

Life Sciences Thematic Services at the Biomedical Research Foundation, Academy of Athens

National End-Users NI4OS-Europe Training - CY
6 June 2022

Dr. Zoe Cournia
Life Sciences Coordinator
Biomedical Research Foundation
Academy of Athens
Greece

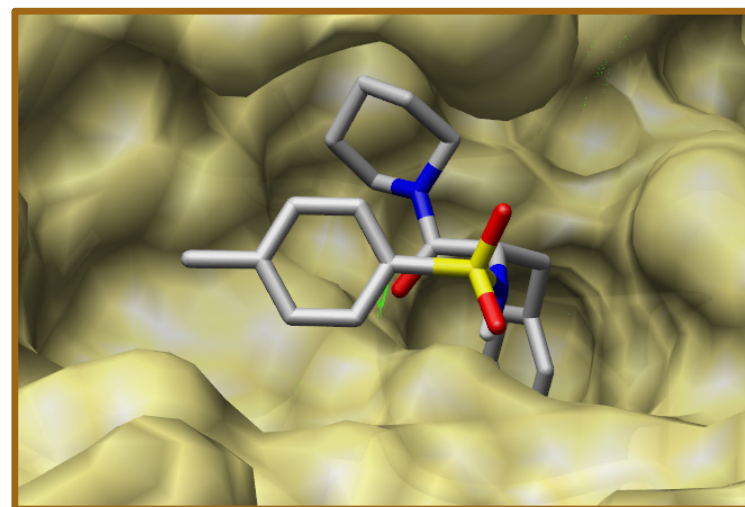
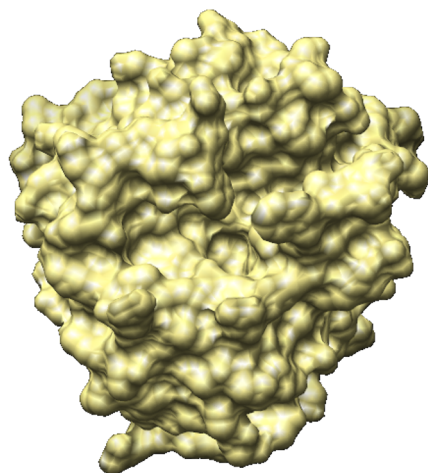
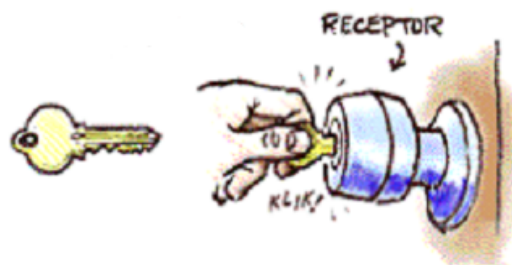


- ❑ ChemBioServer 2.0
- ❑ FEPrepare
- ❑ DREAMM
- ❑ Nanocrystal
- ❑ Ingredio
- ❑ OpenBioMaps
- ❑ REVIGO
- ❑ EEGHUB
- ❑ DICOM
- ❑ MelGene

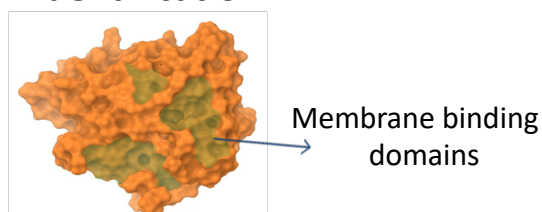
LS Thematic Services: Drug Discovery

- ❑ Identify important genes for a disease
- ❑ Targeting/inactivating genes (proteins) of the pathogen with small molecules = drugs

**PRECISION MEDICINE
TARGETED THERAPY**

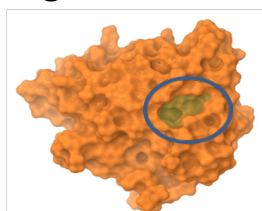


1. Binding Site identification and Membrane binding domain identification

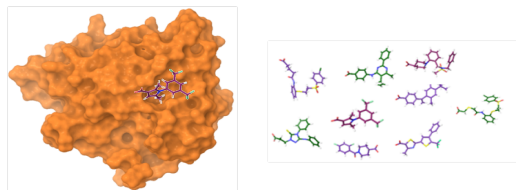


DREAMM

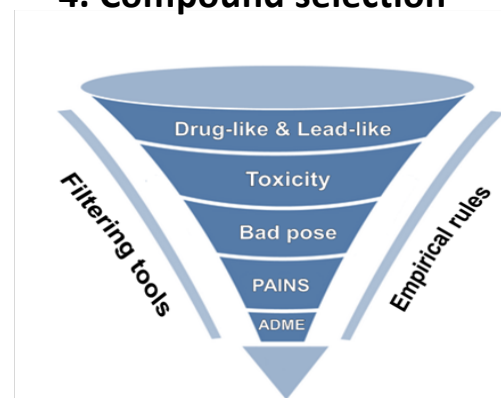
2. Binding Site identification



3. Docking and Scoring



4. Compound selection



CHEMBIOSERVER

6. *In vitro* & *in vivo* assays

7. Lead Optimization

FEPprepare

8. Drug Delivery

Nanocrystal

Drug discovery tools onboarded on NI4OS-Europe

 **EXPLORE**
NI4OS-Europe Catalogue

Thematic services

ChemBioServer is a publicly available web application for effectively **filtering and clustering chemical compounds** used in drug discovery.

<http://chembioserver.vi-seem.eu/>

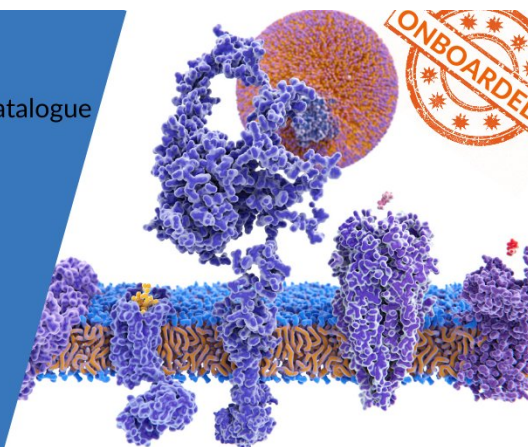


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NI4OS-Europe Catalogue

Thematic services

DREAMM is a novel web-based tool that **predicts the protein-membrane interfaces of peripheral membrane proteins** using ensemble machine learning.

<http://dreamm-ni4os.eu/>

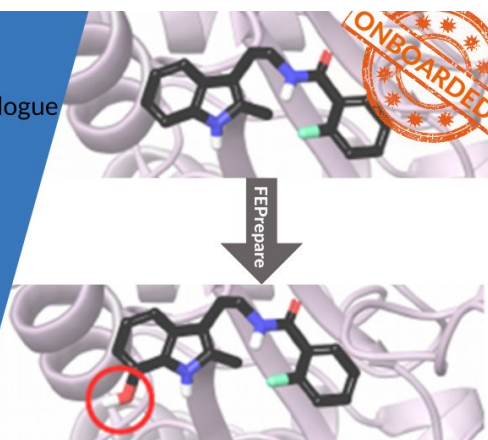


 **EXPLORE**
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Thematic services

FEPPrepare is a webserver, which automates the set-up procedure for performing **NAMD/FEP simulations**.

<http://fepprepare.vi-seem.eu>

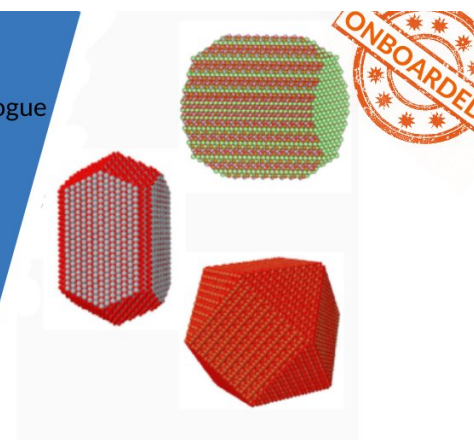


 **EXPLORE**
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Thematic services

NanoCrystal is a novel web-based **crystallographic tool** for the construction of nanoparticles from any material crystal structure.

<http://nanocrystal-seem.eu>



DREAMM: Predicting cavities at protein-membrane interfaces

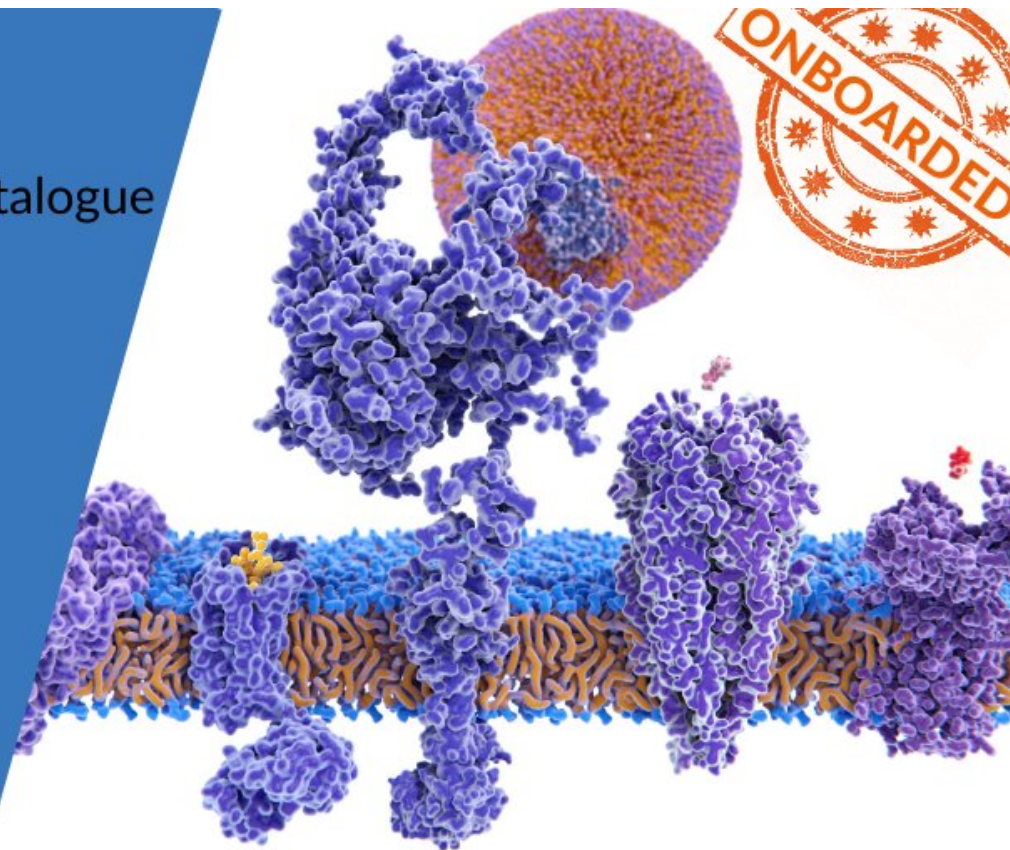


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Thematic services

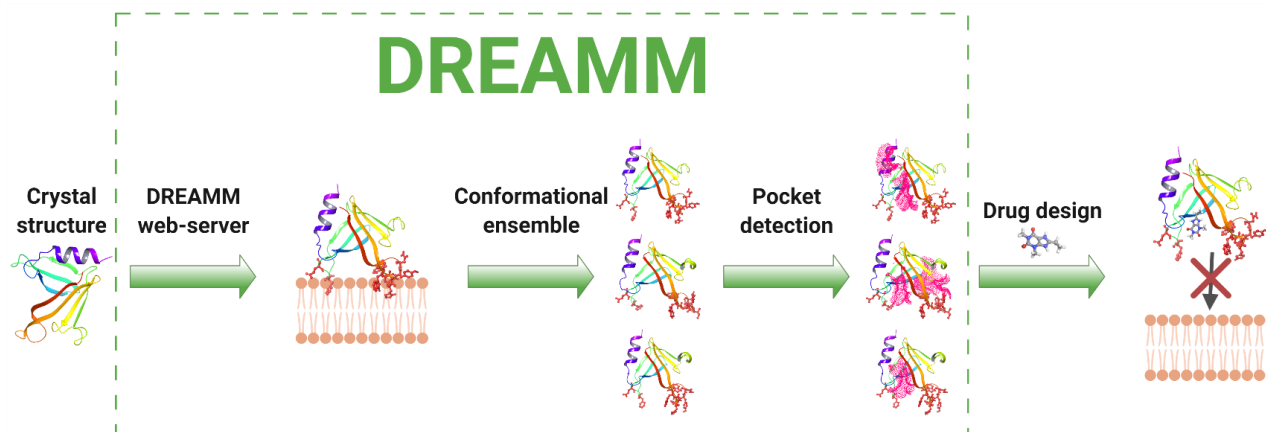
DREAMM is a novel web-based tool that **predicts the protein-membrane interfaces of peripheral membrane proteins** using ensemble machine learning.

<http://dreamm-ni4os.eu/>








DREAMM Main Features

- ❑ Use an ensemble machine learning model that predicts the protein-membrane interfaces of peripheral membrane proteins
- ❑ Predict binding sites in the predicted protein-membrane regions in conformational ensembles using P2Rank
- ❑ Cluster the predicted binding sites for all protein conformations based on the binding sites center coordinates
- ❑ Create a novel web-based tool for predicting and drugging protein-membrane interfaces



DREAMM Video Example

Prediction of protein-membrane in x +

← → ↻   https://dreamm.ni4os.eu/index.php   

Manual

Video example

Download datasets

Check this box to search for binding sites (using P2Rank) near the predicted membrane-penetrating residues in protein ensembles:

PDB ID: and Chain

Upload

OR

Upload PDB file

DREAMM: Predicting cavities at protein-membrane interfaces

- ❑ Information in NI4OS-Europe Agora:
https://catalogue.ni4os.eu/?_=/resources/bc445004-2869-43c9-9ef3-e5aa6b44d2e3
- ❑ Access: <https://dreamm.ni4os.eu/>
- ❑ Training Material:
<https://training.ni4os.eu/mod/scorm/view.php?id=1187>

Chatzigoulas and Cournia, Briefings in Bioinformatics, 2021

ChemBioServer: A drug discovery tool

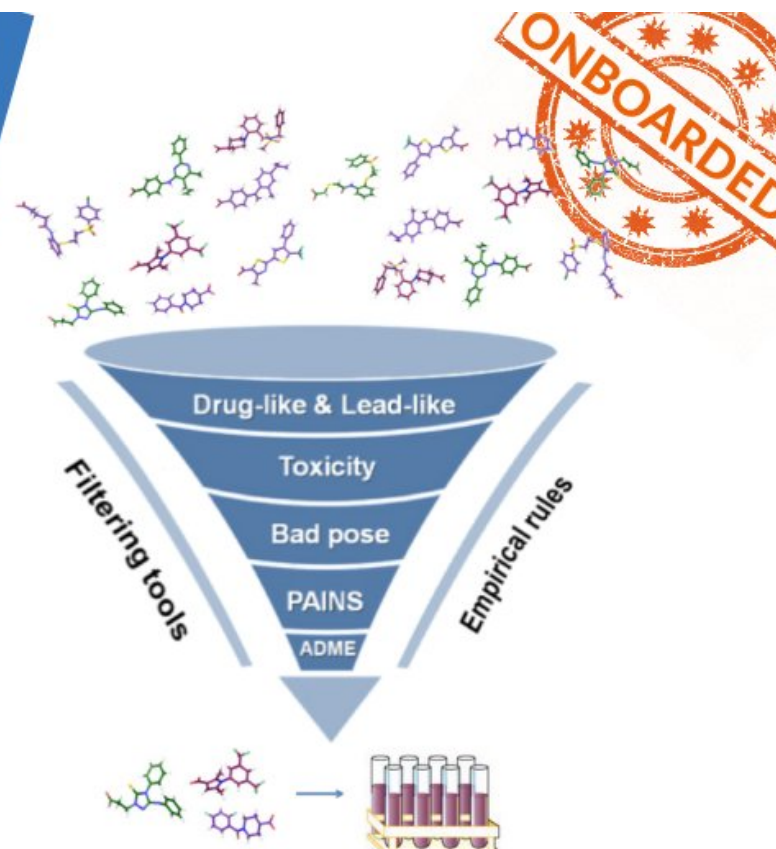


EXPLORE
NI4OS-Europe Catalogue

Thematic services

ChemBioServer is a publicly available web application for effectively **filtering and clustering chemical compounds** used in drug discovery.

<http://chembioserver.vi-seem.eu/>



ChemBioServer Main Features

ChemBioServer 2.0

- Uploading and Browsing Compounds in 2D and 3D.
- Filtering of compounds based on physicochemical properties.
- Substructure filtering of compounds based on custom sdf files.
- Van der Waals filtering using distance and energy tests.
- Toxicity filtering using specific organic toxic roots.
- Cross-Docking molecules.
- Hierarchical clustering with 4 different distances.
- Affinity Propagation clustering, providing exemplars for each cluster.
- Structural Similarity Network Visualization and Analysis.
- Visualization of compounds' properties.

Athanasiadis, Cournia, Spyrou,
Bioinformatics. 2012

Karatzas et al, Spyrou Bioinformatics.
2019

ChemBioServer: A drug discovery tool

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- ❑ Access: <http://chembioserver.vi-seem.eu/>
- ❑ Training Material:
<https://training.ni4os.eu/mod/scorm/view.php?id=1186>

FEPprepare: A lead optimization tool

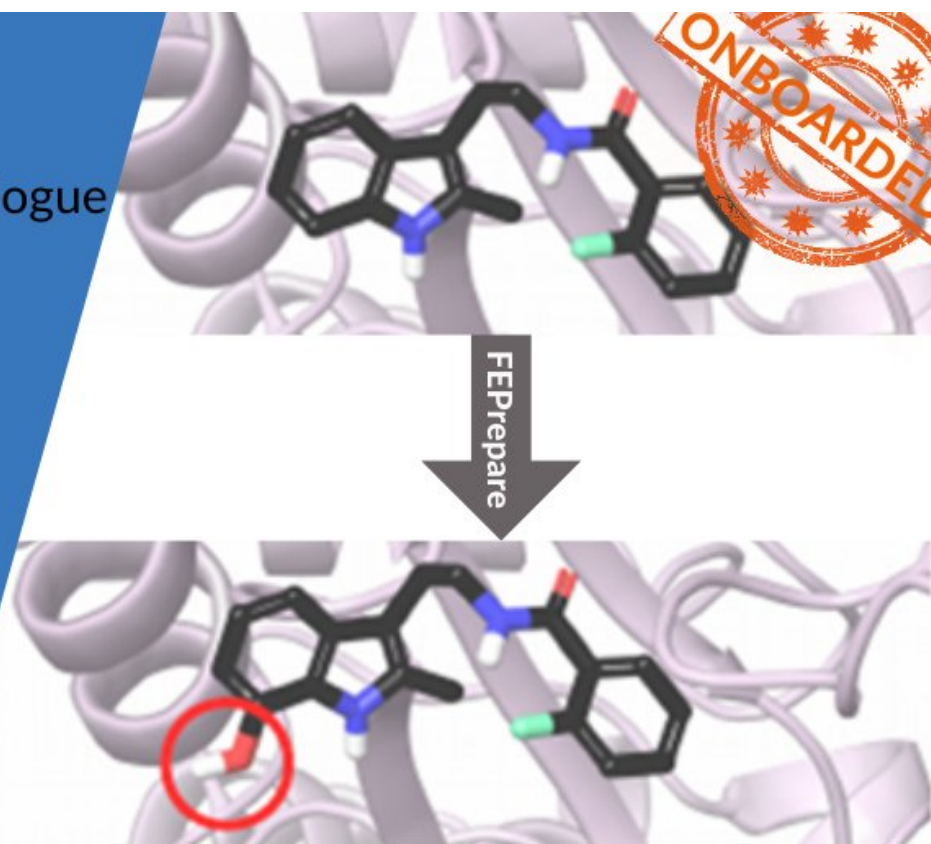


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Thematic services 

FEPprepare is a webserver,
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<http://fepprepare.vi-seem.eu>



FEPPrepare: A lead optimization tool

- Information in NI4OS-Europe Agora:
https://catalogue.ni4os.eu/?_=/resources/4d2f5c58-d32d-46ce-b075-8b278889fe96
- Access: <https://fepprepare.vi-seem.eu/>
- Training
Material <https://training.ni4os.eu/mod/scorm/view.php?id=1183>

Zavitsanou et al... Cournia, J Chem Inf Model 2021

Nanocrystal: construction of nanoparticles for simulation

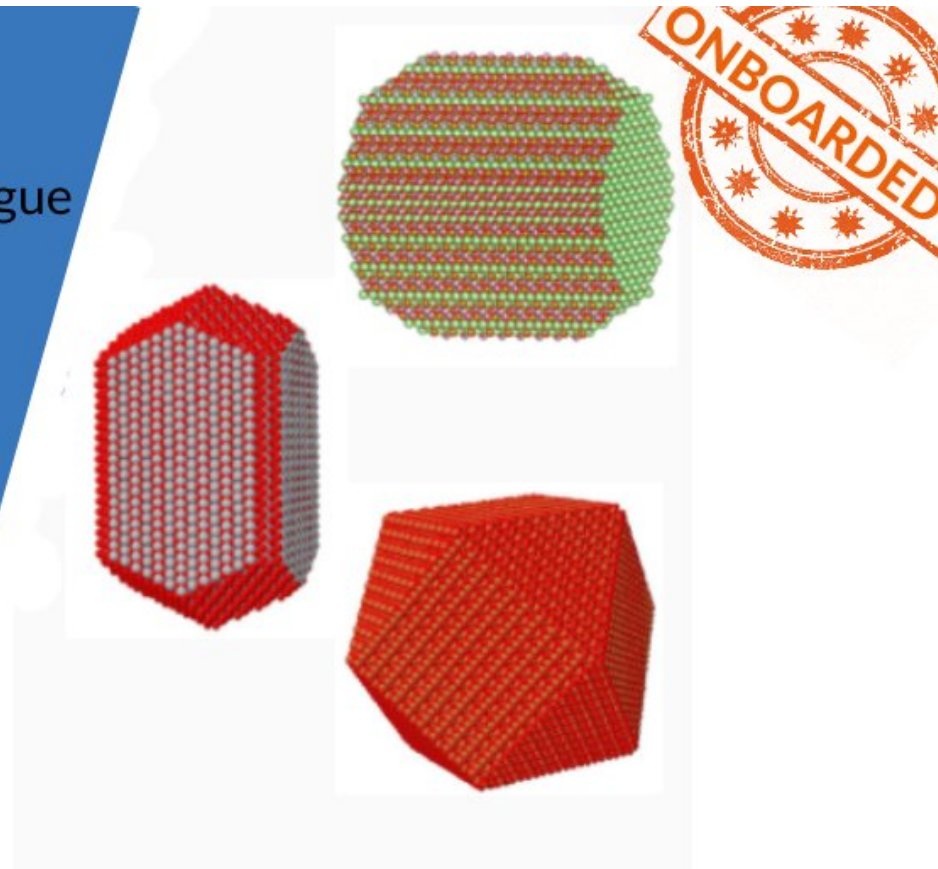


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Thematic services 

NanoCrystal is a novel web-based **crystallographic tool** for the construction of nanoparticles from any material crystal structure.

<http://nanocrystal-seem.eu>



Nanocrystal Video Example

A crystallographic tool for the construction of nanoparticles

This tool constructs nanoparticles for simulation of any material given as input the crystal structure, the size of the nanoparticle, and the preferred growing planes and energies. As a result you have the choice to download the coordinates of the atoms in a .xyz file and a .pdb file. For more information please read our paper or the manual

[Manual](#)[Video example](#)[Download example](#)

Select a .cif file No file selected.

Check this box to create spherical nanoparticle:

Check this box to create stoichiometric nanoparticle:

Choose Miller indices: and the corresponding minimum surface energy:

[Add new Miller indices and energy](#)

Choose maximum radius of nanoparticle in (Å):

Welcome to Nanocrystal. This tool may be used to construct nanoparticles given

the crystal structure as input,

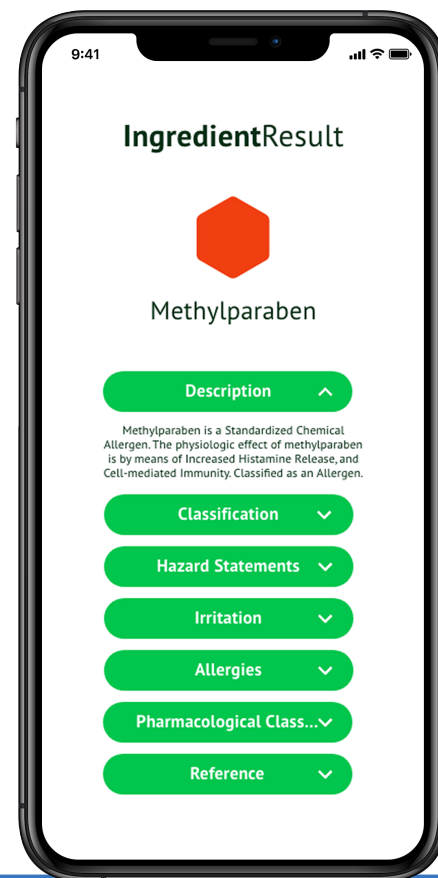
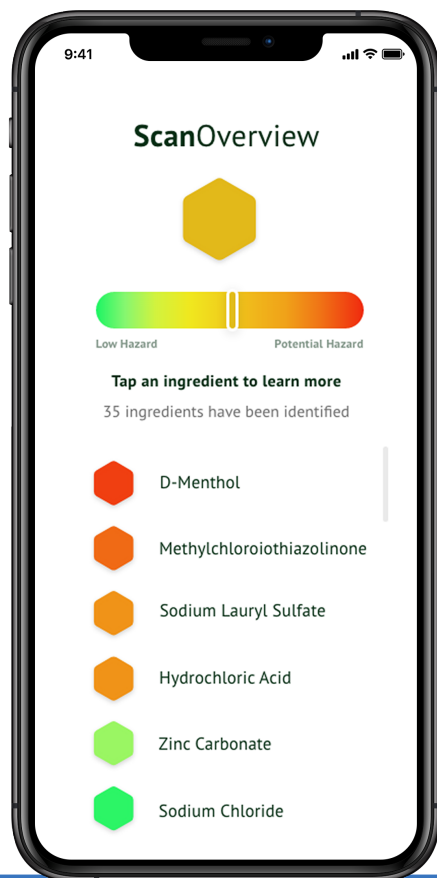
Nanocrystal: construction of nanoparticles for simulation

- ❑ Information in NI4OS-Europe Agora:
https://catalogue.ni4os.eu/?_=/resources/c1f8d7fb-4250-4278-ba8d-4d1df4a85df5
- ❑ Access: <http://nanocrystal-seem.eu>
- ❑ Training Material:
<https://training.ni4os.eu/mod/scorm/view.php?id=1181>

Chatzigoulas and Cournia, J Chem Inf Model, 2018

Ingredio: Users can check if the product has ingredients with potential hazards for human health

Unique proprietary scientific algorithms & scoring function



Level of hazard per ingredient*



* Information sourced from institutional databases



Ingredio Main Features

Feature 1

Develop text mining and Machine Learning algorithms to extract OpenAIRE data linking chemical ingredients of food & cosmetics to potential health hazards

Feature 3

Identifying new chemical ingredients from OpenAIRE data to enrich the OpenAIRE research graph & the Ingredio database

Feature 2

Support the curation of OpenAIRE data with appropriate metadata schemas for efficient integration of information in the OpenAIRE Research Graph

Feature 4

Identify causal relationships of chemical ingredients with hazards using the collected information



Ingredio is FAIR compatible– Reusability: Video Example



Ingredio Application



Enhancing the food & cosmetics OpenAIRE Research Graph for consumer health

Ingredio application is a natural processing language (NLP) application that offers a pipeline of three services related to biomedical text. The application is able to classify biomedical text based on certain features of its content, extract compound names and infer causal relations from the text, however it is experimental and is not meant to replace human curation. It's main use is to showcase how this can be used as a high-throughput and high precision language filtering software for large scale biomedical data. The codebase of the application can be found [here](#).

Usage

While each stage can be used independently, the application facilitates the sequential usage in its three stages (Classification, Entity Extraction and Causality Inference). Each stage involves submitting text. If the query bears results, the text is forwarded to the next stage filling all the required information for the submission of the next stage.

Classification

The classification stage of the application employs different machine learning models that were trained independently with the aim to be able to classify biomedical text according to its relevance with toxicity of compounds found in foods and cosmetics. This stage is based on combining four different [ML algorithms](#) to reach a consensus regarding the classification of the text.

Classify Text

Ingredio: Natural Language Processing to process biomedical text

- Information in NI4OS-Europe Agora:

https://catalogue.ni4os.eu/?_=/resources/7cc4118c-e637-4463-a841-92831e897368

- Access: <https://ingredio.ni4os.eu/>

- Training Material:

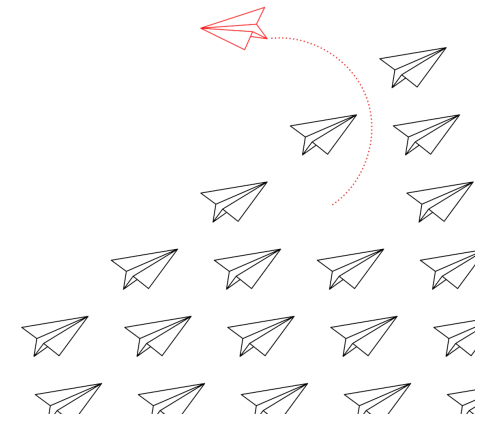
<https://training.ni4os.eu/mod/scorm/view.php?id=1182>

Benefits for researchers using EOSC resources

- ❑ Open data: excellent opportunity for ECRs who often have neither the funding nor the network of a senior scientist
- ❑ Access datasets from colleagues without duplicating data and enable Open Innovation
- ❑ Increased robustness and reliability of scientific work
- ❑ Store, manage, analyze TB of produced data
- ❑ Training on Best Practices for Open Science & FAIR principles for various data
- ❑ More efficient dataset searching based on metadata
- ❑ Onboard web-based thematic services in one common, unified portal
- ❑ Help with evaluation and certification of datasets (e.g. FAIRsFAIR)
- ❑ Gain Visibility
- ❑ Opportunities to collaborate with Pharma Industry opened up for my lab / Networking

Benefits for researchers using EOSC as service providers

- ❑ Publish, share and advertise services & resources
- ❑ Get statistics about access & feedback
- ❑ Free online platform to manage service requests
- ❑ Interact with users more efficiently & understand needs
- ❑ Get support for user authentication
- ❑ Open Service to a wider base
- ❑ Boosts visibility and discoverability → citations → impact
- ❑ Increase computational power of your lab / company with reliable core services



Thanks for your attention!

zcournia@bioacademy.gr