

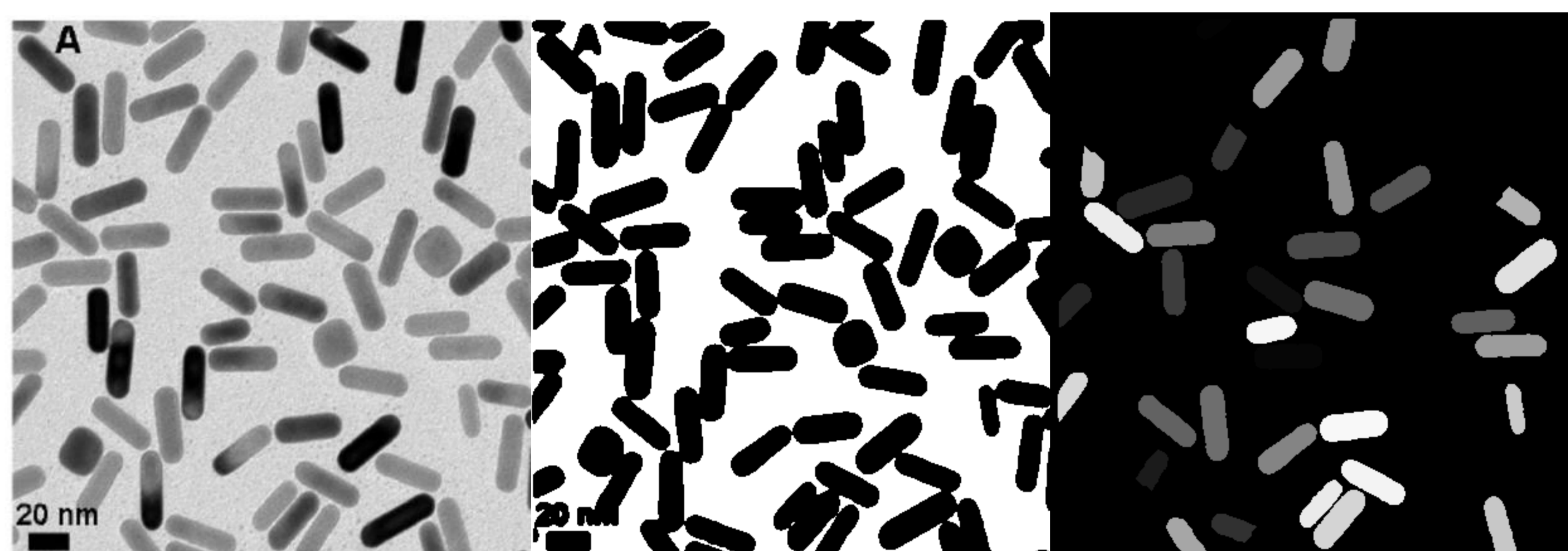
Introduction

NovaMechanics Ltd. (NovaM) is a leading nano- and cheminformatics company offering state of the art computational tools for the combination and exploitation of relevant datasets through the Enalos Cloud Platform. The Enalos Cloud Platform has been integrated with the Horizon's 2020 (H2020) e-infrastructure project NanoCommons making it available to the nanosafety community and its broadest set of stakeholders (enterprise, regulators, insurance and society broadly) via funded calls for Transnational Access (TA), as well as development of demonstration User case studies targeting the key stakeholders (academia, industry, regulators). Our services include machine and deep learning techniques for the extraction of valuable descriptors from ENM and the identification of ENM hazardous effects invisible to the naked eye in organisms (e.g. *D. magna*) from electron microscopy images and predictive modelling tools, e.g. for ENM toxicity, based on open source and in house developed algorithms. These tools can be combined with NovaM's safe by design tools for the design and development of novel, safer and fully functional ENMs.

Case Study 1

Calculation of ENM descriptors from TEM images

- Collaboration with the University of Burgos, Burgos, Spain
- Measure the size and extract image descriptors of nanomaterials of various chemistries, shapes and sizes using the Enalos NanoXtract tool
- Test the tool applicability on ENM with thin layers, images in bright and dark filed, high resolution (STEM) etc.



- Analysis of Au rod-shaped nanomaterials.
- The image is transformed into black and white to assist with ENM tracking.
- Identification and filtering of wrongly identified ENM and outliers.

Description	Values	Standard Deviation
Circularity	0.612359	0.043420
Perimeter [nm]	82.108526	13.604483
Convexity	0.959073	0.008643
Extend	0.630144	0.136092
Diameter [nm]	32.743938	5.671466
Area [nm ²]	311.256657	91.764775
Circularity #2	0.620529	0.044848
Convexity #2	0.959435	0.010182
Eccentricity	0.924059	0.030786
Main Elongation	0.617005	0.066656
Minimum Ferets Diameter [nm]	11.689719	1.319942
Maximum Ferets Diameter [nm]	31.571779	5.678232
Major Axis [nm]	32.791801	6.956281
Minor Axis [nm]	11.889457	1.526955
Boundary Size [nm]	78.743014	13.389894
Boxivity	0.831306	0.053822
Roundness	0.374595	0.070869

- Calculation of 18 size- and surface-related image nanodescriptors

Case Study 3

Read across model for the prediction of ζ -potential

- Collaboration with the University of Burgos, Burgos, Spain
- Application of TEM image nanodescriptors for the prediction of ENM ζ -potential with read-across applicability.

 Nanoinformatics Model for Zeta Potential Prediction Powered by Enalos Cloud Platform
[User Guide](#)

Row ID	Type of core	pH	Main Elongation
1	pure metal	7	0.617

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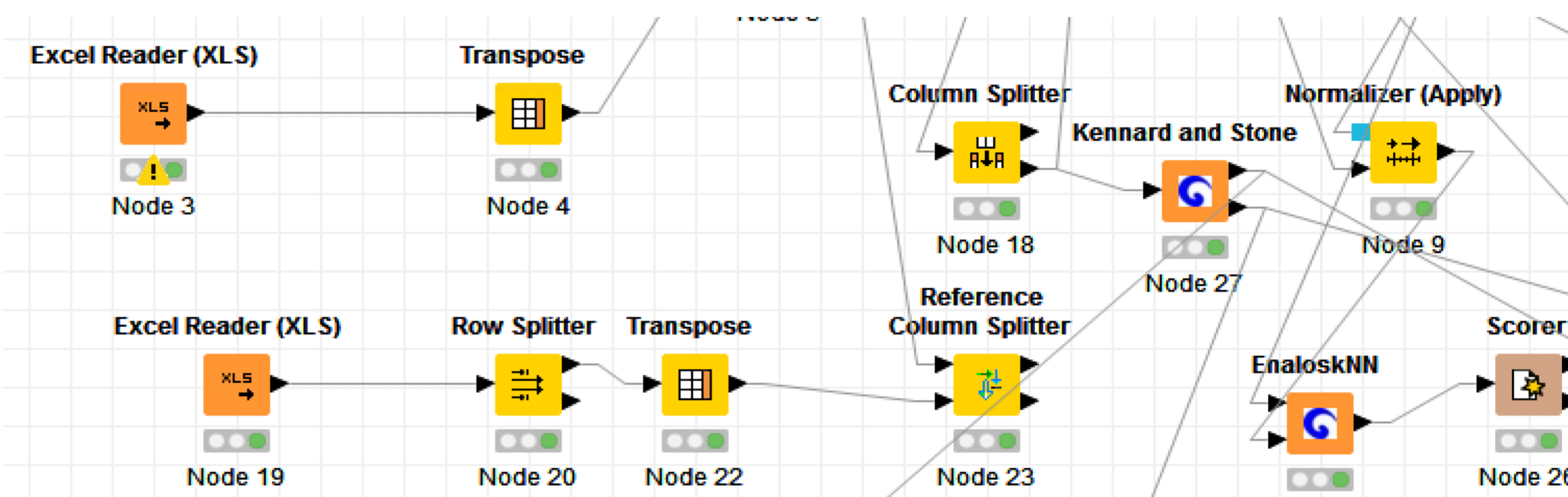
Row ID	Predicted zeta potential [mV]	Reliability
"1"	-0.7625082314807177	"reliable"

- Main elongation extracted from the TEM images through NanoXtract can be used to predict the ENM ζ -potential.
- The predictive model is based on the Enalos implementation of the *k*-closest neighbours algorithm.
- Besides the ζ -potential the model provides information on the reliability of the prediction, i.e. whether the prediction falls within the calculated domain of applicability.

Case Study 2

Genes profiling of cells exposed to carbon nanomaterials

- Collaboration with the Università del Piemonte Orientale "Amedeo Avogadro", Italy
- Studying the effects of cell exposure to carbon-based nanomaterials
- Standardization/normalization of expression profiling data Identification of the most significant Genes
- Malignant Pleural Mesothelioma (MPM) and Normal Paired Lung Parenchyma (NPLP)
- Application of modelling procedures in order to develop a predictive model
- Validation of the predictive model according to OECD principles
- Analysis of expression profiling data obtained from carbon nanomaterials exposed cells



- A detailed computational workflow has been developed using the Konstanz Information Miner (KNIME) data analytics, reporting and integration platform powered by the Enalos+ predictive modelling nodes.
- The available data were split into test and training sets.
- Modelling procedure: Enalos implementation of the *k*-closest neighbours (*k*NN) algorithm providing read-across capabilities.

ID	Gene.symbol	Gene.title
206069_s_at	ACADL	acyl-CoA dehydrogenase, long chain
226228_at	AQP4	aquaporin 4
206068_s_at	ACADL	acyl-CoA dehydrogenase, long chain
211024_s_at	NKX2-1	NK2 homeobox 1
204975_at	EMP2	epithelial membrane protein 2
212741_at	MAOA	monoamine oxidase A

- Dataset included: 41 MPM cells, 48 NPLP cells, 54,675 genes
- Results included the identification of the genes with the most statistically significant genes expression using the GEO2R algorithm
- Development of the predictive model with accuracy of 85%

Conclusions

- Nanoinformatics is a rapidly evolving field in nanosafety and nanotechnology research.
- This field requires a wide suite of tools and workflows to maximise data exploitation and lead to the uncovering of hidden patterns and novel insights regarding the behaviour and effects of ENMs.
- The Enalos Cloud Platform, integrated into the NanoCommons Knowledgebase, offers a wide range of nanoinformatics tools for use by all nanosafety stakeholders.
- Tools include image analysis, predictive modelling and safe-by-design services that are publicly available and easy to use.
- The NanoCommons Transnational Access program offers a great opportunity to take advantage of the Enalos Cloud Platform services, along with support from the NovaMechanics experts free of charge.

Check out our tools and services!

<https://infrastructure.nanocommons.eu/>

Apply for Transnational Access:

<https://www.nanocommons.eu/ta-access/>



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