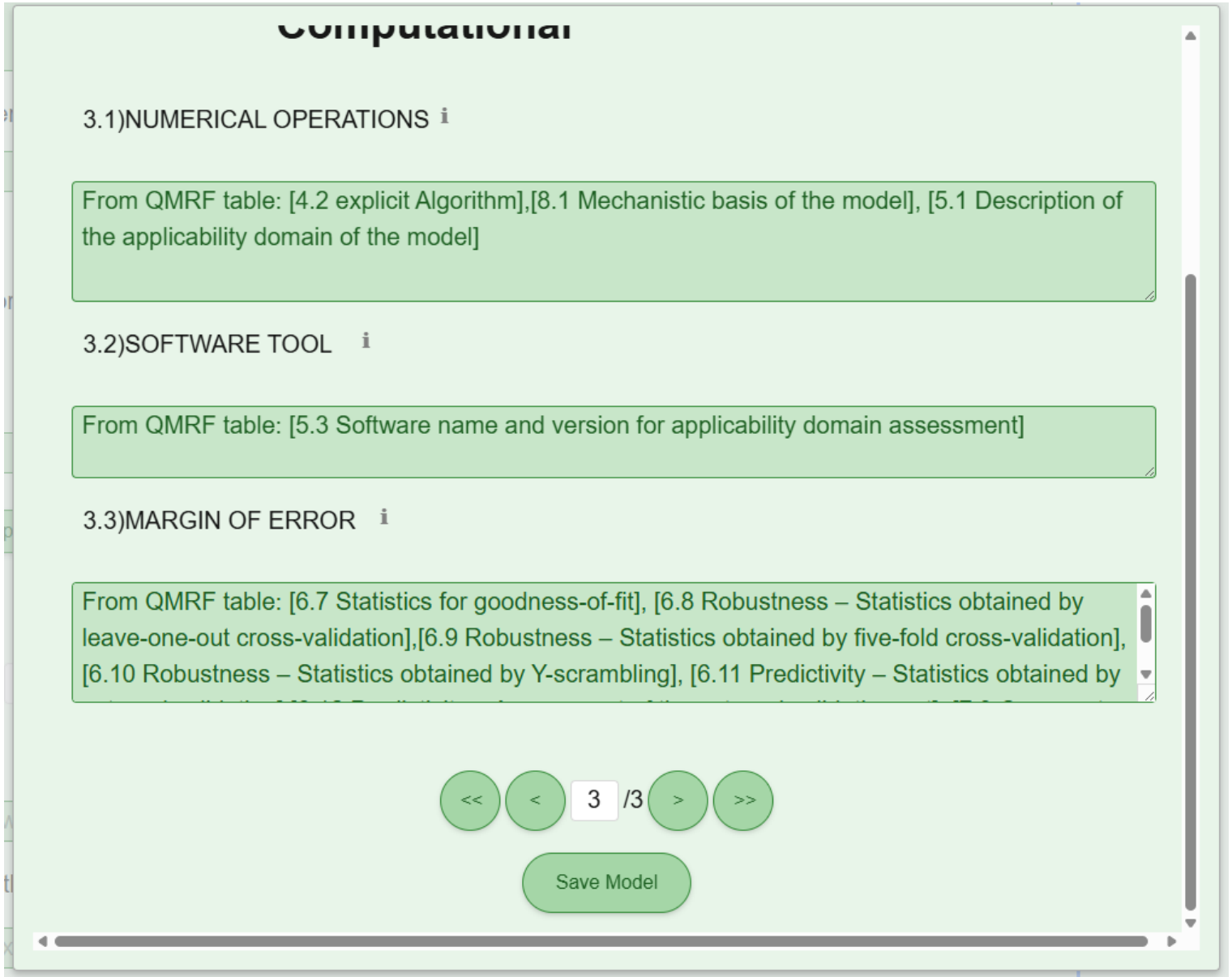
2.8.	Availability of information about the model	The model is proprietary: the source code is confidential; however, the description of the modelling workflow is presented in the original research article, training and test sets are available as supplementary information of the original research article and the model is implemented as a public web service.
2.9.	Availability of another QMRF for exactly the same model	No
3	**Defining the endpoint - OECD Principle 1: "A DEFINED ENDPOINT"**	**PRINCIPLE 1: "A DEFINED ENDPOINT". ENDPOINT refers to any physicochemical, biological, or environmental property / activity / effect that can be measured and therefore modelled. The intent of PRINCIPLE 1 (a (Q)SAR should be associated with a defined endpoint) is to ensure clarity in the endpoint being predicted by a given model, since a given endpoint could be determined by different experimental protocols and under different experimental conditions. It is therefore important to identify the experimental system and test conditions that is being modelled by the (Q)SAR.**
3.1.	Species	Human hepatic cell line (HepaRG)
3.2.	Endpoint	The human hepatoma HepaRG cell line was treated with 89 NPs at 10 different concentrations, and 14 imaging endpoints were measured through a High Throughput Screening (HTS) – High Content Imaging (HCI) study to initially classify NP hazards and identify candidates for further toxicological assessment. The endpoints assessed included cell viability and mitochondrial health by measuring 9 features and the results of the HTS-HCI screening were normalised following the signal-to-noise ratio approach. A threshold of -3 for downward response and +3 for upward response was used, which corresponded to a 99% certainty that the cell behaviour was different from the untreated (negative) control value (cells treated only with medium).
3.3	Comment on endpoint	The normalised values were depicted in a colour-coded heatmap, which reflected the extend of difference of the behaviour from the untreated control (red and blue colours for decreased or increased response, respectively) or indicated similar behaviour to the untreated control (green colour).
3.4.	Endpoint units	The results of the 9 toxicity features were summarised into a single endpoint ("overall") class as follows: NP treatments were classified as "Low effect" if they had a similar response to the negative controls (green labels) in at least 5 measured features (73 NP treatments). Otherwise, NP treatments were classified as "High effect" (red and/or blue label, 37 treatments).
3.5.	Dependent variable	Not applicable
3.6.	Experimental protocol	Information on the experimental protocols can be found in: Joossens, E., Macko, P., Palosaari, T. *et al.* A high throughput imaging database of toxicological effects of nanomaterials tested on HepaRG cells. Sci Data 6, 46 (2019). https://doi.org/10.1038/s41597-019-0053-2
3.7.	Endpoint data quality and variability	Information on the data quality and variability can be found in: Joossens, E., Macko, P., Palosaari, T. *et al.* A high throughput imaging database of toxicological effects of nanomaterials tested on HepaRG cells. Sci Data 6, 46 (2019). https://doi.org/10.1038/s41597-019-0053-2

4	**Defining the algorithm - OECD Principle 2 : "AN UNAMBIGUOUS ALGORITHM"**	**PRINCIPLE 2: "AN UNAMBIGUOUS ALGORITHM". The (Q)SAR estimate of an endpoint is the result of applying an ALGORITHM to a set of structural parameters which describe the chemical structure. The intent of PRINCIPLE 2 (a (Q)SAR should be associated with an unambiguous algorithm) is to ensure transparency in the model algorithm that generates predictions of an endpoint from information on chemical structure and/or physicochemical properties. In this context, algorithm refers to any mathematical equation, decision rule or output approach.**
4.1.	Type of model	Type of model: Ensemble learner (Random Forest)
4.2.	Explicit algorithm	Random Forest: Random forests are supervised ensemble learning algorithms that utilize bagging (bootstrap aggregating) and feature randomness to construct a multitude of decision trees.
4.3.	Descriptors in the model	• Concentration of NPs in μg/mL • The average difference of the common neighbour parameter, CNP, (local crystal structure in a diameter of 3Ang) between core and shell atoms [AD45*] • The average difference of the coordination parameter (neighbouring atoms in a diameter of 5Ang) between core and shell atoms [AD27] • The average difference of the coordination parameter (neighbouring atoms in a diameter of 4Ang) between core and shell atoms [AD22] • The average difference of the coordination parameter (neighbouring atoms in a diameter of 3Ang) between core and shell atoms [AD17] • The average coordination parameter (neighbouring atoms in a diameter of 3Ang) of the shell atoms [AD16] • The average coordination parameter (neighbouring atoms in a diameter of 3Ang) of all atoms [AD14] • The average coordination parameter of all atoms [AD9] • The average difference of the potential energy between core and shell atoms in eV [AD7] • Log10 of all atoms in the surface [AD3] • Log10 of all atoms in the NP [AD1] *This notation is consistent with the relevant publication.
4.4.	Descriptor selection	From the initial pool of descriptors (53 in total), 33 were filtered out using missing values, low variance and correlation filtering (see §6.6). The information gain of all remaining descriptors (20) is calculated and descriptors with zero information gain score are excluded from the modelling, as they are not considered critical for establishing a predictive relationship. Finally, 11 descriptors were selected (see §4.3).
4.5.	Algorithm and descriptor generation	Atomistic simulations. To perform the simulations and acquire the computational descriptors, the size, the shape, and the phase of the NPs were needed.
4.6.	Software name and version for descriptor generation	ASCOT: A Web Tool for the Digital Reconstruction of Energy Minimized Ag, CuO, and TiO_2 Spherical Nanoparticles and Calculation of their Atomistic Descriptors Powered by Enalos SABYDOMA Cloud Platform, https://www.enaloscloud.novamechanics.com/sabydoma/ascot/ For ellipsoid NPs see the NanoConstruct: Nanoparticle Construction Tool Powered by Enalos RiskGONE Cloud Platform, http://enaloscloud.novamechanics.com/riskgone/nanoconstruct/

https://one.oecd.org/document/ENV/CBC/MONO(2023)32/ANN1/en/pdf

QMRF and MODA

QMRF and MODA



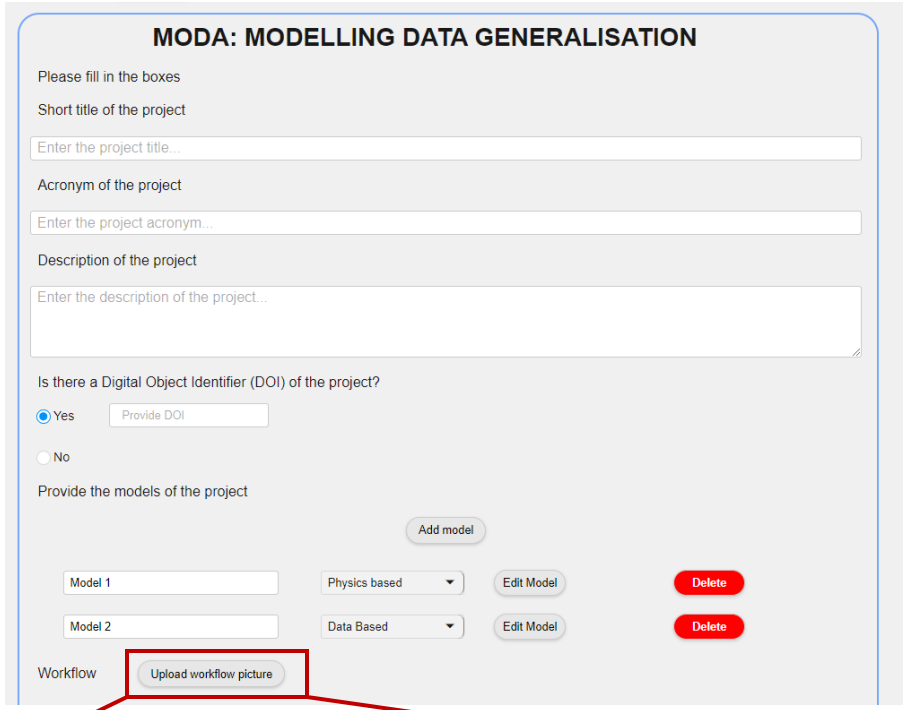
By clicking on the **“Upload Workflow Picture”** button (see the Figure on the right), the user can upload the workflow image which shall create manually based on the information inserted in each model.

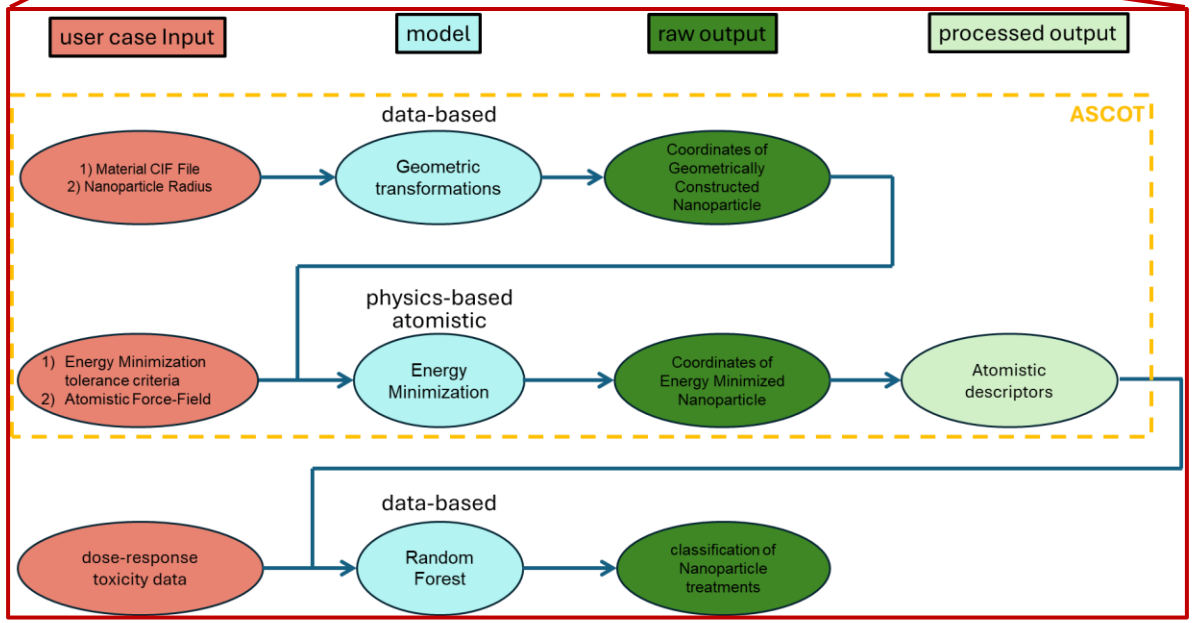
The information in the fields *“Material”*, *“Geometry”* of the **“Aspect”** tab and *“time step”* and *“computational boundary conditions”* in the **“Solver”** tab are the text of the red boxes of the workflow (see bottom right of the figure).

The information inserted in the *“numerical solver”* field of the **“Solver”** tab is shown in the light blue boxes of the workflow (see bottom right of the figure).

The field of “physical quantities” of the “**Physics**” tab is the raw output of the workflow (see the green boxes in the bottom right of the figure).

The field of “processed output” of the **“Post”** tab is the final (processed) output from the model which is written in the light green box of the workflow (see bottom right of figure).





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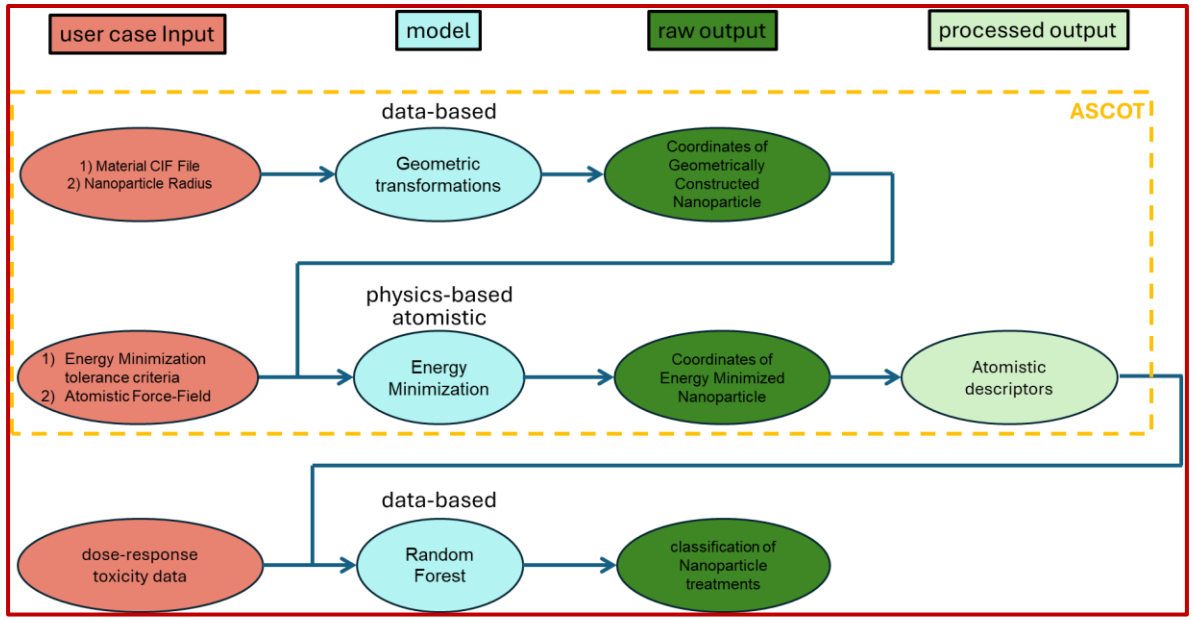
user case Input	model	raw output	processed output
Physics-based a) **"Aspect" tab** "Material", "Geometry" b) **"Solver" tab** "time step" , "computational boundary conditions" Data-based a) **"Data" tab** "Database and type"	Physics-based a) **"Solver" tab** "numerical solver" Data-based a) **"Data" tab** "Equation Type and Name" b) **"Computational" tab** "numerical operations"	Physics-based a) **"Physics" tab** "physical quantities" Data-based a) **"Data" tab** "physical quantities"	Physics-based a) **"Post" tab** "processed output"



By clicking on the **"Upload Workflow Picture"** button (see the Figure on the right), the user can upload the workflow image which shall create manually based on the information inserted in each model.

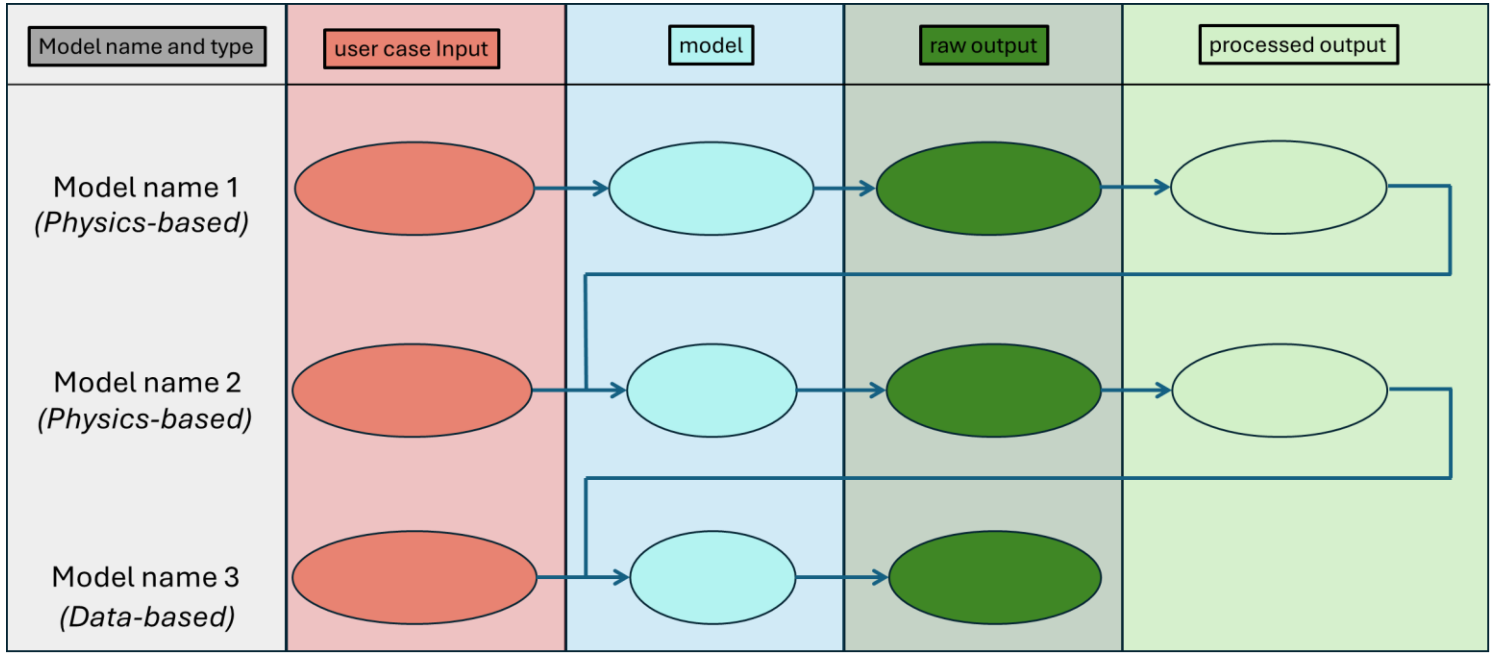
The information in the fields *"Material"*, *"Geometry"* of the **"Aspect"** tab and *"time step"* and *"computational boundary conditions"* in the **"Solver"** tab are the text of the red boxes of the workflow (see bottom right of the figure).

The information inserted in the *"numerical solver"* field of the **"Solver"** tab is shown in the light blue boxes of the workflow (see bottom right of the figure).

The field of "physical quantities" of the "**Physics**" tab is the raw output of the workflow (see the green boxes in the bottom right of the figure).

The field of "processed output" of the **"Post"** tab is the final (processed) output from the model which is written in the light green box of the workflow (see bottom right of figure).

user case Input	model	raw output	processed output
Physics-based a) **"Aspect" tab** "Material", "Geometry" b) **"Solver" tab** "time step" , "computational boundary conditions" Data-based a) **"Data" tab** "Database and type"	Physics-based a) **"Solver" tab** "numerical solver" Data-based a) **"Data" tab** "Equation Type and Name" b) **"Computational" tab** "numerical operations"	Physics-based a) **"Physics" tab** "physical quantities" Data-based a) **"Data" tab** "physical quantities"	Physics-based a) **"Post" tab** "processed output"



By clicking on the **“Upload Workflow Picture”** button (see the Figure on the right), the user can upload the workflow image which shall create manually based on the information inserted in each model.

The information in the fields *“Material”*, *“Geometry”* of the **“Aspect”** tab and *“time step”* and *“computational boundary conditions”* in the **“Solver”** tab are the text of the red boxes of the workflow (see bottom right of the figure).

The information inserted in the *“numerical solver”* field of the **“Solver”** tab is shown in the light blue boxes of the workflow (see bottom right of the figure).

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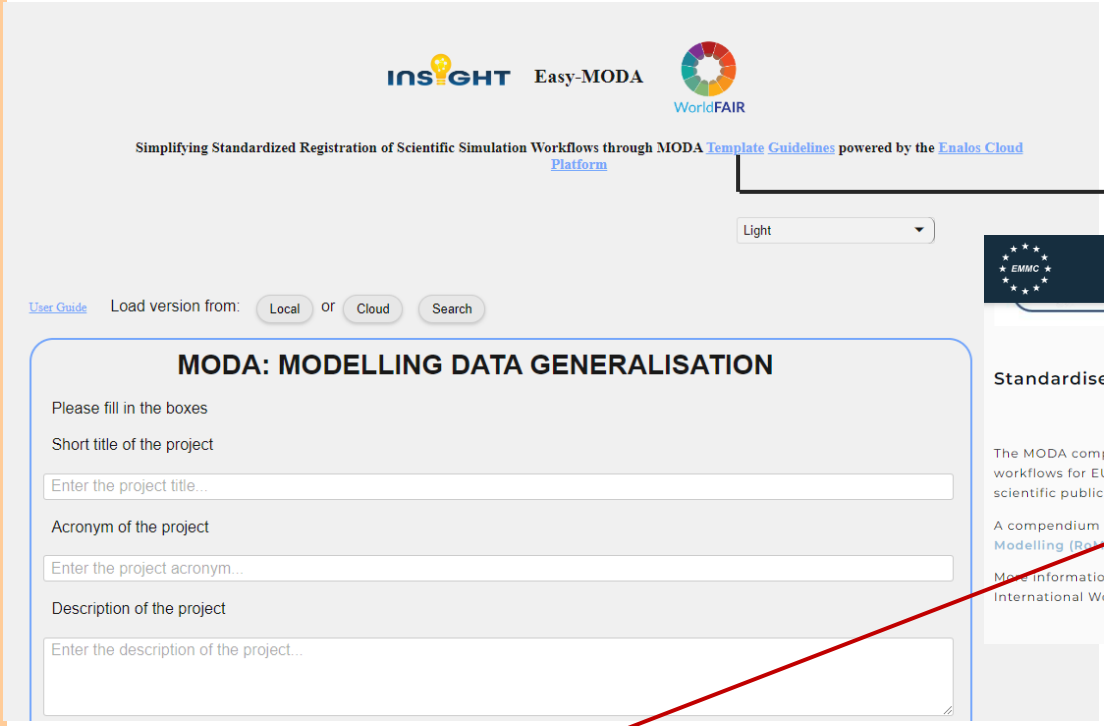
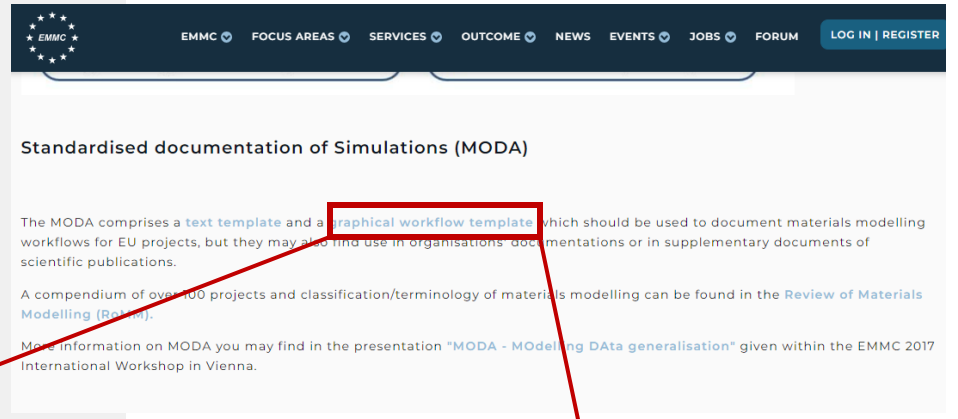
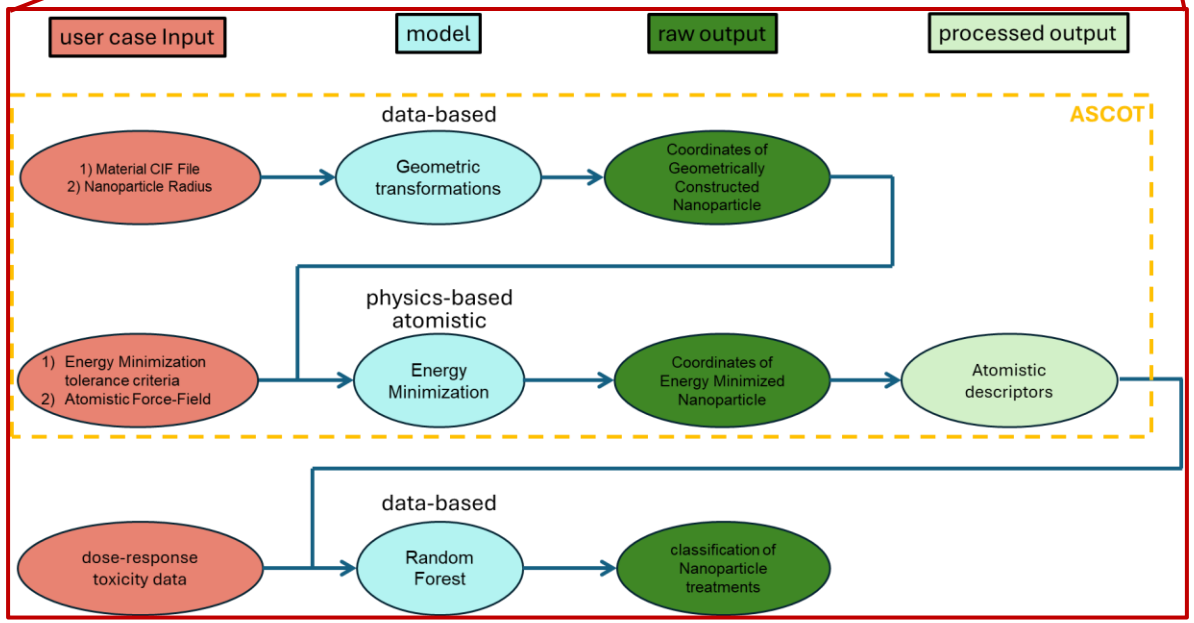


https://emmc.eu/moda/

By clicking this link, the EMMC website appears and Workflow Templates can be downloaded





Moda powered by Enalos Cloud Platform

MODA for

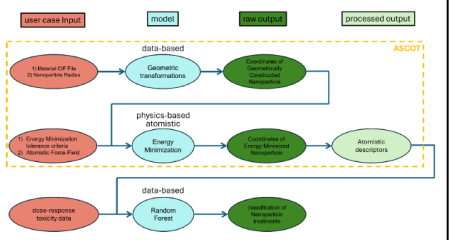
Safety Assessment of Ag, TiO_2, and CuO nanoparticles

Simulated in project:

SafeNanoScope

OVERVIEW of the SIMULATION			
1	USER CASE	Safety Assessment of Ag, TiO_2, and CuO nanoparticles	
2	CHAIN OF MODELS	**Model 1**	construction of energy minimized NP Physics based
		Model 2	autoML Data Based
		Model 3	construction of geometrically constructed NP Data Based
3	PUBLICATION PEER - REVIEWING THE DATA	DOI provided: **No**	
4	ACCESS CONDITIONS	Access type: **Free** Owner of workflow: **NovaMechanics Ltd** Workflow access link: https://www.enaloscloud.novamechanics.com/sabydoma/safenanoscope/	
5	WORKFLOW AND ITS RATIONALE	Traditional (experimental) methods for assessing the nanoparticles (NPs) safety are time-consuming, expensive, and resource-intensive, and raise ethical concerns due to their reliance on animals. To address these challenges, we propose an in silico workflow that serves as an alternative or complementary approach to conventional hazard and risk assessment strategies, which incorporates state-of-the-art computational methodologies. In detail, an automated machine learning (autoML) scheme is developed employing dose-response toxicity data for silver (Ag), titanium dioxide (TiO_2), and copper oxide (CuO) NPs. This model is further enriched with atomistic descriptors using the ASCOT tool to capture the NPs' underlying structural properties. To overcome the issue of limited data availability, synthetic data generation techniques are used. These techniques help in broadening the dataset, thus improving the representation of different NP classes.	

Workflow picture



Each physics-based model used in this simulation is to be documented in four chapters:

1. Aspect of the User Case or system simulated with this model
2. Model: Please make sure the notions Physics Equation and Materials Relation are properly understood.
   - Tightly coupled models can be written up collectively in one set of four tables. To solve tightly coupled PE one matrix is set up and solved in one go.
   - For continuum models the PE is often the conservation equations coded up in bought software packages.
   - Often the MR is established by the modeller.
3. Computational aspects include also a documentation of how the user case specifications are translated into computer language.
4. Post processing documents how the raw output of one simulation is processed into input for the next simulation. This information given under 4.1 in the first model will be the same as the "simulated input" information under 2.4 for the next model. This is the essence of model inter-operability!
5. Pre-processing before the first model can be depicted in pink as it is considered to be part of the user-case.

Each data-based model in this simulation is to be documented in three chapters:

1. Aspect of the User Case or system simulated with this data-based model
2. Data-based Model
3. Computational detail of the datamining operation

MODA

Physics based Model

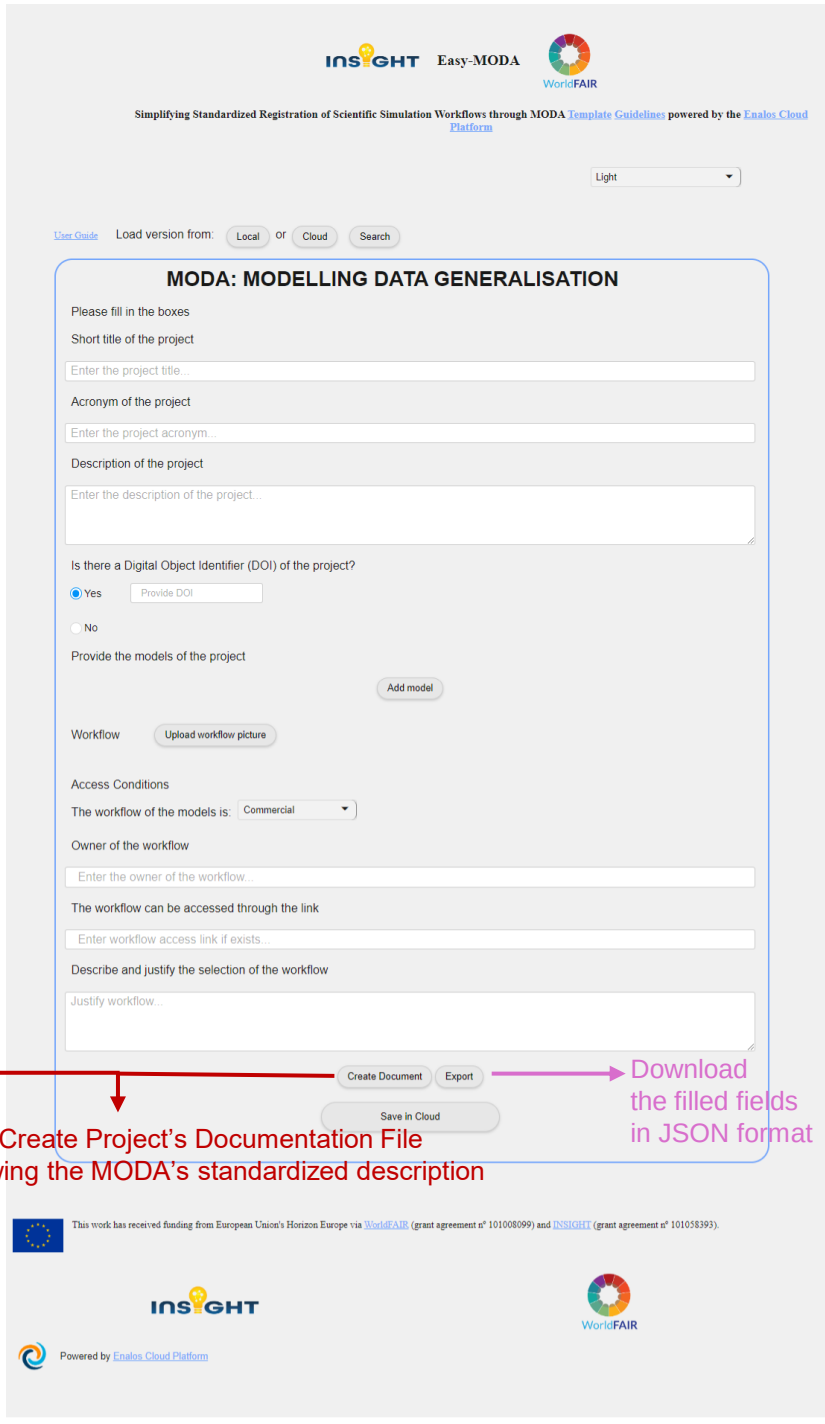
MODEL 1

construction of energy minimized NP

Aspect of the User Case/System to be Simulated		
1.1	**Aspect of the User Case to be simulated**	Digital Construction of energy minimized Ag, TiO_2 and CuO nanoparticles(NPs) having the diameters mentioned in the dataset needed to be enriched and calculation of their atomistic descriptors.
1.2	**Material**	Geometrically constructed Nanoparticles made by model "Construction of Geometrically Constructed NPs after using the following CIF files Ag (Fm-3 m space group, COD ID 1509146), TiO_2 (rutile P42/mnm, COD ID 1532819 and Anatase, I4 1/amd space group, COD ID 1010942), CuO (the space group C12/c1, tenorite, COD ID 1011148)
1.3	**Geometry**	Spherical initially and any shape that is created after the energy minimization procedure.

The Data-based Model			
2.0	**Equation type and name**	Geometrical manipulations were used (e.g. unit cell replication) and an algorithmic procedure mentioned in detail in the section "MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS"	
2.1	**Database and type**	Initial configuration file names Ag(1509146.cif), TiO_2 (1532819.cif and 1010942.cif), CuO (1011148.cif)	
2.2	**Equation**	Hypothesis	Geometrical manipulations were used (e.g. unit cell replication) and an algorithmic procedure mentioned in detail in the section "MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS"
		Physical quantities	Coordinates of atoms of the NP

Computational detail of datamining operation		
3.1	**Numerical Operations**	Geometrical manipulations were used (e.g. unit cell replication) and an algorithmic procedure mentioned in detail in the section "MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS"
3.2	**Software tool**	ASCOT web application (https://www.enaloscloud.novamechanics.com/sabydoma/ascot/)
3.3	**Margin Of Error**	Due to strictly mathematical operations used during the geometrical construction of NP there is no margin of error except the errors may have been inserted due to errors of the inserted input files.



By clicking on the **"Create Document"** button (see the bottom of the right hand side of the figure), the user can get the project's information in pdf format as shown on the left of the figure) structured according to the MODA guidelines.

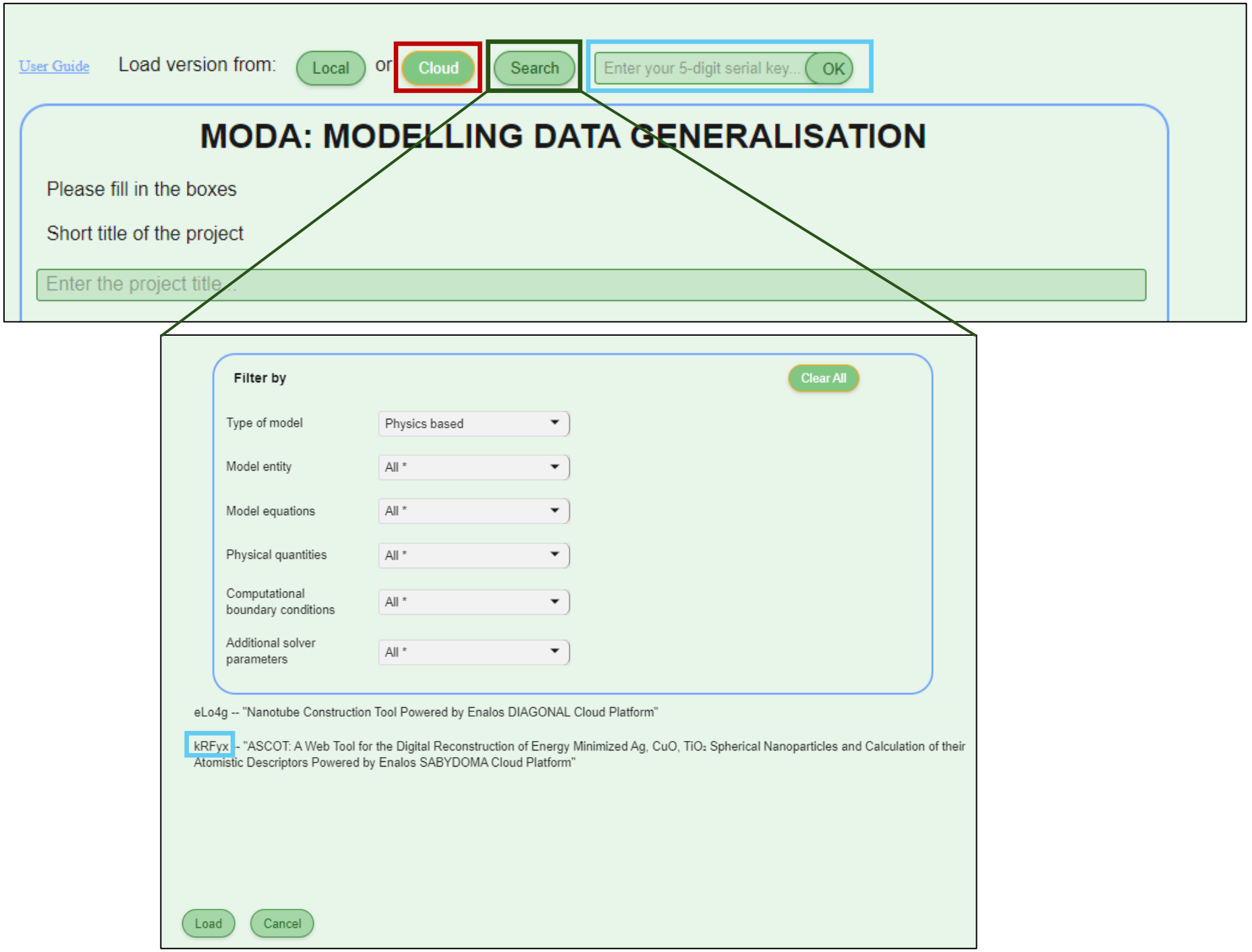
The user can also download a JSON file to save the information of the model(s) in a format compatible with Easy-MODA in order to upload it later.

For any further modification of the document, the user can convert the pdf file to a doc format and manually change it.

By clicking on the **“Cloud”** button (see the Figure on the right), the user can upload a user case from the cloud by inserting its 5-digit serial key .

By clicking on the **“Search”** button (see the Figure on the right), the user can search a user case from the cloud that satisfies specific criteria.

The list of the use cases of the cloud is mentioned at the bottom of the pop-up window. The user can search the list of the available use cases and load them by clicking on them. The first five digits of each model in the list are its serial key.



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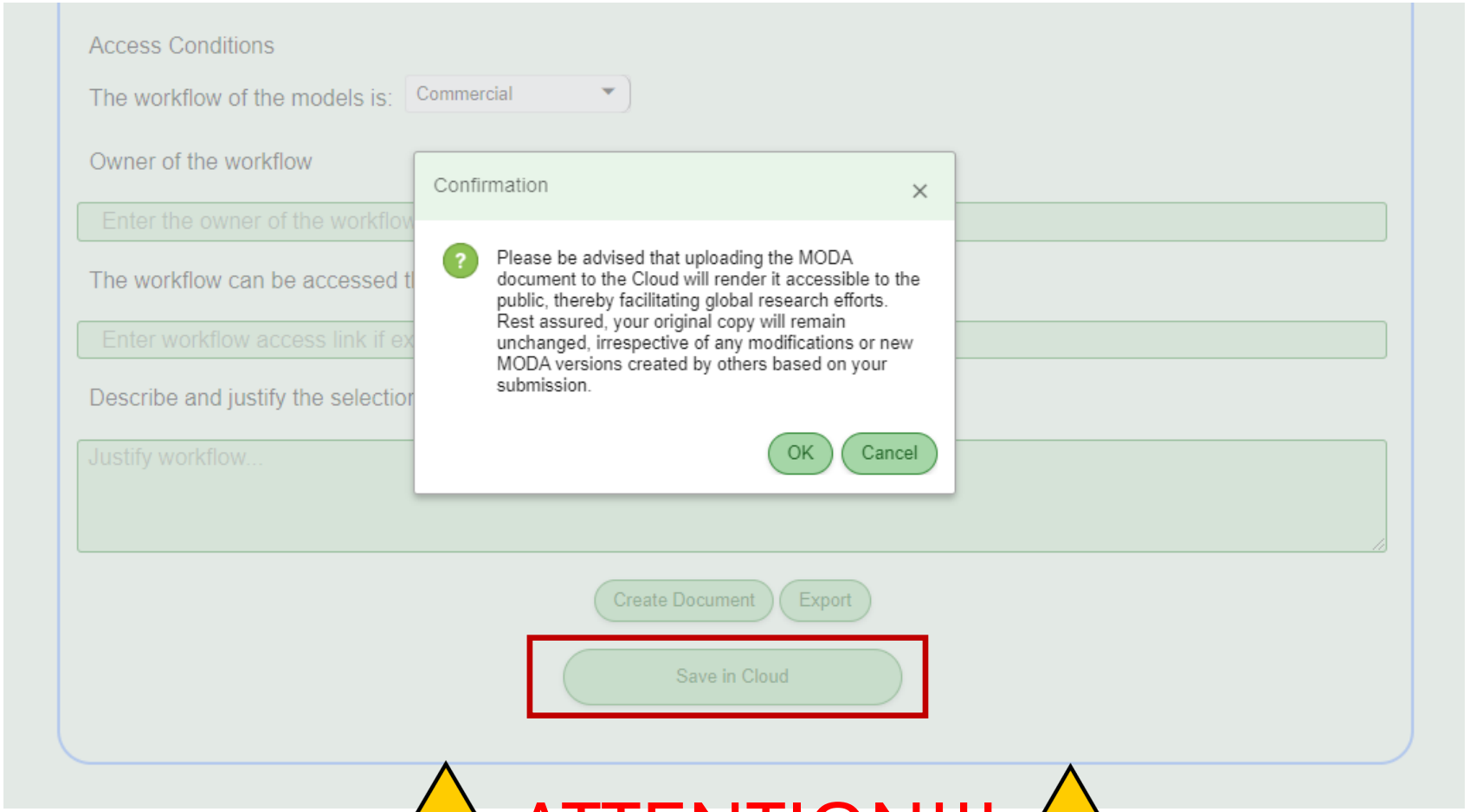

ATTENTION!!!

By clicking on the **“Save in Cloud”** button (see the Figure above), the user can upload the use case MODA documentation in the Cloud where it will remain in cloud permanently. A warning message appears to confirm that the user agrees with the uploading of the MODA document in the cloud.

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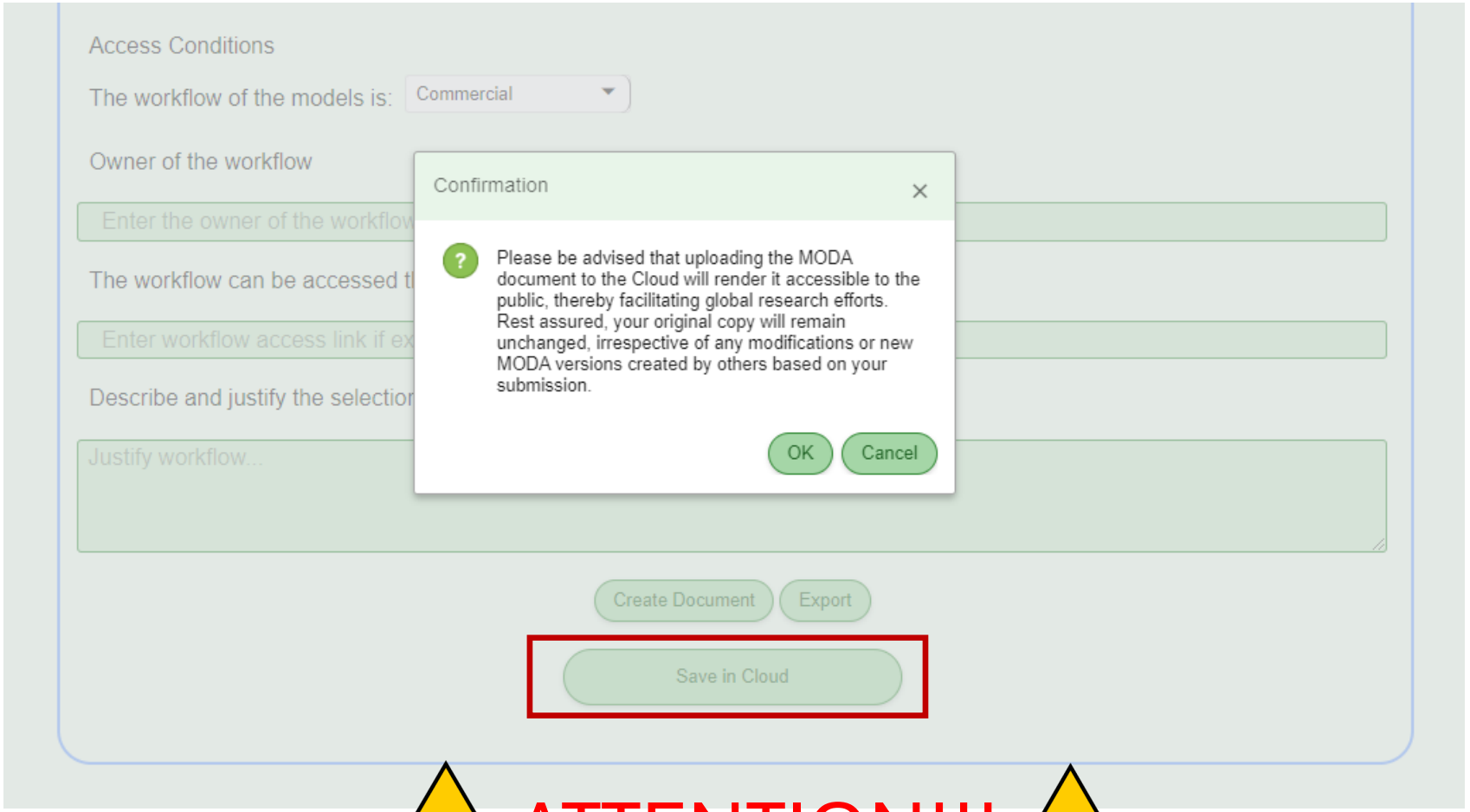

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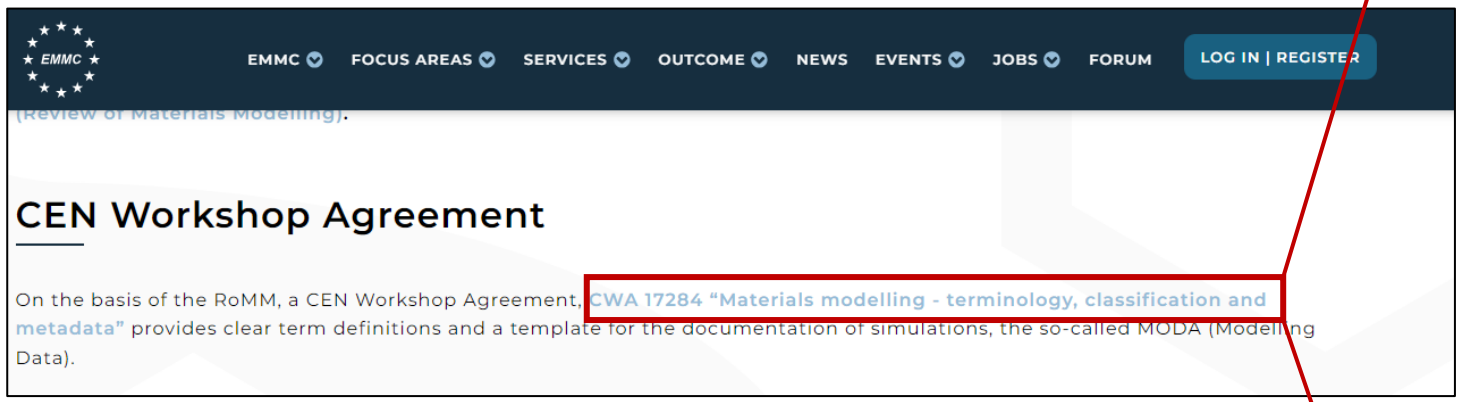
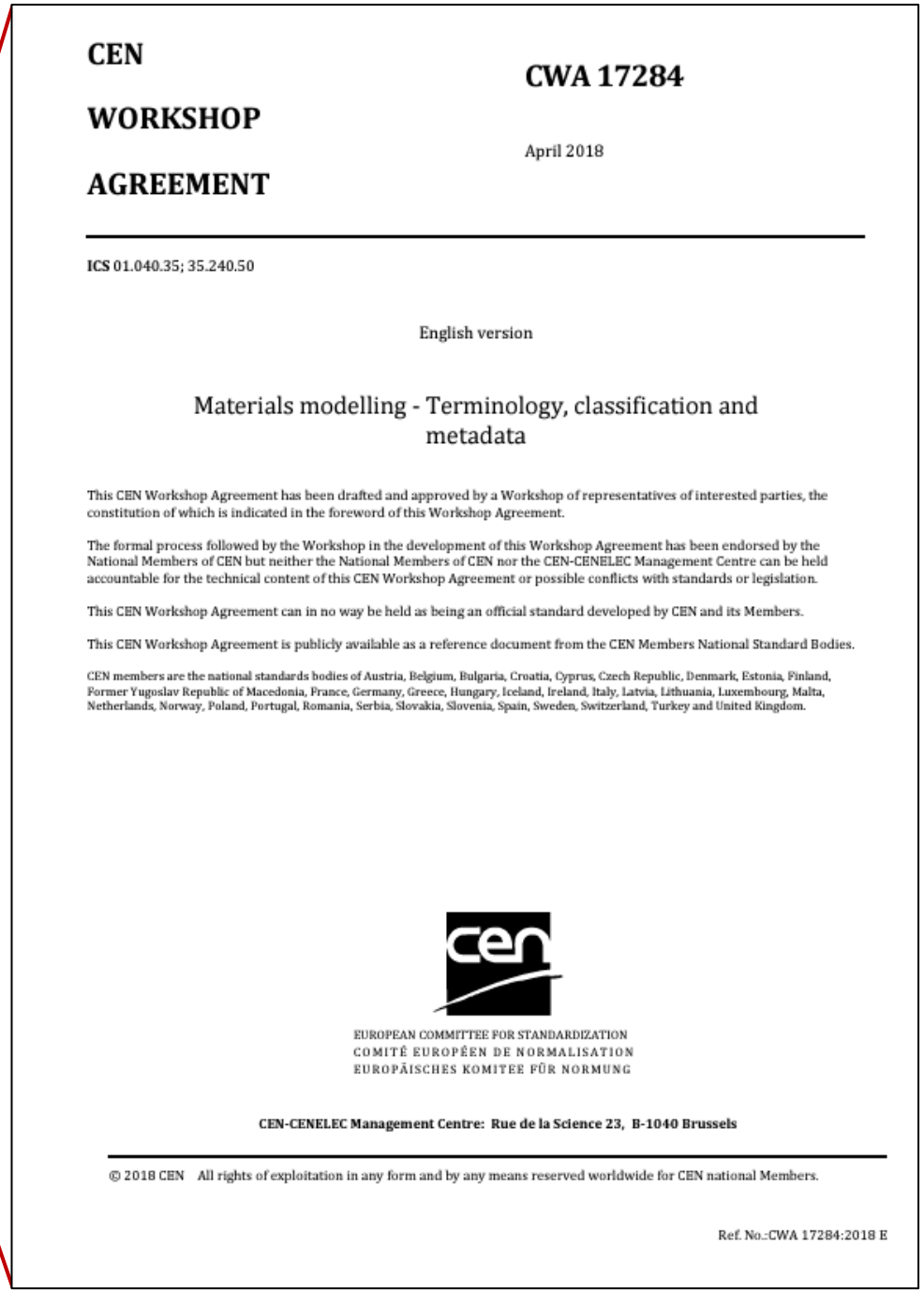
https://emmc.eu/moda/



Easy-MODA complies with the CEN Workshop Agreement (CWA 17284 "Materials modelling - terminology, classification and metadata") which can be found in the EMMC webpage.



CEN WORKSHOP AGREEMENT

CWA 17284

April 2018

ICS 01.040.35; 35.240.50

English version

Materials modelling - Terminology, classification and metadata

This CEN Workshop Agreement has been drafted and approved by a Workshop of representatives of interested parties, the constitution of which is indicated in the foreword of this Workshop Agreement.

The formal process followed by the Workshop in the development of this Workshop Agreement has been endorsed by the National Members of CEN but neither the National Members of CEN nor the CEN-CENELEC Management Centre can be held accountable for the technical content of this CEN Workshop Agreement or possible conflicts with standards or legislation.

This CEN Workshop Agreement can in no way be held as being an official standard developed by CEN and its Members.

This CEN Workshop Agreement is publicly available as a reference document from the CEN Members National Standard Bodies.

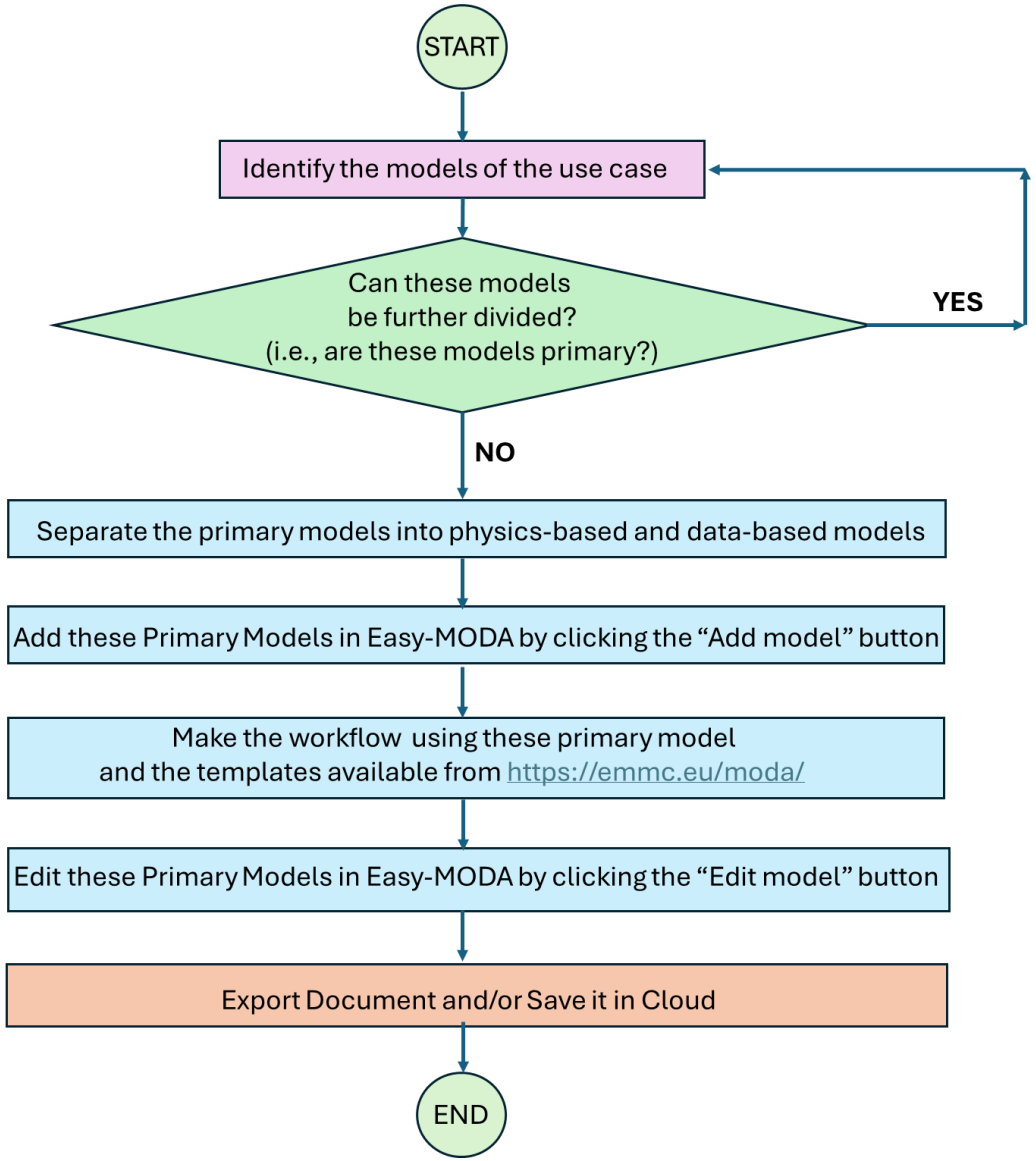
CEN members are the national standards bodies of Austria, Belgium, Bulgaria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, Former Yugoslav Republic of Macedonia, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, Netherlands, Norway, Poland, Portugal, Romania, Serbia, Slovakia, Slovenia, Spain, Sweden, Switzerland, Turkey and United Kingdom.

EUROPEAN COMMITTEE FOR STANDARDIZATION
COMITÉ EUROPÉEN DE NORMALISATION
EUROPÄISCHES KOMITEE FÜR NORMUNG

CEN-CENELEC Management Centre: Rue de la Science 23, B-1040 Brussels

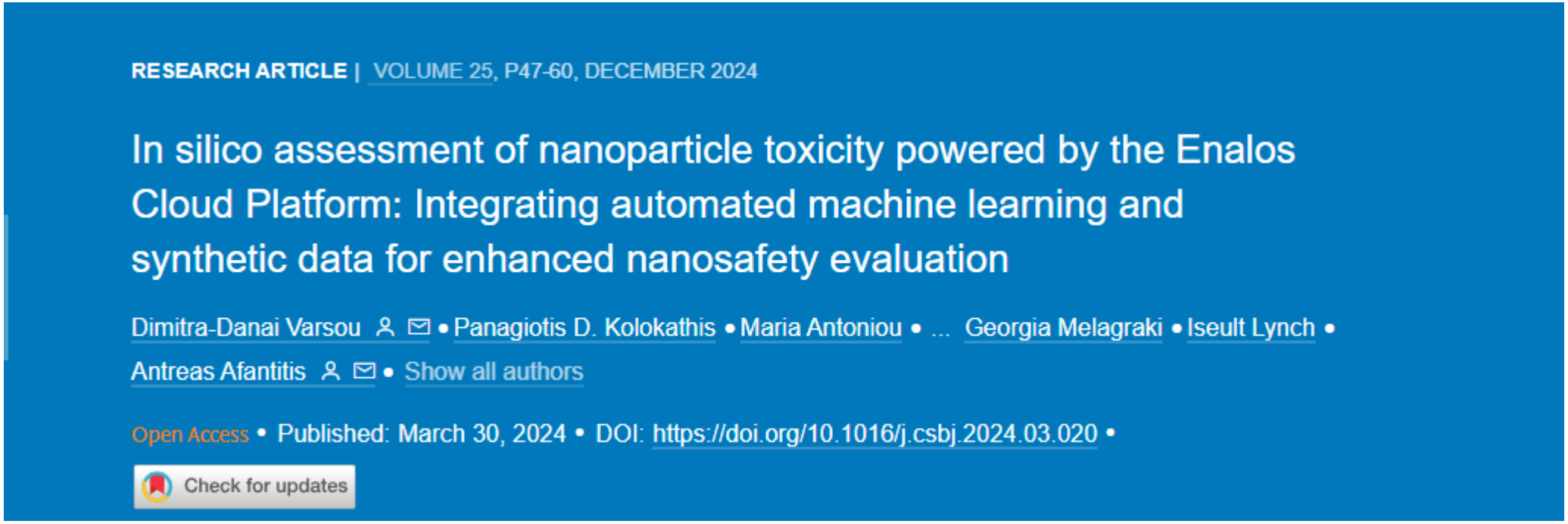
Ref. No.:CWA 17284:2018 E

IDENTIFYING THE WORKFLOW



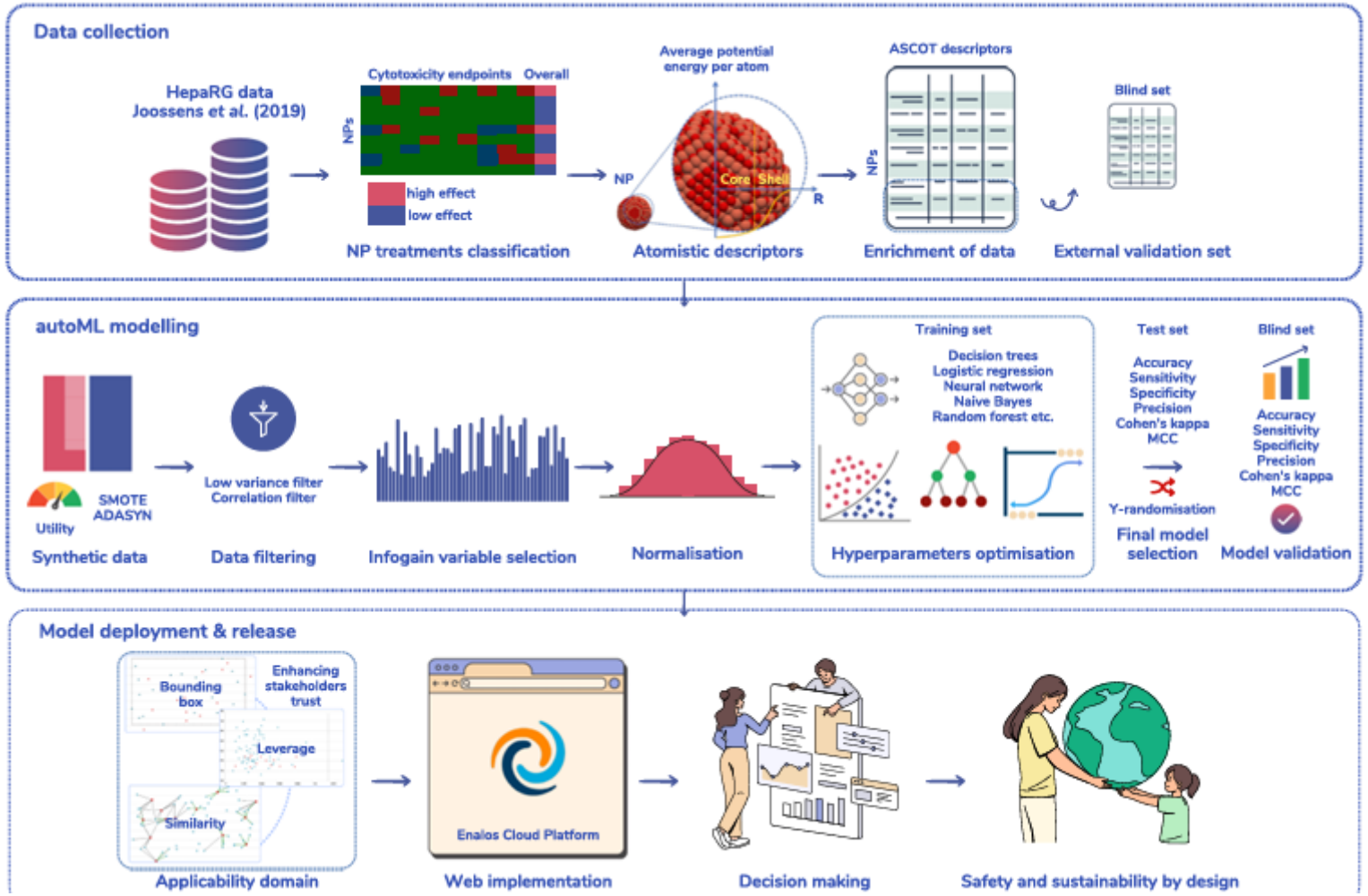
SAFENANOSCOPE

Let’s try to make a MODA documentation for the workflow proposed on the paper:



https://doi.org/10.1016/j.csbj.2024.03.020

SAFENANOSCOPE

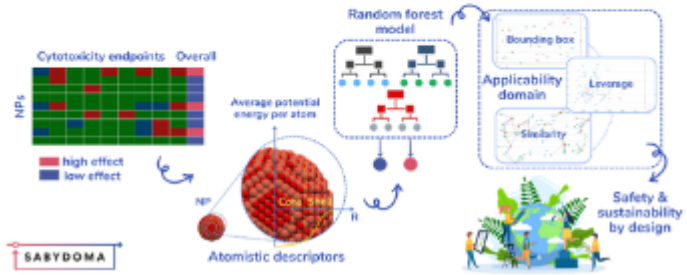


https://doi.org/10.1016/j.csbj.2024.03.020

SAFENANOSCOPE

This tool is based on two tools of Enalos Cloud platform

SafeNanoScope: Ag-TiO_2-CuO safety assessment powered by Enalos SABYDOMA Cloud Platform



This web-application hosts a random forest model for the prediction of the adverse effects class (against HepaRG cell line) of Ag, TiO_2 and CuO nanoparticles (NPs) based on their properties in atomistic level.

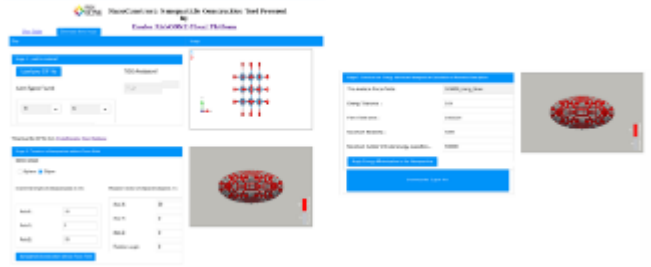
Visit service Publication Documentation Video tutorial

ASCOT

ASCOT is a toolbox for the digital construction of energy minimized Ag, CuO and TiO_2-cored nanoparticles and the calculation of their atomistic descriptors.

Visit service Publication Documentation Video tutorial

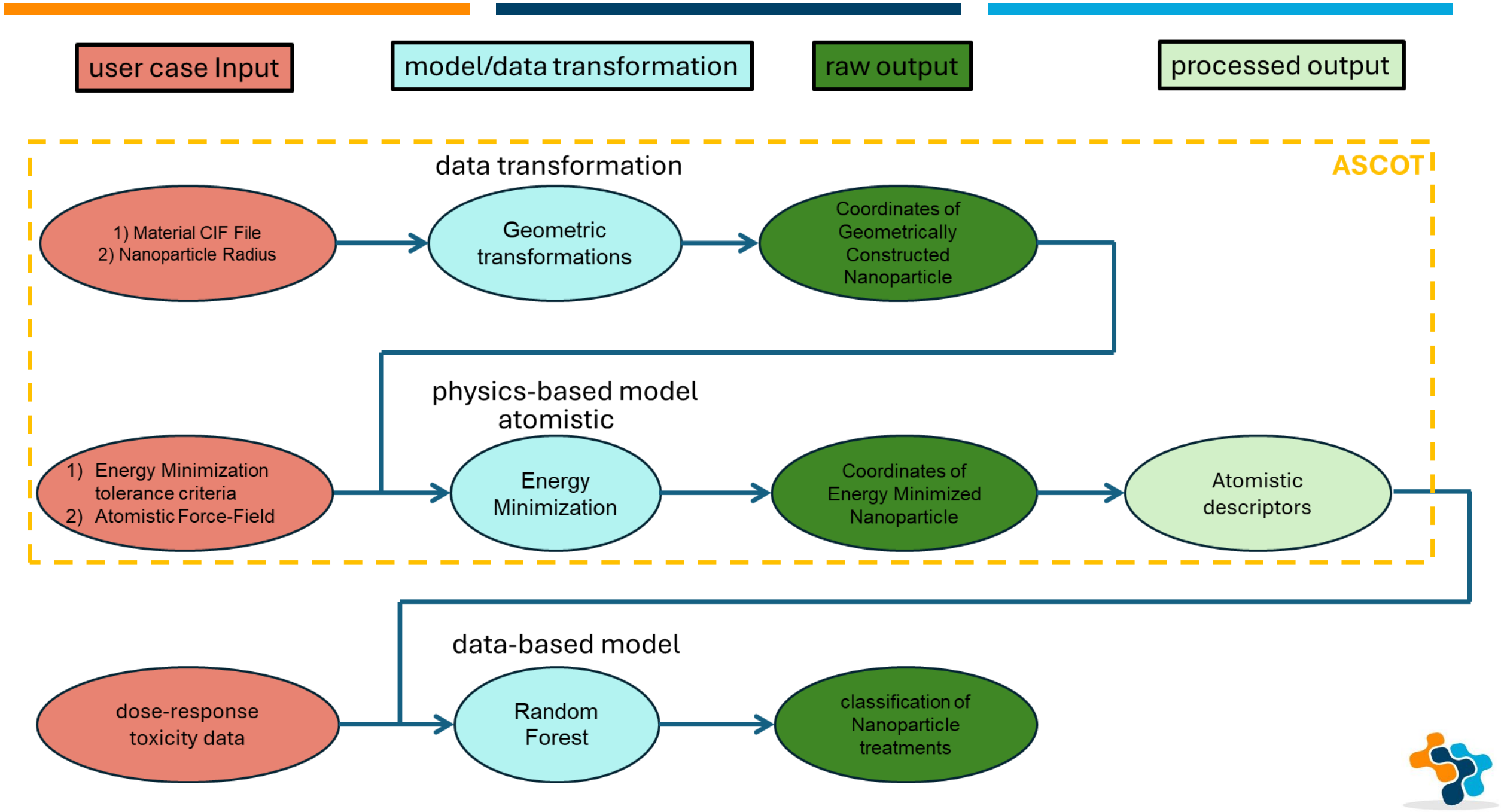
NanoConstruct: Nanoparticle construction tool



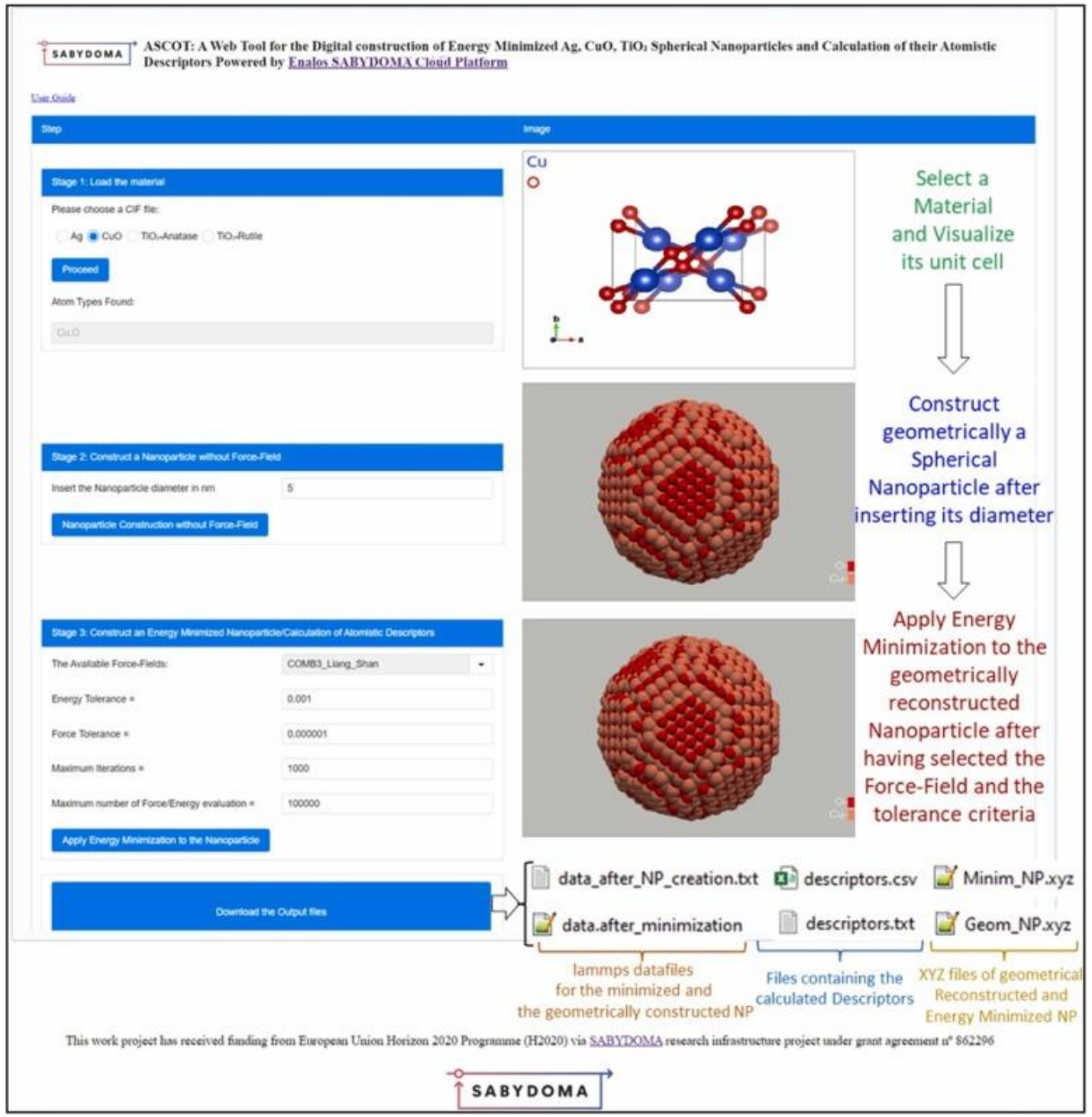
NanoConstruct is a toolbox for the digital reconstruction of energy minimized nanoparticles based on their CIF files and the calculation of their atomistic descriptors.

Visit service Publication Documentation Video tutorial

https://doi.org/10.1016/j.csbj.2024.03.020


user case Input
model/data transformation
raw output
processed output
ASCOT
data transformation
1) Material CIF File
2) Nanoparticle Radius
Geometric transformations
Coordinates of Geometrically Constructed Nanoparticle
physics-based model atomistic
1) Energy Minimization tolerance criteria
2) Atomistic Force-Field
Energy Minimization
Coordinates of Energy Minimized Nanoparticle
Atomistic descriptors
data-based model
dose-response toxicity data
Random Forest
classification of Nanoparticle treatments

ASCOT



https://doi.org/10.1016/j.csbj.2024.03.011

https://doi.org/10.1016/j.csbj.2024.05.039

SAFENANOSCOPE

https://doi.org/10.1016/j.csbj.2024.03.020

Atomistic Descriptors

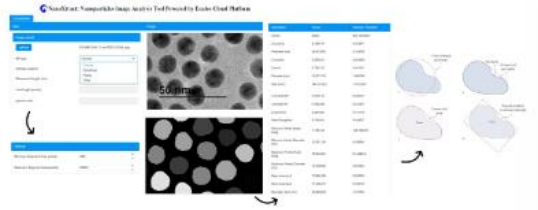
ASCOT

ASCOT is a toolbox for the digital construction of energy minimized Ag, CuO and TiO_2-cored nanoparticles and the calculation of their atomistic descriptors.

```
Cif title: TiO2-Anatase.cif
Nanoparticle Diameter: 50.0
Force Field: COMB3_Liang_Shan
Energy Tolerance: 0.01
Force Tolerance: 1.0E-6
Maximum Iterations: 1000
Maximum number of Force/Energy evaluation: 100000
D1001: Log10 of all atoms in the NP: 3.7766285534201502
D1002: Log10 of all atoms in the core: 1.7075701760979363
D1003: Log10 of all atoms in the surface: 3.7729081949712717
D2001: The average potential energy of all atoms in eV is : -6.102988730909535
D2002: The average potential energy of the core atoms in eV is: -6.701865698743352
D2003: The average potential energy of the shell atoms in eV is: -6.097836449303678
D3001: The average coordination parameter of all atoms is : 6.952667670178959
D3002: The average coordination parameter of the core atoms is: 8.0
D3003: The average coordination parameter of the shell atoms is: 6.9436572199730096
D4001: The diameter of the NP in A is: 50.3228855976518
D4002: The surface area of the NP in A^2 is: 7955.746663212837
D4003: The volume of the NP in A^3 is 66726.02152945993
D4004: Lattice energy of NP in eV: -18.308966192728604
D4005: Lattice energy of bulk material - Lattice energy of NP in eV: 14.271530999825265
D4006: Lattice energy of NP divided by the NP diameter in eV/A: -0.3638298157048242
D4007: Lattice energy of NP divided by the NP surface in eV/A^2: -0.002301351082154084
D4008: Lattice energy of NP divided by the NP volume in eV/A^3: -0.00027439019700350466
D8001: The average CNP of all atoms is : 16.6001092672243
D8002: The average CNP of the core atoms is: 17.477098833325627
D8003: The average CNP of the shell atoms is: 16.592564316503786
D9001: The average first hex parameter of all atoms is : -0.0014286271857610645
D9002: The average first hex parameter of the core atoms is: 0.008899333854380234
D9003: The average first hex parameter of the shell atoms is: -0.0015174811015922377
D9004: The average second hex parameter of all atoms is : -0.000613957609410395
D9005: The average second hex parameter of the core atoms is: -0.0022009973283844755
D9006: The average second hex parameter of the shell atoms is: -0.0006003039276176032
```

Experimental Descriptors

NanoXtract



NanoXtract is a unique online tool for the calculation of 18 image descriptors based on Transmission Electron Microscopy (TEM) images of nanomaterials.

Nanoparticle ID **Descriptors**

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
1	row ID	Circularity	Perimeter	Convexity	Extend	Diameter	Area [nm2	Circularity	Convexity	Eccentricit	Main Elon	Minimum	Maximum	Major Axi:	Minor Axi	Boundary	Boxivity	Roundnes	Solidity
2	Row0	0.865178	46.14902	0.985387	0.789474	14.38322	143.8364	0.878868	0.950599	0.300617	0.030928	13.06162	14.1144	13.85713	13.21617	45.35003	0.790744	0.953745	0.984704
3	Row1	0.855696	46.6998	0.984526	0.768849	14.84731	145.7017	0.869028	0.946945	0.413643	0.07362	13.10927	14.57063	14.27453	12.99609	45.90081	0.783562	0.910439	0.98357
4	Row2	0.849594	46.81681	0.985146	0.757882	14.65663	145.3825	0.86272	0.944557	0.398157	0.09276	13.0254	14.40747	14.20533	13.03079	46.01782	0.776637	0.917317	0.982871
5	Row3	0.843669	46.52012	0.984056	0.74377	14.7874	142.5397	0.856863	0.947767	0.385632	0.080357	13.01215	14.51782	14.02503	12.94023	45.72113	0.774207	0.922653	0.982536
6	Row4	0.803727	54.68382	0.981872	0.726288	17.14866	187.9848	0.813578	0.941049	0.241614	0.046855	15.30504	16.86715	15.70533	15.24002	53.88483	0.737136	0.970372	0.976224
7	Row5	0.840644	49.14524	0.980865	0.771774	15.23592	158.629	0.852839	0.944307	0.330998	0.074108	13.76568	14.95842	14.63003	13.80535	48.34624	0.775083	0.943631	0.975225
8	Row6	0.853722	48.19496	0.985547	0.791	14.82445	154.8884	0.866455	0.944714	0.210374	0	13.89647	14.58295	14.20298	13.88513	47.39597	0.792164	0.977621	0.984717
9	Row7	0.836387	47.747	0.982814	0.762506	15.06738	148.8637	0.84872	0.939394	0.450865	0.09816	13.11904	14.78673	14.57213	13.00696	46.94801	0.778557	0.892592	0.979137
10	Row8	0.87071	46.6856	0.985677	0.764801	14.63552	148.2452	0.884746	0.954324	0.243163	0.009243	13.58284	14.3742	13.94963	13.53094	45.88661	0.793497	0.969986	0.983717
11	Row9	0.849592	46.08636	0.982662	0.757206	14.81974	140.8539	0.863028	0.950751	0.393233	0.038441	12.95051	14.55899	13.9662	12.84106	45.28737	0.767628	0.919439	0.980285
12	Row10	0.849121	47.62999	0.985634	0.784082	14.87886	150.4197	0.861882	0.943721	0.373592	0.020202	13.32798	14.6137	14.36907	13.32865	46.831	0.785171	0.927593	0.983756
13	Row11	0.853858	45.08762	0.983523	0.759211	14.25924	135.4376	0.86769	0.950314	0.433647	0.042821	12.71803	14.02508	13.83383	12.46542	44.28863	0.765034	0.901083	0.980786
14	Row12	0.862395	48.49753	0.985986	0.777981	15.28624	158.5193	0.875552	0.950292	0.416048	0.038835	13.68272	15.04685	14.89815	13.54752	47.69853	0.779249	0.909343	0.983964
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21	Row19	0.858788	49.4478	0.985992	0.752561	15.16636	164.175	0.871711	0.947146	0.177576	0.01232	14.15761	14.93773	14.57429	14.34266	48.64881	0.781681	0.984107	0.985038
22	Row20	0.857924	44.92214	0.98348	0.757237	14.1137	135.0985	0.872022	0.947335	0.306413	0.005855	12.83558	13.85405	13.44265	12.79604	44.12315	0.786903	0.951899	0.982731
23	Row21	0.852512	44.60539	0.98601	0.757671	13.92658	132.3155	0.866454	0.945379	0.377809	0.068716	12.47144	13.70129	13.48908	12.48931	43.8064	0.791815	0.925883	0.984489
24	Row22	0.859501	48.91122	0.985462	0.77319	15.03358	160.6838	0.87231	0.948971	0.231226	0.019417	14.255	14.782	14.5013	14.10832	48.11223	0.774248	0.9729	0.984417
25	Row23	0.85405	47.73281	0.98515	0.754911	15.19265	152.0057	0.867158	0.944973	0.381776	0.05625	13.43877	14.91167	14.47069	13.3746	46.93382	0.788442	0.924255	0.984304
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27	Row25	0.769941	52.73481	0.981048	0.789956	15.98543	167.4766	0.819104	0.925185	0.415542	0.045977	14.01906	15.73639	15.31134	13.92679	50.68887	0.795566	0.909574	0.971362
28	Row26	0.860084	48.35212	0.985986	0.734658	15.24181	157.1826	0.873486	0.949308	0.364681	0.082192	13.38309	14.96175	14.66059	13.65096	47.55313	0.805459	0.931133	0.984813
29	Row27	0.832226	49.67594	0.982608	0.765178	15.85763	160.4344	0.843916	0.943318	0.381324	0.024584	13.96301	15.5912	14.86497	13.7418	48.87695	0.767273	0.924442	0.974197
30	Row28	0.841091	46.03789	0.983269	0.733395	14.44067	139.1383	0.854343	0.942923	0.345883	0.027256	12.9886	14.15886	13.74082	12.89271	45.2389	0.80227	0.938278	0.980115
31	Row29	0.855001	43.4069	0.982419	0.793431	14.01796	125.5925	0.869347	0.953374	0.449008	0.022222	11.98486	13.80573	13.37774	11.95339	42.60791	0.794886	0.893528	0.981372
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33	Row31	0.830205	49.54473	0.983783	0.752198	15.54699	159.2075	0.841977	0.936316	0.347271	0.018039	13.88246	15.29081	14.70246	13.78744	48.74574	0.784902	0.937765	0.979563
34	Row32	0.868765	45.43865	0.984452	0.761737	14.44067	140.046	0.883159	0.952583	0.360318	0.016731	12.95412	14.15886	13.82577	12.89708	44.63966	0.783445	0.932829	0.983882
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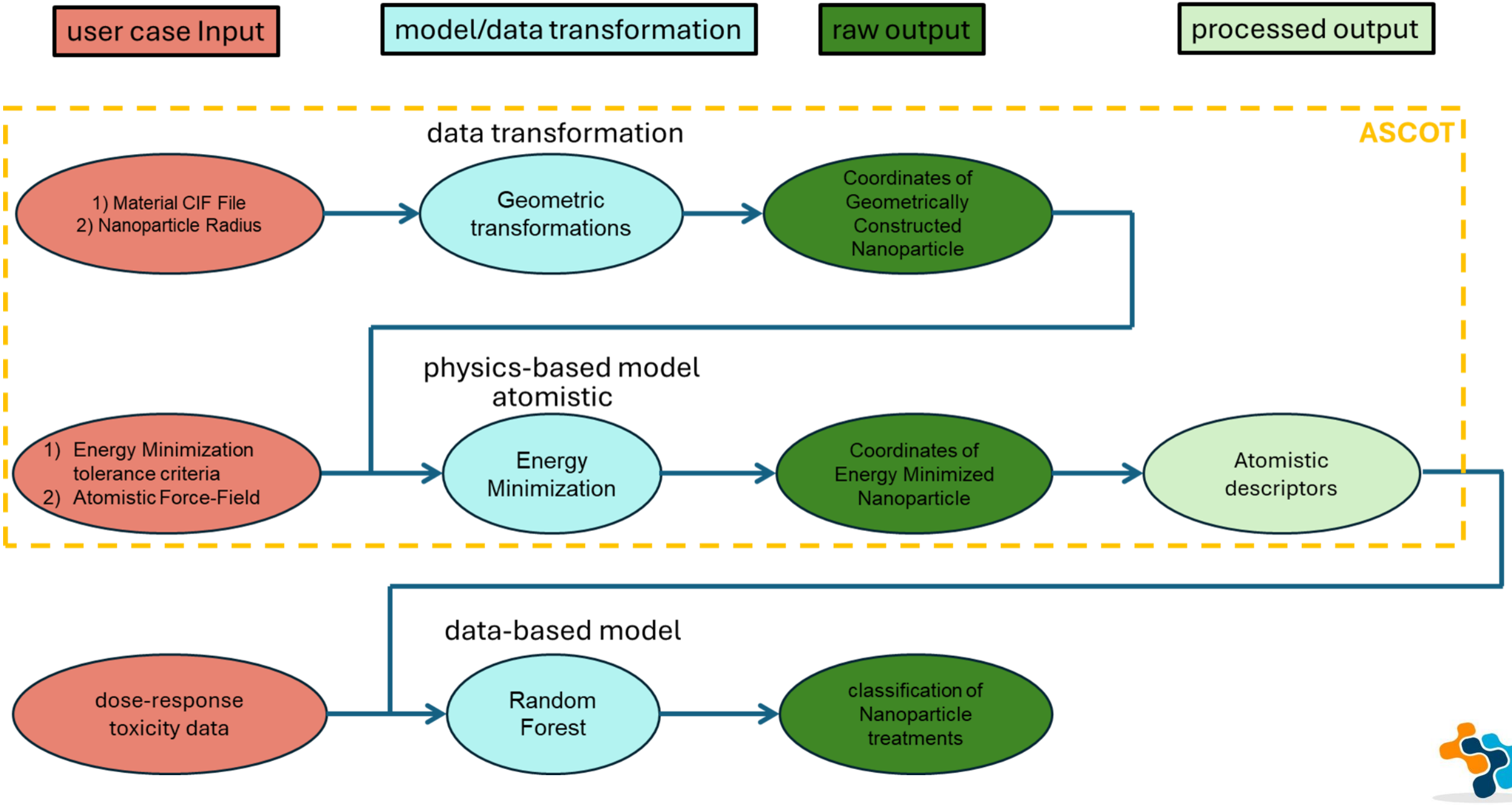
descriptorValuesPerComponents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raw output
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ASCOT
data transformation
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1) Energy Minimization tolerance criteria
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Energy Minimization
Coordinates of Energy Minimized Nanoparticle
Atomistic descriptors
data-based model
dose-response toxicity data
Random Forest
classification of Nanoparticle treatments

UANANODOCK

JCIM JOURNAL OF CHEMICAL INFORMATION AND MODELING

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Application Note

UANanoDock: A Web-Based *UnitedAtom* Multiscale Nanodocking Tool for Predicting Protein Adsorption onto Nanoparticles

Julia Subbotina,* Panagiotis D. Kolokathis, Andreas Tsoumanis, Nikolaos K. Sidiropoulos, Ian Rouse, Iseult Lynch, Vladimir Lobaskin, and Antreas Afantitis*

Cite This: *J. Chem. Inf. Model.* 2025, 65, 3142–3153

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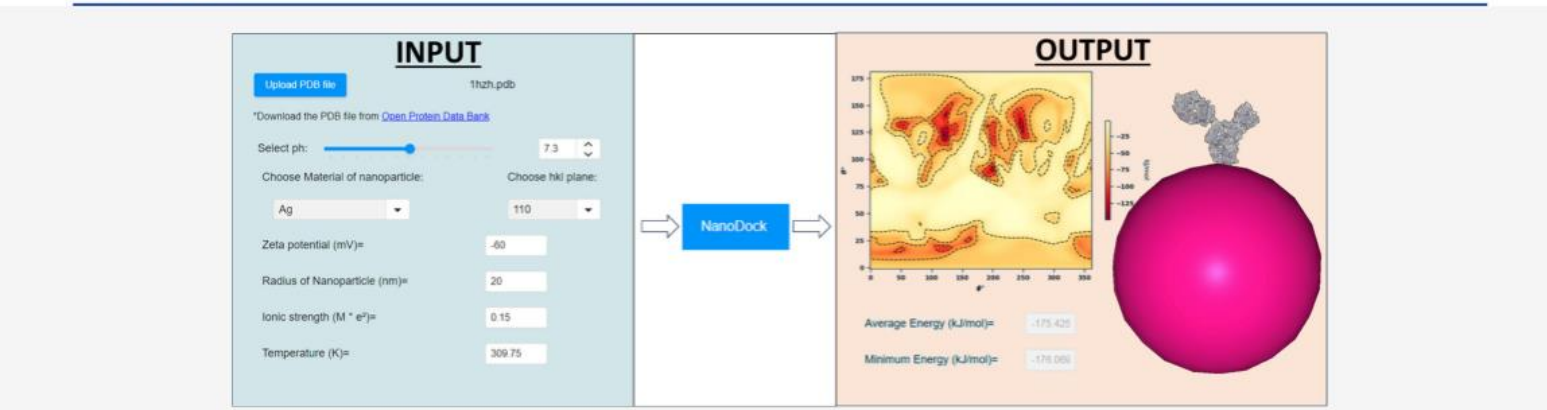

https://doi.org/10.1021/acs.jcim.4c02292

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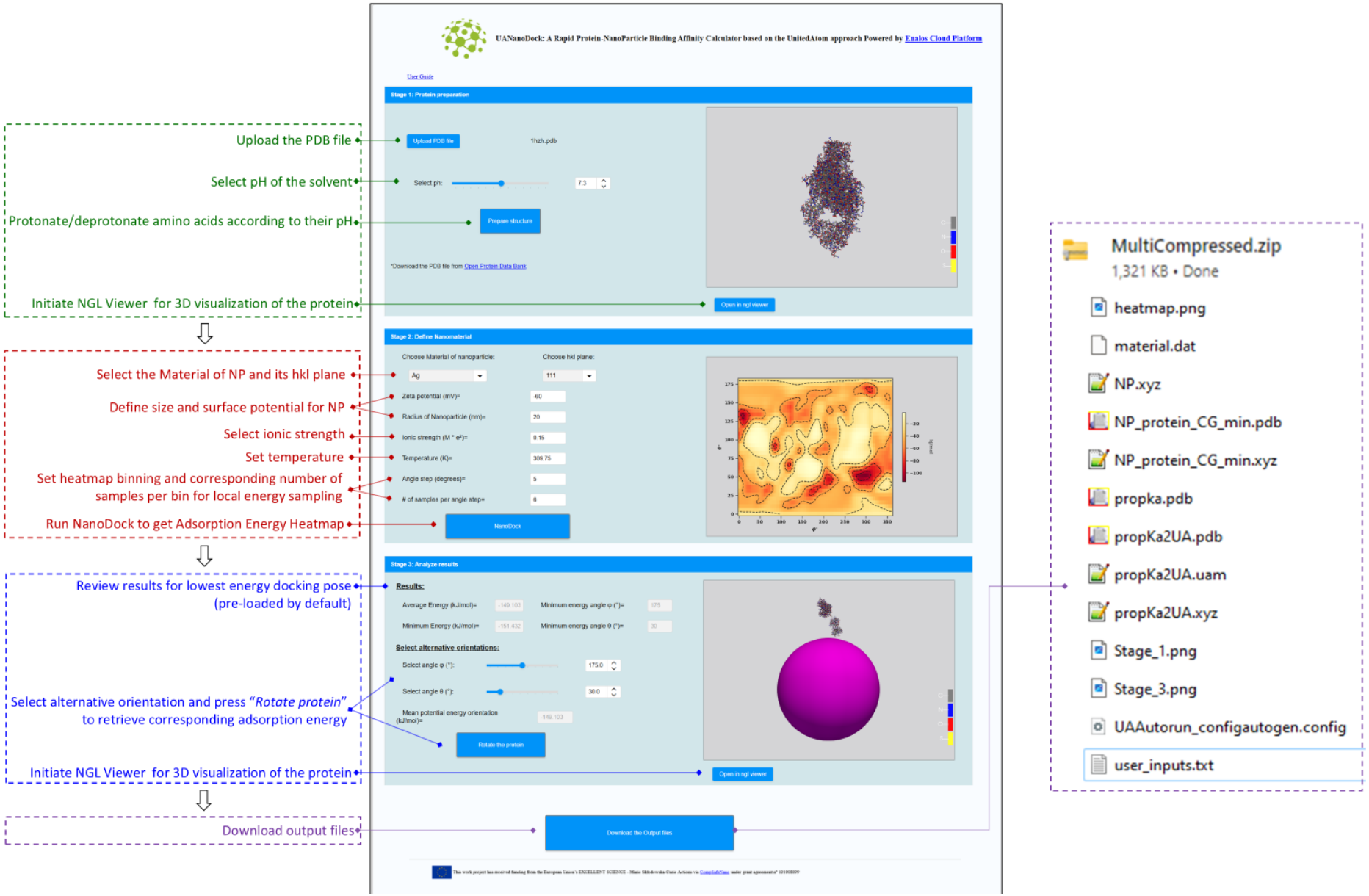
Upload the PDB file
Select pH of the solvent
Protonate/deprotonate amino acids according to their pH
Initiate NGL Viewer for 3D visualization of the protein
Select the Material of NP and its hkl plane
Define size and surface potential for NP
Select ionic strength
Set temperature
Set heatmap binning and corresponding number of samples per bin for local energy sampling
Run NanoDock to get Adsorption Energy Heatmap
Review results for lowest energy docking pose (pre-loaded by default)
Select alternative orientation and press "Rotate protein" to retrieve corresponding adsorption energy
Initiate NGL Viewer for 3D visualization of the protein
Download output files
UANanoDock: A Rapid Protein-NanoParticle Binding Affinity Calculator based on the UnitedAtom approach Powered by Enalos Cloud Platform
User Guide
Stage 1: Protein preparation
Upload PDB file
1hzh.pdb
Select ph:
7.3
Prepare structure
*Download the PDB file from Open Protein Data Bank
Open in ngl viewer
Stage 2: Define Nanomaterial
Choose Material of nanoparticle:
Ag
Choose hkl plane:
111
Zeta potential (mV)=
-60
Radius of Nanoparticle (nm)=
20
Ionic strength (M * e²)=
0.15
Temperature (K)=
309.75
Angle step (degrees)=
5
# of samples per angle step=
6
NanoDock
Stage 3: Analyze results
Results:
Average Energy (kJ/mol)=
-149.103
Minimum energy angle φ (°)=
175
Minimum Energy (kJ/mol)=
-151.432
Minimum energy angle θ (°)=
30
Select alternative orientations:
Select angle φ (°):
175.0
Select angle θ (°):
30.0
Mean potential energy orientation (kJ/mol)=
-149.103
Rotate the protein
Open in ngl viewer
Download the Output files
MultiCompressed.zip
1,321 KB • Done
heatmap.png
material.dat
NP.xyz
NP_protein_CG_min.pdb
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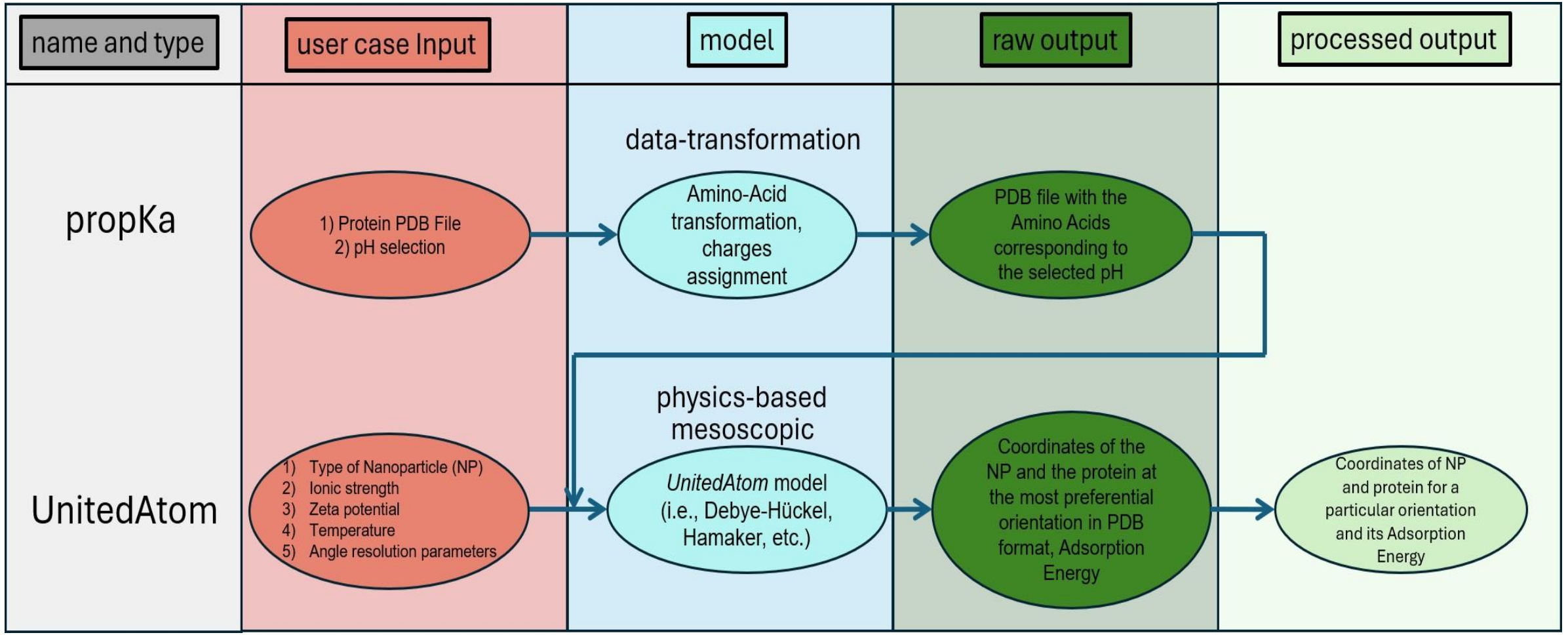

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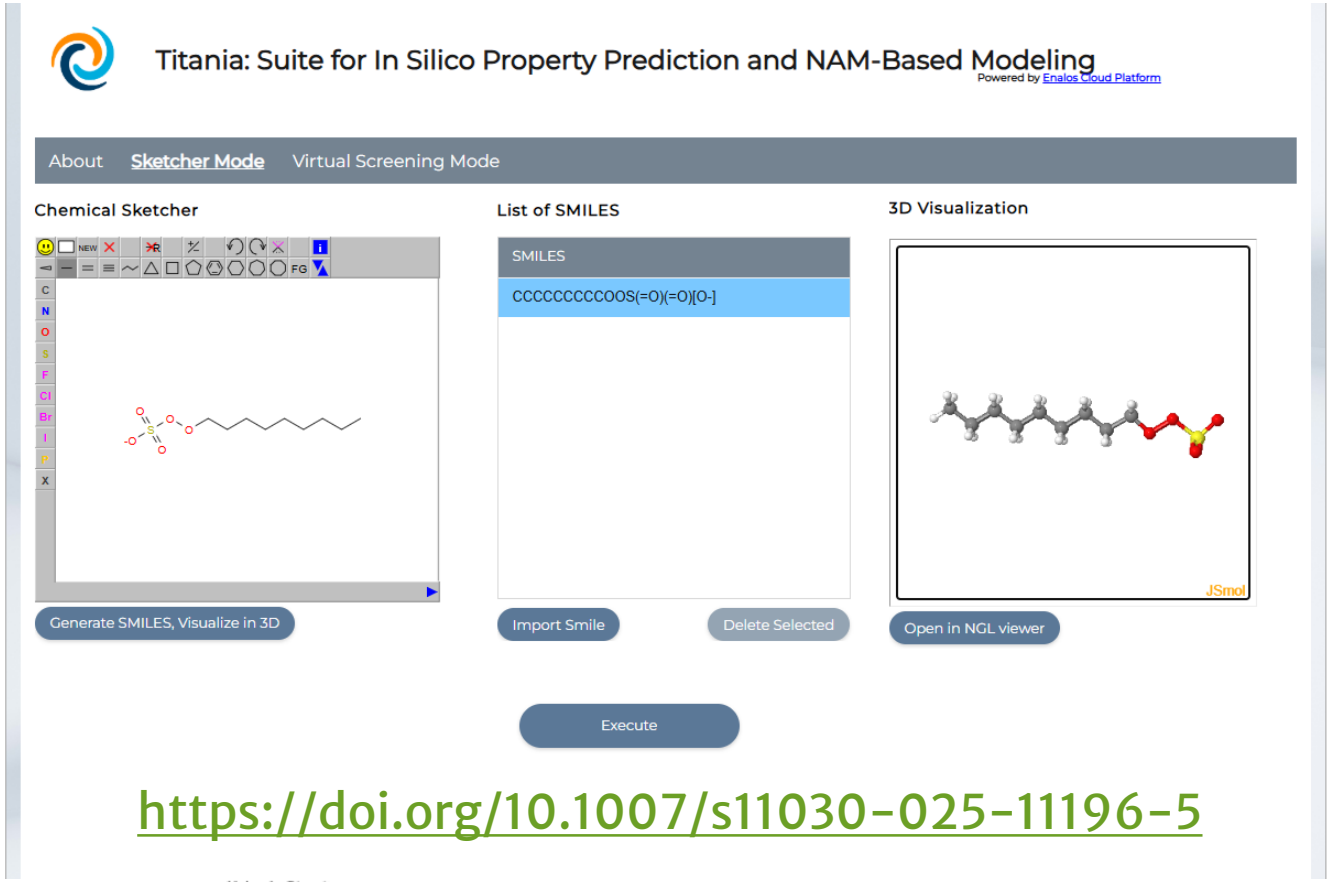


https://doi.org/10.1007/s11030-025-11196-5

Molecular Diversity
https://doi.org/10.1007/s11030-025-11196-5

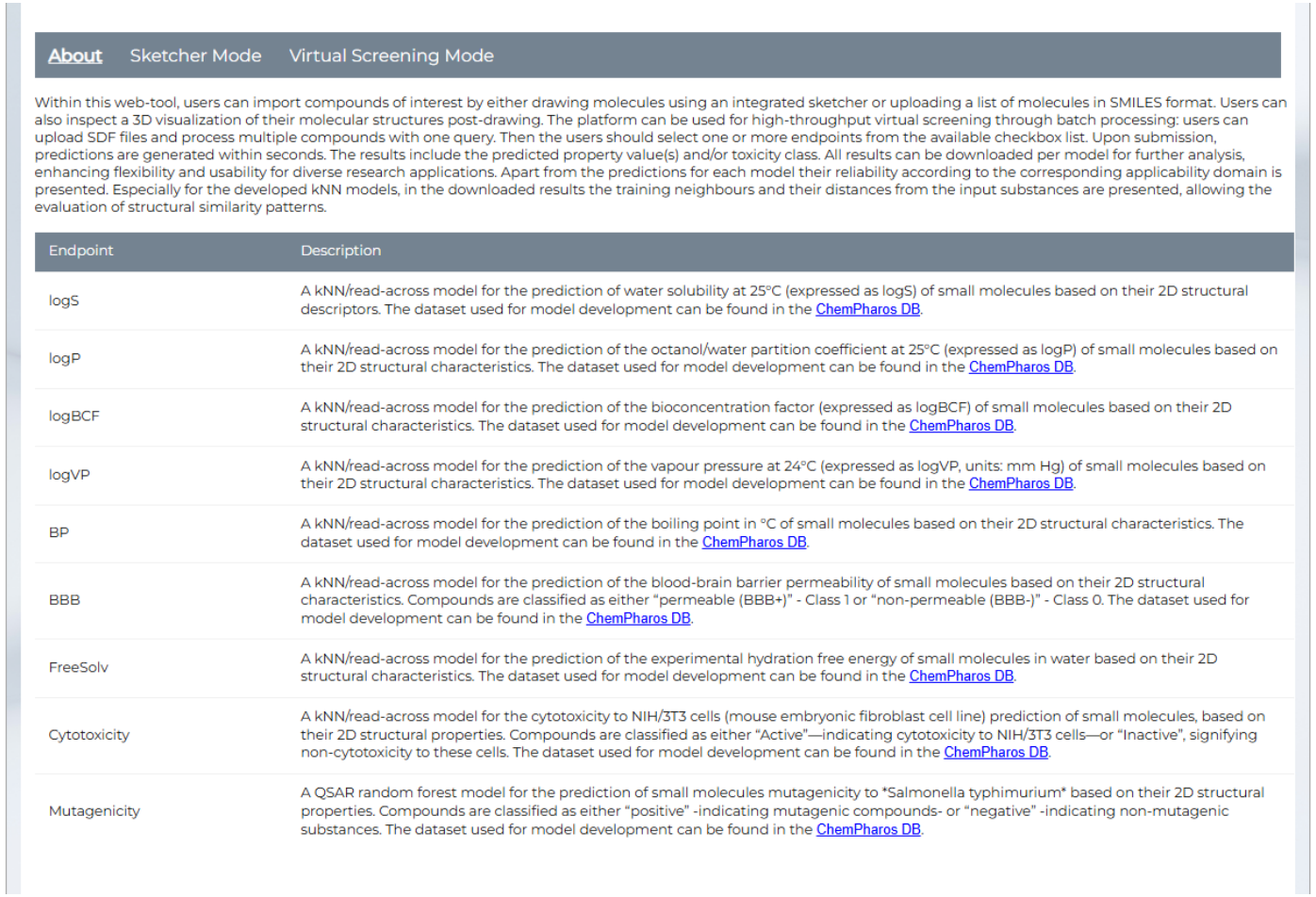
ORIGINAL ARTICLE

Titania: an integrated tool for in silico molecular property prediction and NAM-based modeling

Nikoletta-Maria Koutroumpa[1,2,3] · Maria Antoniou[1,3,4] · Dimitra-Danai Varsou[3,5] · Konstantinos D. Papavasileiou[3,5] · Nikolaos K. Sidiropoulos[3,5] · Christoforos Kyprianou[1] · Andreas Tsoumanis[1,3,5] · Haralambos Sarimveis[2] · Iseult Lynch[6] · Georgia Melagraki[7] · Antreas Afantitis[1,3,5]

Received: 16 February 2025 / Accepted: 12 April 2025

TITANIA



About Sketcher Mode Virtual Screening Mode

Within this web-tool, users can import compounds of interest by either drawing molecules using an integrated sketcher or uploading a list of molecules in SMILES format. Users can also inspect a 3D visualization of their molecular structures post-drawing. The platform can be used for high-throughput virtual screening through batch processing: users can upload SDF files and process multiple compounds with one query. Then the users should select one or more endpoints from the available checkbox list. Upon submission, predictions are generated within seconds. The results include the predicted property value(s) and/or toxicity class. All results can be downloaded per model for further analysis, enhancing flexibility and usability for diverse research applications. Apart from the predictions for each model their reliability according to the corresponding applicability domain is presented. Especially for the developed kNN models, in the downloaded results the training neighbours and their distances from the input substances are presented, allowing the evaluation of structural similarity patterns.

Endpoint	Description
logS	A kNN/read-across model for the prediction of water solubility at 25°C (expressed as logS) of small molecules based on their 2D structural descriptors. The dataset used for model development can be found in the ChemPharos DB.
logP	A kNN/read-across model for the prediction of the octanol/water partition coefficient at 25°C (expressed as logP) of small molecules based on their 2D structural characteristics. The dataset used for model development can be found in the ChemPharos DB.
logBCF	A kNN/read-across model for the prediction of the bioconcentration factor (expressed as logBCF) of small molecules based on their 2D structural characteristics. The dataset used for model development can be found in the ChemPharos DB.
logVP	A kNN/read-across model for the prediction of the vapour pressure at 24°C (expressed as logVP, units: mm Hg) of small molecules based on their 2D structural characteristics. The dataset used for model development can be found in the ChemPharos DB.
BP	A kNN/read-across model for the prediction of the boiling point in °C of small molecules based on their 2D structural characteristics. The dataset used for model development can be found in the ChemPharos DB.
BBB	A kNN/read-across model for the prediction of the blood-brain barrier permeability of small molecules based on their 2D structural characteristics. Compounds are classified as either "permeable (BBB+)" - Class 1 or "non-permeable (BBB-)" - Class 0. The dataset used for model development can be found in the ChemPharos DB.
FreeSolv	A kNN/read-across model for the prediction of the experimental hydration free energy of small molecules in water based on their 2D structural characteristics. The dataset used for model development can be found in the ChemPharos DB.
Cytotoxicity	A kNN/read-across model for the cytotoxicity to NIH/3T3 cells (mouse embryonic fibroblast cell line) prediction of small molecules, based on their 2D structural properties. Compounds are classified as either "Active"—indicating cytotoxicity to NIH/3T3 cells—or "Inactive", signifying non-cytotoxicity to these cells. The dataset used for model development can be found in the ChemPharos DB.
Mutagenicity	A QSAR random forest model for the prediction of small molecules mutagenicity to *Salmonella typhimurium* based on their 2D structural properties. Compounds are classified as either "positive" -indicating mutagenic compounds- or "negative" -indicating non-mutagenic substances. The dataset used for model development can be found in the ChemPharos DB.

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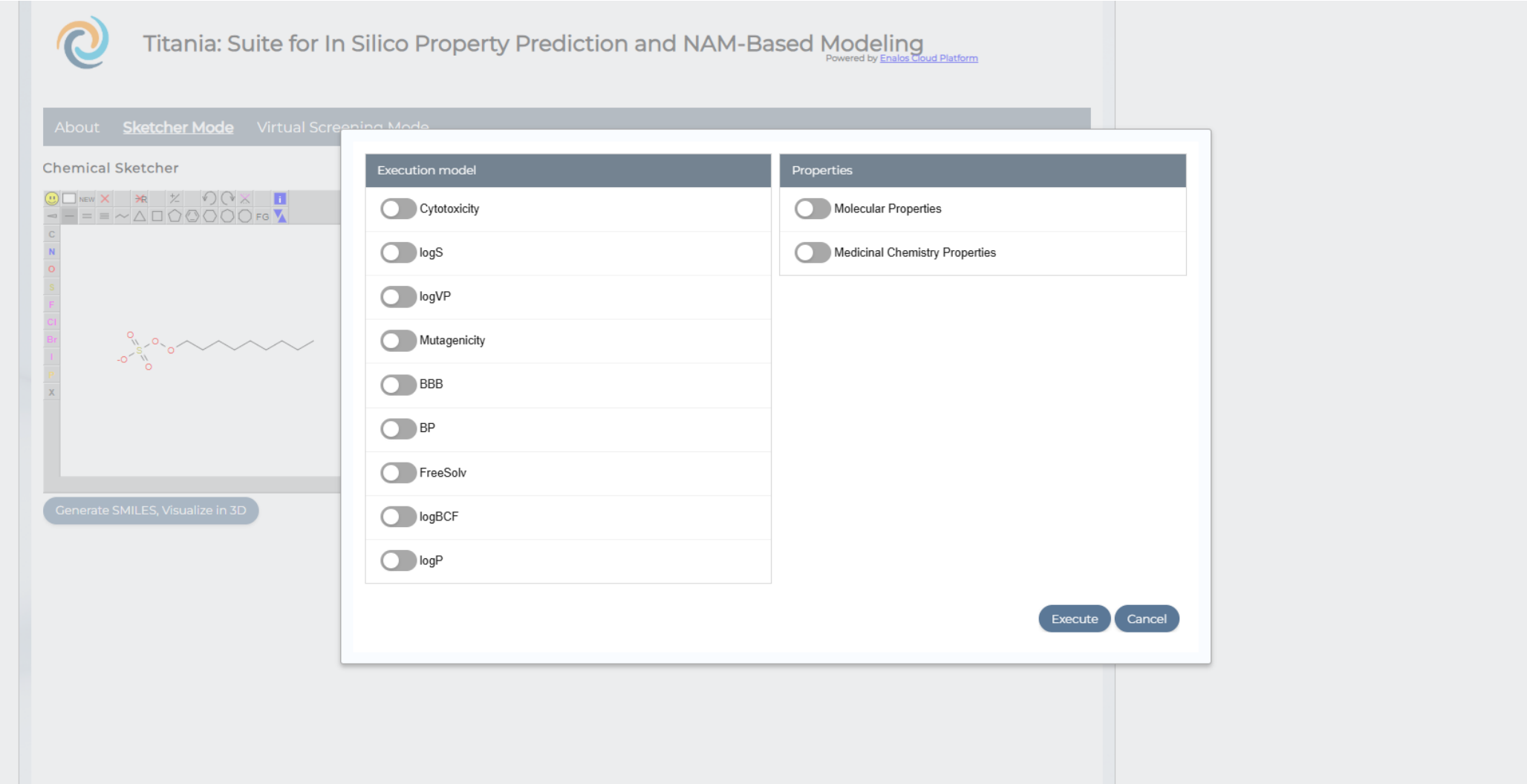

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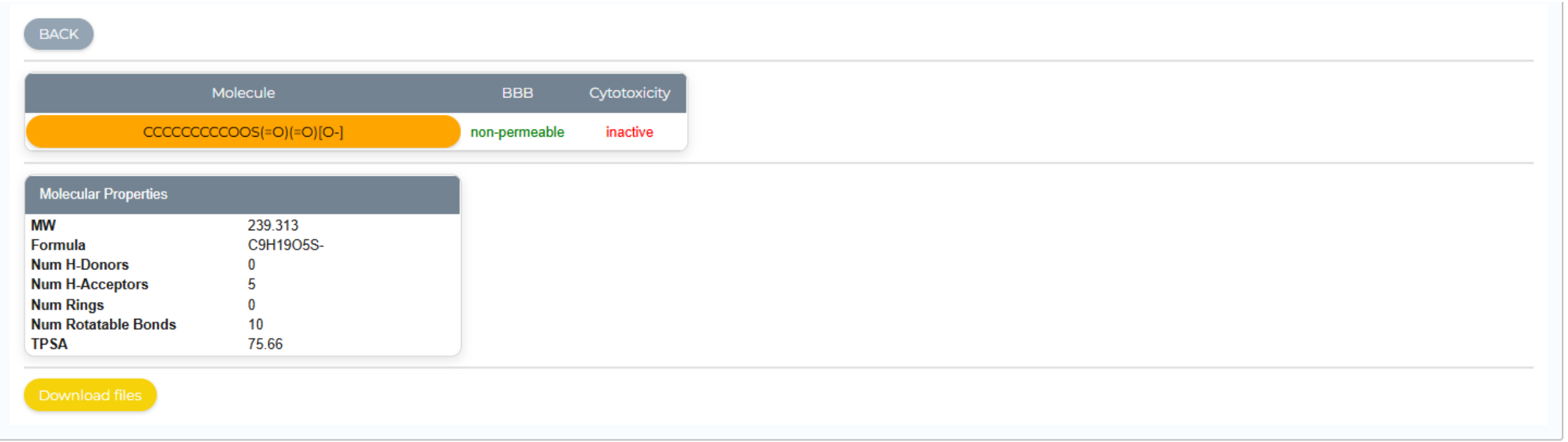

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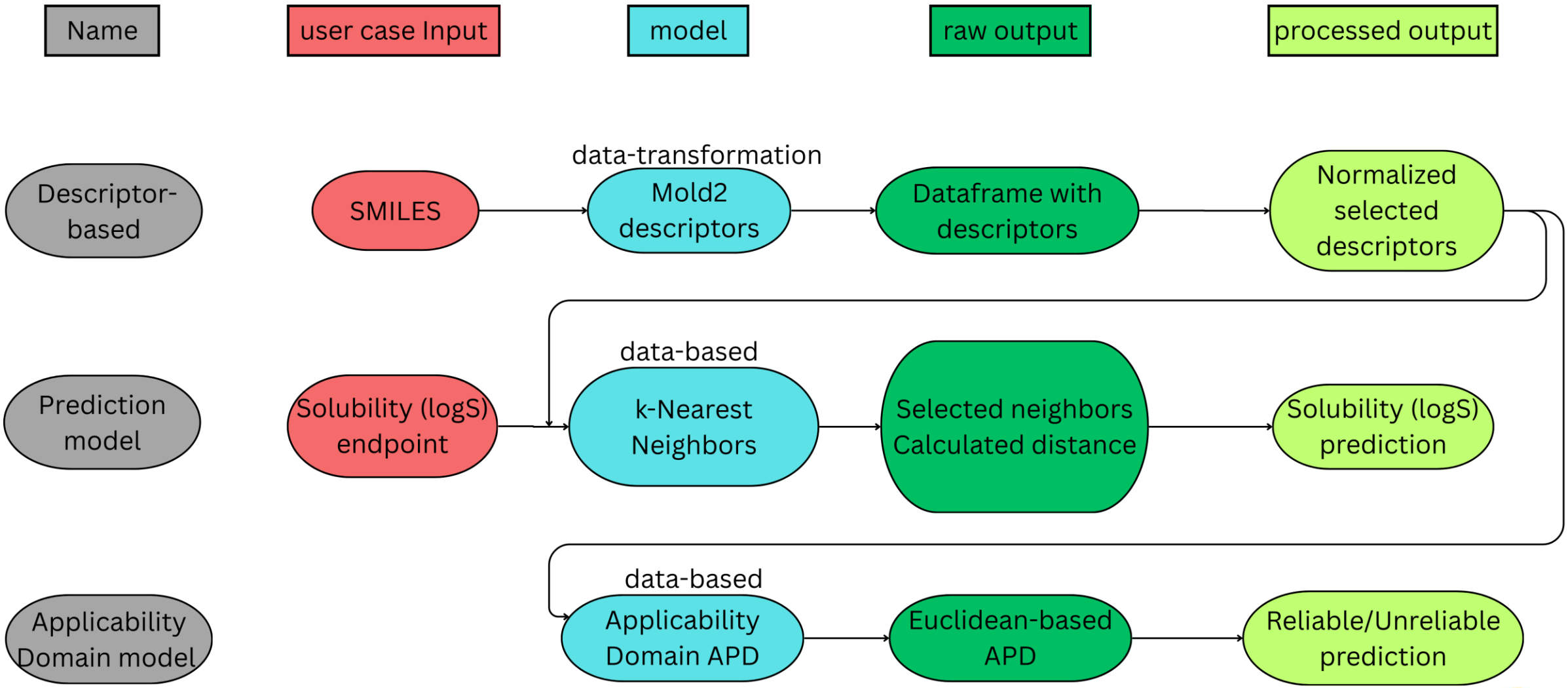

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Functions menu

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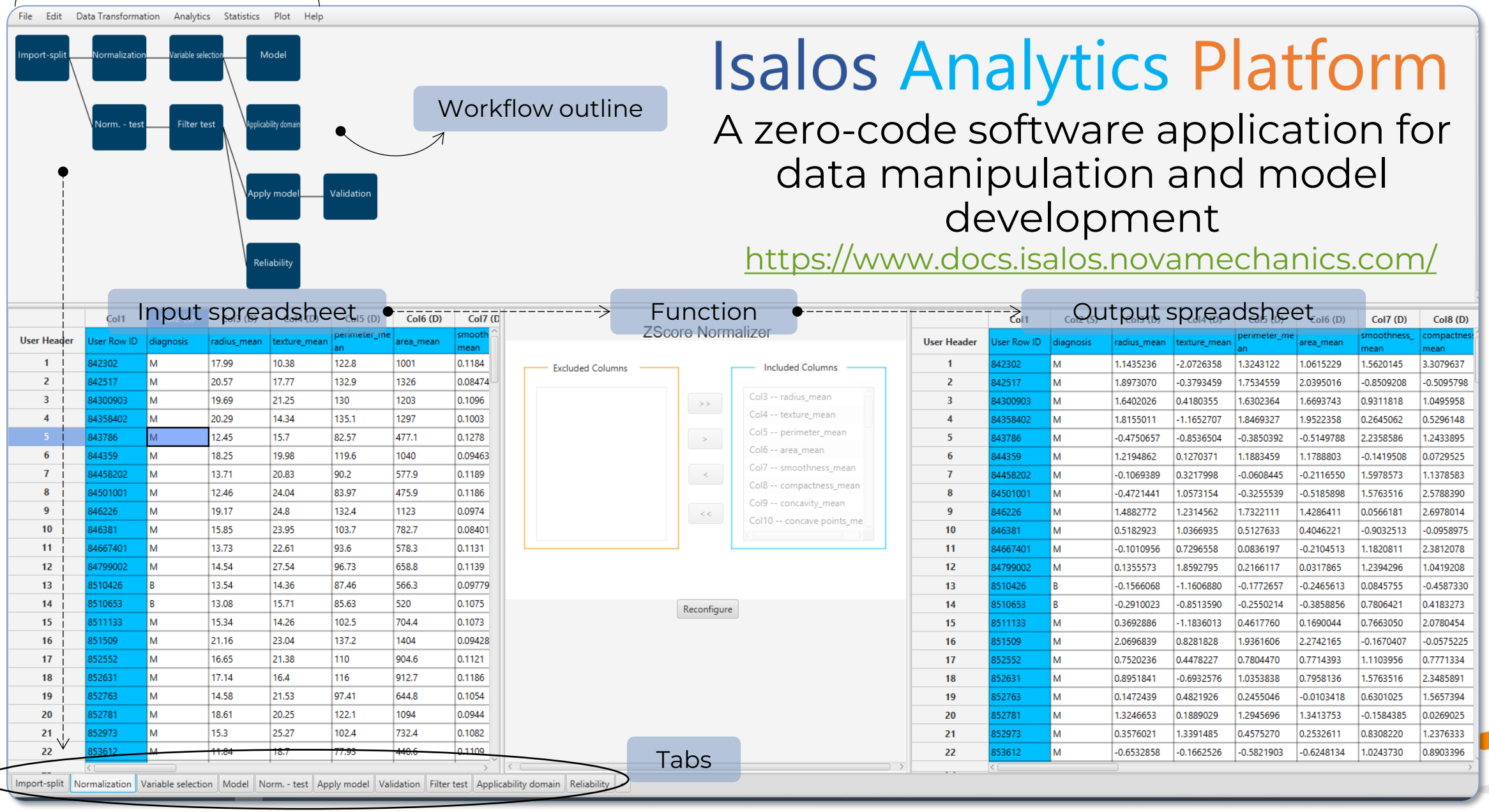

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User Header	User Row ID	diagnosis	radius_mean	texture_mean	perimeter_mean	area_mean	smoothness_mean
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2	842517	M	20.57	17.77	132.9	1326	0.08474
3	84300903	M	19.69	21.25	130	1203	0.1096
4	84358402	M	20.29	14.34	135.1	1297	0.1003
5	843786	M	12.45	15.7	82.57	477.1	0.1278
6	844359	M	18.25	19.98	119.6	1040	0.09463
7	84458202	M	13.71	20.83	90.2	577.9	0.1189
8	84501001	M	12.46	24.04	83.97	475.9	0.1186
9	846226	M	19.17	24.8	132.4	1123	0.0974
10	846381	M	15.85	23.95	103.7	782.7	0.08401
11	84667401	M	13.73	22.61	93.6	578.3	0.1131
12	84799002	M	14.54	27.54	96.73	658.8	0.1139
13	8510426	B	13.54	14.36	87.46	566.3	0.09779
14	8510653	B	13.08	15.71	85.63	520	0.1075
15	8511133	M	15.34	14.26	102.5	704.4	0.1073
16	851509	M	21.16	23.04	137.2	1404	0.09428
17	852552	M	16.65	21.38	110	904.6	0.1121
18	852631	M	17.14	16.4	116	912.7	0.1186
19	852763	M	14.58	21.53	97.41	644.8	0.1054
20	852781	M	18.61	20.25	122.1	1094	0.0944
21	852973	M	15.3	25.27	102.4	732.4	0.1082
22	853612	M	11.84	18.7	77.93	440.6	0.1109

	Col1	Col2 (S)	Col3 (D)	Col4 (D)	Col5 (D)	Col6 (D)	Col7 (D)	Col8 (D)
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15	8511133	M	0.3692886	-1.1836013	0.4617760	0.1690044	0.7663050	2.0780454
16	851509	M	2.0696839	0.8281828	1.9361606	2.2742165	-0.1670407	-0.0575225
17	852552	M	0.7520236	0.4478227	0.7804470	0.7714393	1.1103956	0.7771334
18	852631	M	0.8951841	-0.6932576	1.0353838	0.7958136	1.5763516	2.3485891
19	852763	M	0.1472439	0.4821926	0.2455046	-0.0103418	0.6301025	1.5657394
20	852781	M	1.3246653	0.1889029	1.2945696	1.3413753	-0.1584385	0.0269025
21	852973	M	0.3576021	1.3391485	0.4575270	0.2532611	0.8308220	1.2376333
22	853612	M	-0.6532858	-0.1662526	-0.5821903	-0.6248134	1.0243730	0.8903396

FUTURE IMPROVEMENTS

Directly incorporating the QMRF report into MODA template by uploading the QMRF File

Increasing the dependency depth based on user selections.

Automated filling of the MODA workflow Figure based on the input of the user.

Upload already developed scientific workflows into Easy-MODA and store them in the Easy-MODA database

Include all updates to the MODA documentation introduced by EMMC

Integration with CHADA

CONCLUSIONS

Easy-MODA is a freely accessible web tool open to all users which is hosted in the Enalos Cloud Platform .

Registration of use cases/projects (MODA-based metadata regarding the models) is achieved in a cloud from which the use cases can be retrieved and searched according to user-defined criteria

Modification of previously stored workflows/models

Easy-MODA ensures that every relevant detail is captured in a harmonised and standardised manner, enhancing clarity and consistency across the scientific community and improving model interoperability and reusability (consistent with the FAIR principles).

The flexibility of Easy-MODA offers users the ability to customise fields as needed, to modify or expand the pre-filled fields to document unconventional workflows.

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Software/web server article

Easy-MODA: Simplifying standardised registration of scientific simulation workflows through MODA template guidelines powered by the Enalos Cloud Platform

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QUESTIONS?