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

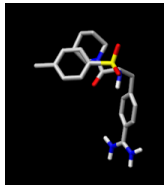
NI4OS-Europe on-boarded/candidate LS Thematic Services

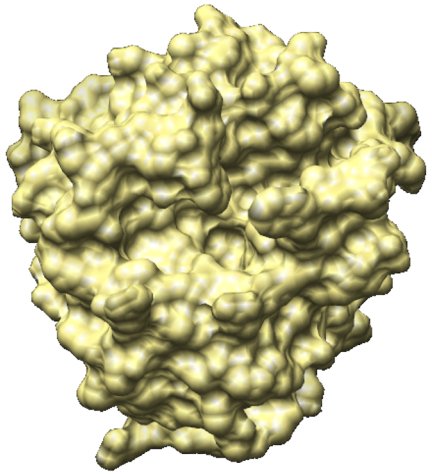
- ChemBioServer 2.0
- FEPrepare
- DREAMM
- Nanocrystal
- Ingredio
- OpenBioMaps
- REVIGO
- EEGHUB
- DICOM
- MelGene

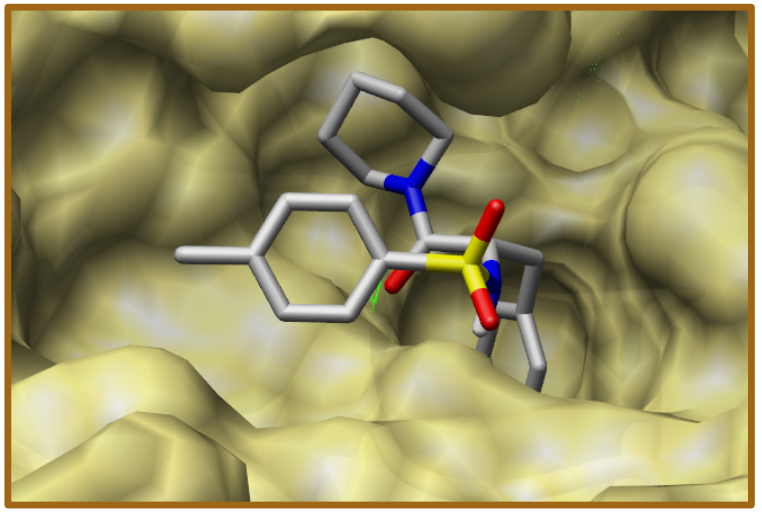
LS Thematic Services: Drug Discovery

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

PRECISION MEDICINE
TARGETED THERAPY

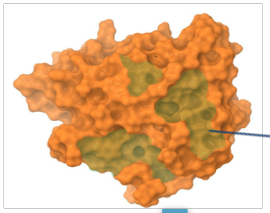






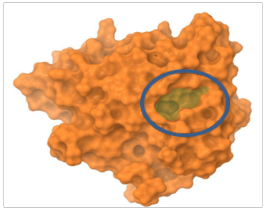
LS Thematic Services: Drug Discovery

1. Binding Site identification and Membrane binding domain identification

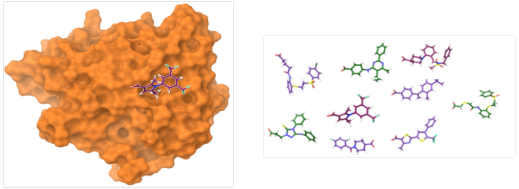


DREAMM

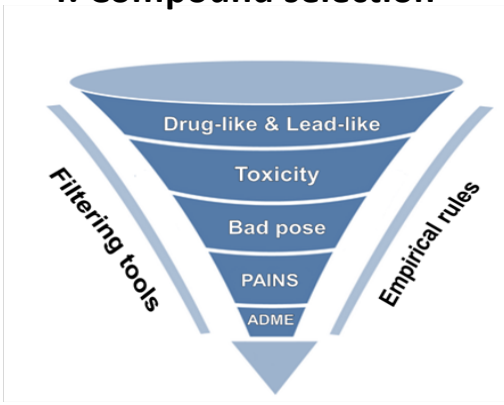
2. Binding Site identification



3. Docking and Scoring



4. Compound selection



CHEMBIOSERVER

6. *In vitro & in vivo* assays

7. Lead Optimization

FEPrepare

8. Drug Delivery

Nanocrystal

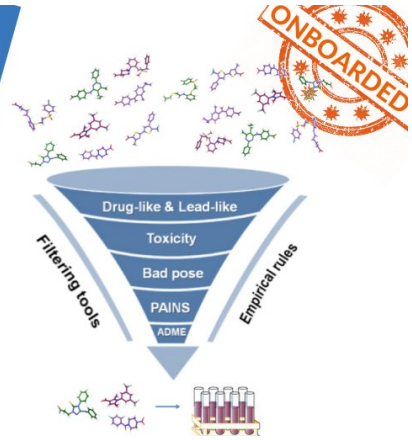
Drug discovery tools onboarded on NI4OS-Europe

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/

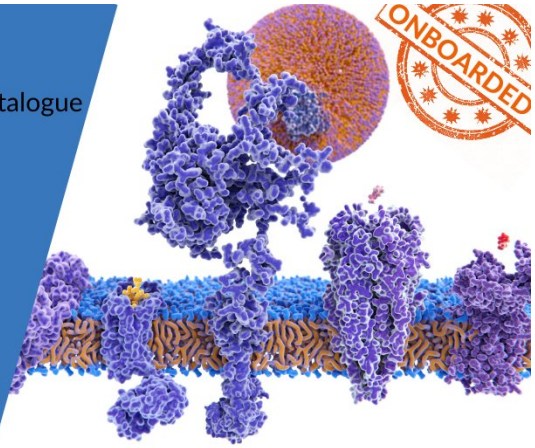


EXPLORE
NI4OS-Europe Catalogue

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/

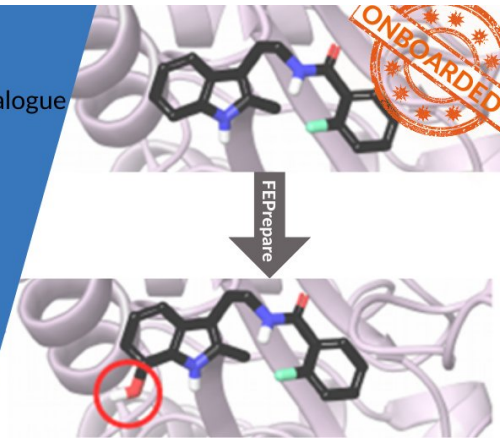


EXPLORE
NI4OS-Europe Catalogue

Thematic services

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

http://feprepare.vi-seem.eu

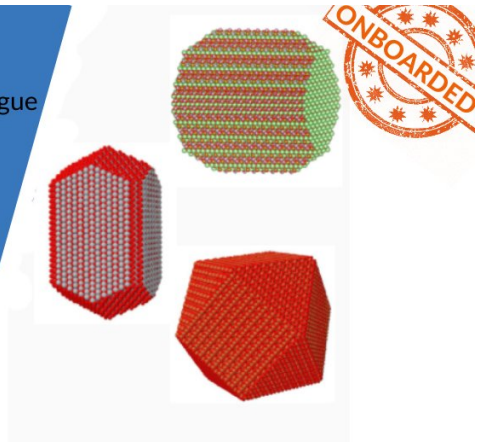


EXPLORE
NI4OS-Europe Catalogue

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

NI4OS Europe

EXPLORE
NI4OS-Europe Catalogue

Thematic services

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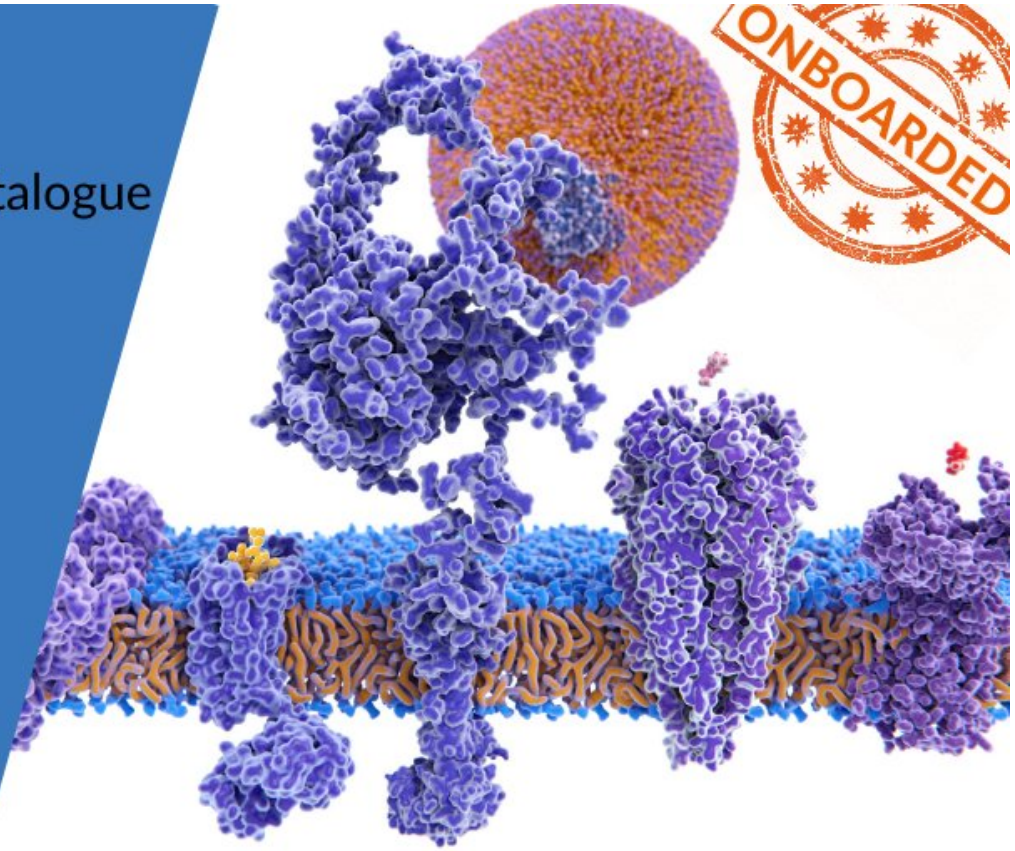
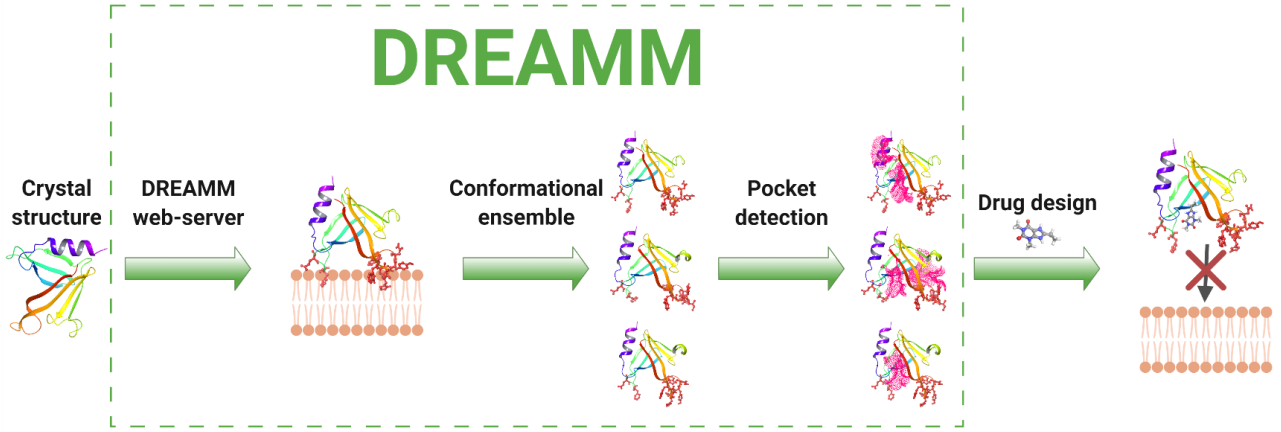
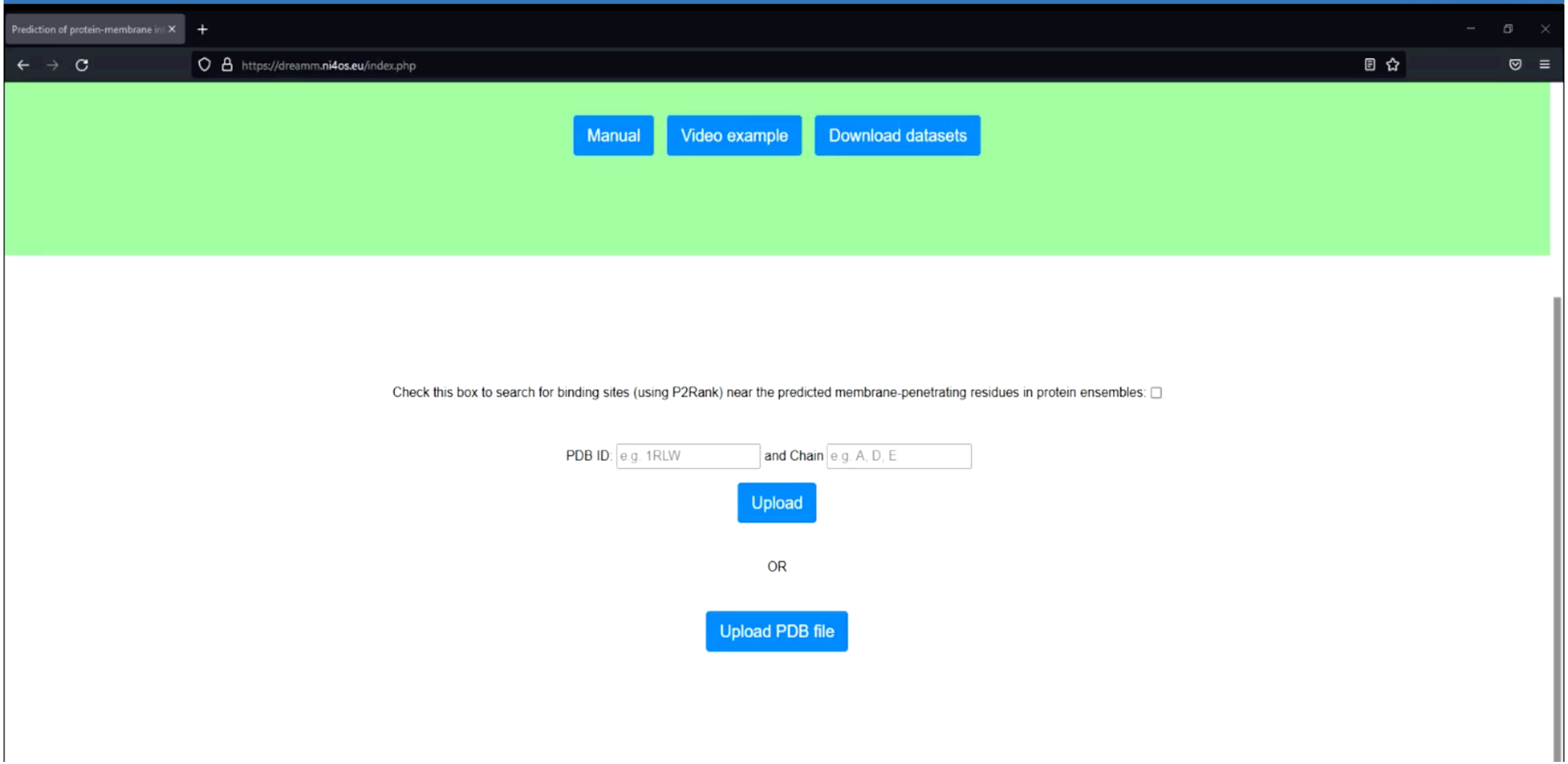


DREAMM Main Features

- 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



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

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NI4OS-Europe Catalogue

Thematic services

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

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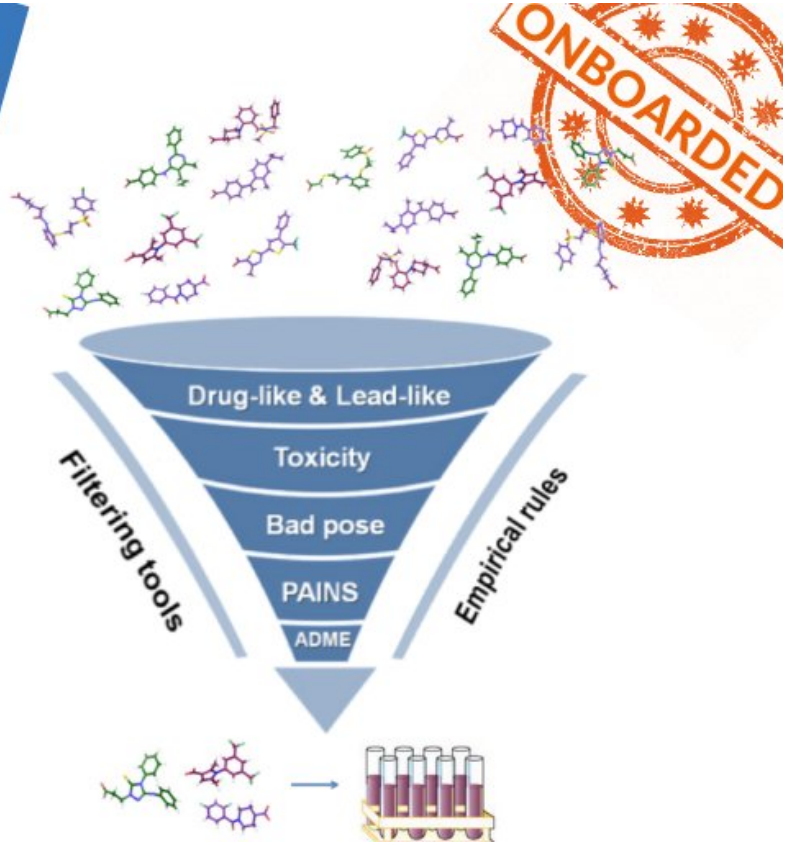


ChemBioServer Main Features

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.

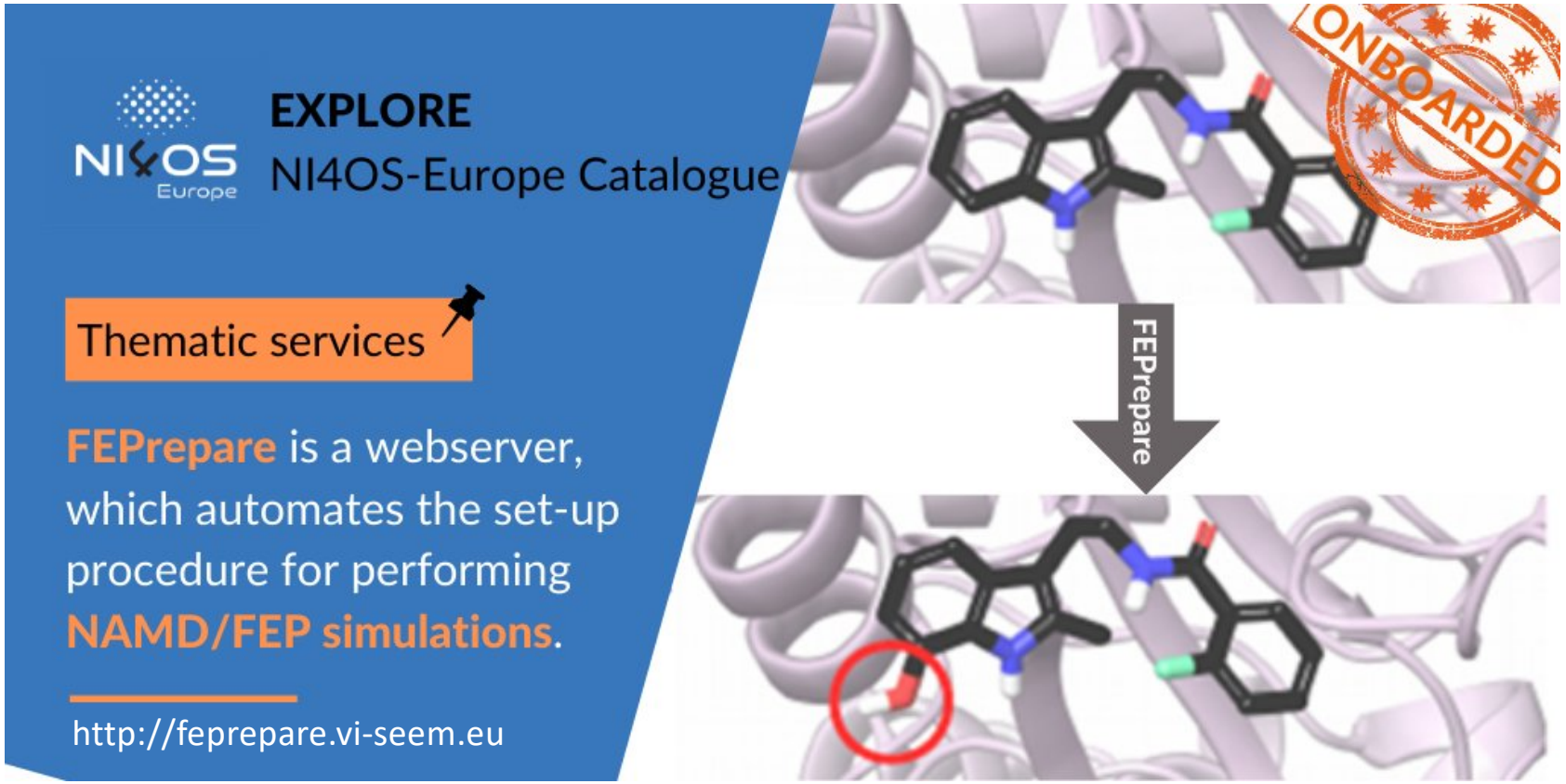
Athanasiadis, Cournia, Spyrou, Bioinformatics. 2012

Karatzas et al, Spyrou Bioinformatics. 2019

ChemBioServer: A drug discovery tool

- Information in NI4OS-Europe Agora: https://catalogue.ni4os.eu/?_=/resources/d06512f9-b287-4452-8a2f-5742eccb44c4
- Access: http://chembioserver.vi-seem.eu/
- Training Material: https://training.ni4os.eu/mod/scorm/view.php?id=1186

FEPrepare: A lead optimization tool



FEPrepare: A lead optimization tool

- Information in NI4OS-Europe Agora: https://catalogue.ni4os.eu/?_=/resources/4d2f5c58-d32d-46ce-b075-8b278889fe96
- Access: https://feprepare.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

NI4OS Europe

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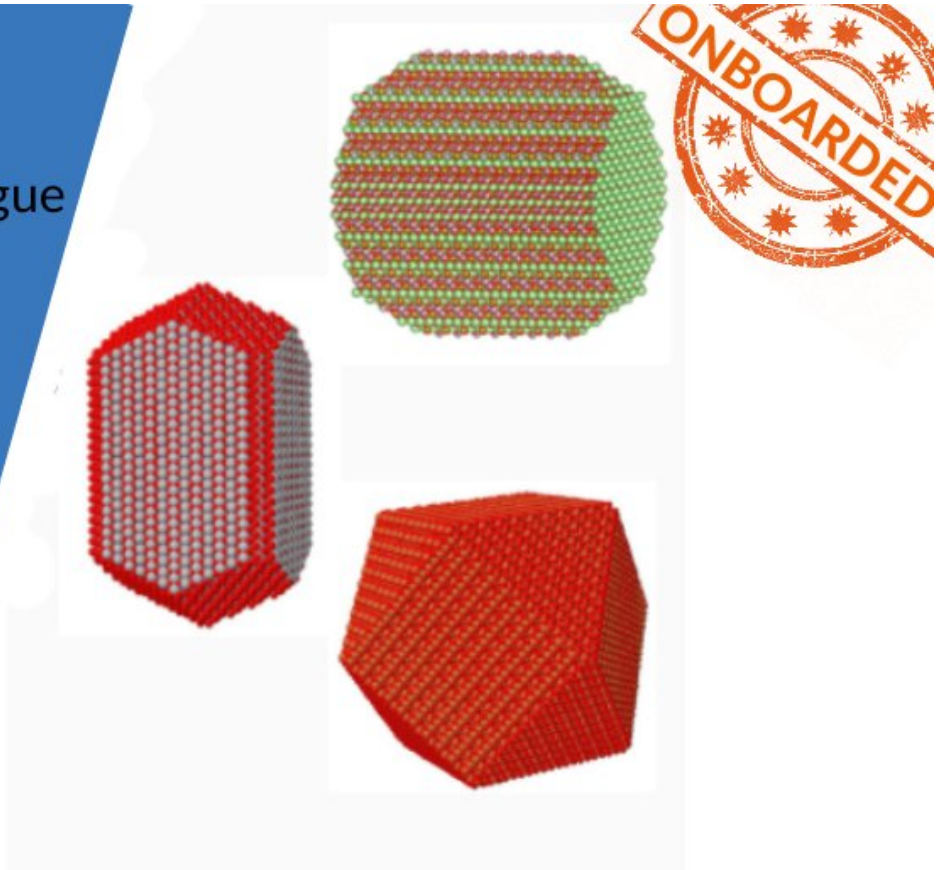
NI4OS-Europe Catalogue

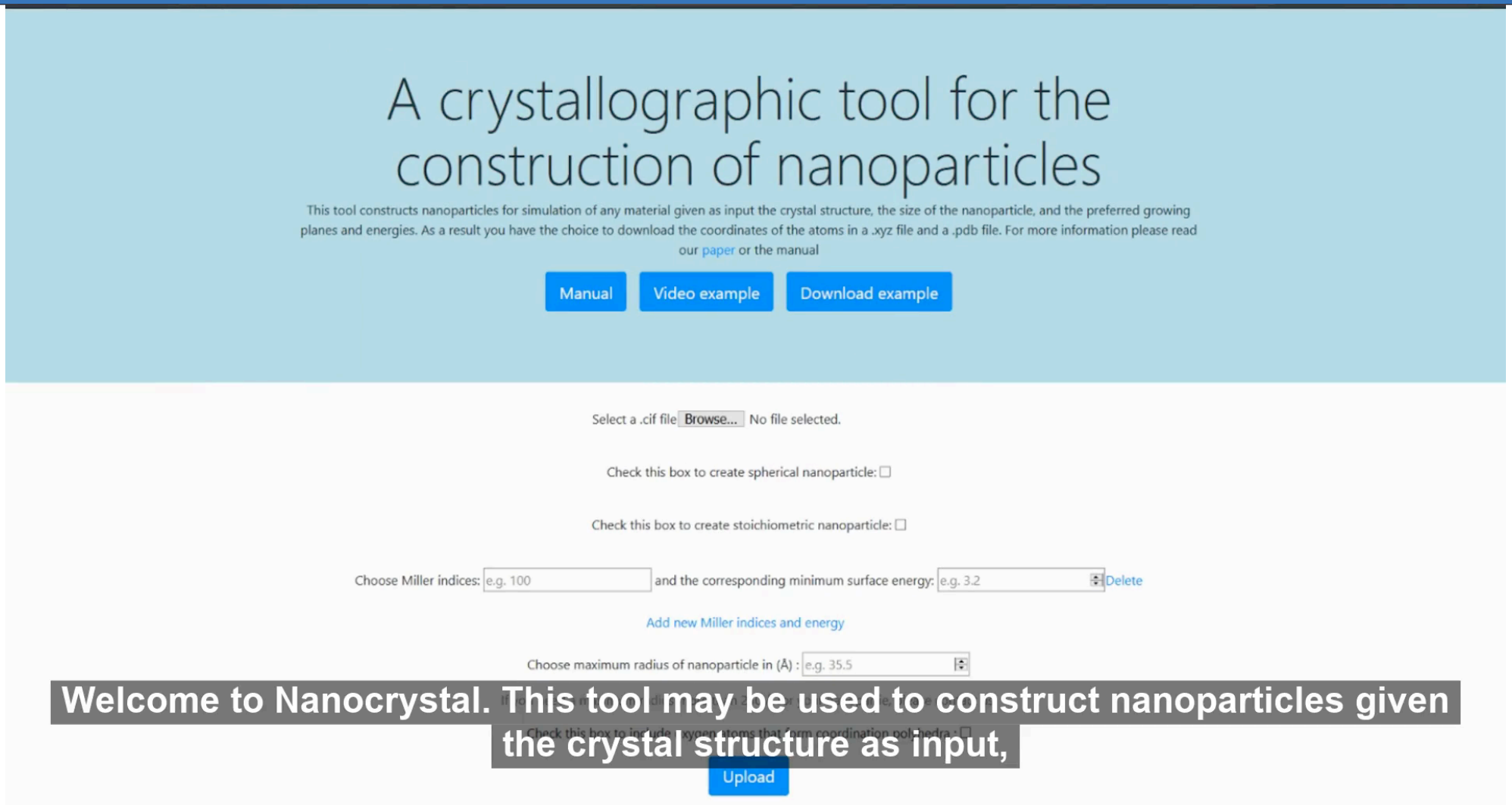
Thematic services

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



Welcome to Nanocrystal. This tool may be used to construct nanoparticles given the crystal structure as input,

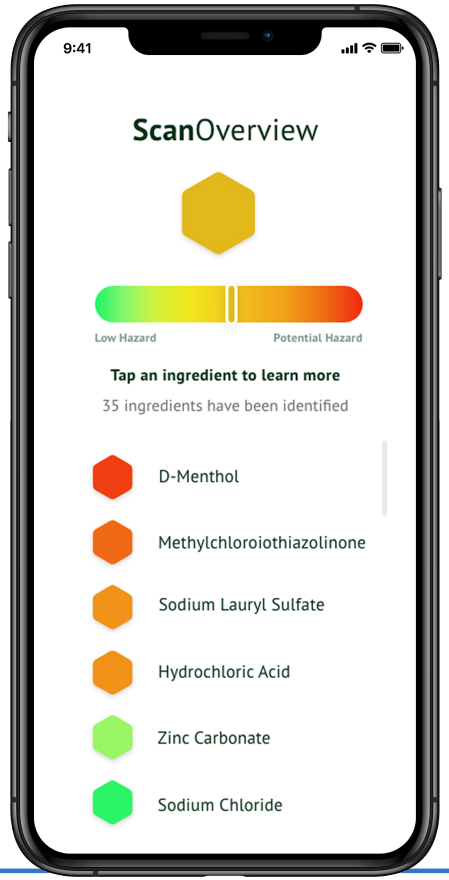
Nanocrystal: construction of nanoparticles for simulation

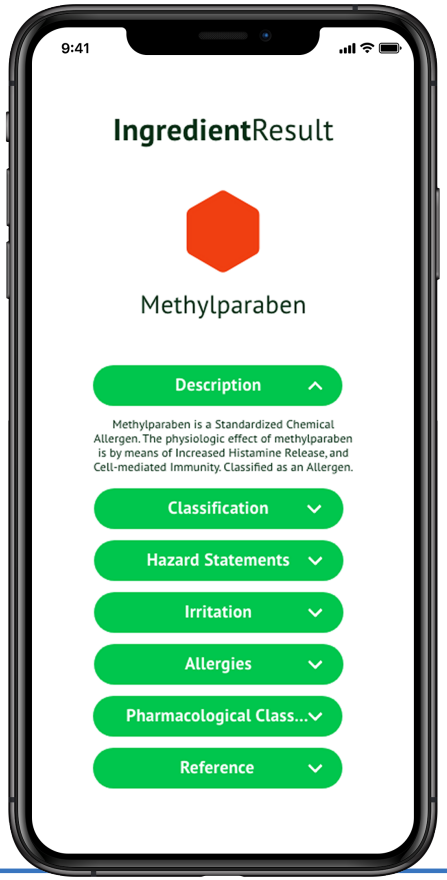
- Information in NI4OS-Europe Agora: https://catalogue.ni4os.eu/?_=/resources/c1f8d7fb-4250-4278-ba8d-4d1df4a85df5
- Access: http://nanocrystal-seem.eu
- Training Material: https://training.ni4os.eu/mod/scorm/view.php?id=1181

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*

European Commission

CosIng COSMETIC INGREDIENTS & SUBSTANCES

NATIONAL INSTITUTES OF HEALTH

PubChem

*** Information sourced from institutional databases**

OpenAIRE

Ingredio Main Features

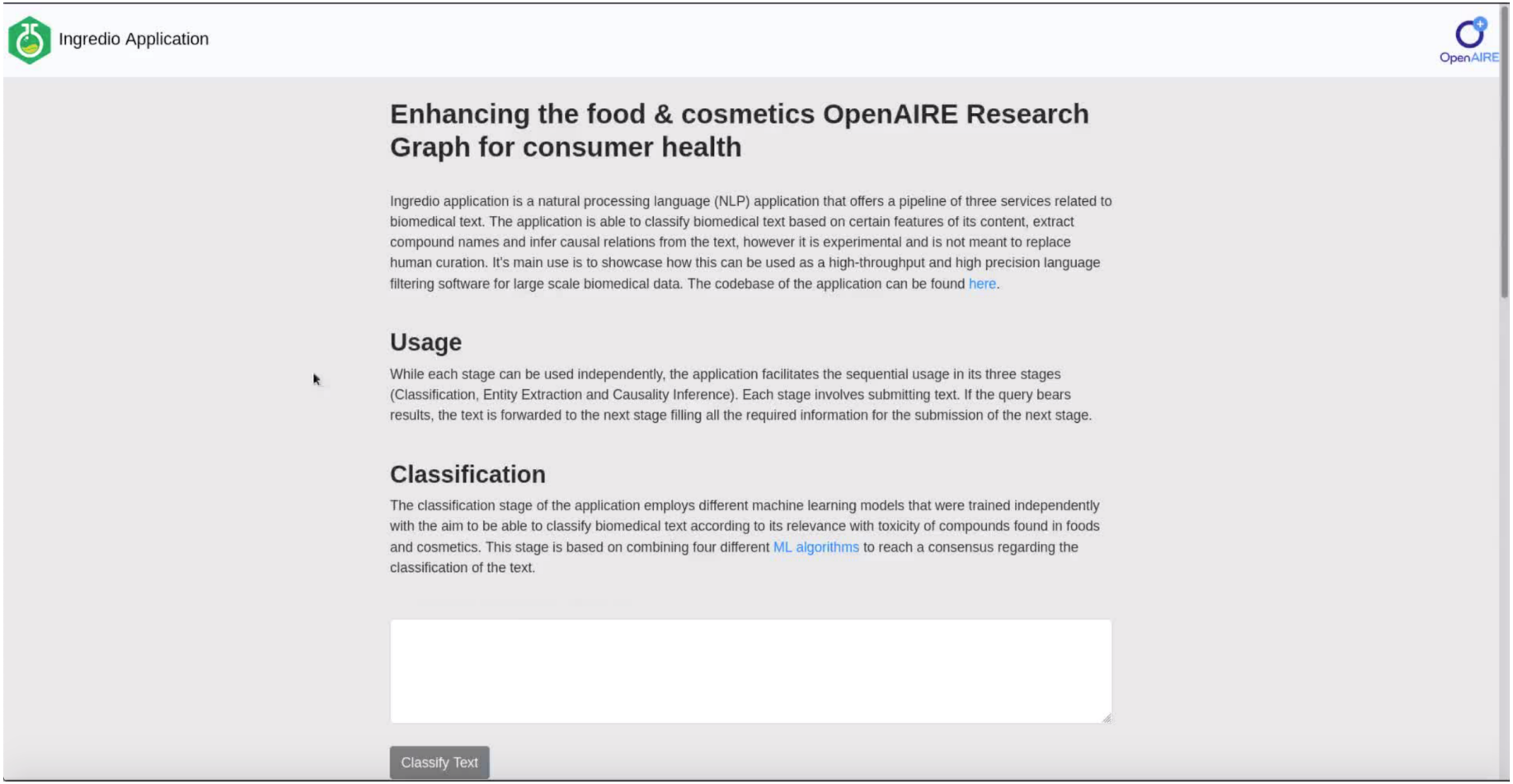
Feature 1
Develop text mining and Machine Learning algorithms to extract OpenAIRE data linking chemical ingredients of food &cosmetics to potential health hazards

Feature 2
Support the curation of OpenAIRE data with appropriate metadata schemas for efficient integration of information in the OpenAIRE Research Graph

Feature 3
Identifying new chemical ingredients from OpenAIRE data to enrich the OpenAIRE research graph & the Ingredio database

Feature 4
Identify causal relationships of chemical ingredients with hazards using the collected information

Ingredio is FAIR compatible– Reusability: Video Example



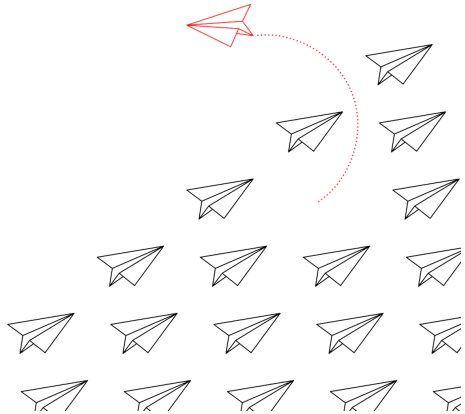
Ingredio: Natural Language Processing to process biomedical text

- 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