Nanoinformatics TAs services: NanoCommons KNIME nodes

Will they blend?

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NovaMechanics Ltd

Cheminformatics & Nanoinformatics Excellence

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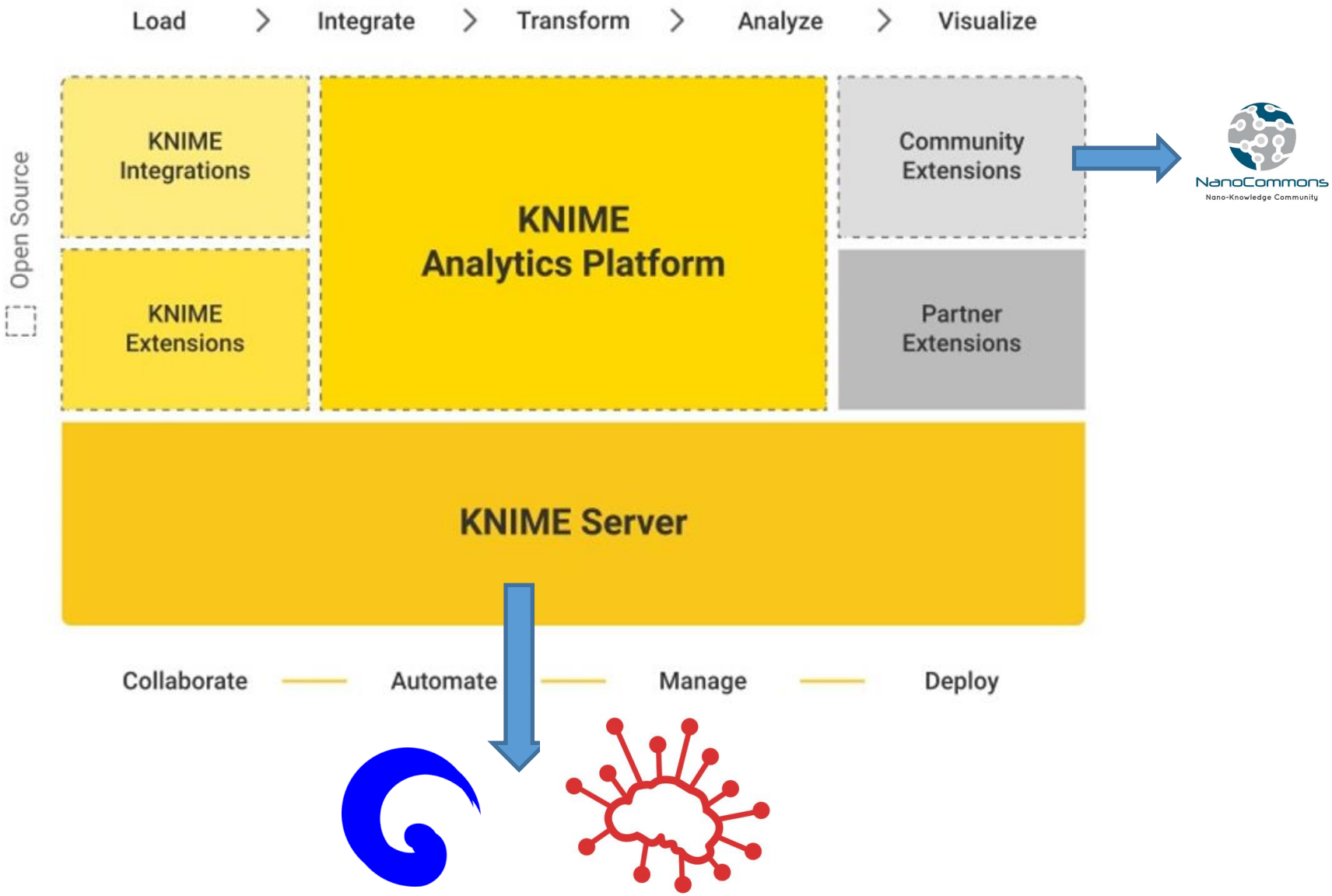
Interactive online Workshop: If you want to go far go together –
Collaborative Research supported by NanoCommons Transnational Access

What is KNIME Analytics Platform

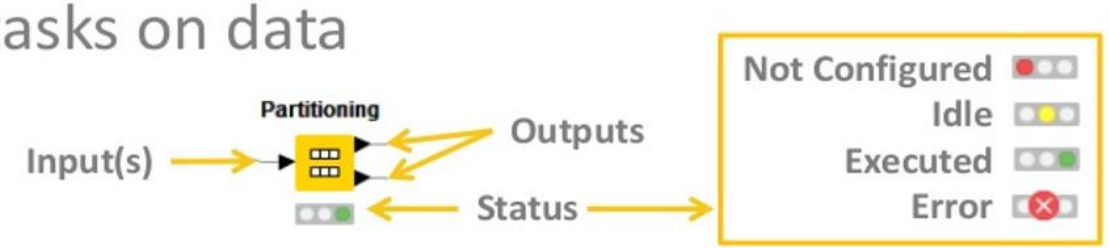
- A free tool for data analysis, manipulation, visualization and reporting
- Based on the graphical programming paradigm
- Provides a diverse array of extensions:
  - Text Mining
  - Chem/Nano informatics
  - Big Data
  - Many integrations, such as Java, R, Python, Weka etc.

KNIME Software

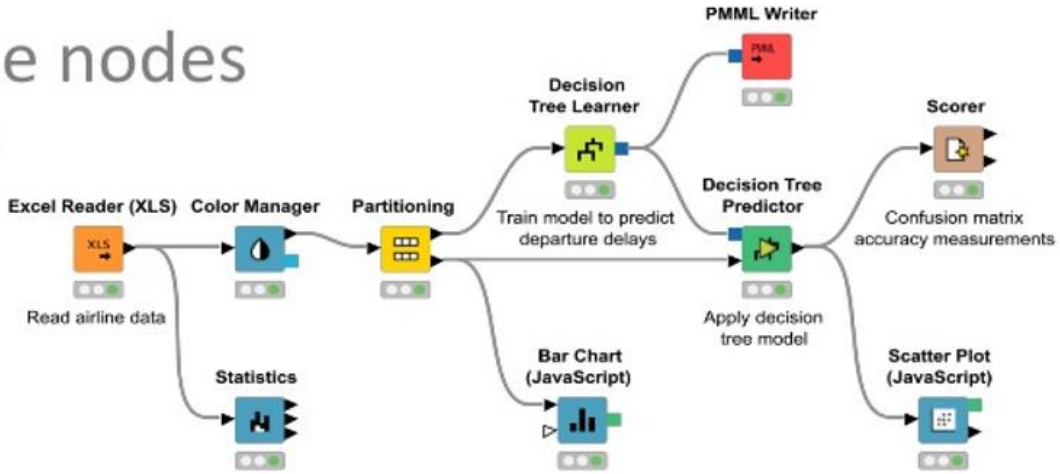


Visual KNIME workflows

Nodes perform tasks on data

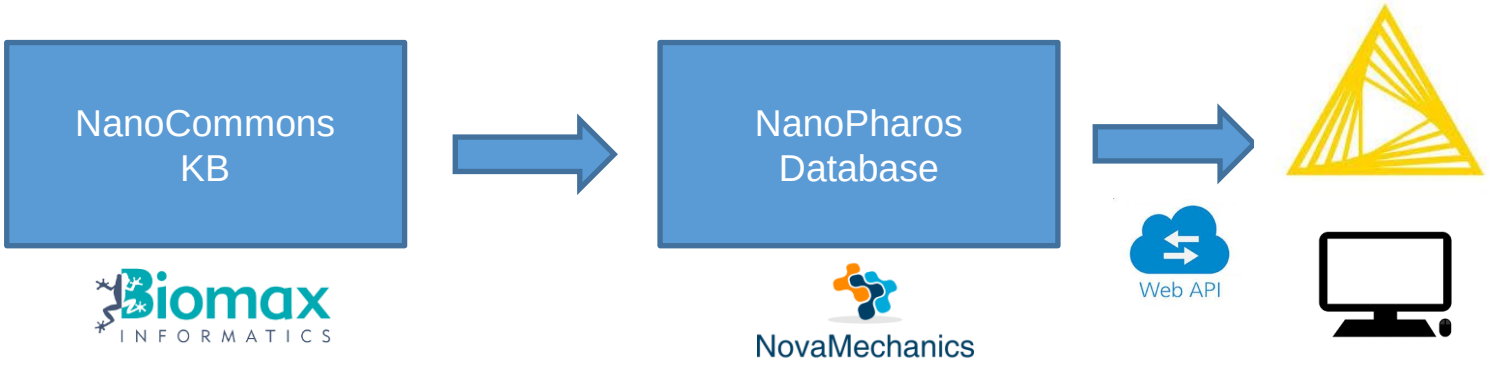


Workflows combine nodes to model data flow



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

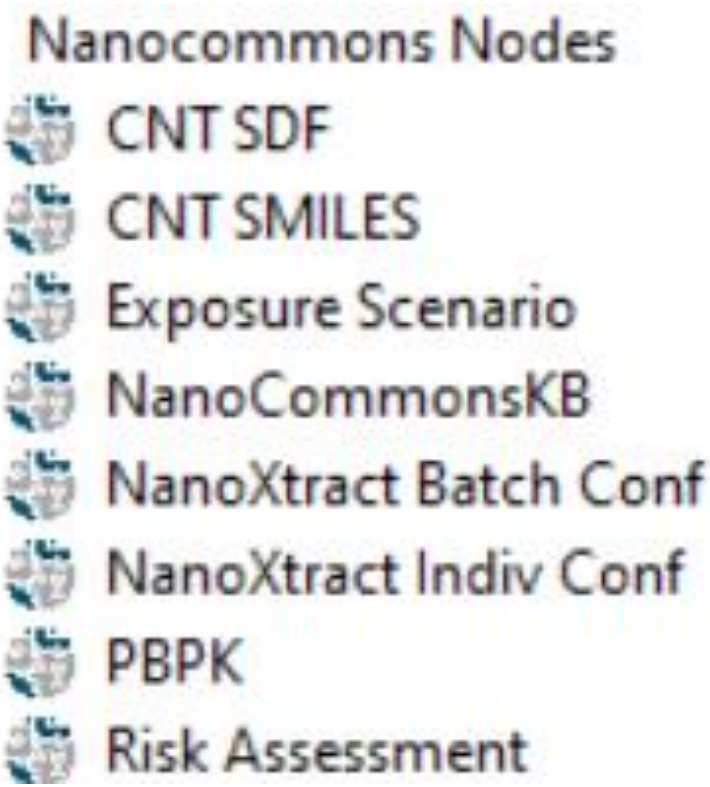
Antreas Afantitis [1], Andreas Tsoumanis [1], Georgia Melagraki [1]

Affiliations + expand

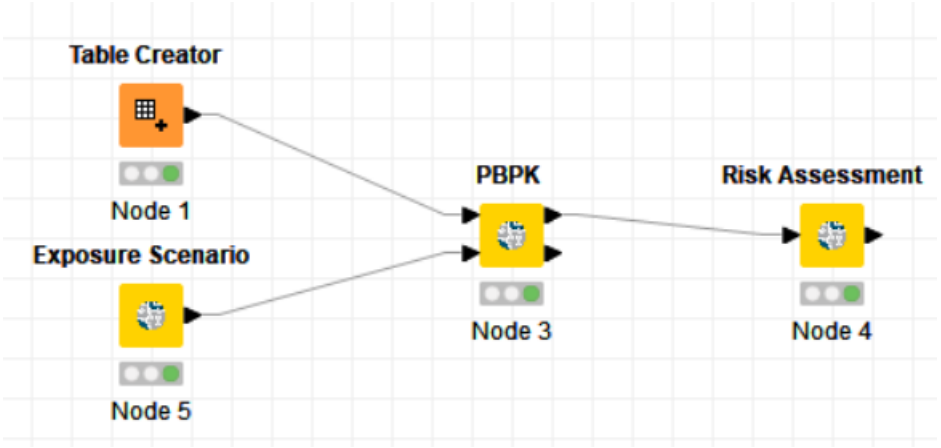
PMID: 32718281 DOI: 10.2174/0929867327666200727114410

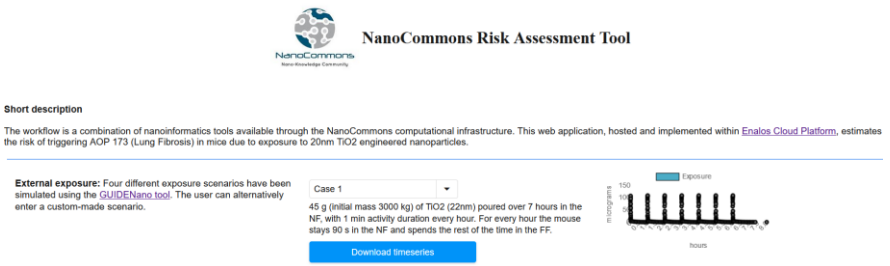
KNIME Implementation - NanoCommons Nodes

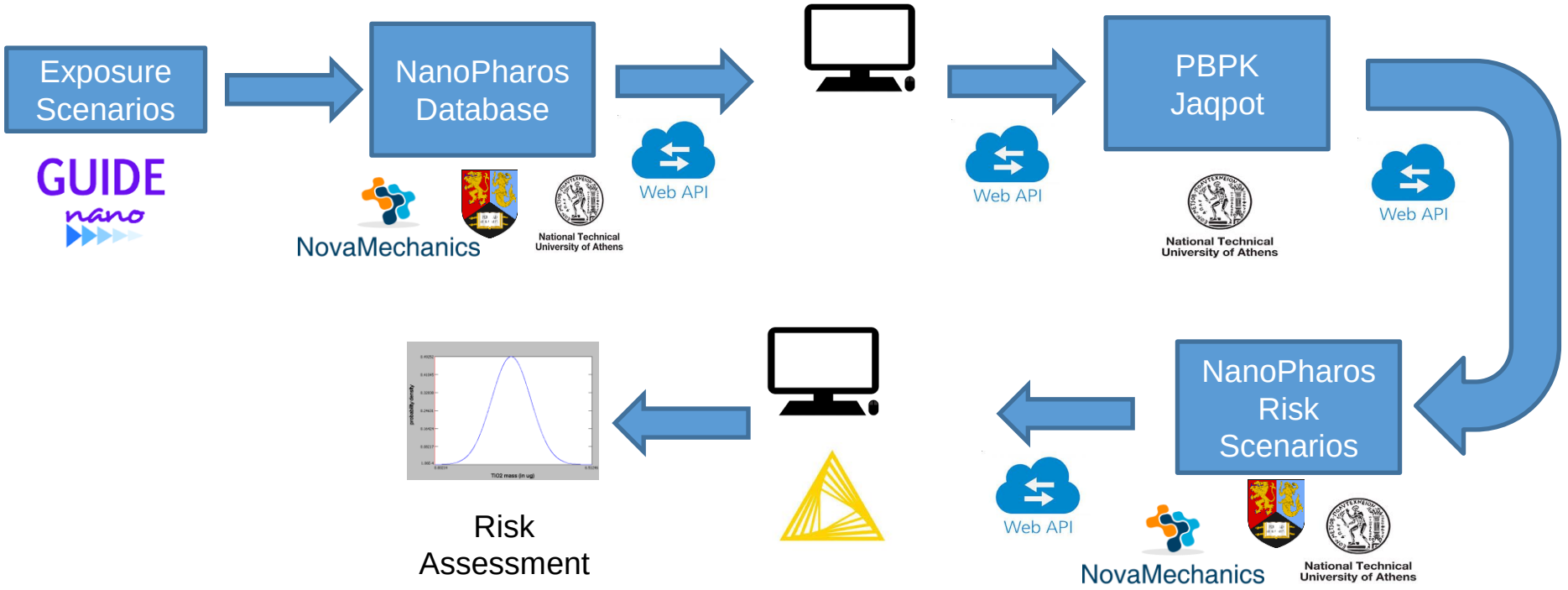
- Our computational tools through NanoCommons KNIME nodes can make some very useful operations available as extensions for KNIME platform.
- NanoCommons Nodes can be combined with custom made workflows and external nanoinformatics tools combined with state of the art modeling techniques (WEKA, R, TensorFlow,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



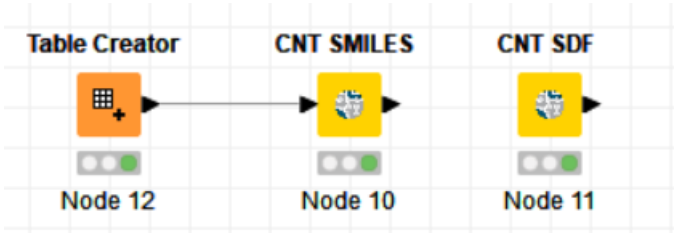
NanoCommons Risk Assessment Tool

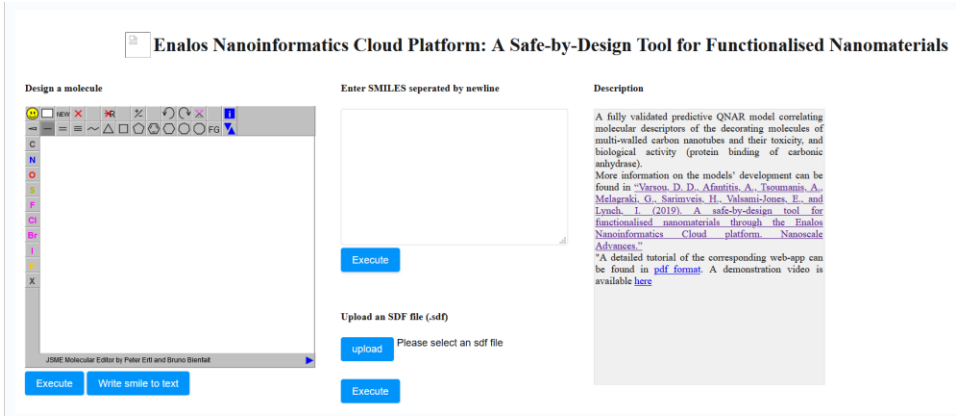


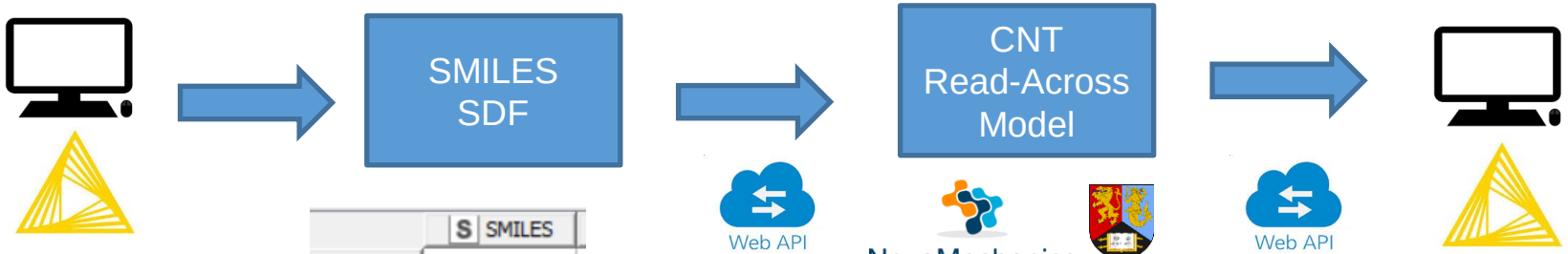




A Safe-by-Design Tool for Functionalised Nanomaterials



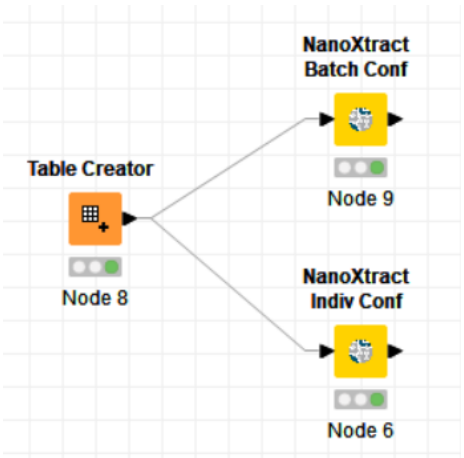


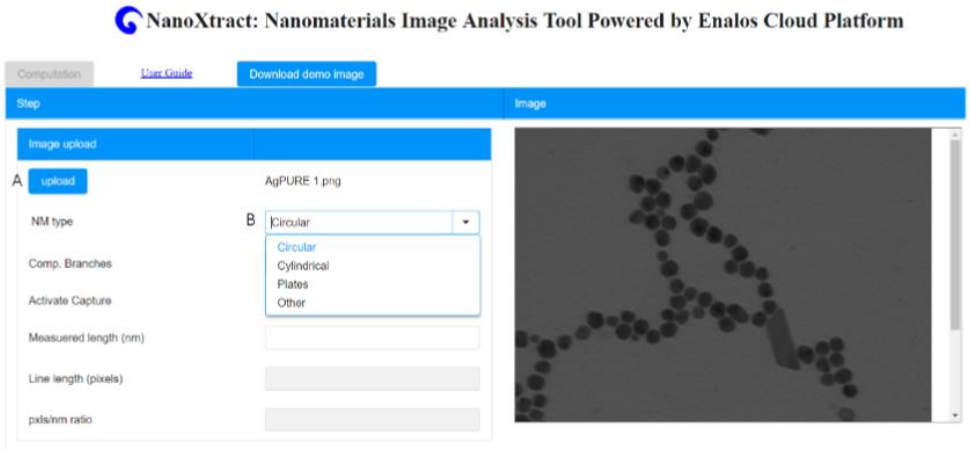


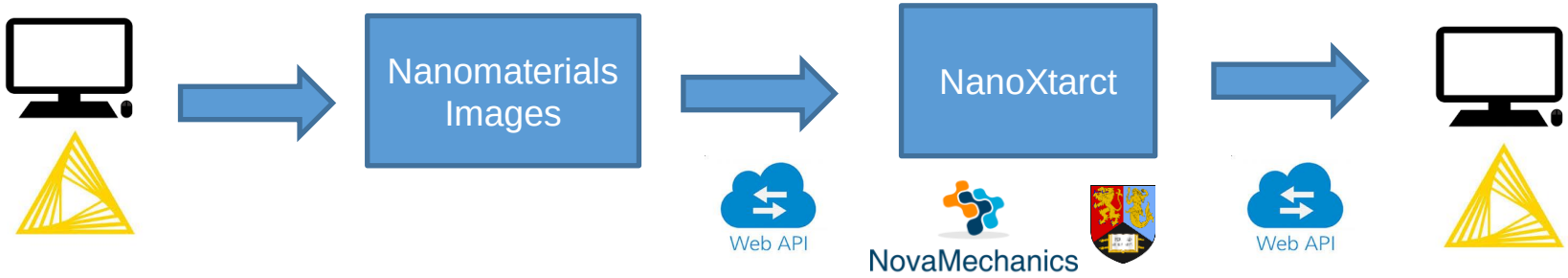
	S SMILES
Row0	CCC
Row1	CCCCC
Row2	CCCCCC

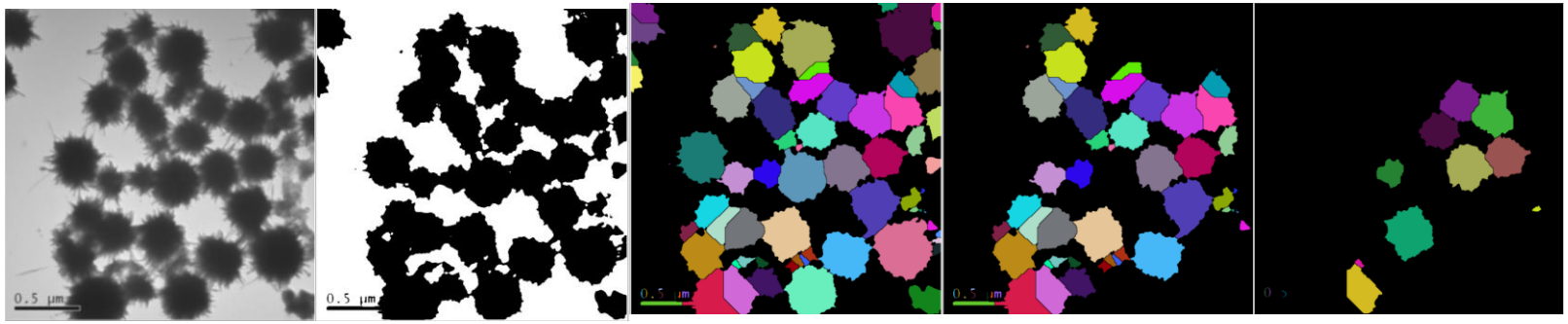
S id	S activity	S activityNN1	D distanc...	S activityNN2	D distanc...	
Row0	binder	c1cccc(c1)C(O)=O	3.675	c1cccc(c1)C(Oc1ccc(cc1)CC(C(N(CCCC)CCCC)=O)NC(Cc1ccccc1)=O)=O	3.768	c
Row1	binder	c1cccc(c1)C(O)=O	1.916	c1cccc(c1)C(Oc1ccc(cc1)CC(C(N(CCCC)CCCC)=O)NC(Cc1ccccc1)=O)=O	1.94	c
Row2	binder	c1cccc(c1)C(Oc1...	1.901	c1cccc(c1)C(Oc1ccc(cc1)CC(C(Nc1ccccc1)=O)NC(Cc1ccccc1)=O)=O	1.98	c

NanoXtract: Nanomaterials Image Analysis Tool









Enalos+ nodes for access to small molecule databases

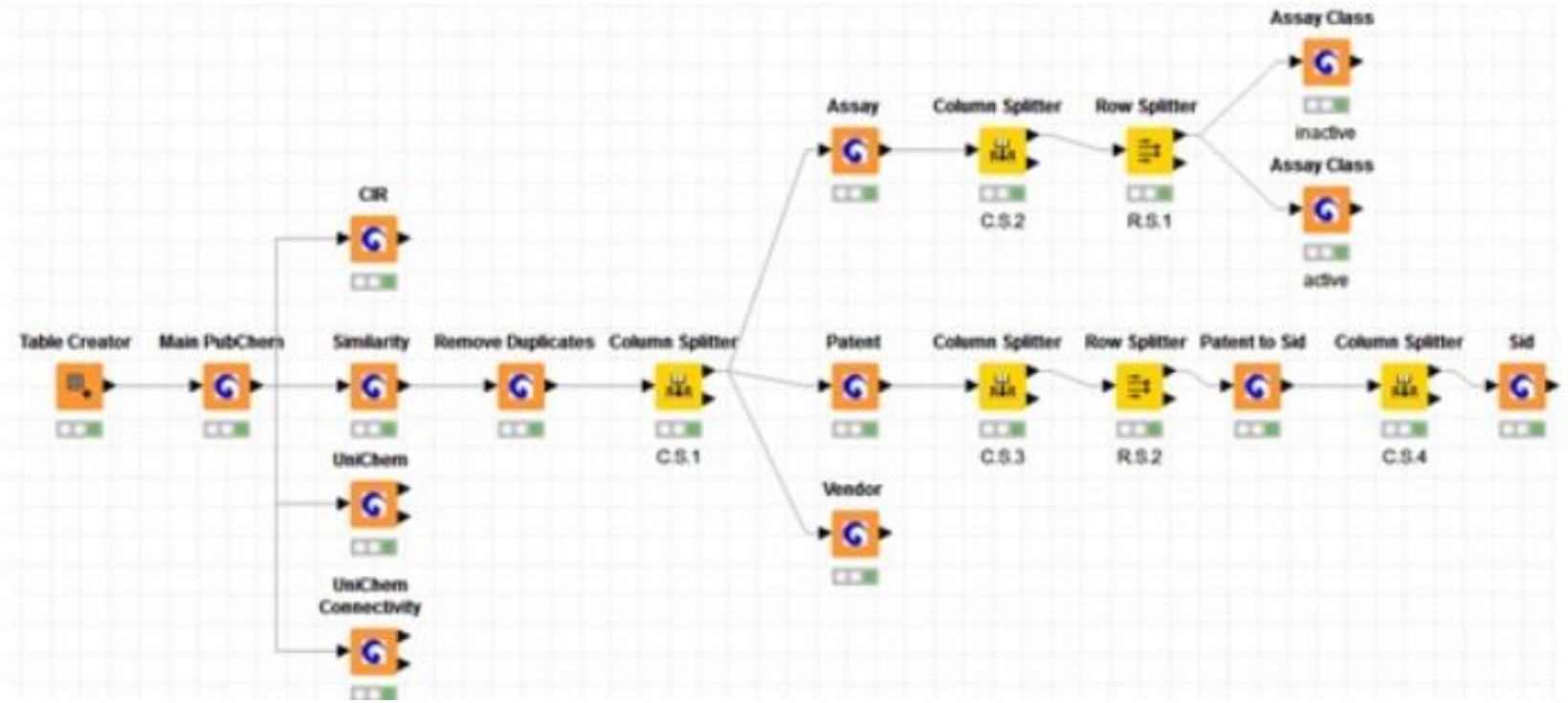
- PubChem
  - Assay
  - Assay Class
  - Main PubChem
  - Patent
  - Patent to Sid
  - Sid
  - Similarity
  - Vendor

UniChem

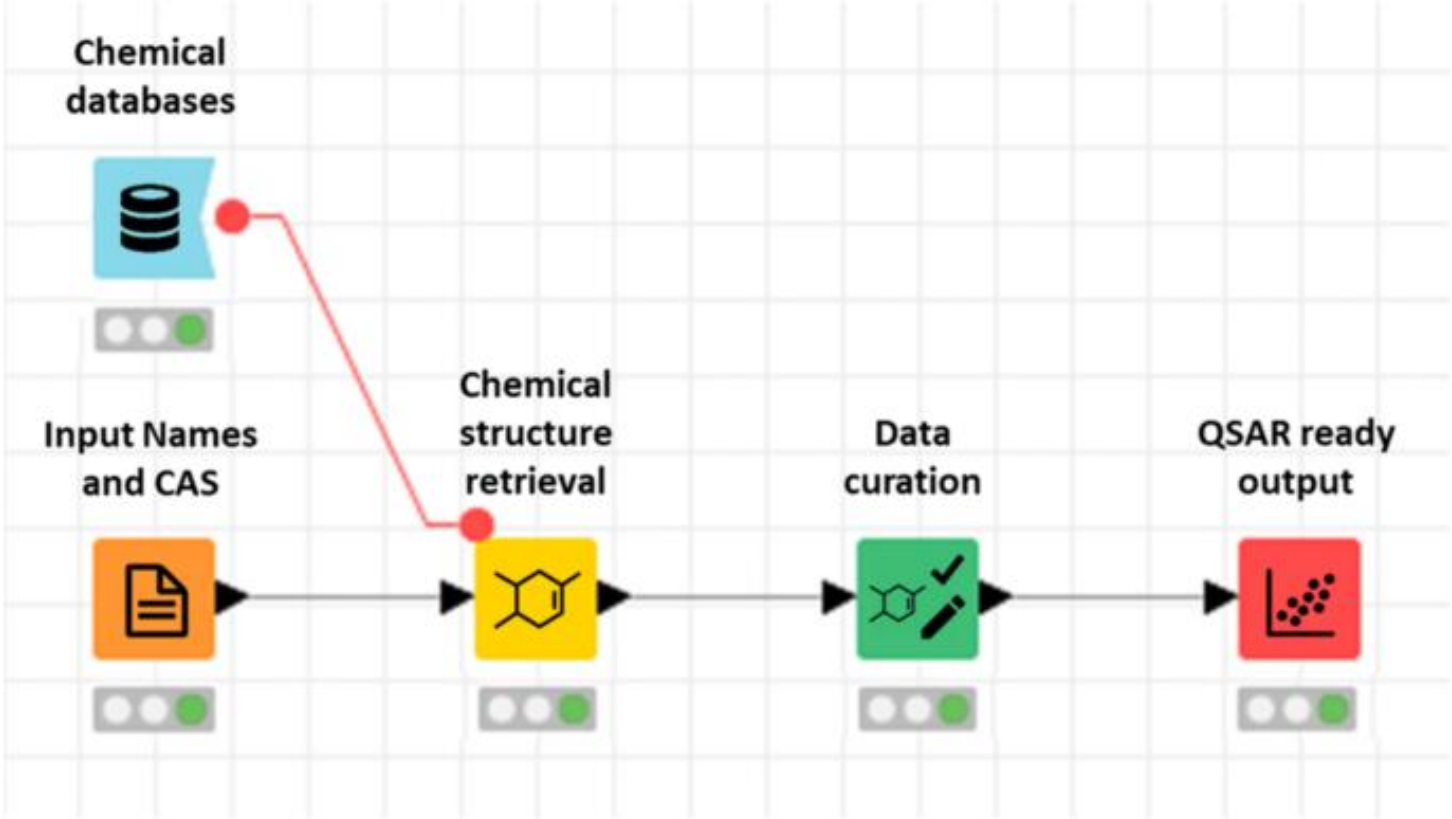
Access to 31 chemical databases :
e.g ChEMBL,PubChem, DrugBank, KEGG, ZINC, BindinDB, eMolecules, IBM patents, SureChEMBL etc

NIH
National Institutes of Health

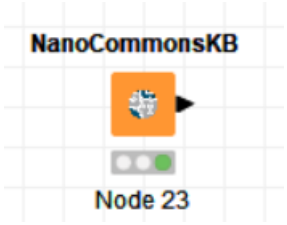
Blend >35 databases together with the aid of InChi

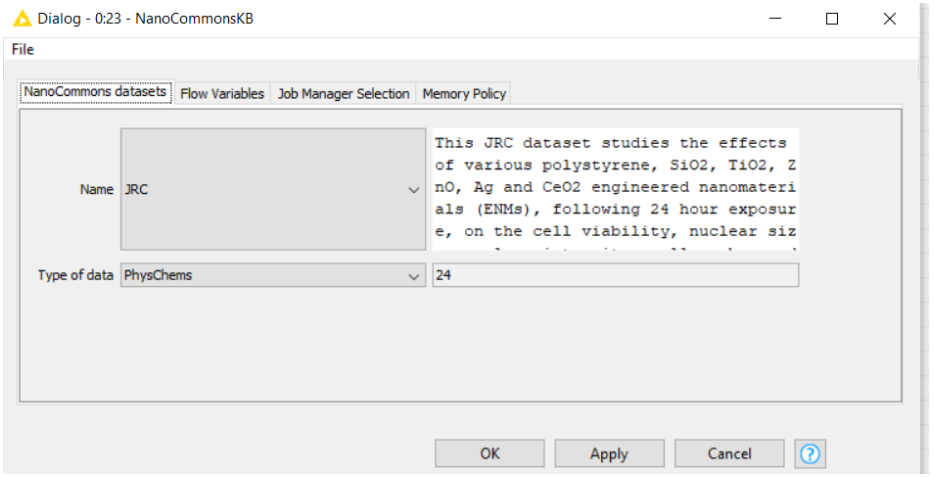


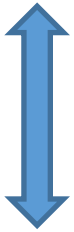
Small molecules paradigm

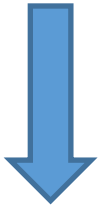


Nanomaterials paradigm









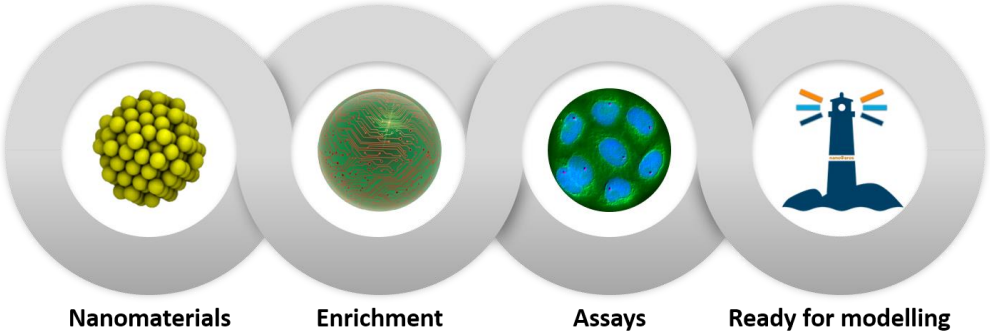
Nanocommons - NanoSolveIT NInChI Server

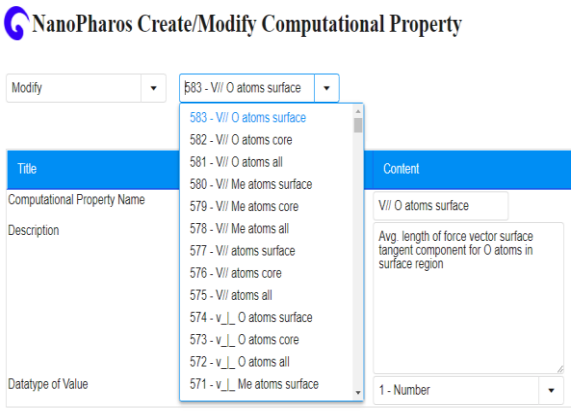
The nanomaterial is being built with a layered architecture from core to outer layers

Composition	Morphology	Size (nm)	Crystal layer	Chirality layer	
	Sphere	d	None	n,m	+

NInChI

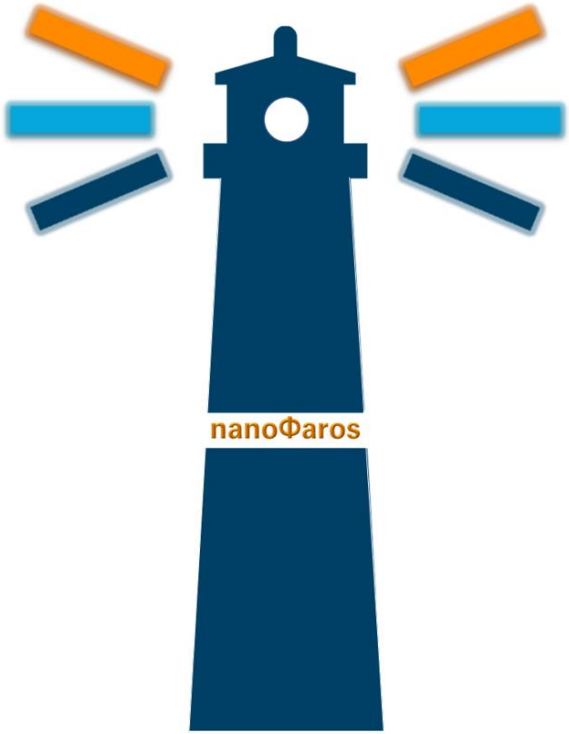
NanoPharos database: Ready-for-modelling datasets for the development of in silico Alternative Testing Strategies and Integrated Approaches to Testing and Assessment





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

Available at:
https://db.nanopharos.eu/Queries/Datasets.zul

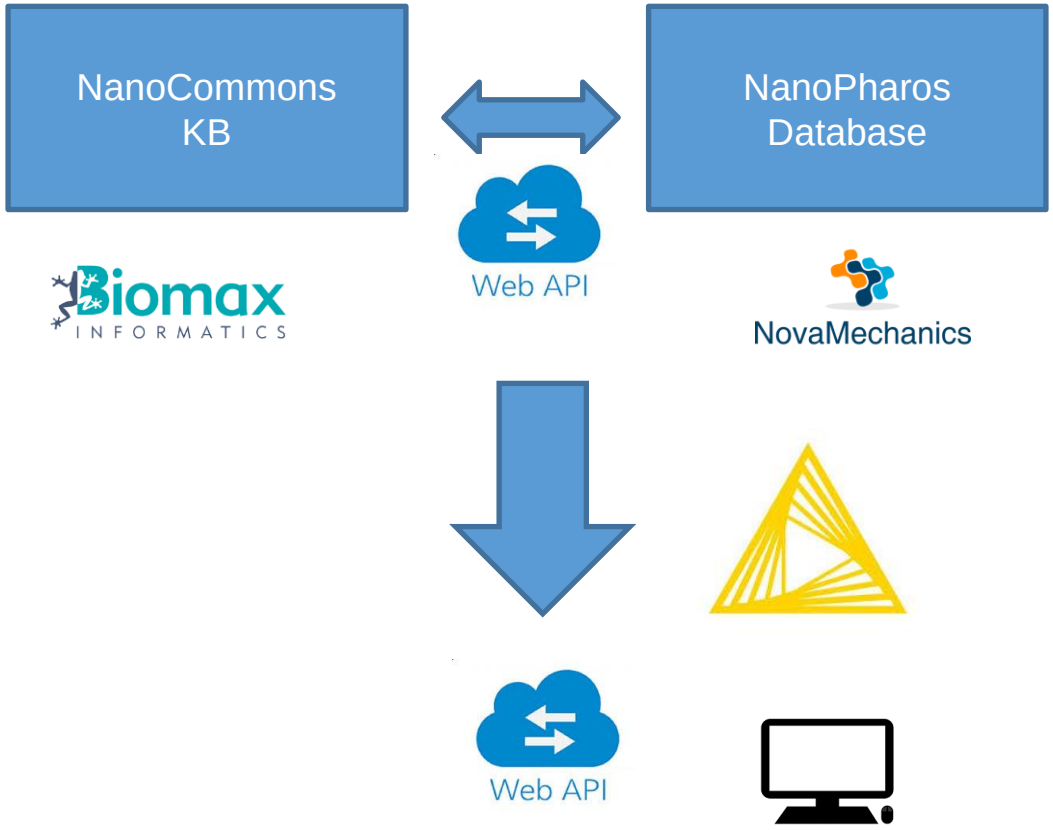


NanoSolveIT
H2020 Nanoinformatics Project

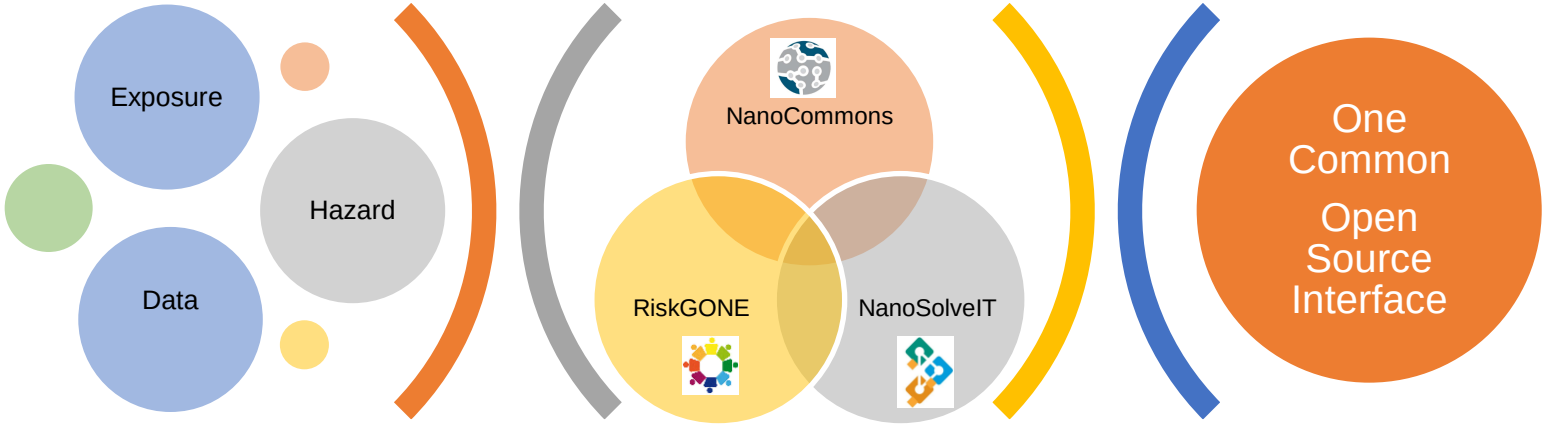
NanoCommons
Nano-Knowledge Community

Future developments, stay tuned

- Full integration of NanoCommons KB with NanoPharos database



NanoCommons KNIME nodes



NanoCommons APIs

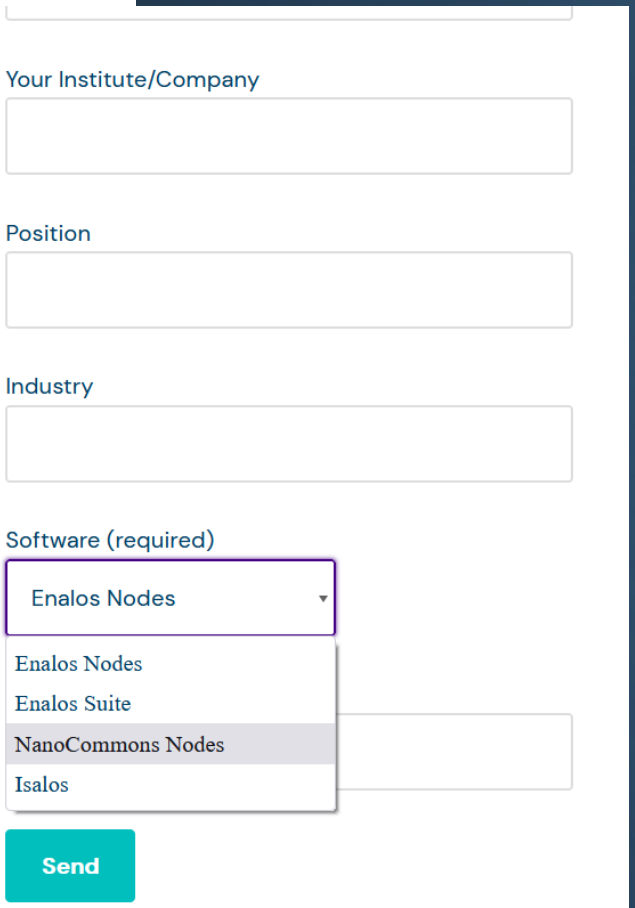
Will They Blend?

Integrated Solutions

New Entry:
CompSafeNano

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



NanoCommons
Nano-Knowledge Community

Thank you

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Cheminformatics & Nanoinformatics Excellence

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