



NovaMechanics
Cheminformatics & Nanoinformatics Excellence

Nanoinformatics TAs services: NanoCommons KNIME nodes

Will they blend?

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NovaMechanics Ltd

Cheminformatics & Nanoinformatics Excellence

www.novamechanics.com

Interactive online Workshop: If you want to go far go together –
Collaborative Research supported by NanoCommons Transnational Access



What is KNIME Analytics Platform

A free tool for data analysis, manipulation, visualization and reporting

Based on the graphical programming paradigm

Provides a diverse array of extensions:

Text Mining

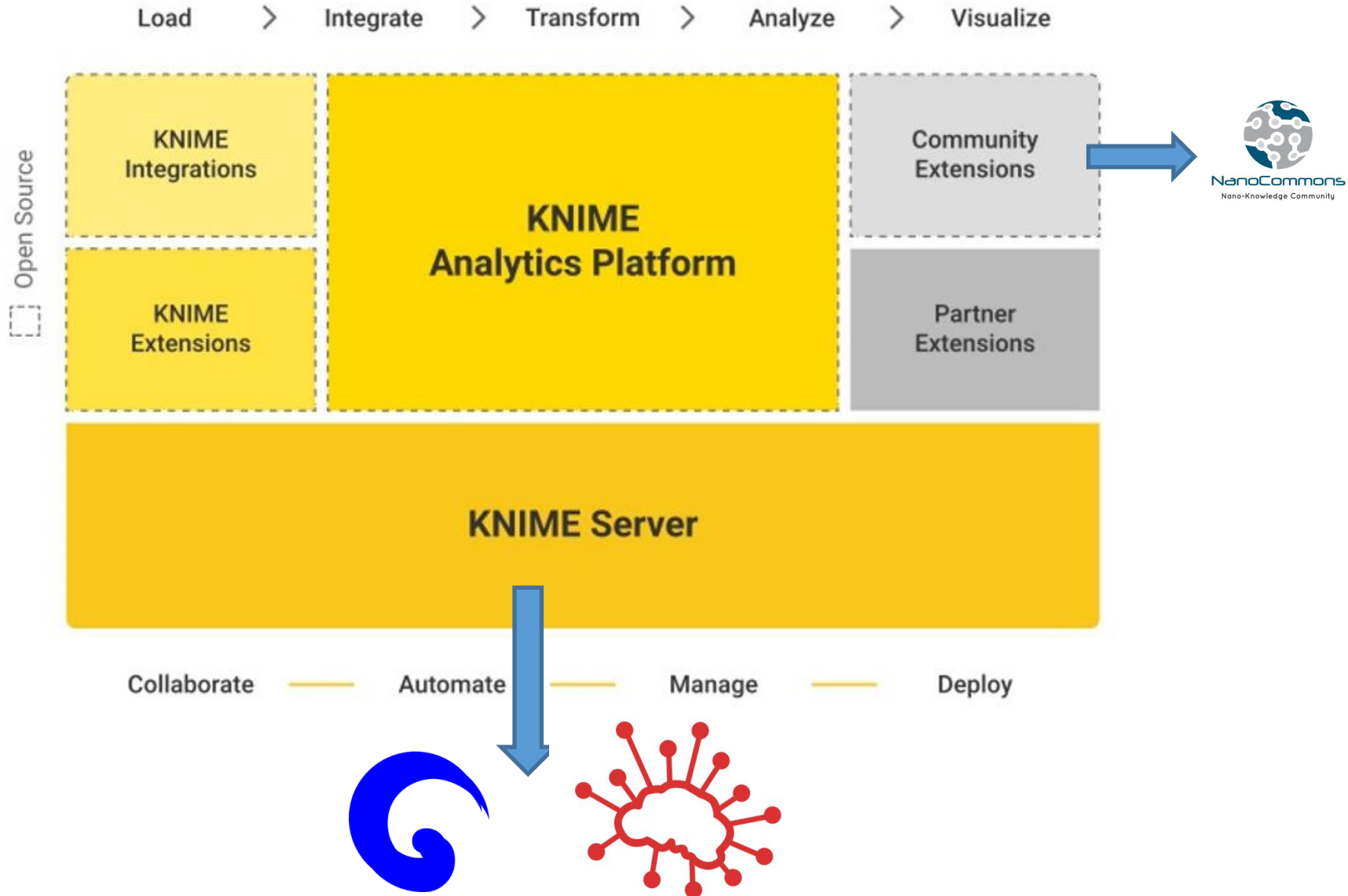
Chem/Nano informatics

Big Data

Many integrations, such as Java, R, Python, Weka etc.



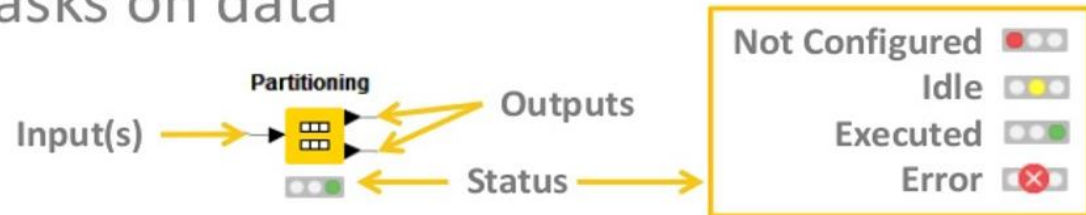
KNIME Software



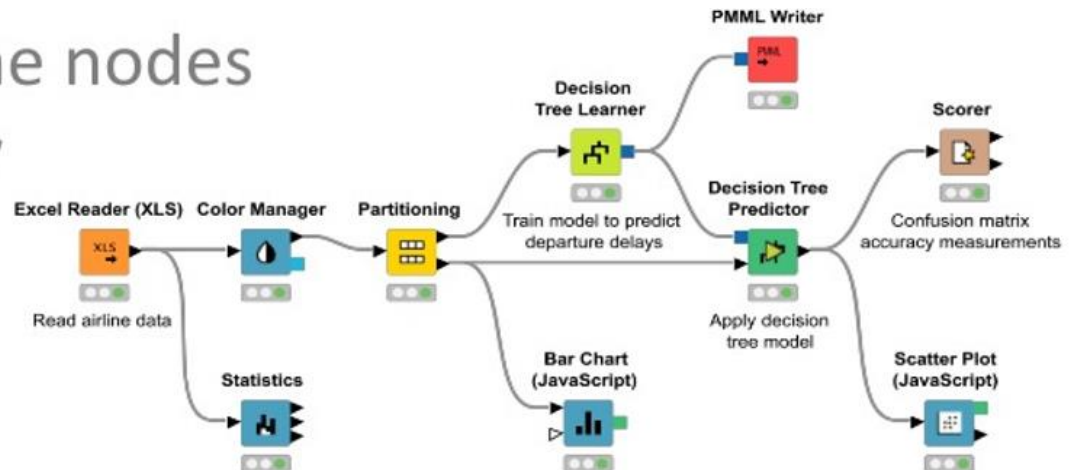


Visual KNIME workflows

Nodes perform tasks on data



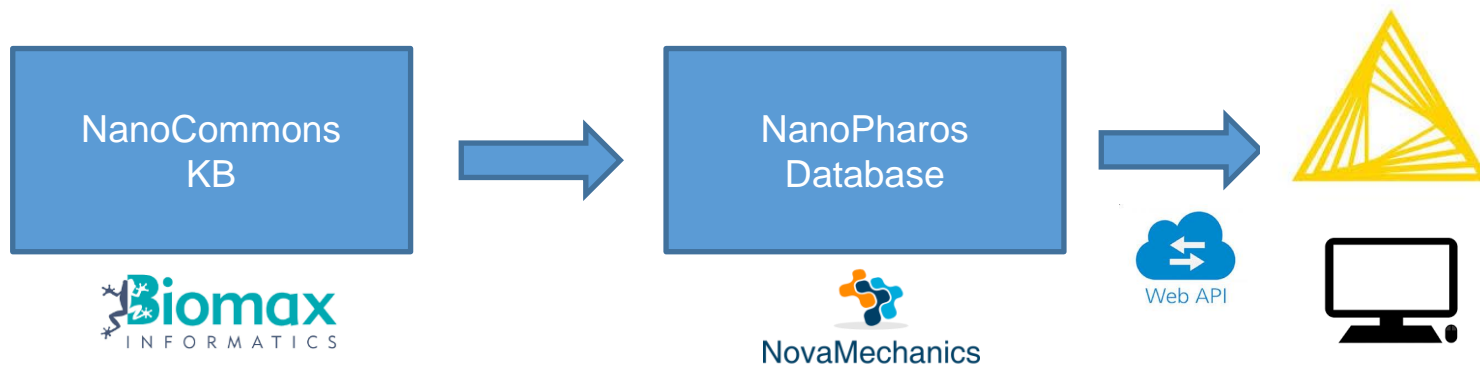
Workflows combine nodes to model data flow





First NanoCommons KNIME Node

- Released Jan 2020
- Available for access through [TA](#): Enalos KNIME data retrieving workflow for *in silico* modelling
- Now a new version is available



> *Curr Med Chem.* 2020;27(38):6523-6535. doi: 10.2174/0929867327666200727114410.

Enalos Suite of Tools: Enhancing Cheminformatics and Nanoinfor - matics through KNIME

Antreas Afantitis ¹, Andreas Tsoumanis ¹, Georgia Melagraki ¹

Affiliations + expand









PMID: 32718281 DOI: 10.2174/0929867327666200727114410



KNIME Implementation - NanoCommons Nodes

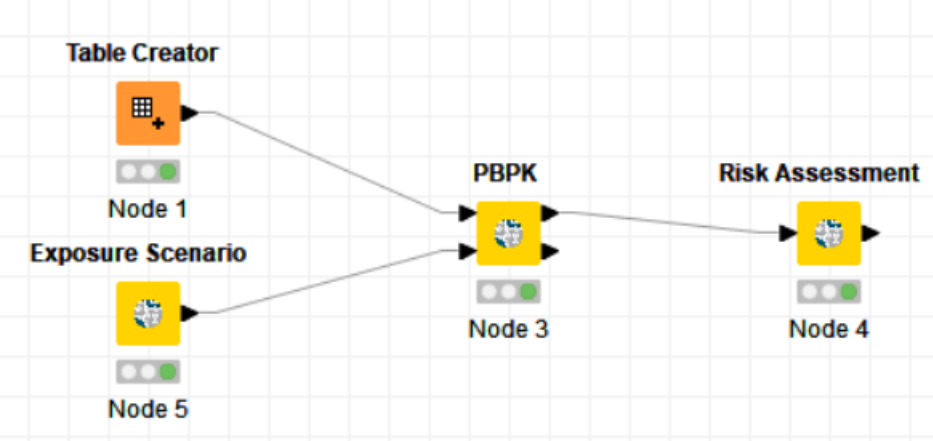
- Our computational tools through NanoCommons KNIME nodes can make some very useful operations available as extensions for KNIME platform.
- NanoCommons Nodes can be combined with custom made workflows and external nanoinformatics tools combined with state of the art modeling techniques (WEKA, R, TensorFlow, etc.).

Nanocommons Nodes

-  CNT SDF
-  CNT SMILES
-  Exposure Scenario
-  NanoCommonsKB
-  NanoXtract Batch Conf
-  NanoXtract Individ Conf
-  PBPK
-  Risk Assessment



NanoCommons Risk Assessment Tool



NanoCommons Risk Assessment Tool

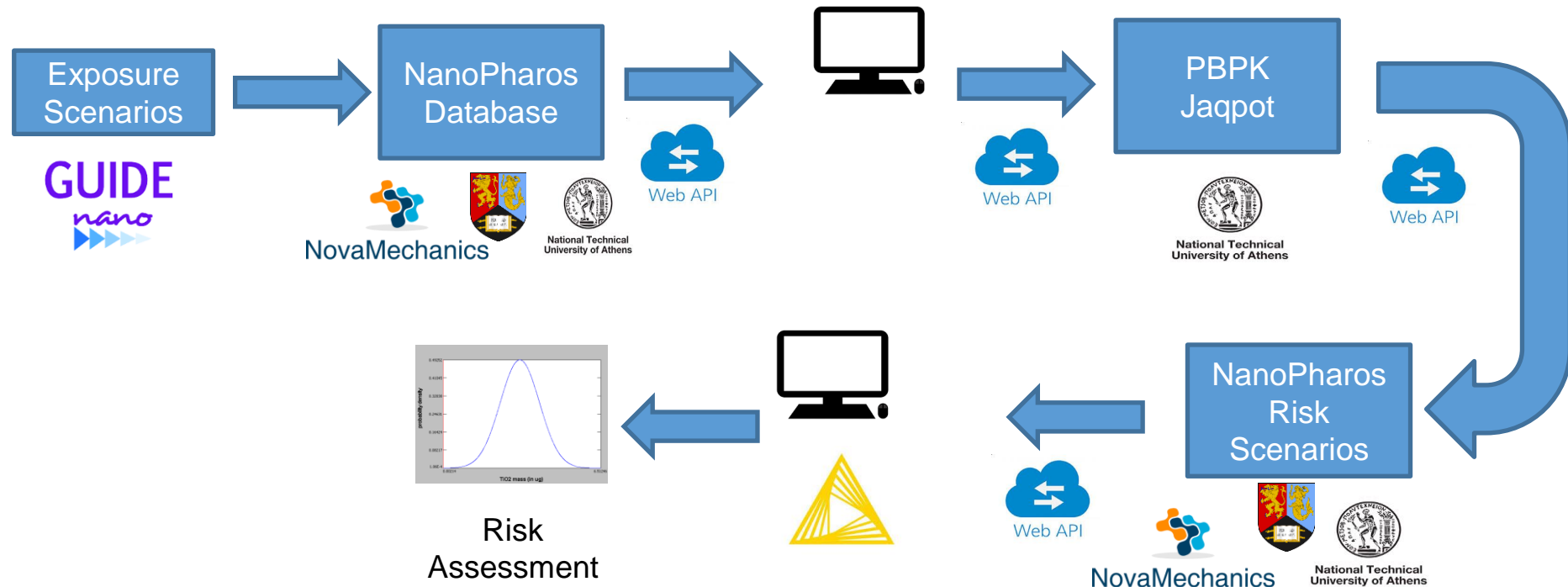
Short description

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

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

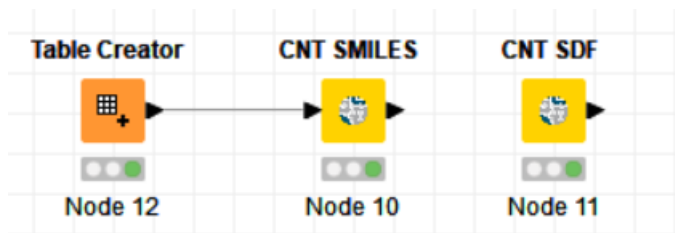
Case 1
45 g (initial mass 3000 kg) of TiO2 (22nm) poured over 7 hours in the NF, with 1 min activity duration every hour. For every hour the mouse stays 90 s in the NF and spends the rest of the time in the FF.

[Download timeseries](#)





A Safe-by-Design Tool for Functionalised Nanomaterials



Enalos Nanoinformatics Cloud Platform: A Safe-by-Design Tool for Functionalised Nanomaterials

Design a molecule

Enter SMILES separated by newline

Description

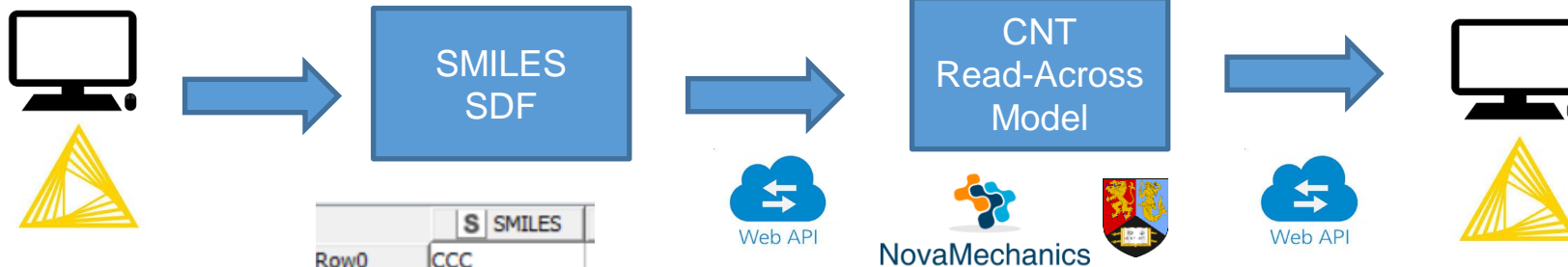
A fully validated predictive QNAR model correlating molecular descriptors of the decorating molecules of multi-walled carbon nanotubes and their toxicity, and biological activity (protein binding of carbonic anhydrase). More information on the models' development can be found in "Varou, D. D., Afanitis, A., Tsoumias, A., Melagraki, G., Sarimis, H., Vlahmi-Jones, E., and Lynch, I. (2019). A safe-by-design tool for functionalised nanomaterials through the Enalos Nanoinformatics Cloud platform. *Nanoscale Advances*." A detailed tutorial of the corresponding web-app can be found in [pdf format](#). A demonstration video is available [here](#).

Execute

Upload an SDF file (.sdf)

upload Please select an sdf file

Execute

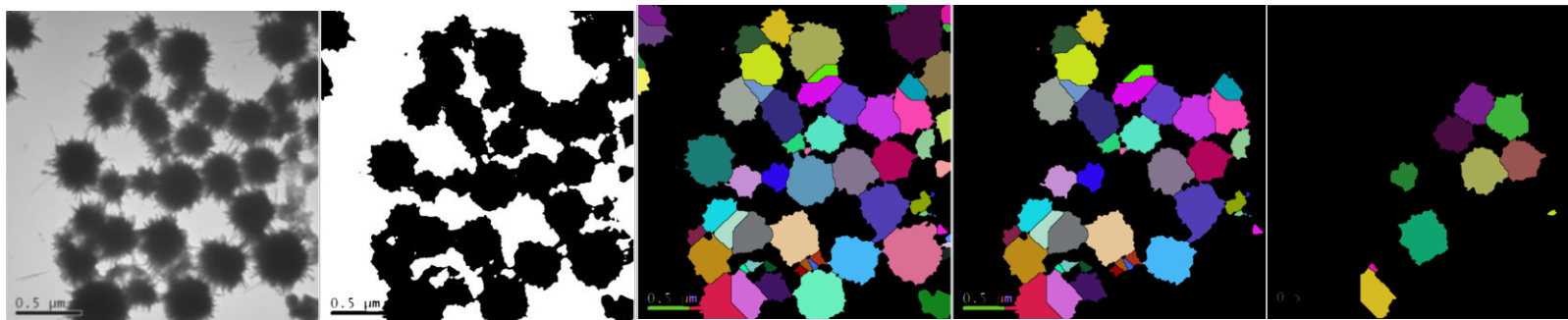
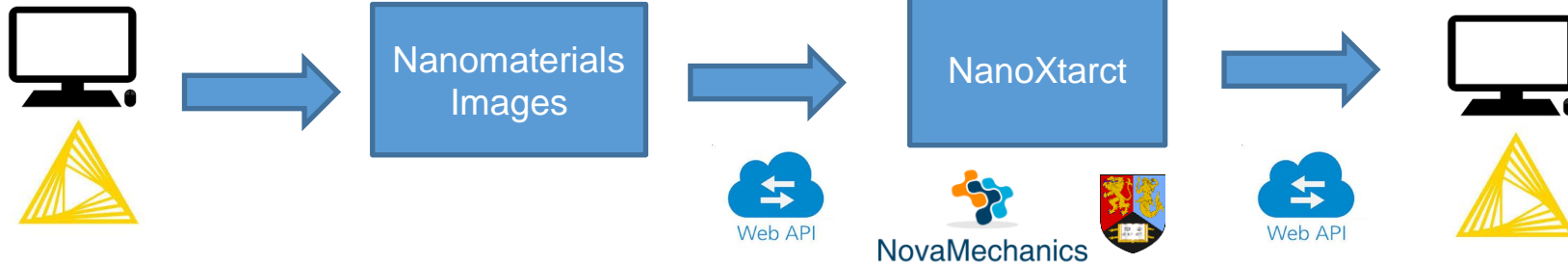
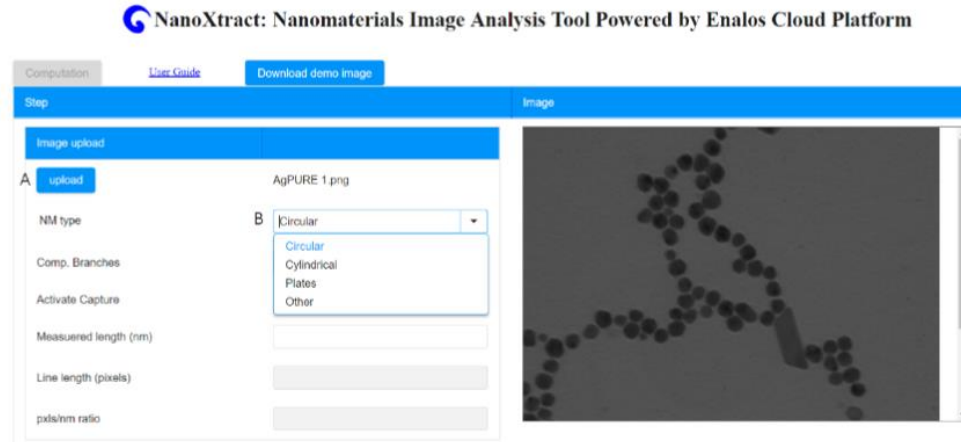
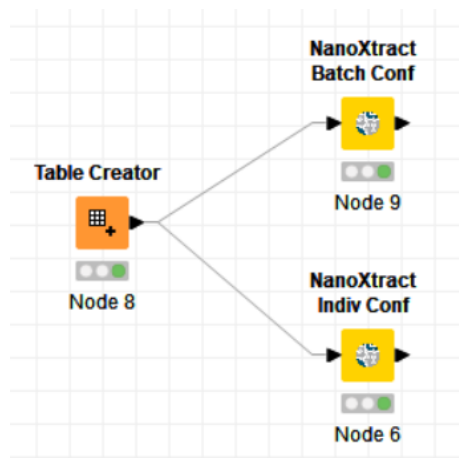


	S	SMILES
Row0		CCC
Row1		CCCC
Row2		CCCCC

S	id	S	activity	S	activityNN1	D	distanc...	S	activityNN2	D	distanc...
	Row0		binder		c1cccc(c1)C(O)=O		3.675		c1cccc(c1)C(Oc1cccc(cc1)CC(C(N(CCCC)CCCC)=O)NC(Cc1cccc1)=O)=O		3.768
	Row1		binder		c1cccc(c1)C(O)=O		1.916		c1cccc(c1)C(Oc1cccc(cc1)CC(C(N(CCCC)CCCC)=O)NC(Cc1cccc1)=O)=O		1.94
	Row2		binder		c1cccc(c1)C(Oc1...		1.901		c1cccc(c1)C(Oc1cccc(cc1)CC(C(Nc1cccc1)=O)NC(Cc1cccc1)=O)=O		1.98












NanoXtract: Nanomaterials Image Analysis Tool





Enalos+ nodes for access to small molecule databases

- ▲  PubChem
 -  Assay
 -  Assay Class
 -  Main PubChem
 -  Patent
 -  Patent to Sid
 -  Sid
 -  Similarity
 -  Vendor



UniChem

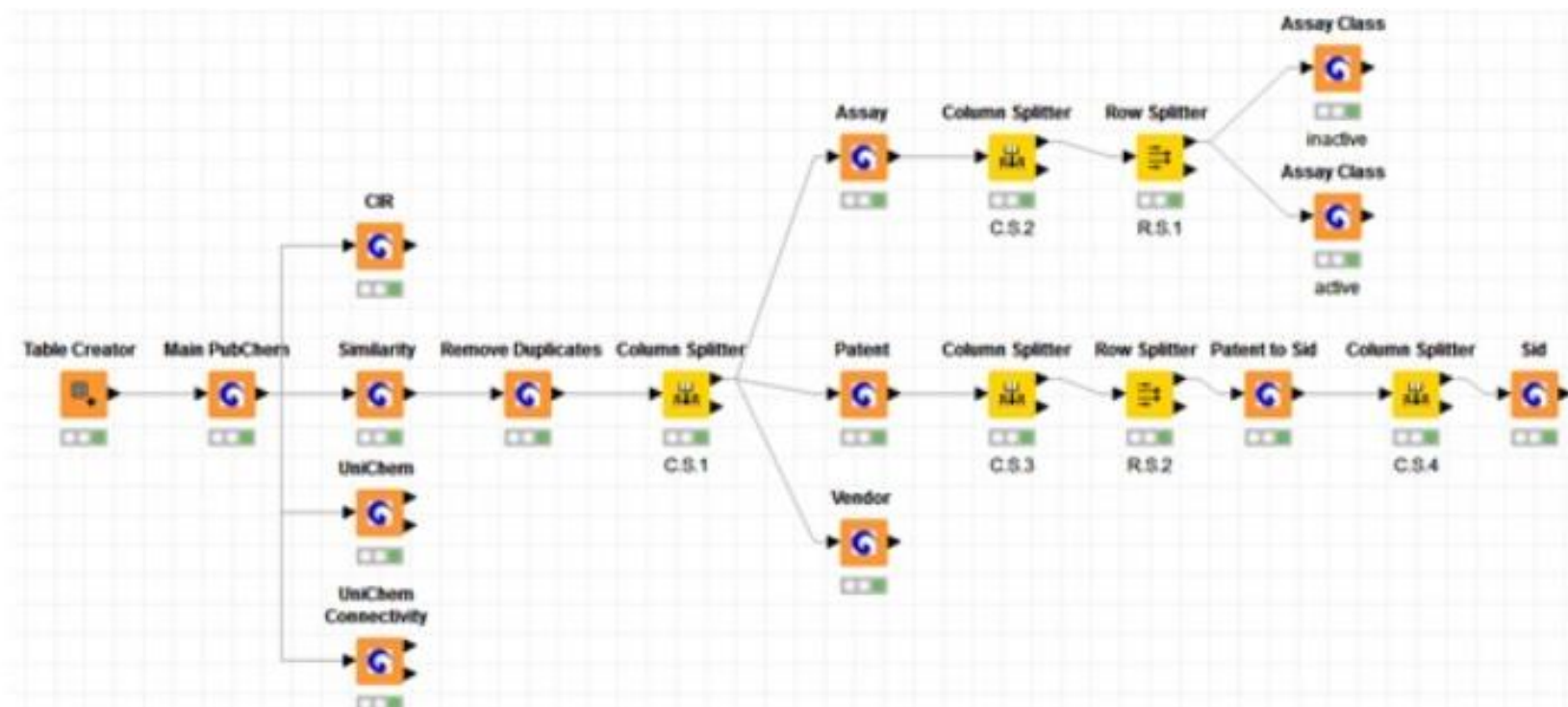
Access to 31 chemical databases :
e.g ChEMBL, PubChem, DrugBank, KEGG, ZINC,
BindinDB, eMolecules, IBM patents, SureChEMBL etc



National Institutes
of Health

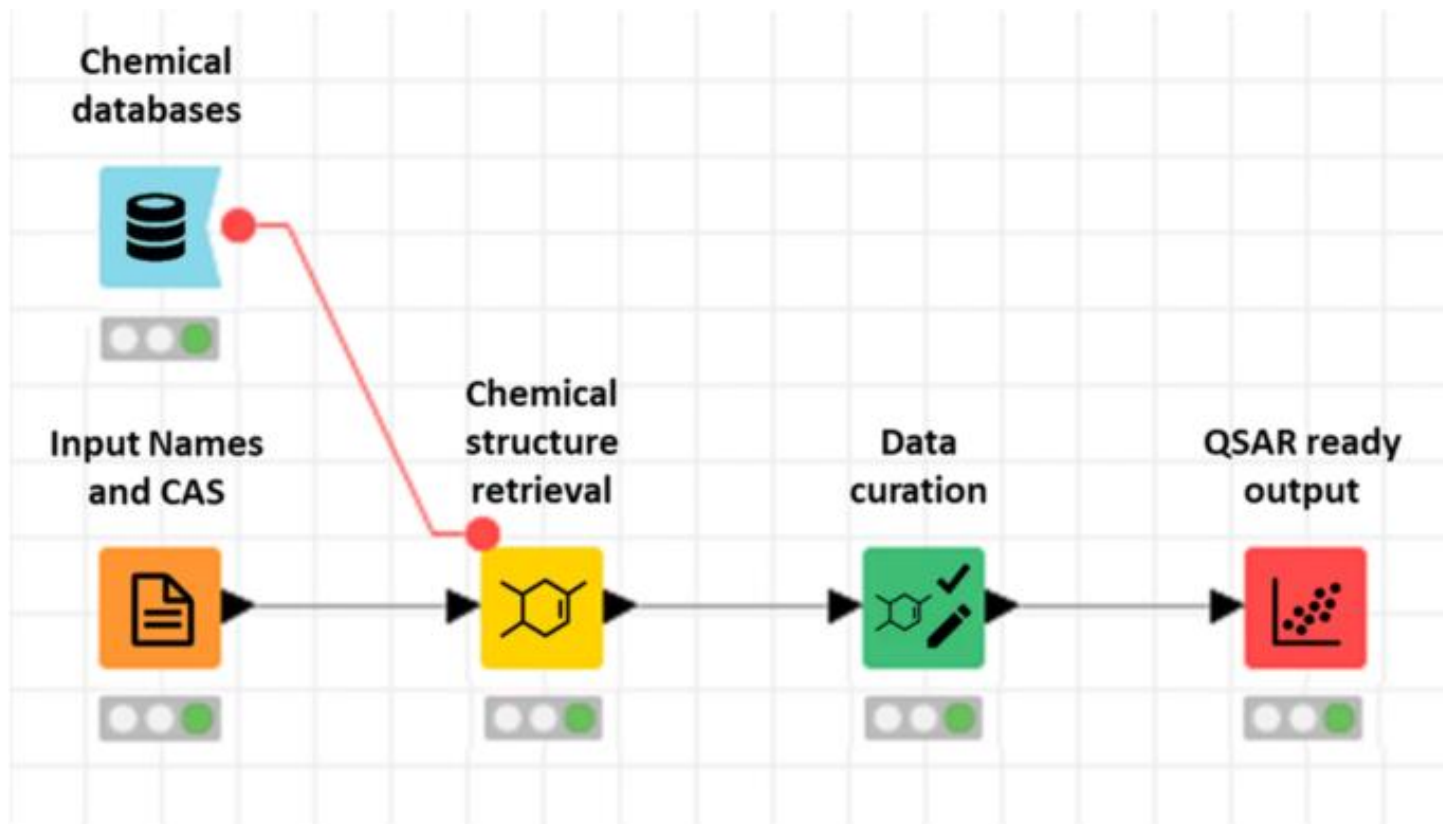


Blend >35 databases together with the aid of InChi



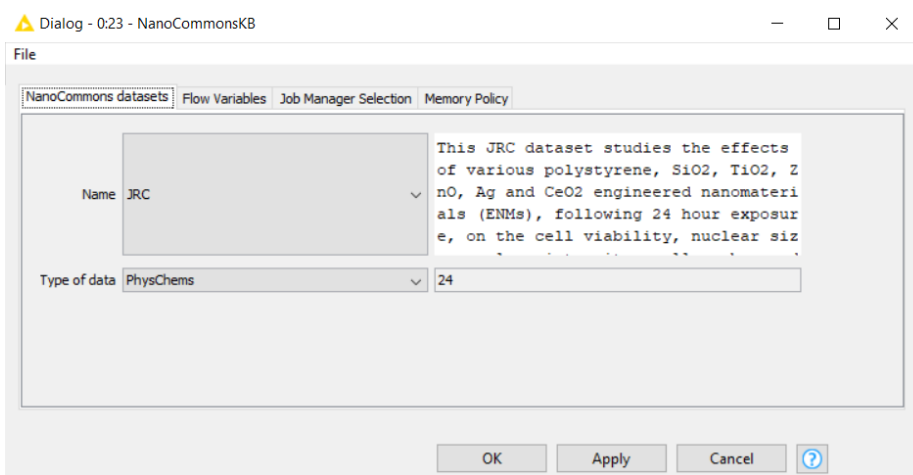
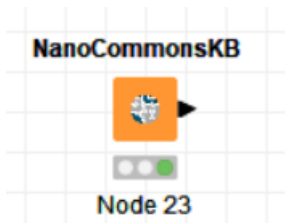


Small molecules paradigm





Nanomaterials paradigm



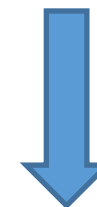
Nanocommons - NanoSolveIT NInChI Server



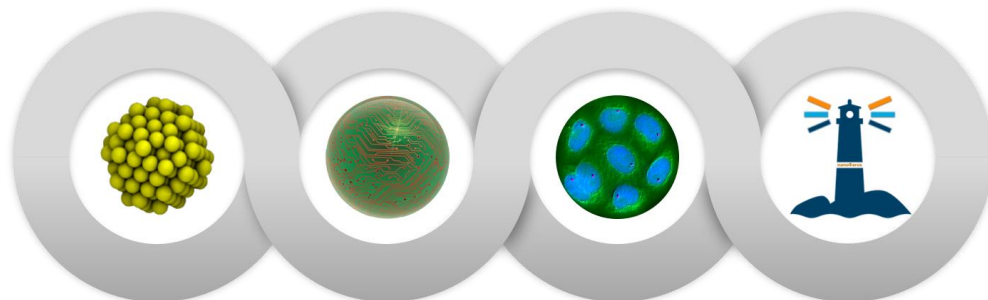
The nanomaterial is being built with a layered architecture from core to outer layers

Composition	Morphology	Size (nm)	Crystal layer	Chirality layer	
<input type="text"/>	Sphere <input type="button" value="v"/>	d <input type="text"/>	None <input type="button" value="v"/>	n,m <input type="text"/>	<input type="button" value="+"/>

NInChI



NanoPharos database: Ready-for-modelling datasets for the development of in silico Alternative Testing Strategies and Integrated Approaches to Testing and Assessment

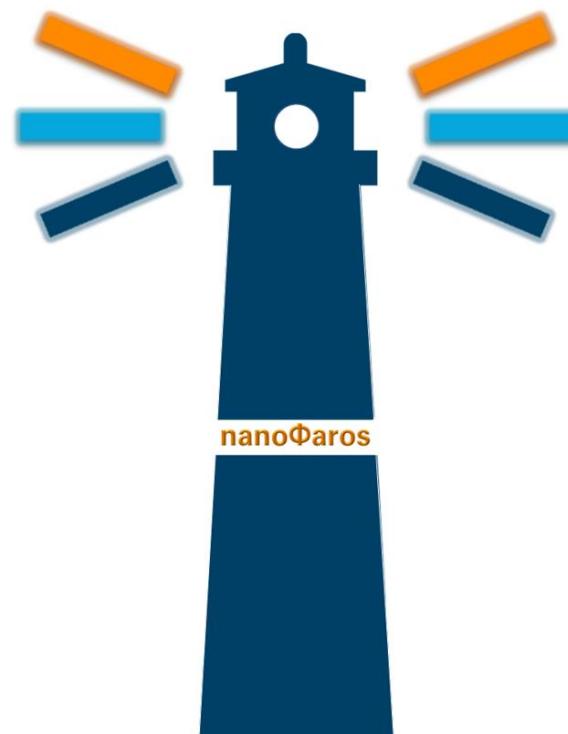


Nanomaterials

Enrichment

Assays

Ready for modelling



NanoPharos Create/Modify Computational Property

Modify	583 - V// O atoms surface	
Title	583 - V// O atoms surface	Content
Computational Property Name	582 - V// O atoms core	V// O atoms surface
Description	581 - V// O atoms all	Avg. length of force vector surface tangent component for O atoms in surface region
	580 - V// Me atoms surface	
	579 - V// Me atoms core	
	578 - V// Me atoms all	
	577 - V// atoms surface	
	576 - V// atoms core	
	575 - V// atoms all	
	574 - v__ O atoms surface	
	573 - v__ O atoms core	
	572 - v__ O atoms all	
Datatype of Value	571 - v__ Me atoms surface	1 - Number

The nanoPharos database concept provides the users with structured, harmonised and ready for modelling datasets

Available at:

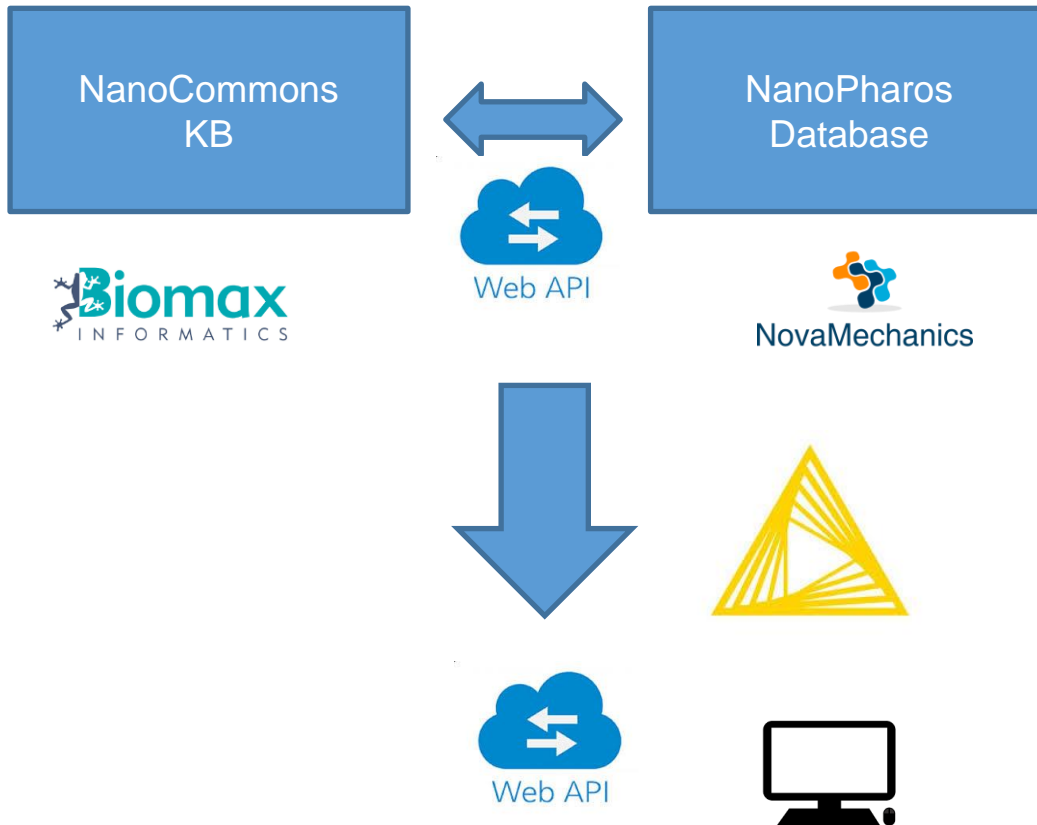
<https://db.nanopharos.eu/Queries/Datasets.zul>





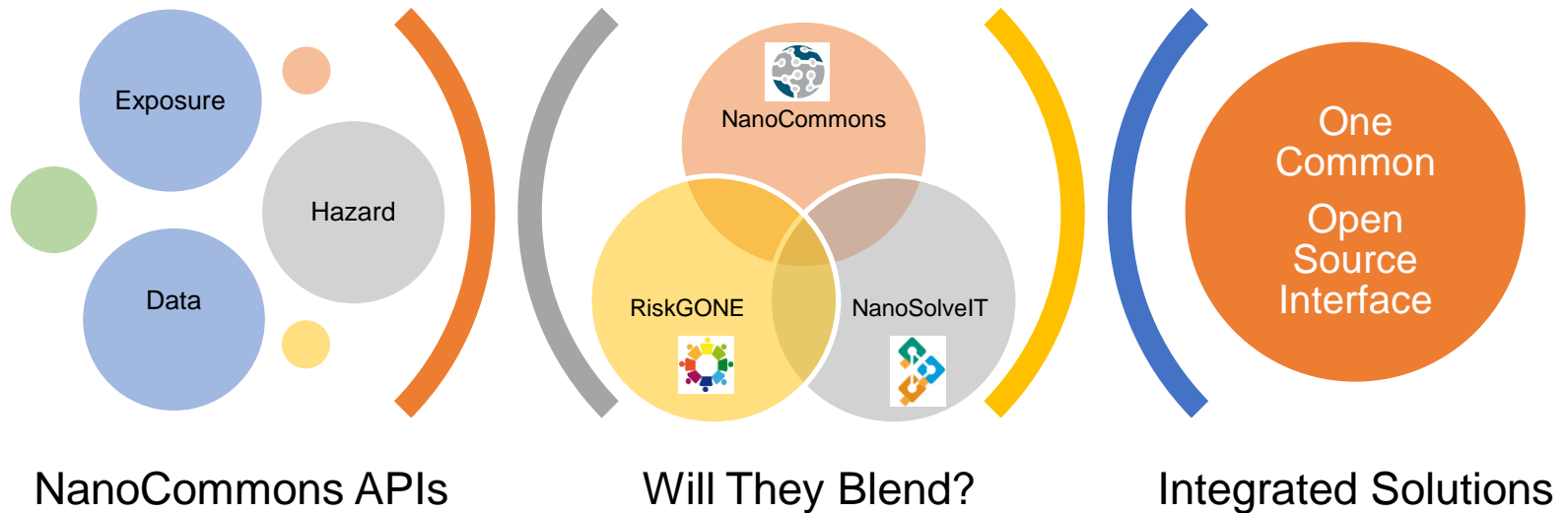
Future developments, stay tuned

- Full integration of NanoCommons KB with NanoPharos database





NanoCommons KNIME nodes





Would you like to test them?

- Apply for a TA at: <https://www.nanocommons.eu/ta-access/>
- Then visit: <https://licenses.novamechanics.com/> to get the license and download the nodes

Your Institute/Company

Position

Industry

Software (required)

Enalos Nodes ▾

Enalos Nodes

Enalos Suite

NanoCommons Nodes

Isalos



NanoCommons
Nano-Knowledge Community

Thank you



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Nicosia, Cyprus

