Enalos Cloud Platform: A Unified Cheminformatics, Nanoinformatics and Advanced Materials Platform

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1. Introduction

The high stakes involved in developing new drugs and advanced materials make the development of alternative and reliable computer models (*in silico* models) an absolute necessity. These models can significantly aid in risk assessment of chemicals, drugs, and materials (engineered nanomaterials and advanced materials), saving time and resources spent in the experimental assessment processes. Nonetheless, there is a disconnect; many existing models for predicting the toxicity effects or other properties of small molecules and (nano)materials have not reached the wider scientific community or achieved regulatory acceptance. To bridge this gap, all models need to be made readily available through user-friendly platforms and fully documented in terms of their modelling approaches and the basis for prediction. This will empower a broader range of researchers and streamline decision-making in the design process.

2. Methods

The Enalos Cloud Platform (http://www.enaloscloud.novamechanics.com/) addresses the need for a user-friendly interface that can produce, in just a few steps and with minimum experimental inputs, toxicity predictions and property calculations for chemical structures, advanced and/or engineered (nano)materials through web-services [1]. The platform integrates reliable, open-source software like KNIME, WEKA, ImageJ, R, Python, LAMMPS, DeepChem etc., alongside proprietary tools (e.g., Enalos+ nodes which are purposefully designed to bridge these tools and facilitate streamlined computational workflows). Predictions and calculations are performed shortly after data input and are accompanied by an indication of their reliability based on the results (applicability domains) of the fully validated models running in the background. The produced results can be downloaded for further analysis and exploration contributing in this way to increased model transparency and accessibility. Depending on the model

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used, the results can even provide insights into material properties at the microscopic or macroscopic levels and their similarities to other substances.

3. Results

Enalos Cloud Platform Platform (Figure 1) is a user-friendly online portal offering 46 cutting-edge tools for researchers in material design, drug discovery, and nanosafety. The computational tools and models were developed in the context of 8 EU-funded projects. These web-services, categorized for easy exploration (i.e., cheminformatics, nanoinformatics, materials engineering, image analysis, exposure and biokinetics models), allow users of all backgrounds (including those with no programming skills) to leverage advanced models for tasks like material property simulation, virtual drug candidate screening, and sustainable material design, all through a carefully designed interface allowing for simple and effective use. For instance, users interested in materials design can employ the *Nanotube construction tool* for the digital construction of energy minimized nanotubes of single layer materials and for the calculation of their atomic descriptors [2], and the *NanoConstruct* tool for the digital reconstruction of energy minimized spherical and ellipsoid nanoparticles based on their CIF files [3]. Users interested in the design of safe and sustainable nanomaterials can employ the *SafeNanoScope* tool [4] and the *Ecotox read-across* models [5] to assess the adverse effects of their materials against human liver cells (HepaRG) and the waterflea *Daphnia Magna*, respectively.

The web-services provided through Enalos Cloud Platform are completely free and accessible, with no need for logins. They come with thorough learning resources, including user guides and video tutorials, and most are supported by scientific publications explaining their development (e.g., modelling steps, validation results, data resources, used software) as well as full documentation according to the standard QSAR model report format as required by the European Chemicals Agency as part of the criteria for regulatory acceptance. This openness allows users to understand the underlying scientific models and the creation process, fostering trust in the service's results.

4. Conclusions

While robust *in silico* models are crucial for efficient drug and material design, their accessibility remains a hurdle for the wider stakeholders' community (e.g., experimentalists, regulatory agencies, etc.). This is because using these models often requires working within programming environments and writing scripts, which can be challenging for those without a programming background. The Enalos Cloud Platform bridges this gap by offering a user-friendly web interface for validated models built upon robust open-source software. This ensures transparency and fosters trust in the results, which include rapid properties and toxicity predictions. By making these powerful tools accessible, the Enalos Cloud Platform empowers researchers to streamline material design and accelerate scientific discovery.

Figure 1: Screenshot of the Enalos Cloud Platform web-services page showing a selection of the available predictive models and web-services.

5. References

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