



NovaMechanics
Cheminformatics & Nanoinformatics Excellence

NInChI prototype Server

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Enalos+ nodes for access to small molecule databases

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



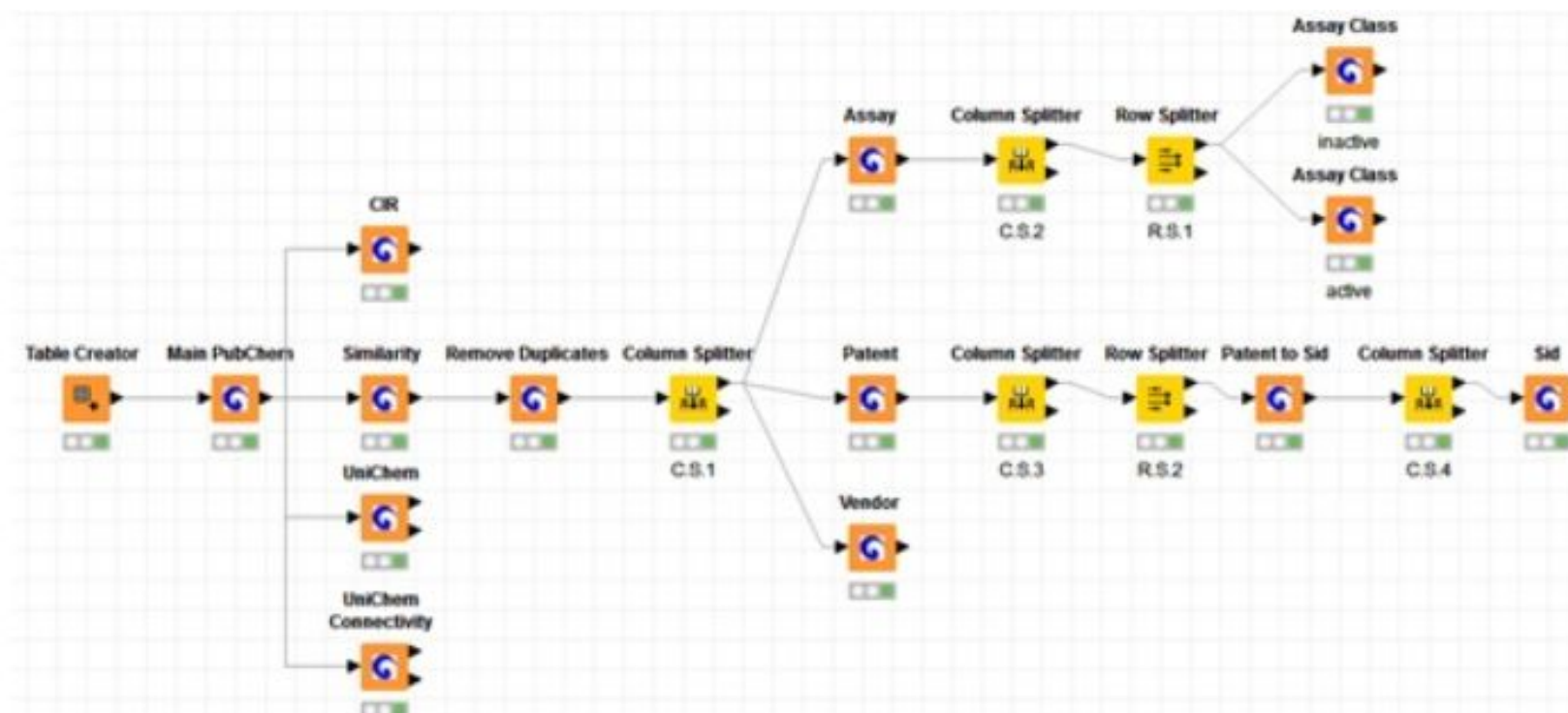
Access to >40 chemical databases :
e.g ChEMBL, PubChem, DrugBank, KEGG, ZINC,
BindinDB, eMolecules, IBM patents, SureChEMBL etc



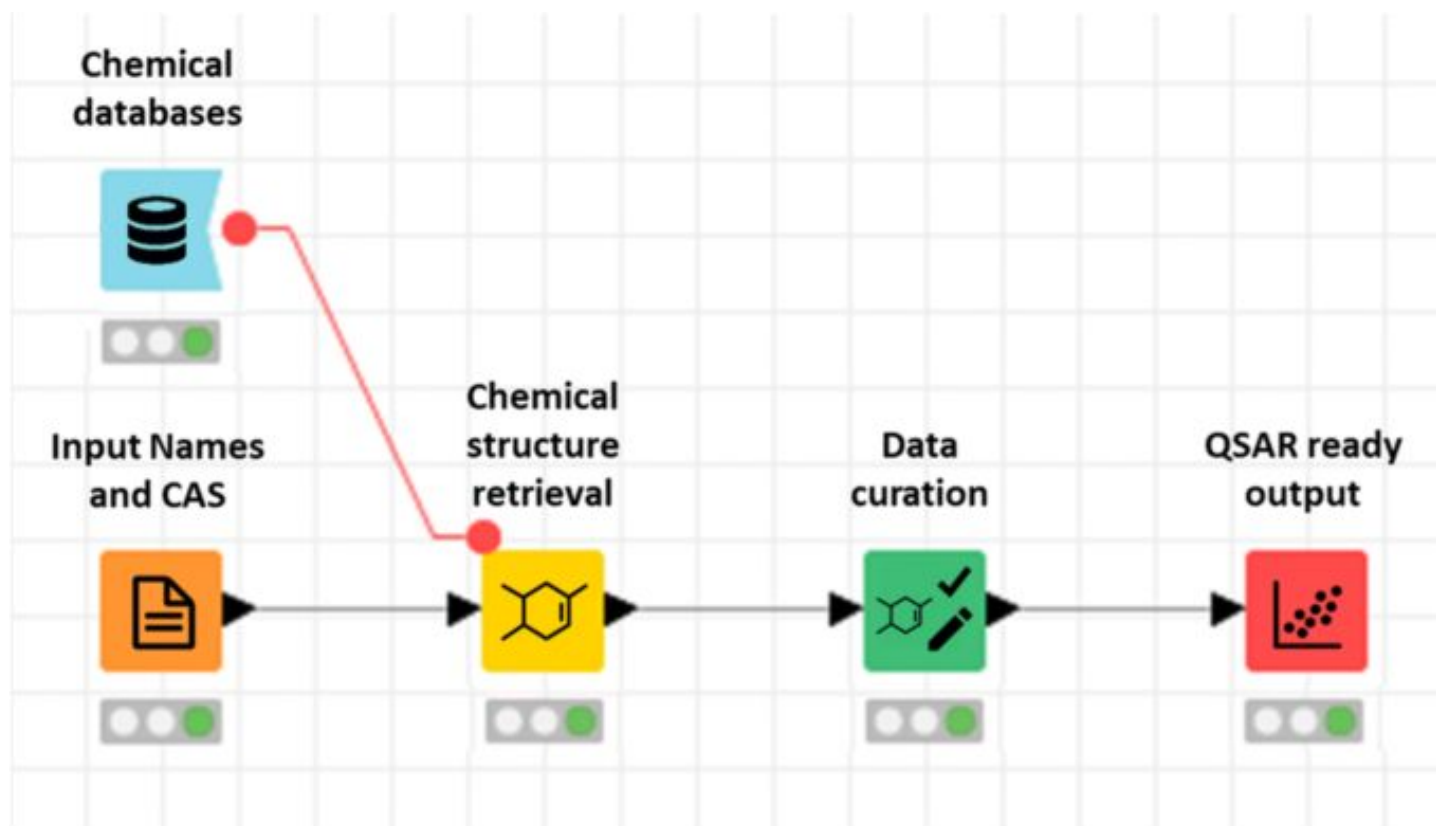
National Institutes
of Health



Blend >50 databases together with the aid of InChi

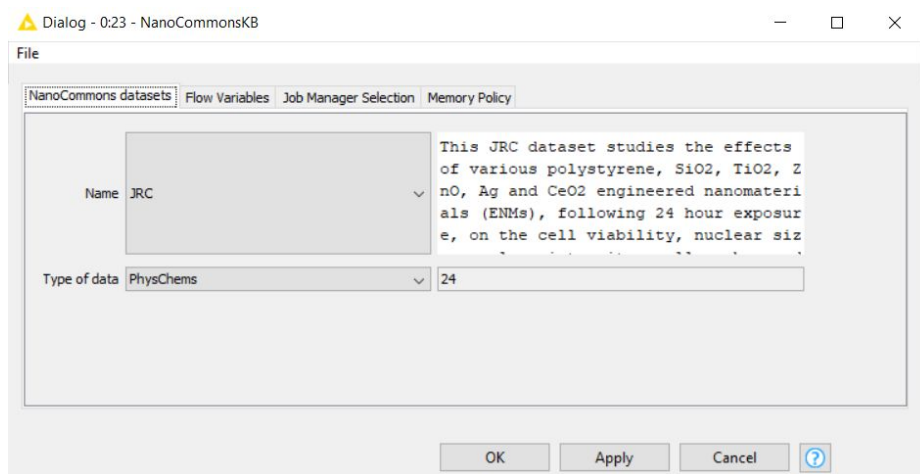
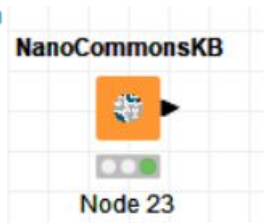
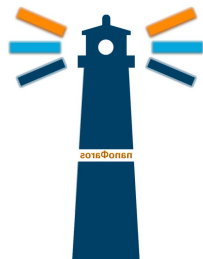


Small molecules paradigm





Nanomaterials paradigm



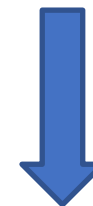
Nanocommons - NanoSolveIT NInChI Server



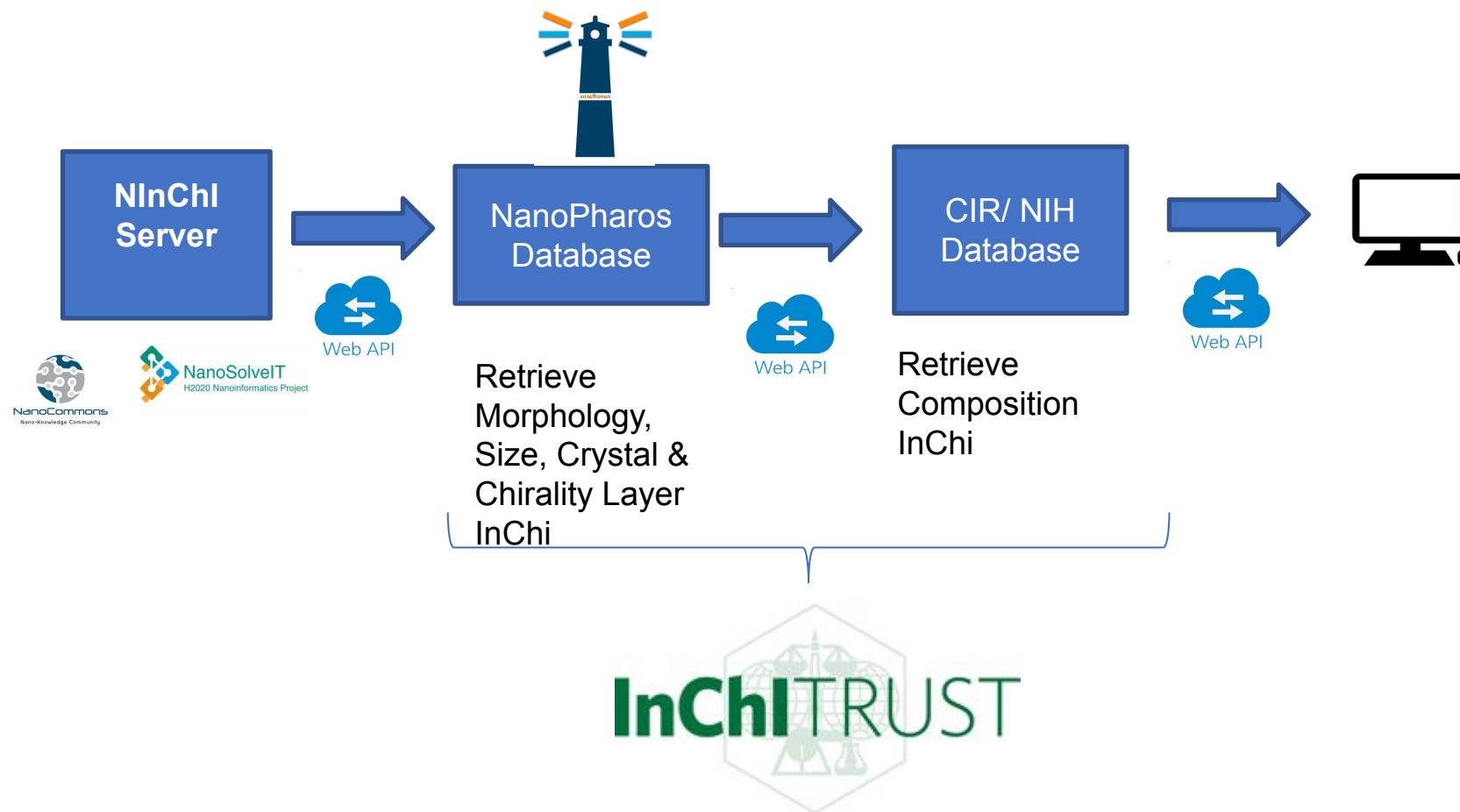
The nanomaterial is being built with a layered architecture from core to outer layers

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



Technical implementation



Future Plans: Include these steps in the InChi software

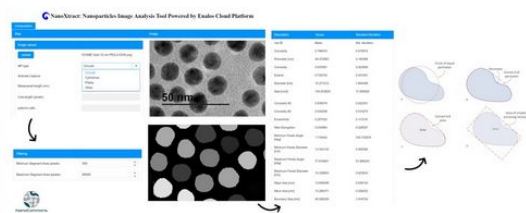


Enalos Cloud Platform

Dedicated NanoCommons webpage:

<http://www.enaloscloud.novamechanics.com/nanocommons.html>

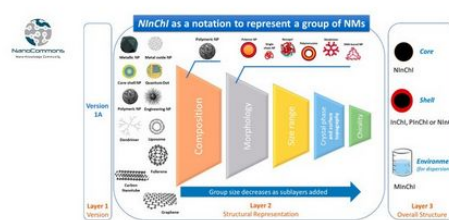
NanoXtract image analysis tool



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

[Visit service](#) [Relevant publication](#) [Documentation](#) [API](#)

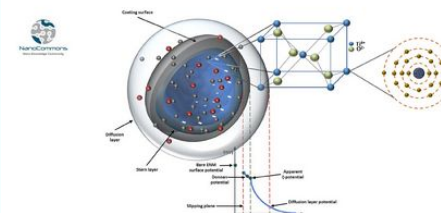
NInChI: InChI generation for nanomaterials



This tool enables the generation of NInChI for a nanomaterial (NM) of preference, assuming that the NM is specified following the inside-to-outside structure approach.

[Visit service](#) [Relevant publication](#) [Documentation](#) [API](#)

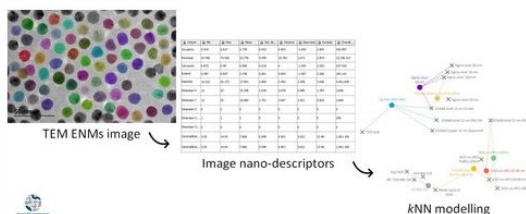
MS3bD zeta potential model



This web service provides the functionality to predict the zeta-potential in water of individual or a set of engineered nanomaterials based on physicochemical and molecular properties.

[Visit service](#) [Relevant publication](#) [Documentation](#) [API](#)

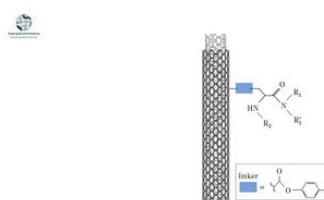
Image nanodescriptors zeta-potential model



A *k*NN/read-across model for the prediction of nanomaterials (NMs) zeta-potential based on the NM type of core, main elongation and medium's pH value.

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Safe-by-design tool for functionalised NMs



Two predictive QNAR/*k*NN models for the assessment of decorated multi-walled carbon nanotubes (MWCNTs) biological and toxicological profile.

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NanoCommons risk assessment tool



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.

[Visit service](#) [Relevant publication](#) [Documentation](#) [API](#)



NInChI server

Dedicated NanoCommons webpage:

<http://www.enalosccloud.novamechanics.com/nanocommons/NInChI/>



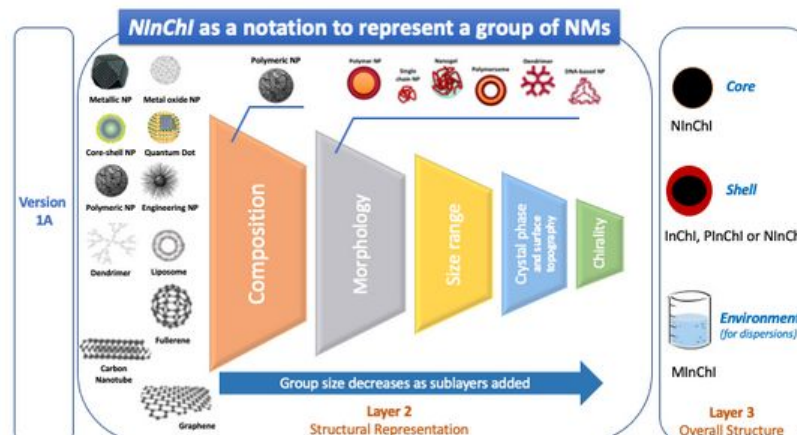
Nanocommons - NanoSolveIT NInChI Server



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NInChI





Thank for your attention

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Nicosia – Athens