

OpenRiskNet

RISK ASSESSMENT E-INFRASTRUCTURE

Integration of toxicology and risk assessment services into the EOSC marketplace

powered by OpenRiskNet and NanoCommons

Thomas Exner, Edelweiss Connect, Basel, Switzerland

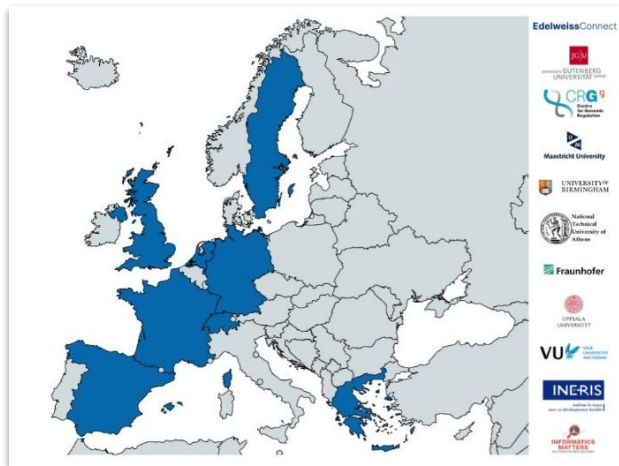
OpenRiskNet: Open e-Infrastructure to Support Data Sharing, Knowledge Integration and *in silico* Analysis and Modelling in Risk Assessment
Project Number 731075



Acknowledgements

OpenRiskNet - 2015-2019 (Grant Agreement 731075) project was funded by the European Commission within Horizon 2020 Programme

Project partners:



P1 Edelweiss Connect GmbH, Switzerland (EwC)

P2 Johannes Gutenberg-Universität Mainz, Germany (JGU)

P3 Fundacio Centre De Regulacio Genomica, Spain (CRG)

P4 Universiteit Maastricht, Netherlands (UM)

P5 The University Of Birmingham, United Kingdom (UoB)

P6 National Technical University Of Athens, Greece (NTUA)

P7 Fraunhofer Gesellschaft Zur Foerderung Der Angewandten Forschung E.V., Germany (Fraunhofer)

P8 Uppsala Universitet, Sweden (UU)

P9 Medizinische Universität Innsbruck, Austria (MUI)

P10 Informatics Matters Limited, United Kingdom (IM)

P11 Institut National De L'environnement Et Des Risques INERIS, France (INERIS)

P12 Vrije Universiteit Amsterdam, Netherlands (VU)

Acknowledgements

NanoCommons - 2018-2021 (Grant Agreement 731032) receives funding from the European Union Horizon 2020 Programme

- P1 - UoB - The University of Birmingham
- P2 - EwC - Edelweiss Connect GmbH
- P3 - NERC CEH - Natural Environment Research Council
- P4 - NTUA - National Technical University of Athens
- P5 - NUID UCD - National University of Ireland Dublin - University College Dublin
- P6 - LEITAT - ACONDICIONAMIENTO TARRASENSE ASSOCIACION
- P7 - BfR - Bundesinstitut für Risikobewertung
- P8 - BIONANONET - BioNanoNet
- P9 - PLUS - Universitat Salzburg / Paris Lodron University of Salzburg
- P10 - NM - NovaMechanics Ltd
- P11 - BIOMAX - BIOMAX Informatics AG
- P12 - UM - Universiteit Maastricht
- P13 - DU - Duke University
- P14 - OSU - Oregon State University



Risk assessment is important

U.S. LEGAL NEWS APRIL 6, 2020 / 11:01 PM / 13 DAYS AGO

Special Report: Doctors embrace drug touted by Trump for COVID-19, without hard evidence it works

Michael Erman, Deena Beasley

NEW YORK/LOS ANGELES (Reuters) — Trump has persistently promoted as a matter of weeks become a standard of care for the pandemic — though doctors prescribe

CORONAVIRUS | 39,069 views | Mar 25, 2020, 01:34pm EDT

Study Shows Hydroxychloroquine Is Ineffective Against COVID-19 — So What Now?

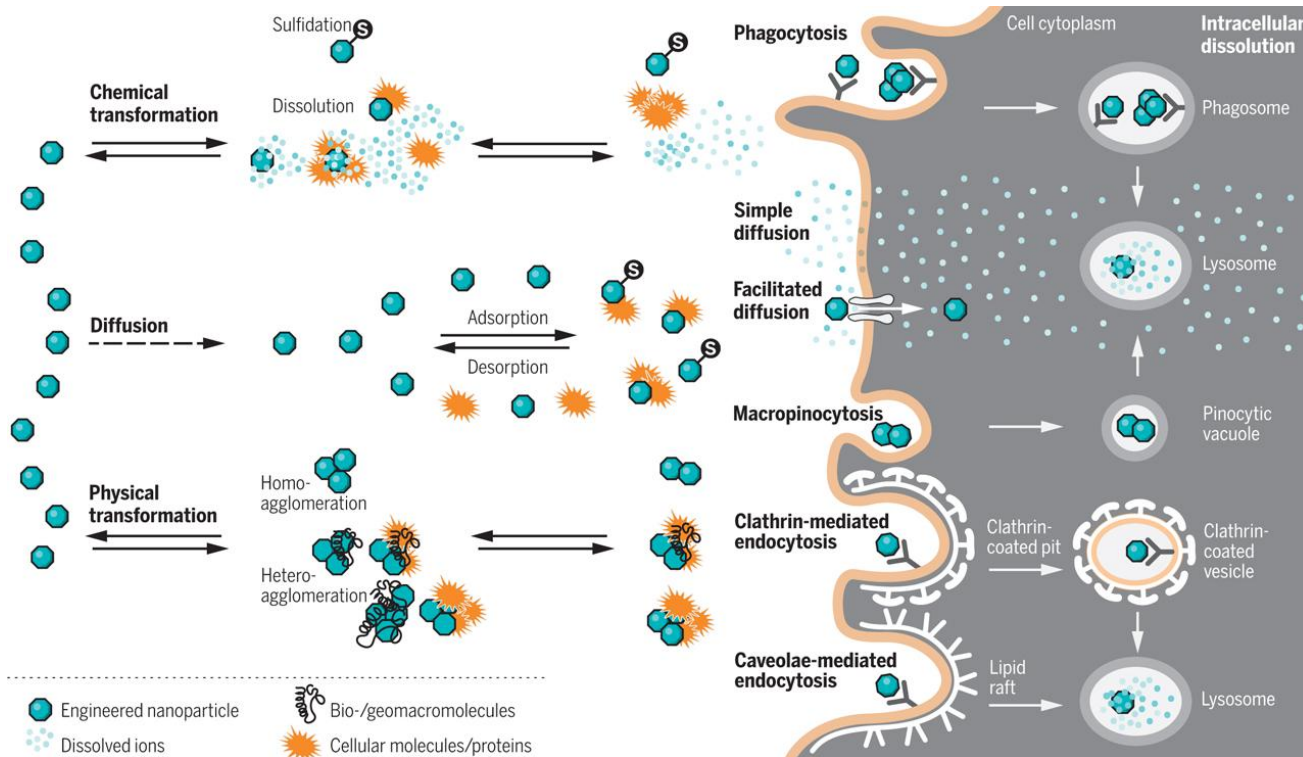
Navarro: "Virtually Every" COVID-19 Patient In New York Is Given Hydroxychloroquine

Posted By Tim Hains
On Date April 6, 2020

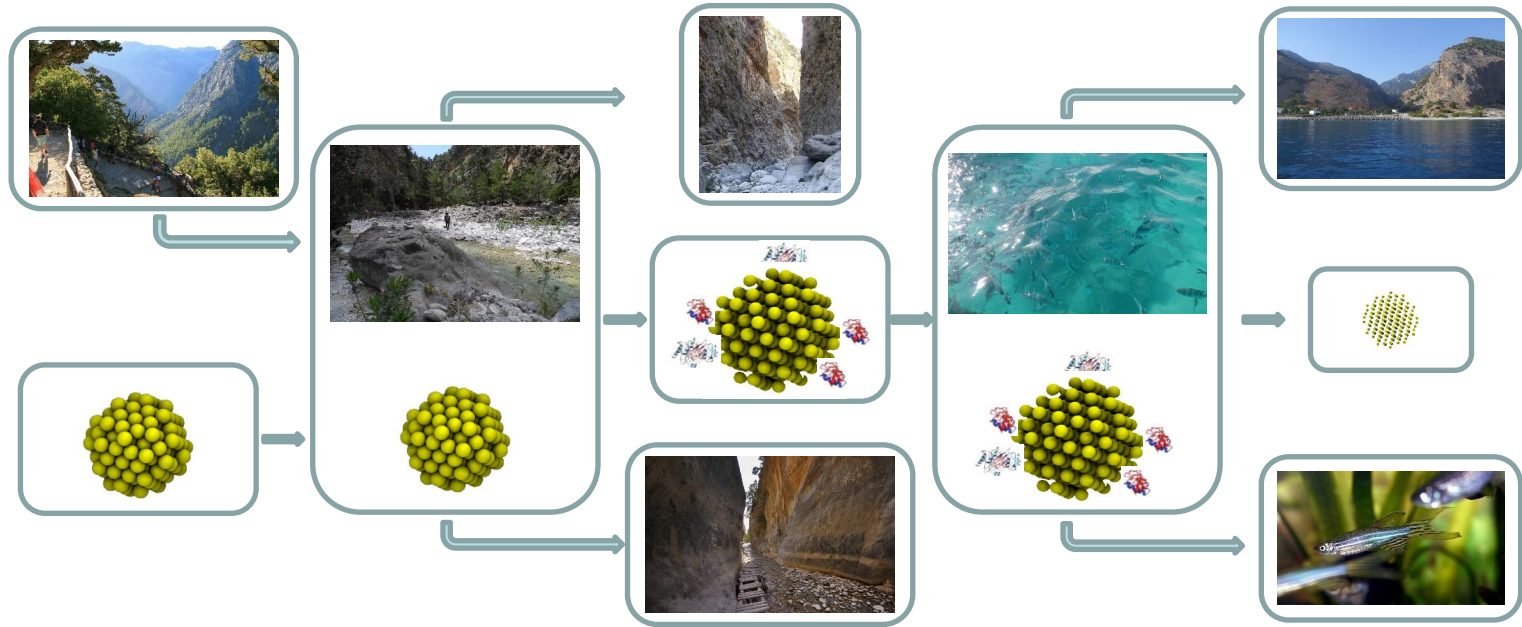


clinical trial from China on the use of treatment for Covid-19 have shown no health outcomes between the control group and the experimental drug.

Paradigm shift towards a mechanistic science

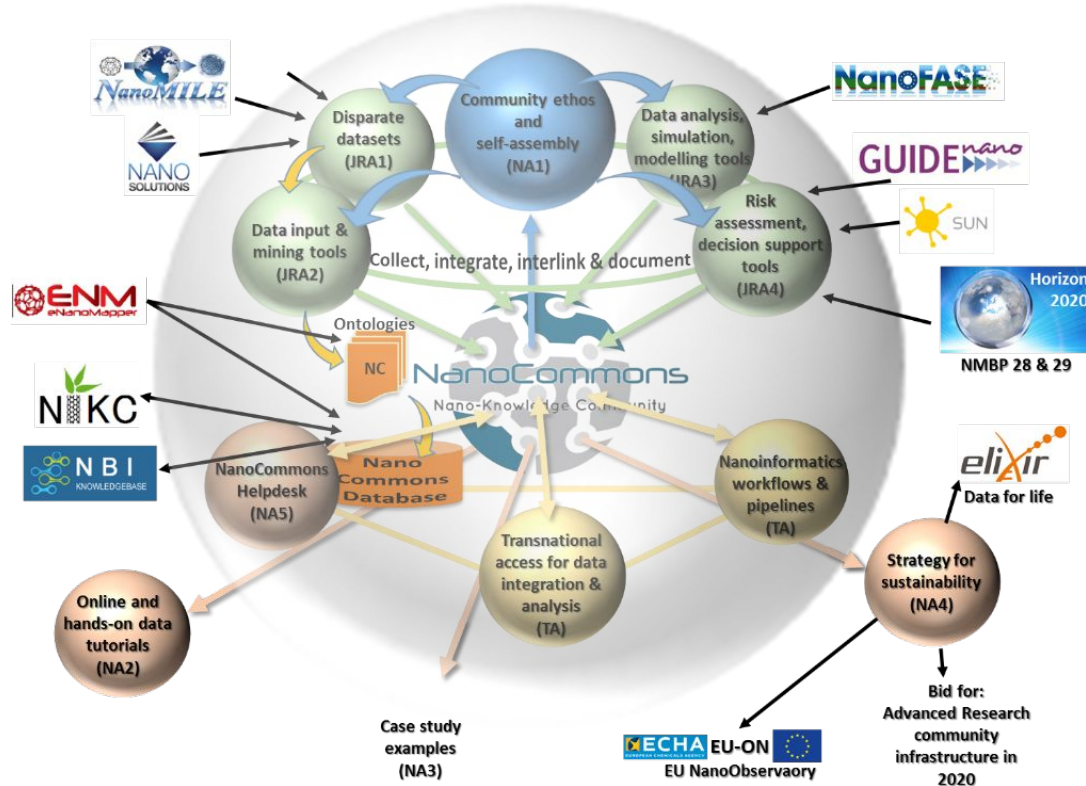


Nanomaterials transformation

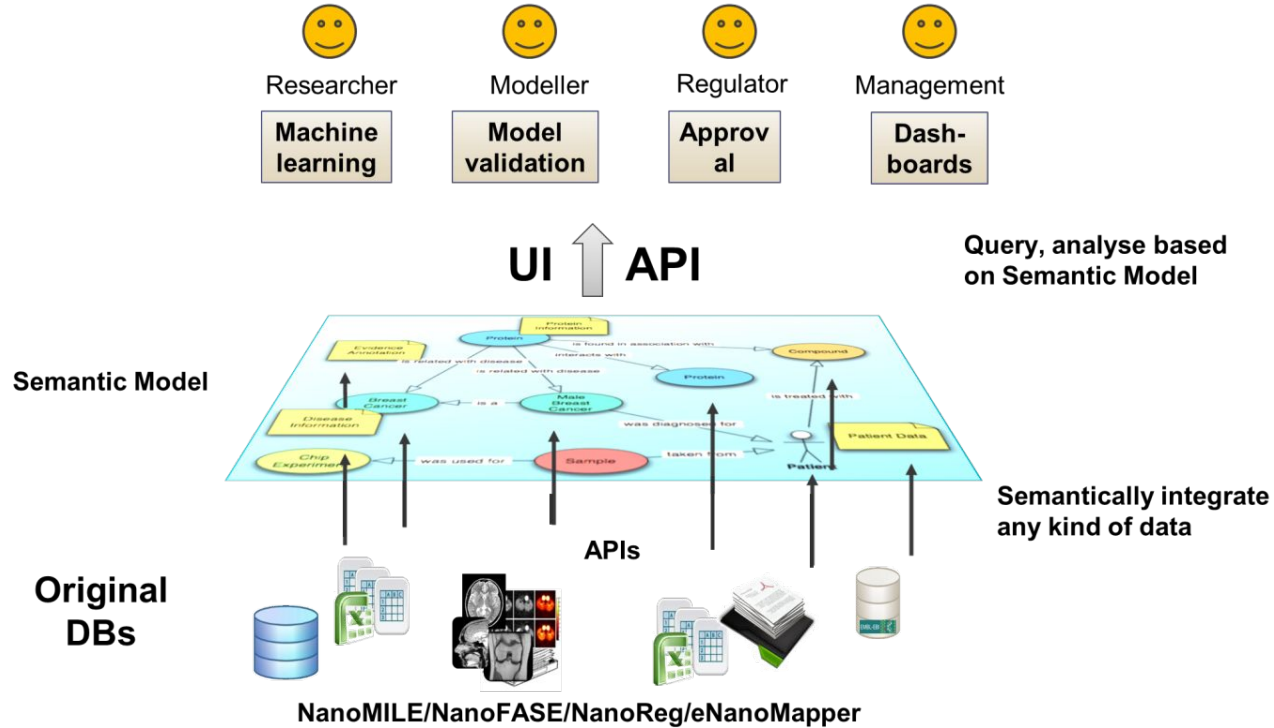


- A released nanomaterial will change itself and affect its surrounding environment

Data harmonization and interoperability



Data harmonization and interoperability



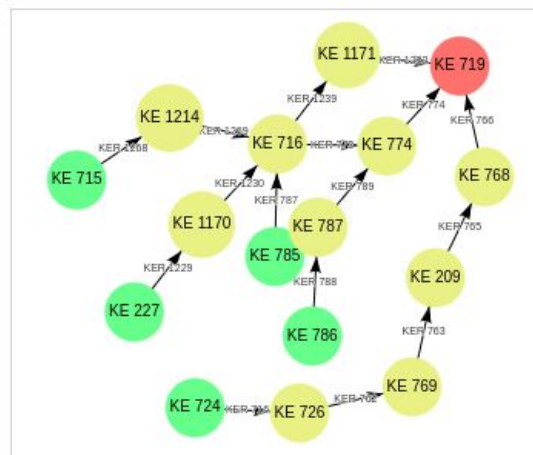
Workflow development

```

for MIE in MIEs:
    net.add_node(MIE, color = 'lightgreen', size = 50, shape = 'circle', font = '26px arial black', title = KEtitle[MIE])
for KE in KEs2:
    net.add_node(KE, color = 'whaki', size = 50, shape = 'circle', font = '26px arial black', title = KEtitle[KE])
for AO in AOs:
    net.add_node(AO, color = 'salmon', size = 50, shape = 'circle', font = '26px arial black', title = KEtitle[AO])

for KER in KERs:
    sparqlquery = '''
SELECT ?KE_UP_ID ?KE_DOWN_ID
WHERE(
?KER_URI a aopo:KeyEventRelationship; rdfs:label ?KER_ID; aopo:has_upstream_key_event ?KE_UP_URI; aopo:has_downstream_key_event ?KE_DOWN_URI.
?KE_UP_URI rdfs:label ?KE_UP_ID.
?KE_DOWN_URI rdfs:label ?KE_DOWN_ID.
FILTER (?KER_ID = '''+?KER+'''))
'''
    aopwikisparql.setQuery(sparqlquery)
    aopwikisparql.setReturnFormat(JSON)
    results = aopwikisparql.query().convert()
    for result in results['results']['bindings']:
        net.add_edge(result['?KE_UP_ID']['value'], result['?KE_DOWN_ID']['value'], width = 2, color = 'black', label = KER, arrows = 'to')

net.show('mygraph.html')
Iframe(src='./mygraph.html', width=700, height=600)
    
```



Goals of EOSC-hub EAP project

- 1) OpenRiskNet services should be findable and directly accessible on the EOSC platform
- 2) EOSC users should be able to acquire direct access to all the OpenRiskNet services
- 3) Usage of EOSC cloud and storage resources should guarantee long-term sustainability

- <https://eosc-hub.eu/research-communities/integration-toxicology-and-risk-assessment-services-eosc-marketplace>
- <https://wiki.eosc-hub.eu/display/EOSC/Integration+of+toxicology+and+risk+assessment+services+into+the+EOSC+marketplace>

1) Service catalogue

OpenRiskNet services



About Governance Services & Resources Policy EOSCI

Enter keywords Category Service type User type Targeted

Home

OpenRiskNet e-infrastructure

Nano-QSAR to predict cytotoxicity of metal and metal oxide nanoparticles

Korea Institute of Technology NanoQSAR model

KIT (Korea Institute of Toxicology) Nano-QSAR models were implemented for prediction of cytotoxicity caused by metal and metal oxide nanoparticles. A Binary classification model was using the Logistic regression ...

Provided by: Korea Institute of Toxicology (KIT)

Type: Trained model, Model

Applicability domain: Computational modelling, Toxicology, Predictive toxicology

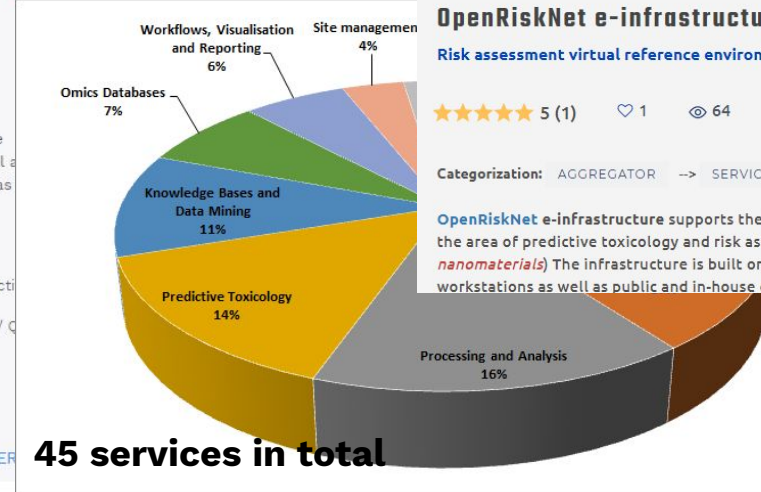
Topic: Predictive modelling, Structure-activity relationship (SAR / QSAR), Risk assessment, Nano safety

✓ For end-users

✓ For developers

DETAILS → VISIT SERVICE

Daphnia magna nanotox



OpenRiskNet e-infrastructure

Risk assessment virtual reference environment for data integration, analysis and modelling

★★★★★ 5 (1) 1 64

Categorization: AGGREGATOR → SERVICES-DATA-APPLICATIONS-SOFTWARE

OpenRiskNet e-infrastructure supports the harmonisation and improved interoperability of data and software tools in the area of predictive toxicology and risk assessment (e.g. for chemicals, cosmetic ingredients, therapeutic agents or nanomaterials). The infrastructure is built on virtual research environments (VRE), which can be deployed to workstations as well as public and in-house cloud infrastructures. Services providing data, analysis, modelling and

ToxCast/Tox21 V3.2

ToxCast and Tox21 datasets (raw and summary) extracted

ToxPlanet

Our platform searches the content from 500+ websites

www.openrisknet.org

2) User management

OpenRiskNet e-infrastructure

Welcome to The OpenRiskNet reference site.
This page provides a landing page for end users that lists the available resources. This page is manually updated when new resources become available.

Login and Policies

You need to register to be able to log in and access some services and agree to our Terms of use and Privacy policy.

- [Login instructions](#)
- [Privacy policy](#)
- [Terms of use](#)

OpenRiskNet and Thrid-Party Workflow Managers and Scripting Tools

- [Squonk Computational Notebook](#)
- [Jupyter Notebooks](#)

Please note that the jupyter notebook containers are large and needs some time to be deployed. Please refresh the reload button of your browser until the interface is appearing. [Example workflows can be accessed here.](#)

Graphical User Interface Access to OpenRiskNet Applications

- [Lazar Toxicity Predictions](#)

OPENRISKNET

Log In

Username or email

Password

Log In

LinkedIn

GitHub

Elxir AAI

3) Cloud resources

OpenRiskNet e-infrastructure

Welcome to The OpenRiskNet reference site.

This page provides a landing page for end users that lists the available resources. The page is manually updated when new resources become available.

- 1 bastion node with 4 CPU cores and 8GB RAM
- 1 master node with 8 CPU cores and 32GB RAM
- 1 infrastructure node with 8 CPU cores and 32GB RAM
- 3 worker nodes with 60 CPU cores and 96GB RAM
- Storage as attached physical volumes, exposed as NFS volumes

→ [Sqonk Computational Notebook](#)

→ [Jupyter Notebooks](#)

Please note that the jupyter notebook containers are large and needs some time to be deployed. Please press the "refresh" button of your browser until the interface is appearing. [Example workflows can be accessed here.](#)

Graphical User Interface Access to OpenRiskNet Applications

→ [Lazar Toxicity Predictions](#)

The top part of the image shows a Grafana dashboard with four panels: CPU Utilisation, CPU Saturation (Load1), Memory Utilisation, and Memory Saturation (Swap I/O). The CPU panels show usage for nodes like cloudv199.zdv.uni-mainz.de and cloudv201.zdv.uni-mainz.de. The Memory panels show usage in MB.

The bottom part shows a Jupyter Notebook interface with the following code and output:

```
# of the node to the correct URL of the service endpoint so it can be queried there directly - but
this
# only works if the id has been assigned correctly by the service author, otherwise you get an ano
ymous node id
?&?relativeendpointpath ?&endpointnode.
?&endpointnode ?&verb ?&endpointverbnode.

# Go one level down into the parameters section and match if the id of the parameter
# is the ontology term that we are looking for. Alternatively you could match based on
# text or a regex here so you can find services where the parameter has not been tagged
# with this ontology term but then you rely on text based matching.
?&endpointverbnode or:nparameters <http://semanticscience.org/resource/CHEMINF_000018>
}...

In [4]: response = requests.get("https://registry.prod.openrisknet.org/api/sparql", params={"query": quer
y})

In [5]: response.raise_for_status()

In [6]: json = response.json()
#pprint.pprint(json)

In [7]: def mapServiceResult(serviceDict):
    result = pandas.DataFrame(data=serviceDict['Result']][1]['ResultValues'], columns=serviceDict
['Result']][1]['Variables'])
    return serviceDict['ServiceName'], result

In [8]: dictOfDataframes = dict(map(mapServiceResult, json))

In [9]: for key, value in dictOfDataframes.items():
    display(key)
    display(value)
```

The output shows a table of service results:

endpointnode	relativeendpointpath	endpointverbnode	n1	n2	verb
					'Lazar REST Service'
					'EPA-ToxCastV3.1-ACEA_ER_80hr_summary_top1'
					'MetPred'
					'JGU WEKA REST Service'
					'ChemIDConvert - Chemical identifier conversion service'

Goals of EOSC-hub EAP project

- 1) OpenRiskNet services should be findable and directly accessible on the EOSC platform
- 2) EOSC users should be able to acquire direct access to all the OpenRiskNet services
- 3) Usage of EOSC cloud and storage resources should guarantee long-term sustainability
- 4) **Interactions with other infrastructures to improve interoperability**

Time planning

Q1:

- scouting of currently available OpenRiskNet services
- definition of a plan to insert suitable OpenRiskNet services into EOSC catalogue
- scouting of the resources for long-term support of OpenRiskNet services

Q2:

- integration of EOSC AAI into OpenRiskNet services
- definition of the transfer procedure and exchange format for the “synchronization” of OpenRiskNet and EOSC catalogues
- feasibility study for “automatic” import of services from OpenRiskNet catalogue into EOSC catalogue
- deployment of OpenRiskNet services on EOSC cloud resources

Q3:

- integration of a preliminary subset of OpenRiskNet services into EOSC catalogue
- defining approaches for better harmonisation and interoperability of OpenRiskNet services with other service providers on EOSC by discussing and reviewing successful implementations performed in other EOSC-hub Early Adopter Programme activities
- management and update of deployed services

Q4:

- finalising the deployment of the “architecture” of OpenRiskNet service catalogue within EOSC marketplace, standing the outcomes of Q1, Q2, and Q3
- management and update of deployed services