Easy access to QSAR modelling

Introduction to NanoCommons

- Consulting/support/training along data life cycle
- TA call open for tool integration

Introduction to QSAR Predictive Modelling by Jaqpot

- Haralambos Sarimveis, NTUA, GR

Guided tour through Jaqpot easy-accessed by Google Colab Notebooks

- Hands-on Training by Philip Doganis, NTUA, GR
- Break-out support by Periklis Tsiros, Pantelis Karatzas, Jason Sotiropoulos, NTUA, GR
- Q&A

Martin Himly (PLUS)
Chair WG-A Education, Training, Communication

www.nanosafetycluster.eu

NanoCommons Training, 2021-04-13, #nanocommons

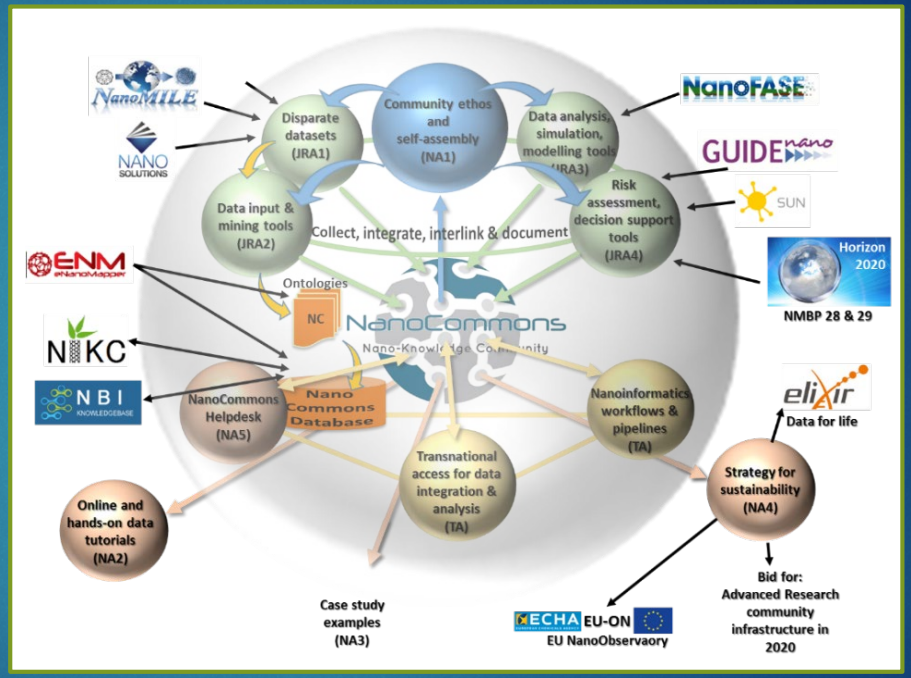
These projects have received funding from the European Union Horizon 2020 Programme (H2020) under grant agreements no. 731032 & 814572.
CC-BY 4.0 International

The idea – problem & solution

Nanotechnologies are a major area of **investment & growth for the European economy**

Knowledge and **data** remain **fragmented** and inaccessible **hampering progress**

Read-across approaches are currently absent for NMs, but would reduce the cost and time of nanosafety research and regulation



NanoCommons is creating an **e-infrastructure** platform for reproducible science, **enhancing data integration & enabling nanoinformatics workflows** to address these gaps

NanoCommons is **integrating and developing tools and services** for use by the nanomaterials communities and beyond

NanoCommons provides **Consultancy & Trainings** covering the entire nanosafety data life cycle:

These tools & services can be **accessed** through the **NanoCommons Transnational Access (TA) scheme**

☞ info@nanocommons.eu

NanoCommons User Guidance Handbook

Home / e-Infrastructure / NanoCommons User Guidance Handbook

NanoCommons
Nano-Knowledge Community

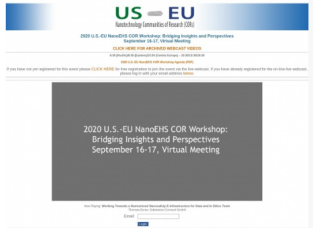
NanoSolveIT

Overview | Data management | Nanoinformatics | Workflows | Electronic lab notebooks | Ontologies

NanoCommons – How can we help you?

Download [2.19 MB]

☞ www.nanocommons.eu



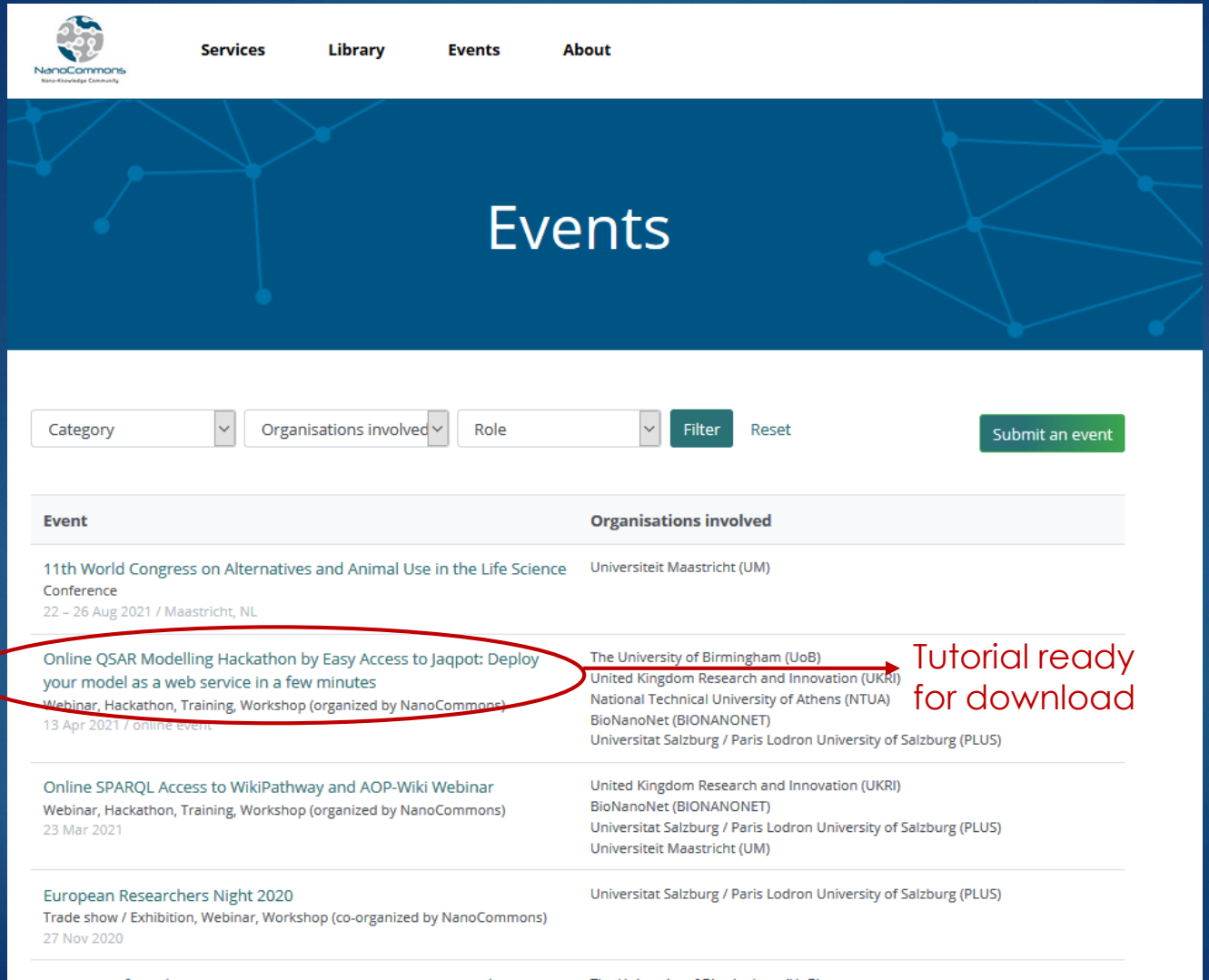
Working Towards a Harmonized Nanosafety E-Infrastructure for Data and In Silico Tools, 2020 U.S.-EU NanoEHS COR Workshop: Bridging Insights and Perspectives, September 16-17, Virtual Meeting

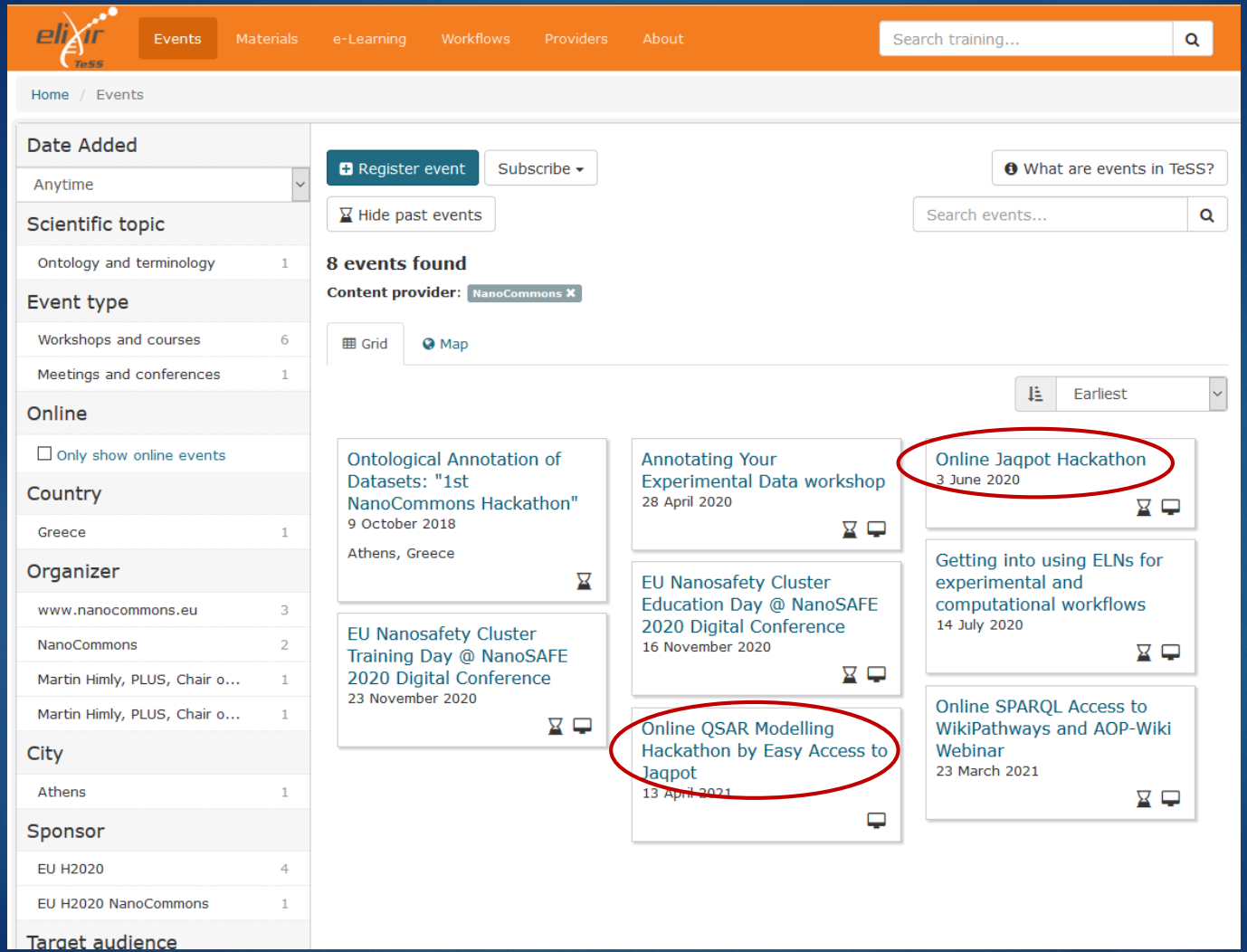
You can still register to see the recordings.

Intro to NanoCommons by Martin Himly, PLUS (at the Jaqpot Hackathon)

Online training tools for nanosafety assessment – NanoCommons for

NanoSafety Cluster


Services
Library
Events
About
Events
Category
Organisations involved
Role
Filter
Reset
Submit an event
Event
Organisations involved
11th World Congress on Alternatives and Animal Use in the Life Science
Conference
22 – 26 Aug 2021 / Maastricht, NL
Universiteit Maastricht (UM)
Online QSAR Modelling Hackathon by Easy Access to Jaqpot: Deploy your model as a web service in a few minutes
Webinar, Hackathon, Training, Workshop (organized by NanoCommons)
13 Apr 2021 / online event
The University of Birmingham (UoB)
United Kingdom Research and Innovation (UKRI)
National Technical University of Athens (NTUA)
BioNanoNet (BIONANONET)
Universitat Salzburg / Paris Lodron University of Salzburg (PLUS)
Tutorial ready for download
Online SPARQL Access to WikiPathway and AOP-Wiki Webinar
Webinar, Hackathon, Training, Workshop (organized by NanoCommons)
23 Mar 2021
United Kingdom Research and Innovation (UKRI)
BioNanoNet (BIONANONET)
Universitat Salzburg / Paris Lodron University of Salzburg (PLUS)
Universiteit Maastricht (UM)
European Researchers Night 2020
Trade show / Exhibition, Webinar, Workshop (co-organized by NanoCommons)
27 Nov 2020
Universitat Salzburg / Paris Lodron University of Salzburg (PLUS)



NanoCommons
Nano-Knowledge Community

NanoSolveIT

NanoSafety Cluster

June 3, 2020

Presentation Open Access

Online Jaqpot Hackathon - Take your research from the bench to the community by making your models available as a web service

Martin Himly (PLUS); Iseult Lynch; Dieter Maier; Philip Doganis

Under the subtitle **"Take your research from the bench to the community by making your models available as a web service",** attendees learned how to use the ***Jaqpot*** suite and python to go from data to model, starting from a common CSV file.

Jaqpot is a computational platform for ***in silico*** modelling of chemical compounds, that provides both access to its services both over a User Interface (GUI) and an Application Programming Interface (API). It is a cloud-ready application that uses the benefits of Java, R and Python, having incorporated functionality by various established and open-source machine learning and data analysis toolkits, while algorithms in any programming algorithm can be added to Jaqpot.

Attached you find the following presentations:

1. Intro to NanoCommons by Martin Himly, PLUS

2. Electronic Lab Notebooks by Iseult Lynch, UoB

3. NanoCommons Knowledgebase by Dieter Maier, Biomax

4. Jaqpot Suite by Philip Doganis, NTUA

Preview

Edit

New version

Communities

EU NanoSafety Cluster Remove

H2020 Infrastructure Project NanoCommons Remove

The Allergy-Cancer-BioNano Research Center at the University of Salzburg Remove

58 views

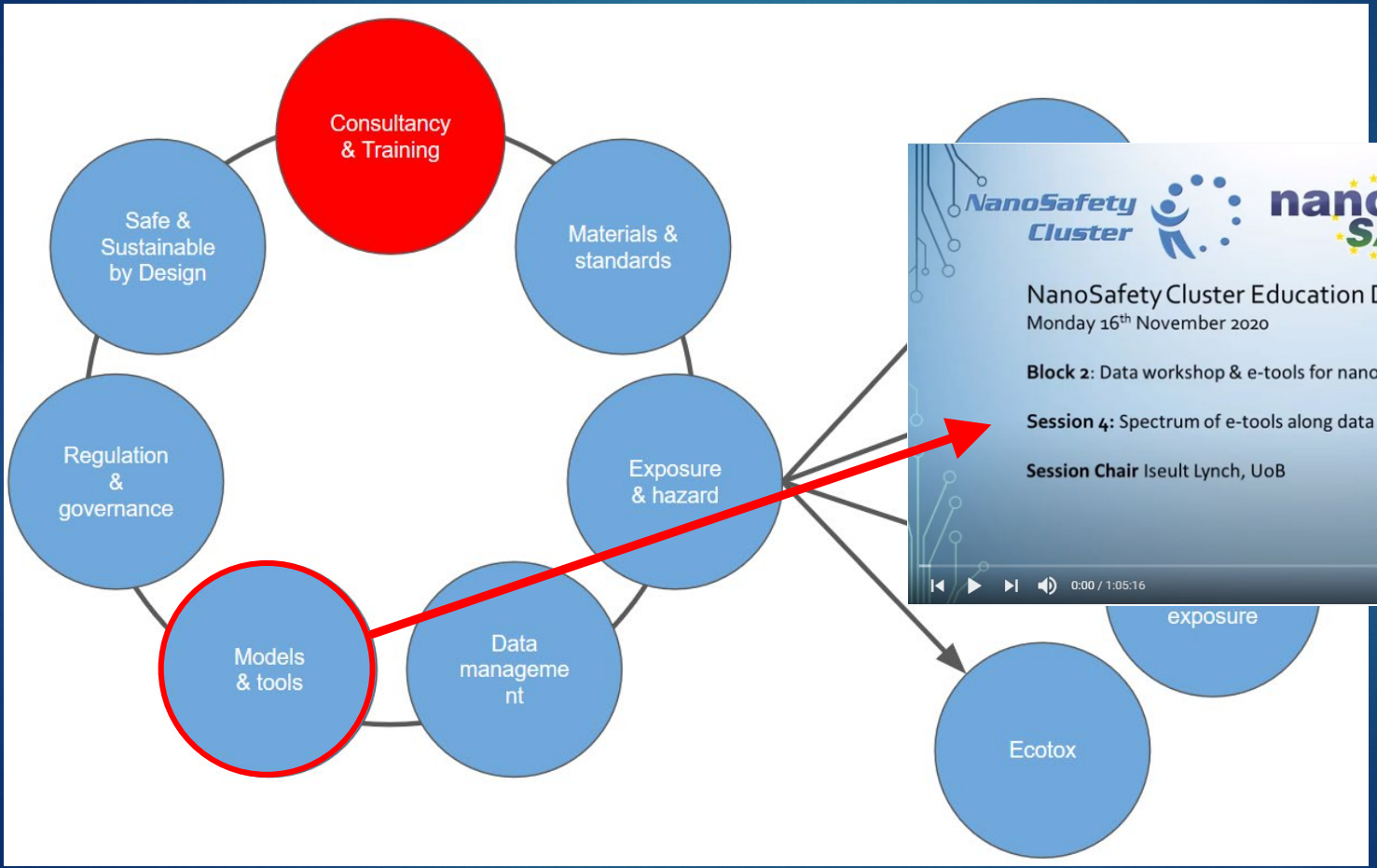
58 downloads

See more details...

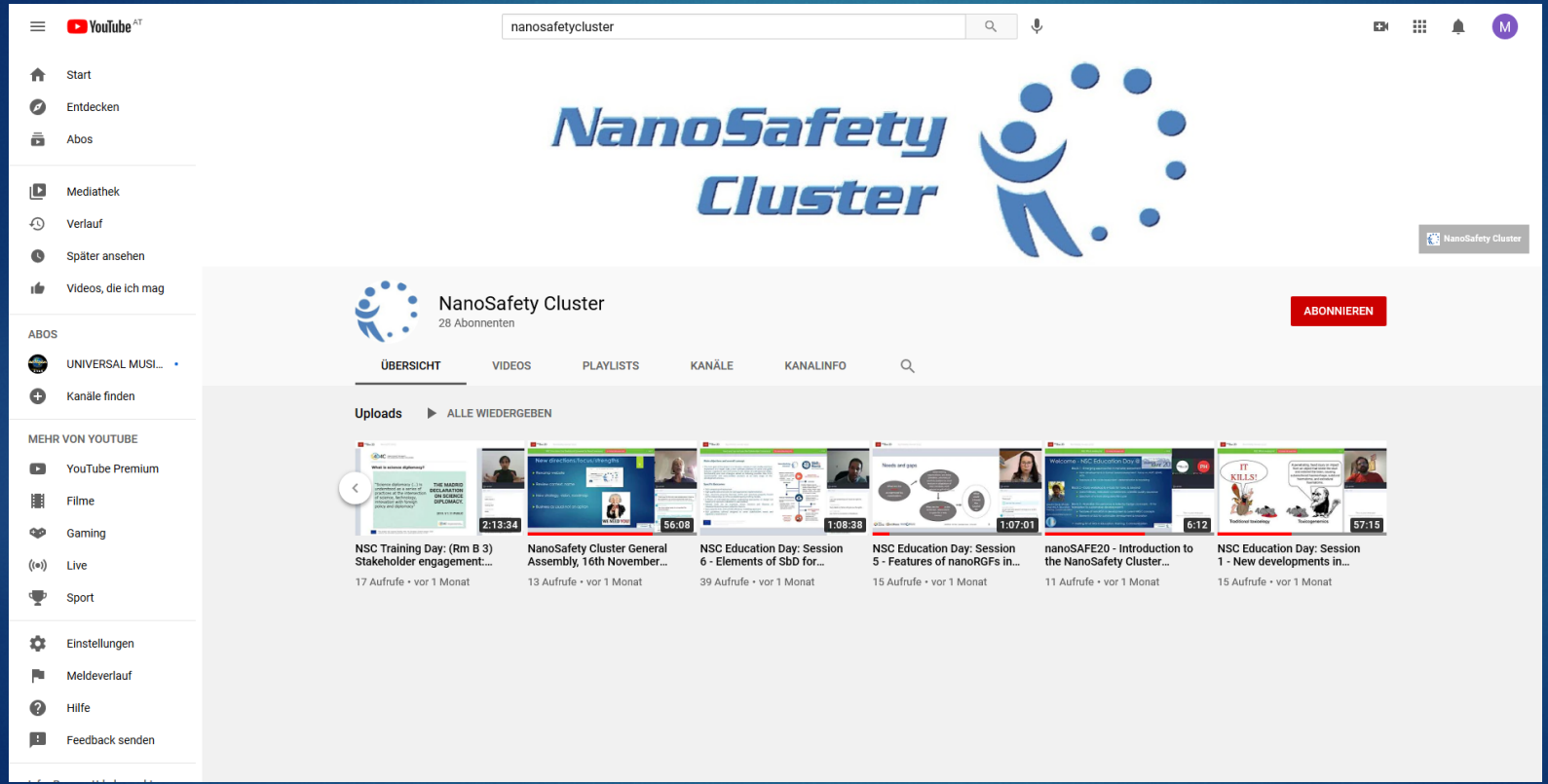
Indexed in OpenAIRE

Publication date:
June 3, 2020

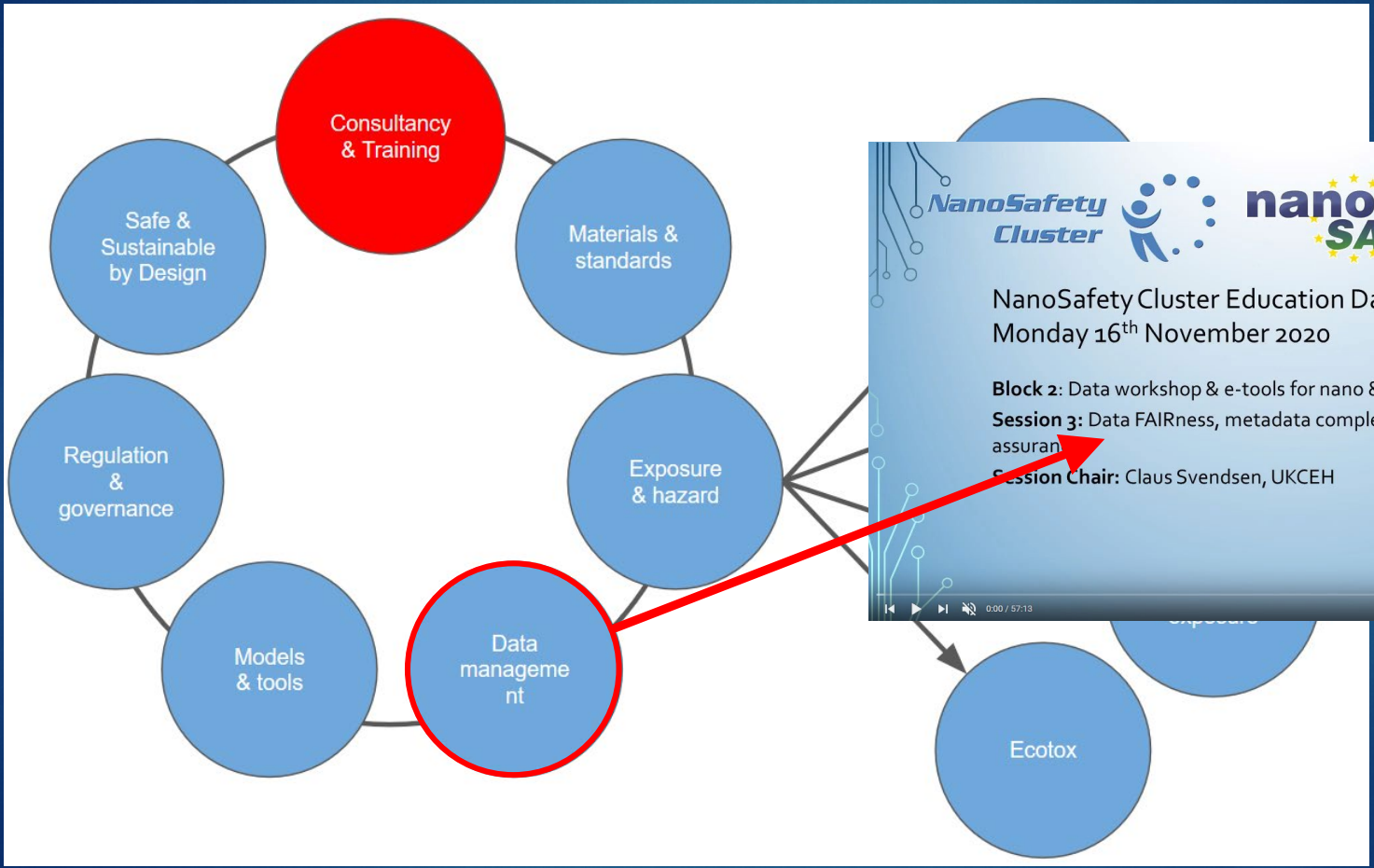
...aligned with the EU NSC WGs

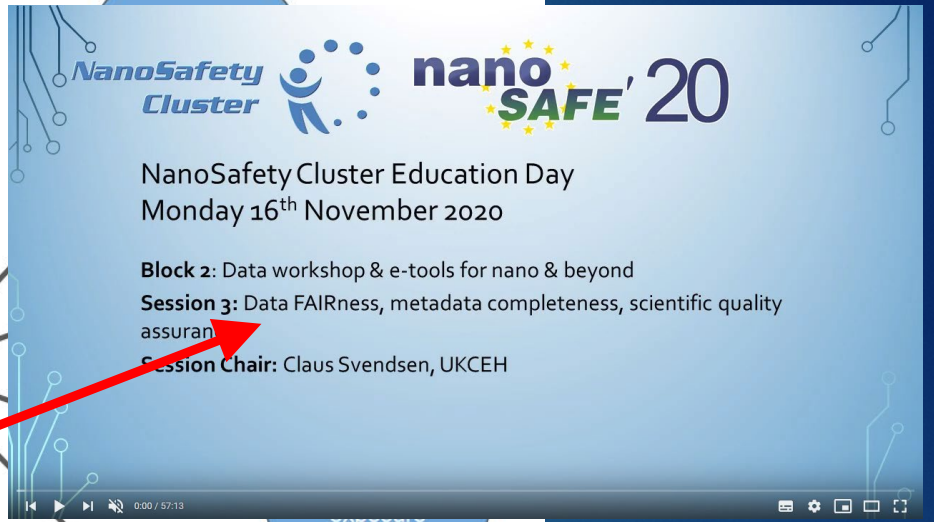


☞ NanoCommons & NSC YouTube channels



...aligned with the EU NSC WGs





Data FAIRness

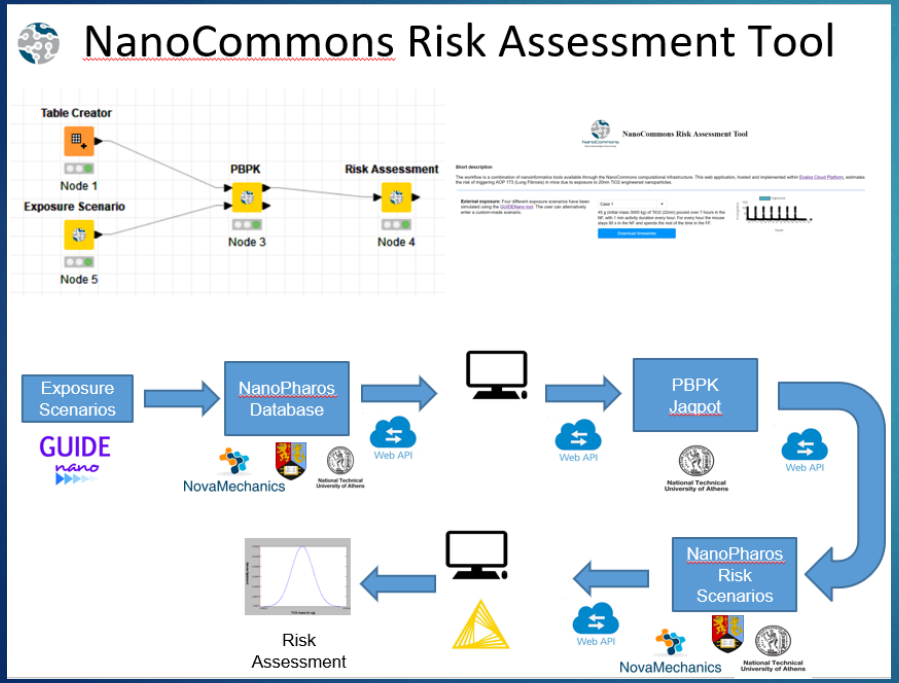
- **To remove barriers** for nanosafety **regulatory and industry** processes
- To develop an **integrated knowledgebase** to facilitate development and application of regulatory tools such as **grouping & read-across**
- To create an **interconnected community** *via* a **FAIR data single market**
- To enable **full exploitation of EU-funded research data** & promotion of **data-driven innovation** leading to **positive socioeconomic impact**

NanoCommons
Nano-Knowledge Community

NanoSolveIT

NanoSafety Cluster

Calling all nanosafety tools developers!



NanoSafety Tools support – interoperability, sustainability, containerisation, integration into nanosafety workflows (KNIME, Jaqpot, Enalos, *etc*.) ☞ APIs, GUIs,...

NanoCommons is offering funded support for **integration of tools** (predictive models, PBPK modelling applications, computational pipelines, databases, decision trees, *etc*.) with the NanoCommons e-infrastructure, to support interoperability and long-term sustainability of the nanosafety community outputs *via* a *toolbox of community accepted standards*.

☞ info@nanocommons.eu

User Guidance Handbook @ www.nanocommons.eu

- https://www.nanocommons.eu/e-infrastructure/user-guidance-handbook/

Training events and materials @ NanoCommons Infrastructure

- https://infrastructure.nanocommons.eu/events/

NanoCommons @ ELIXIR TeSS

- https://tess.elixir-europe.org/content_providers/nanocommons#events

NanoCommons community @ Zenodo

- https://zenodo.org/communities/nanocommons

NanoCommons Channel @ YouTube

- https://www.youtube.com/channel/UCuawpRvXNpglwyeItefTctw

mailing list of WG-A Education, Training, Communication

- www.nanosafetycluster.eu

Enjoy, good success & thank you for interest in our training event!

Online QSAR Modelling Hackathon by Easy Access to Jaqpot
Deploy your model as a web service in a few minutes

Philip Doganis, Harry Sarimveis

School of Chemical Engineering, National Technical University Of Athens, Greece

A place to

deploy discuss

share use

models

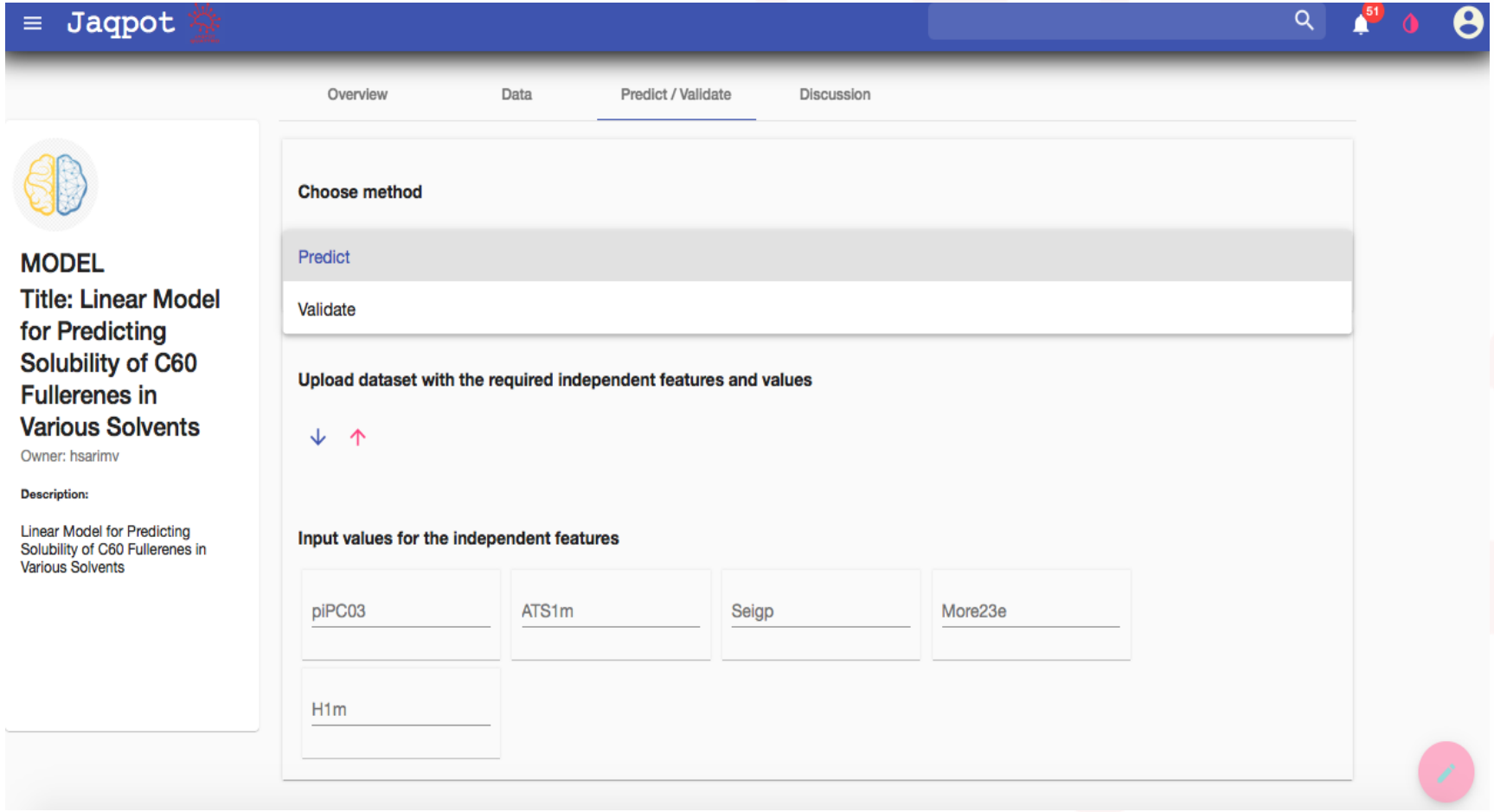
Jaqpot in a nutshell

- **Develop models** on various runtimes and **deploy** them as web services in seconds
- **Validate** your models and **generate predictions** with a user friendly interface
- Make them **transparent** to the users with flexible **documentation** methods
- **Share** your models and make them **accessible** to selected users, collaborators, or groups
- **Integrate** them with your applications within seconds
- Meet your **scalability** requirements

Goal of the Hackathon

- At the end of this hackathon, each participant will have reproduced a **web implementation of a nanoQSAR model** in the Jaqpot platform **in a matter of minutes**.
- The model predicts successfully the **solubility of C60 Fullerene** in Various Solvents and was originally presented in the following publication:
  Farhad Gharagheizi & Reza Fareghi Alamdari (2008) A Molecular-Based Model for Prediction of Solubility of C60 Fullerene in Various Solvents. **Fullerenes, Nanotubes, and Carbon Nonstructures**, 16:1, 40-57, DOI: 10.1080/15363830701779315. https://www.tandfonline.com/doi/full/10.1080/15363830701779315
- Use of Google Colab notebooks will allow you to complete the implementation **without installing any software or application** in your local machines.

Jaqpot user interface



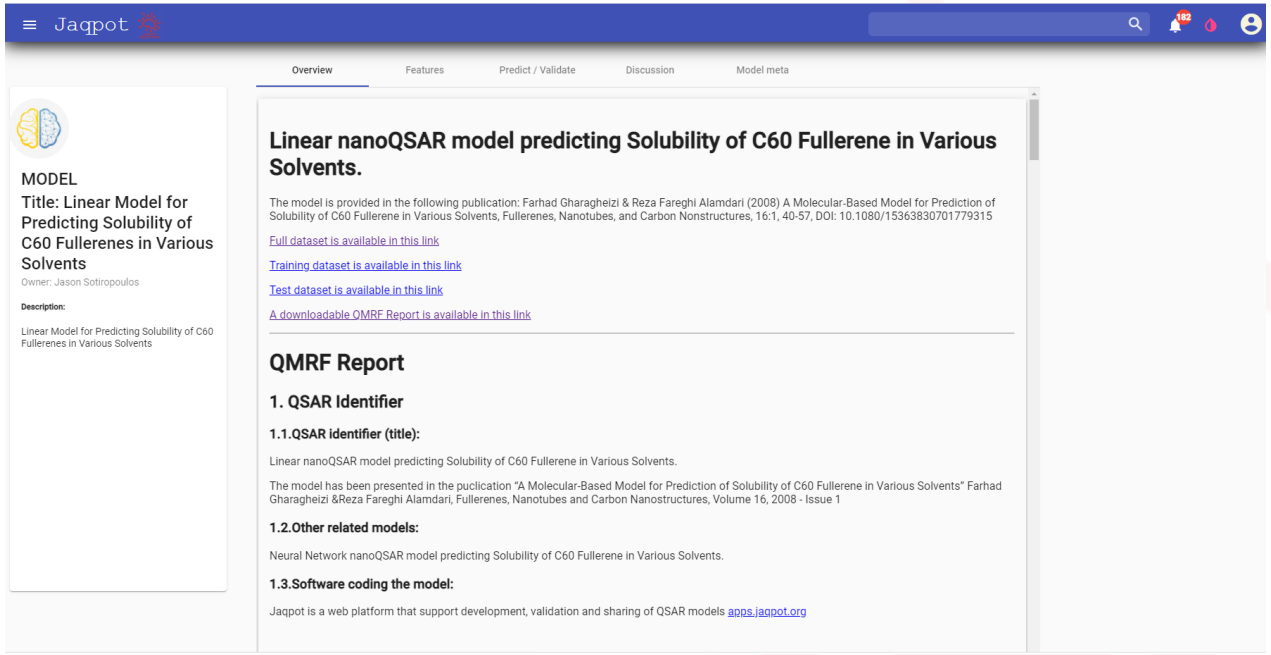
Predict-validate tab

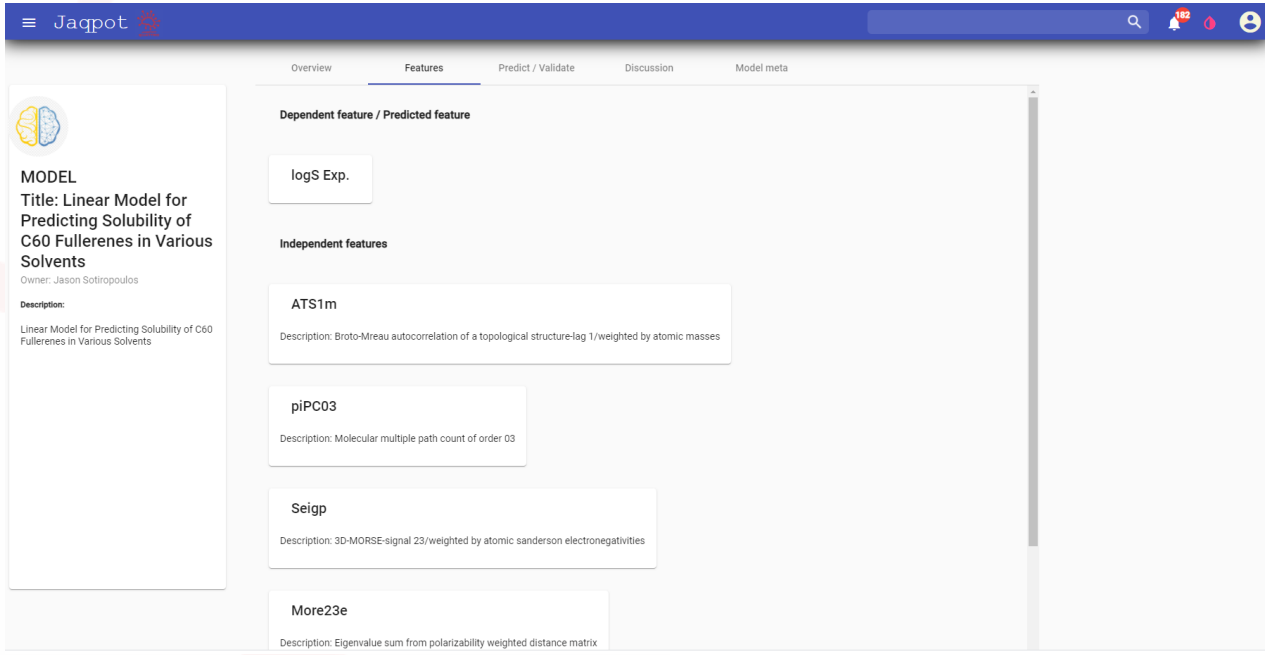
1. **Create predictions**
   a. by manually entering values
   b. CSV datasets using Jaqpot-generated template

1. **Validate model performance:**

   using an external validation dataset as input in CSV format

Model description



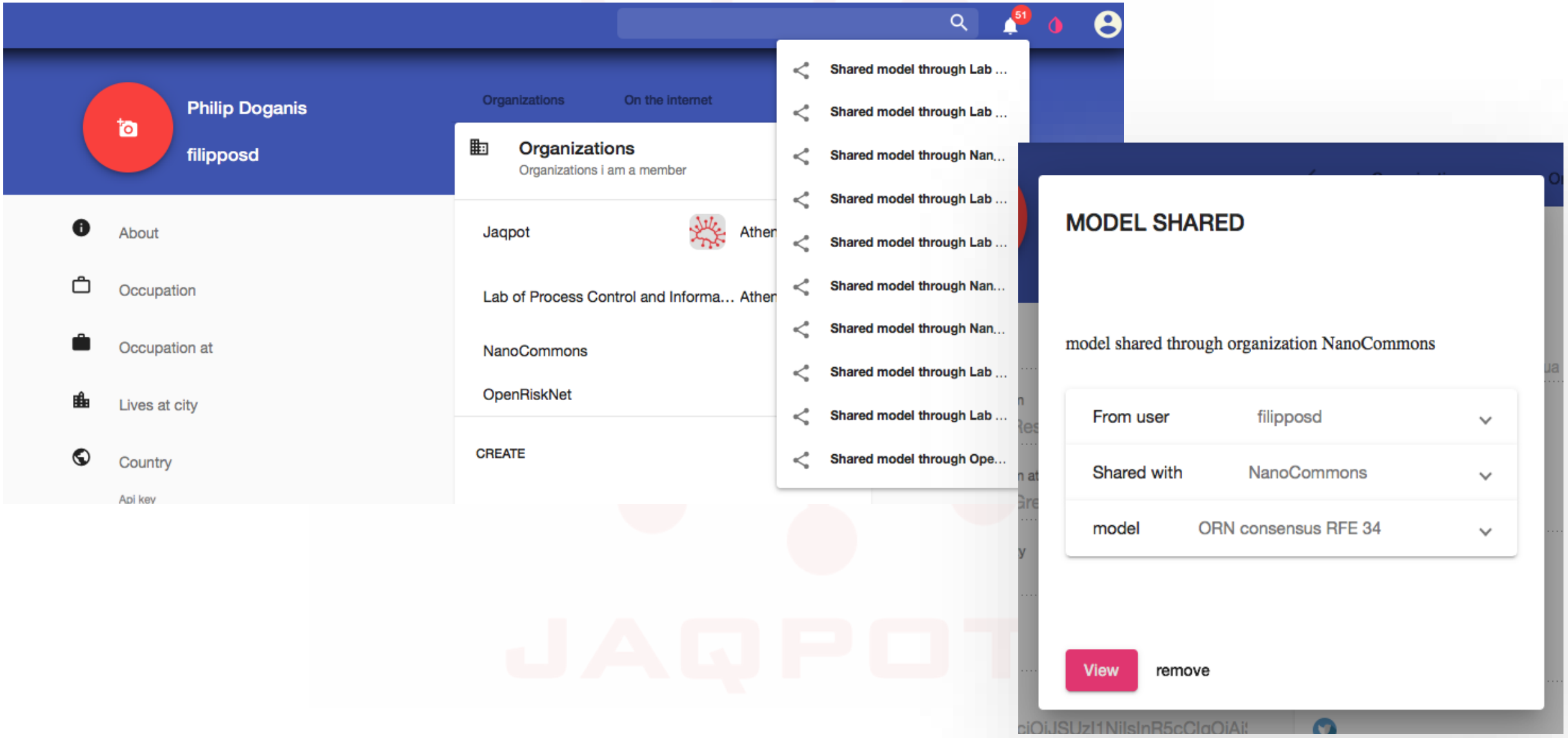


Information on the model can be provided in Markdown:
https://www.markdownguide.org/basic-syntax/

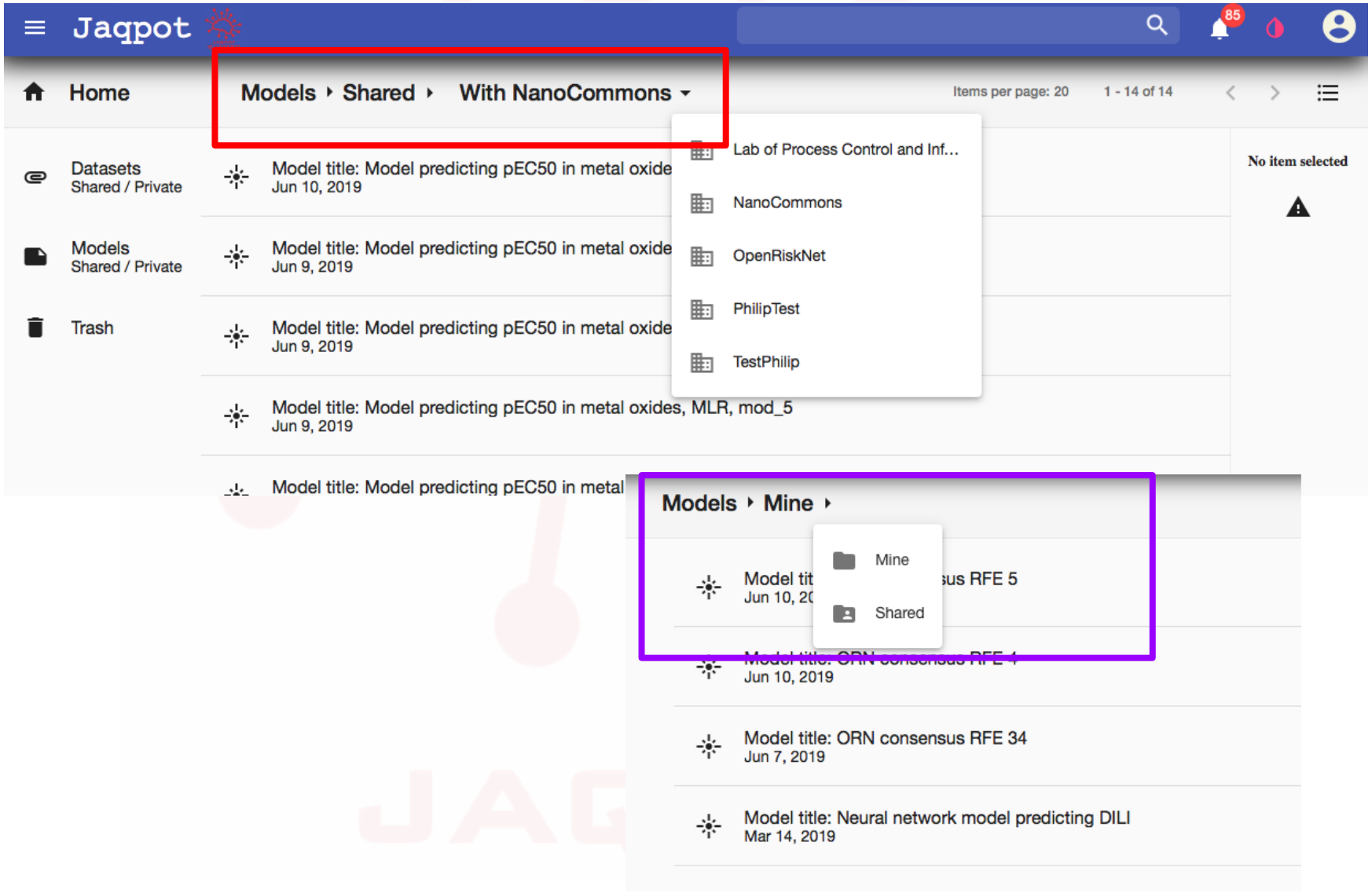
Feature documentation is a critical part of a model interpretation.
Model features can be documented with

- Description
- Units
- Ontological classes

Sharing of resources

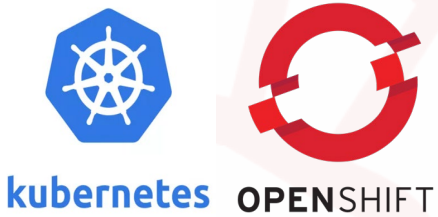


Shared space



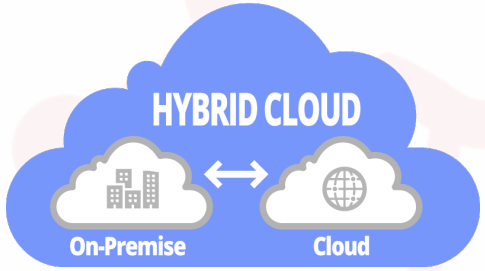
Meet the scalability requirements

All Jaqpot services are running through containers. Consists of REST microservices that can be scaled to meet the requirements of the infrastructure.



Kubernetes allows the container management and incorporates high availability of the services. It can be deployed on any public, private or hybrid cloud. Jaqpot services can run on any such system

Jaqpot can support any solution. It can be deployed on any infrastructure. Public / Private or On-Premise.

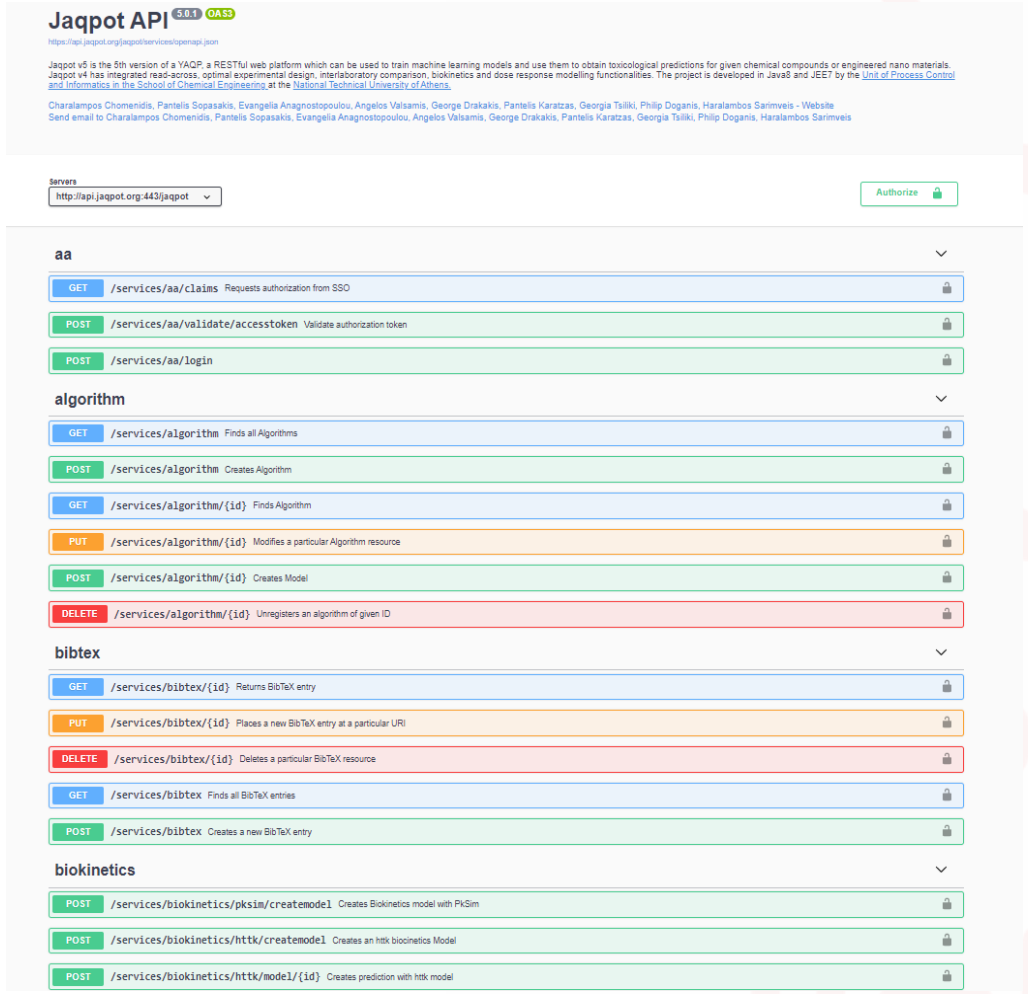


An open source software product to allow OpenID Connect single sign-on with Identity Management and Access Management aimed at modern applications and services.
Variety of user or identity providers can be integrated. From google to LDAP and Kerberos to meet the security needs of an organization

Right now integrated with

Under the stewardship of:

Integration through Application Programming Interfaces (APIs)

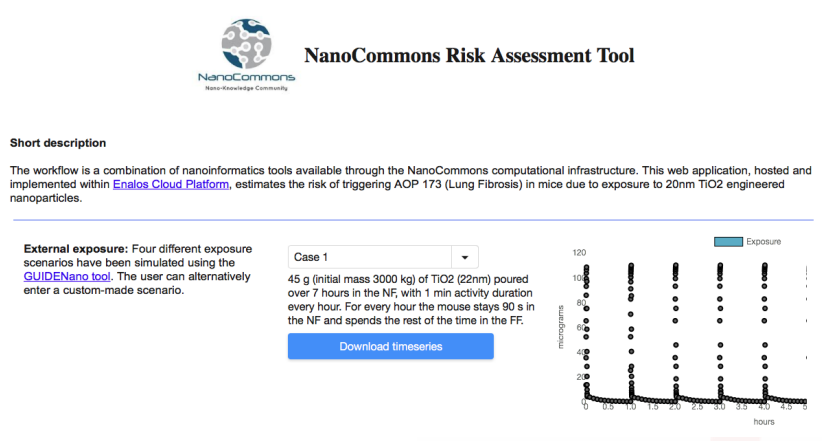


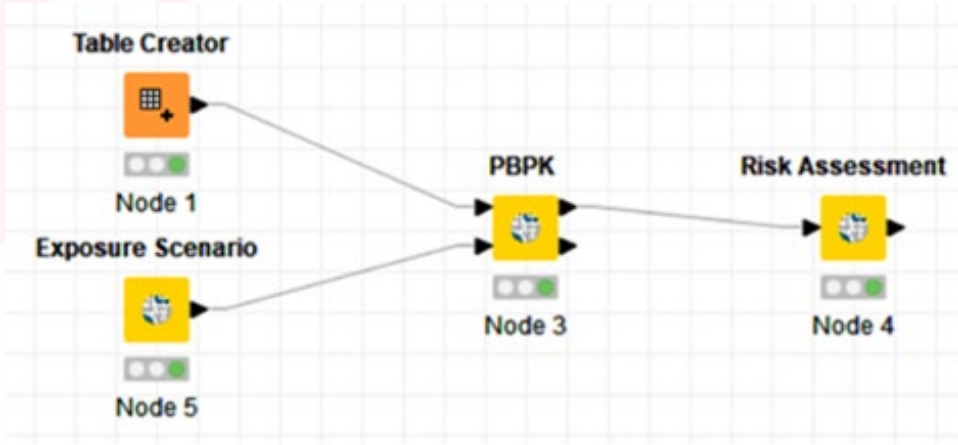
API clients

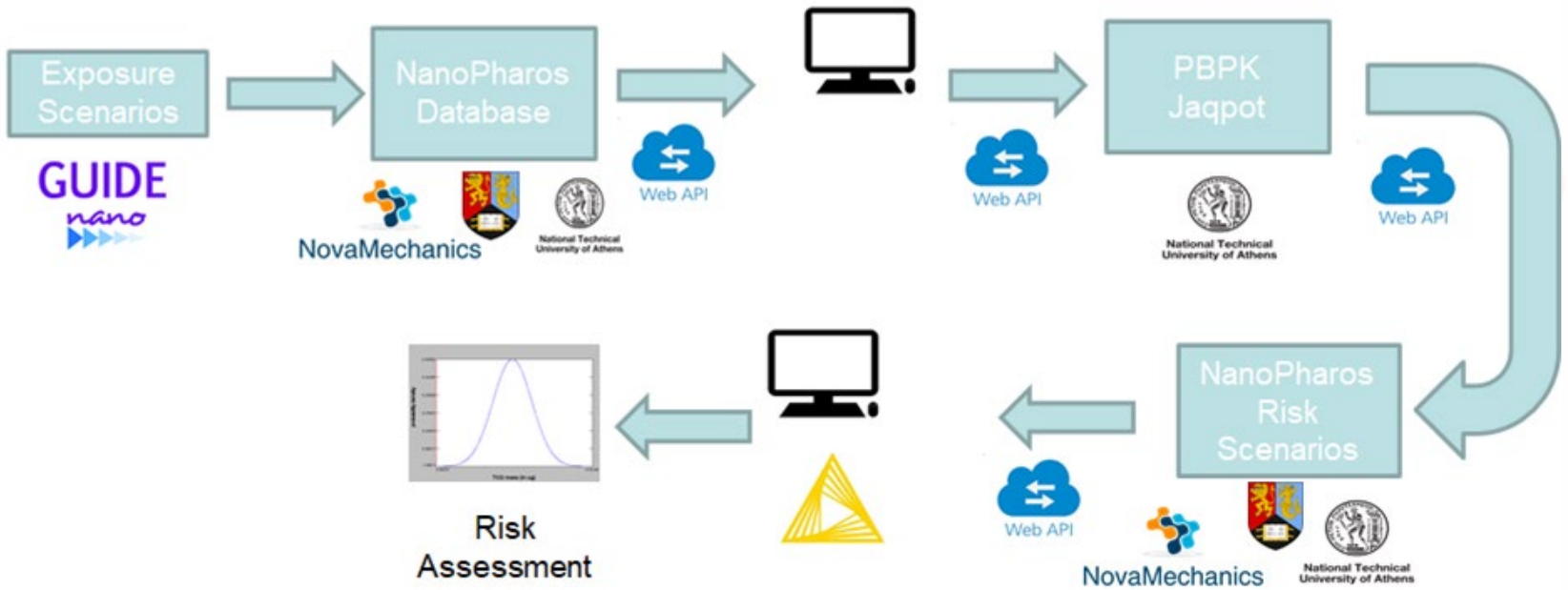
- Nuget Package (.NET): https://www.nuget.org/packages/JaqpotNet/1.0.0
- Go(lang) Package: https://github.com/euclia/gojaqpot
- Java: https://search.maven.org/artifact/xyz.euclia/jaqpotj/0.0.1/jar
- Javascript Package: https://www.npmjs.com/package/@euclia/jaqpot-client
- Python Package: https://pypi.org/project/jaqpotpy/

https://api.jaqpot.org/jaqpot/swagger/

Jaqpot integrated applications and services: NanoCommons Risk Assessment Tool

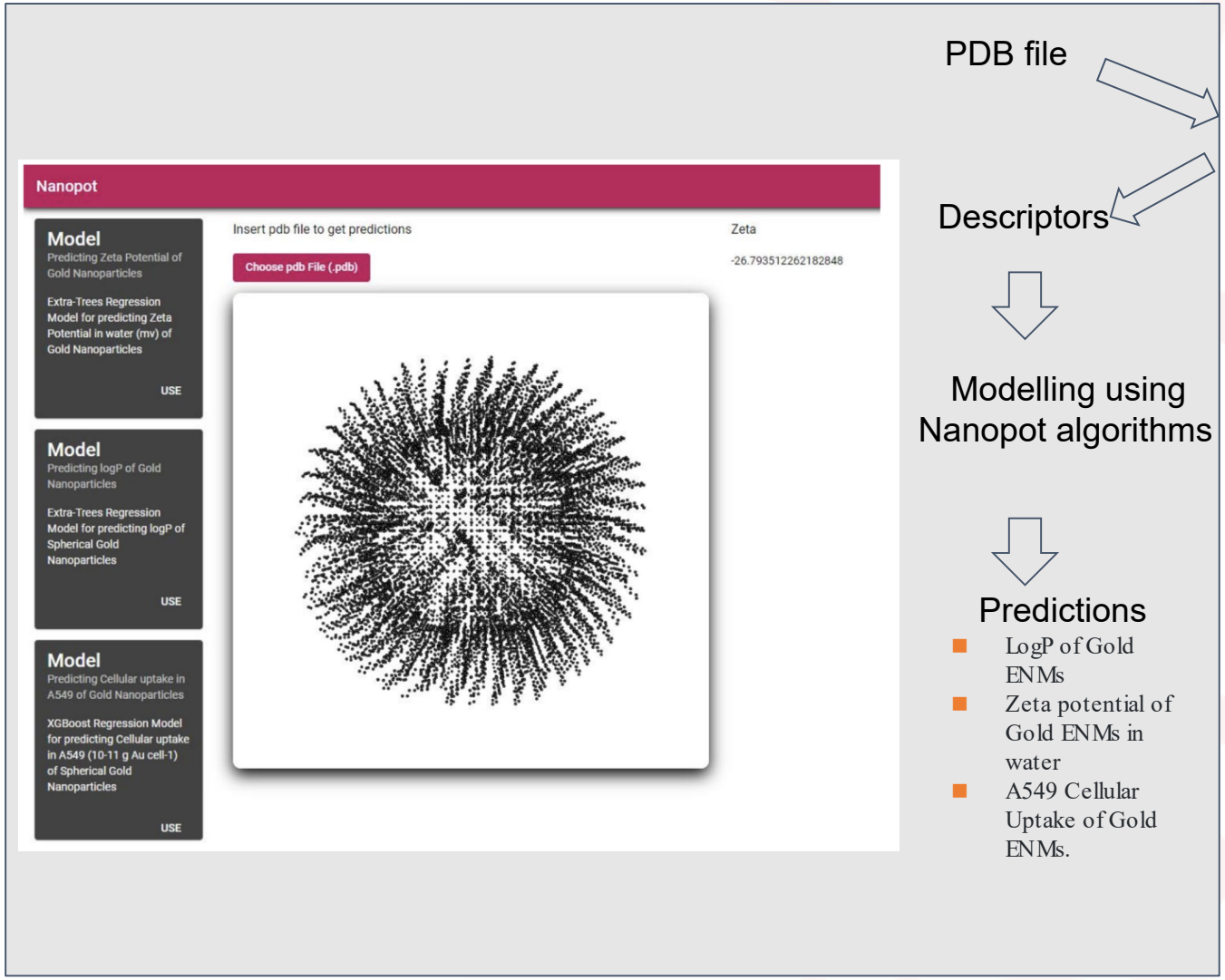






http://enaloscloud.novamechanics.com/nanocommons/exposure/

Jaqpot integrated applications and services: Nanopot



PDB file

Descriptors

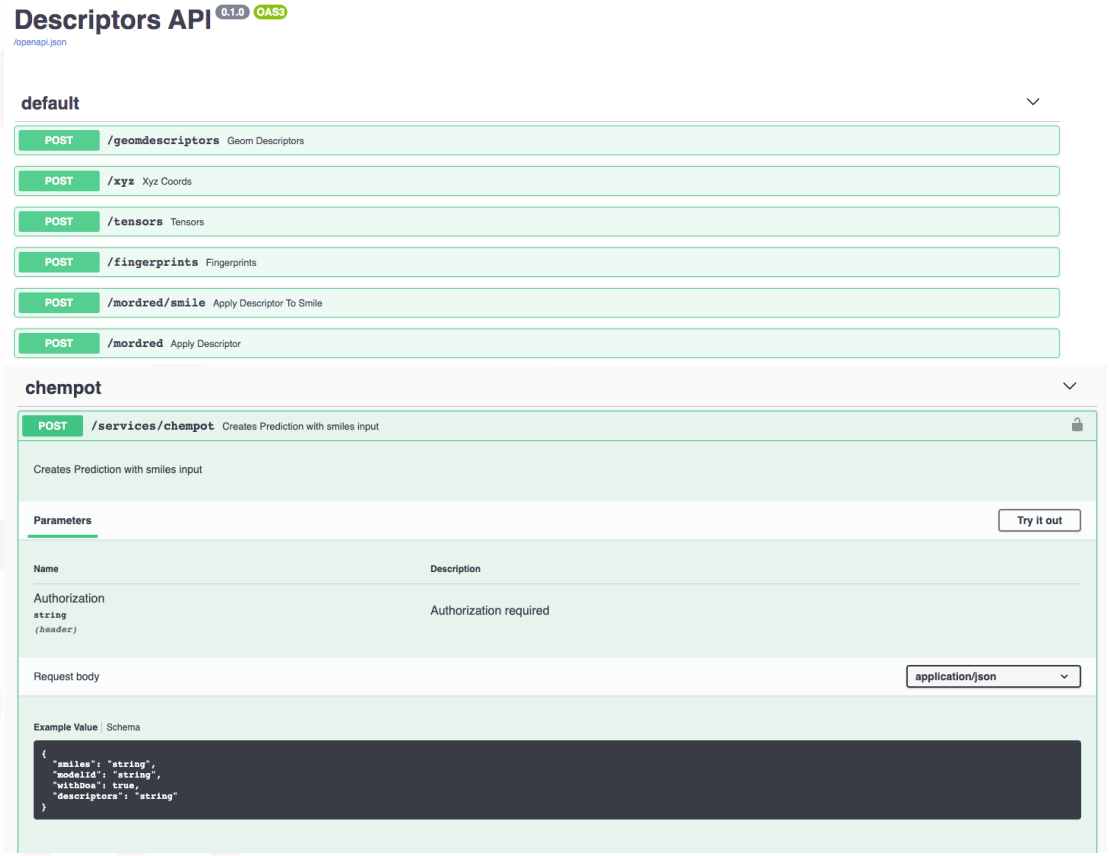
Geometric descriptors API

Modelling using Nanopot algorithms

Predictions

- LogP of Gold ENMs
- Zeta potential of Gold ENMs in water
- A549 Cellular Uptake of Gold ENMs.

Nanopot integrates the Jaqpot API to generate predictions for Engineered Nanomaterials with the use of PDB files.
https://nanopot.cloud.nanosolveit.eu/



SMILES also can be used as input to the API and be integrated with the available clients

How Jaqpot can serve your needs

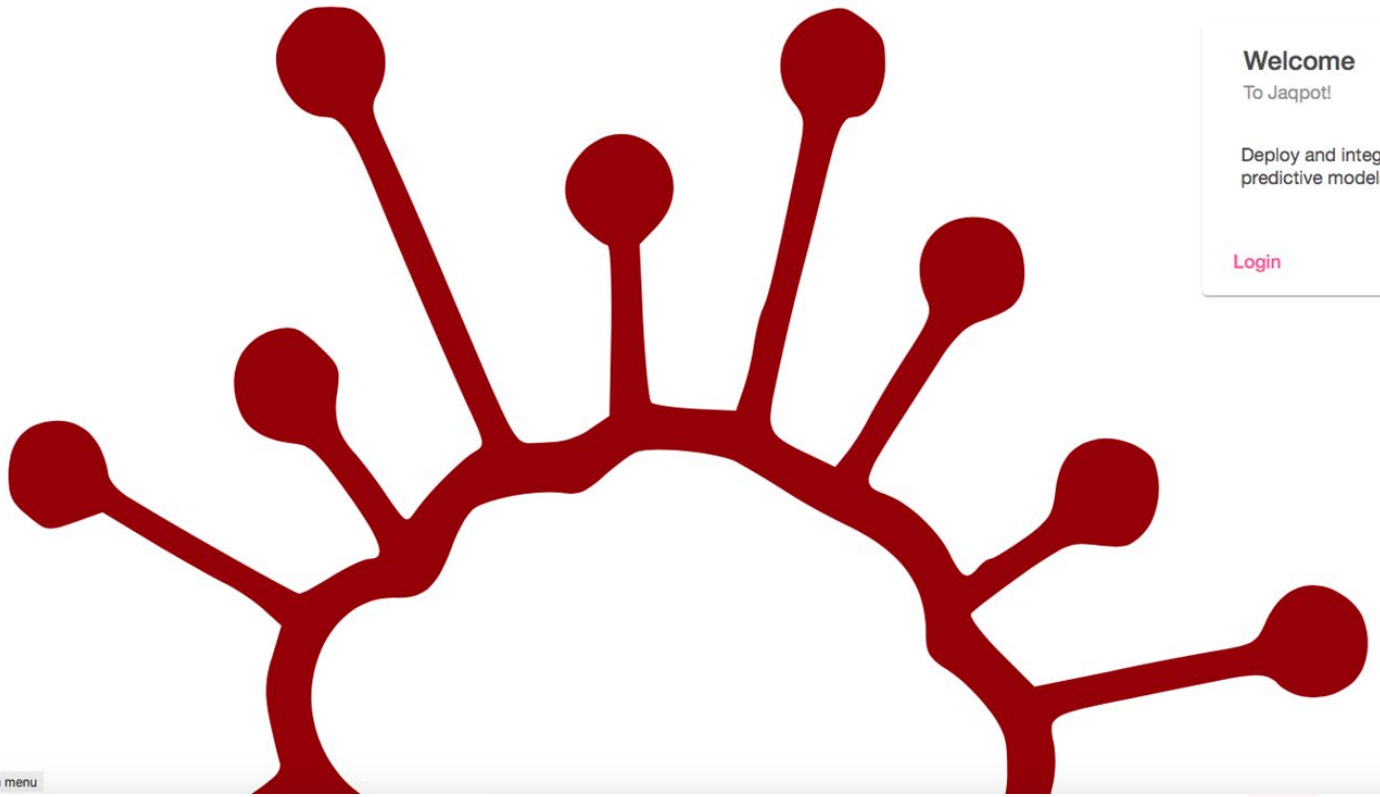
- **Publish your model** as web services
- Provide **ready-to-use implementations** of your models as supporting material to your publications
- **Collaborate** with your partners and colleagues
- **Share models** within your group, project or organisation and **disseminate** them to the community or to the general public
- **Embed and integrate Jaqpot models** into other applications and workflows via API clients.
- Use Jaqpot as your **modelling environment**

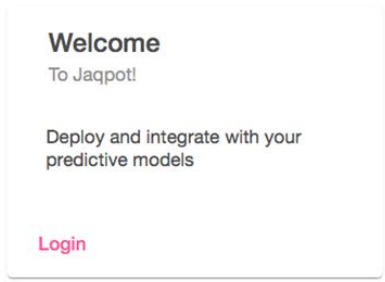
Useful links:

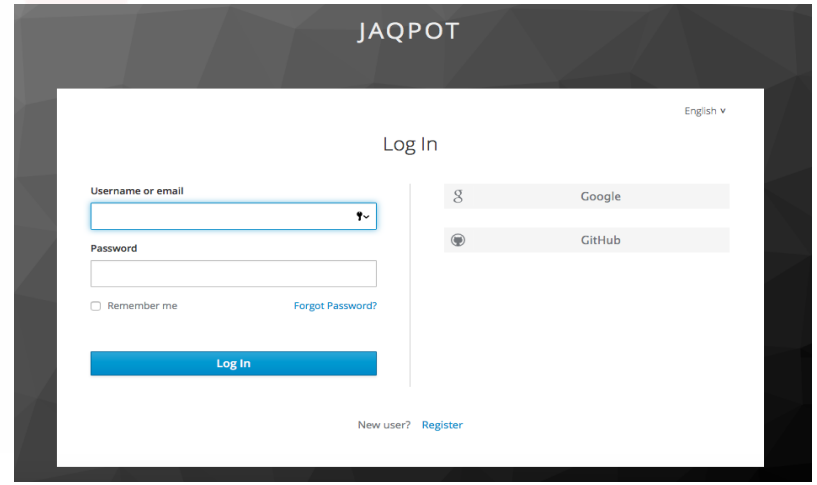
Jaqpot web platform	https://app.jaqpot.org/home
Jaqpot accounts application	https://accounts.jaqpot.org/
Jaqpot technical documentation	https://www.jaqpot.org/
Jaqpot swagger API documentation	https://api.jaqpot.org/jaqpot/swagger/
Jaqpot tutorials	Jaqpot5 - User accounts Jaqpot5: How to manage and use organisations Jaqpot5: How to access and use an existing predictive model Jaqpot5: How to deploy a predictive model using the jaqpotpylibrary Jaqpot5: How to simulate biodistribution scenarios using custom PBPK models

Jaqpot core development team

Sarimveis Haralambos	Professor, Unit of Process Control& Informatics, School of Chemical Engineering, National Technical University Of Athens, Greece
Doganis Philip	Senior Researcher, Laboratory & Teaching Staff
Karatzas Pantelis	Doctoral Researcher, Head Developer
Tsiros Periklis	Doctoral Researcher
Sotiropoulos Jason	Doctoral Researcher




Welcome
To Jaqpot!
Deploy and integrate with your predictive models
Login


JAQPOT
English
Log In
Username or email
Password
Remember me
Forgot Password?
Log In
Google
GitHub
New user?
Register

Thank you

JAQPOT

NanoCommons

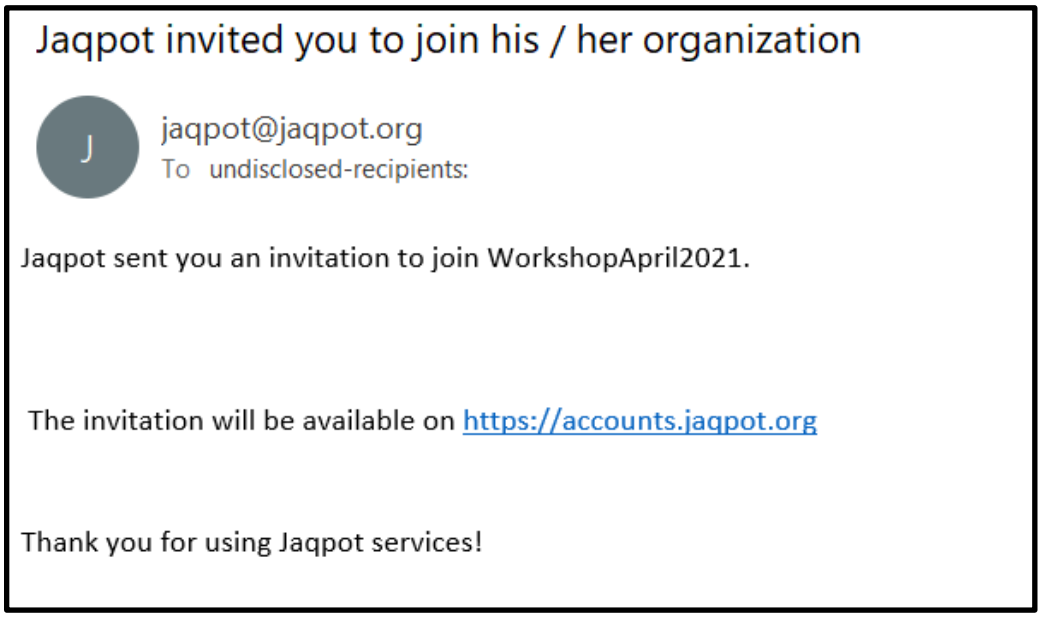
Nano-Knowledge Community

Online QSAR Modelling Hackathon by Easy Access to Jaqpot: Deploy your model as a web service in a few minutes

Tue, Apr 13, 2021 3:00-4:30 PM CEST

Preparing for the hackathon

We have already sent an invitation to all hackathon participants to join the Jaqpot organisation **WorkshopApril2021**, which will be used during the hackathon (please check your spam folder).


Jaqpot invited you to join his / her organization

J

jaqpot@jaqpot.org

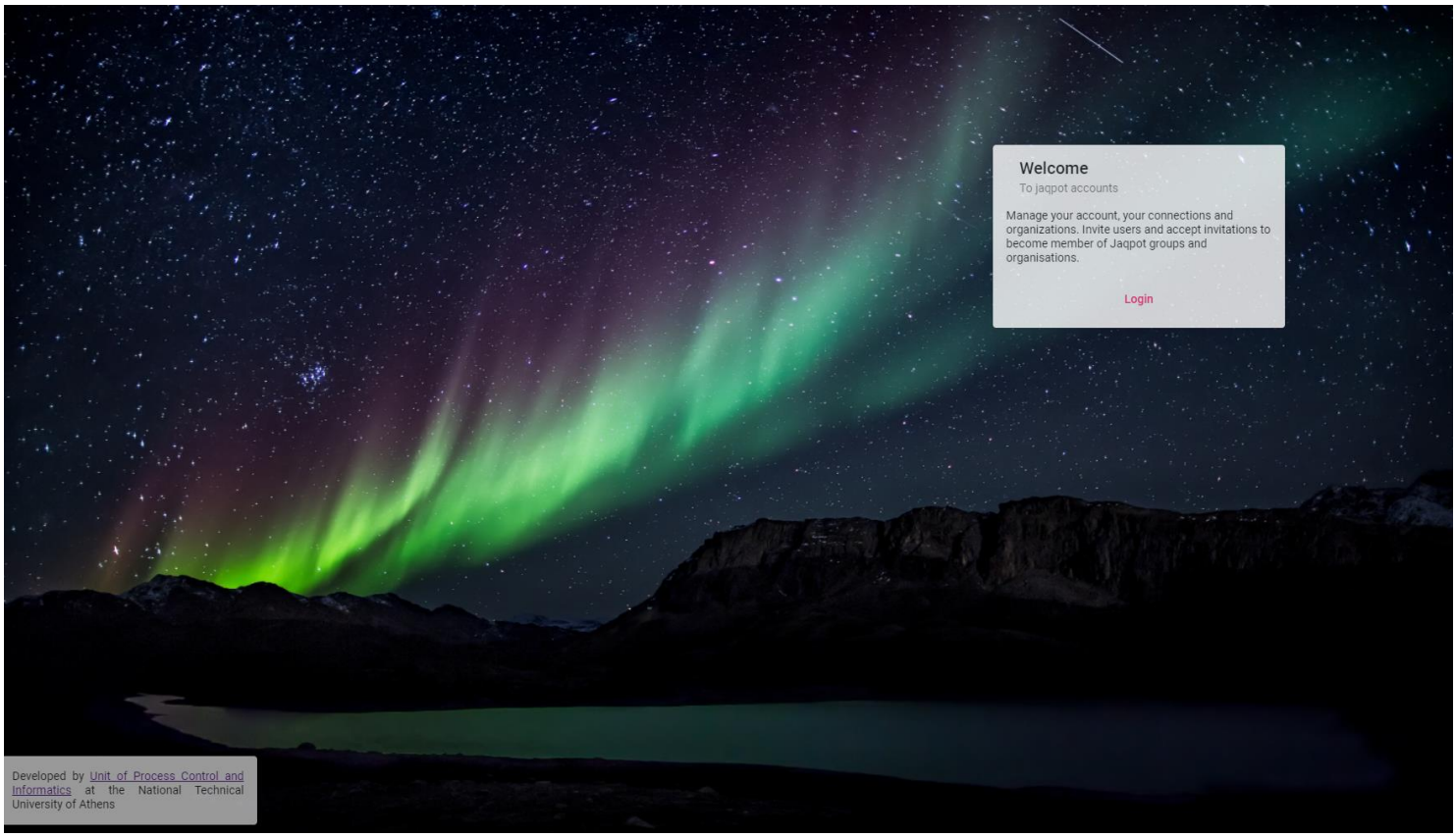
To undisclosed-recipients:

Jaqpot sent you an invitation to join WorkshopApril2021.

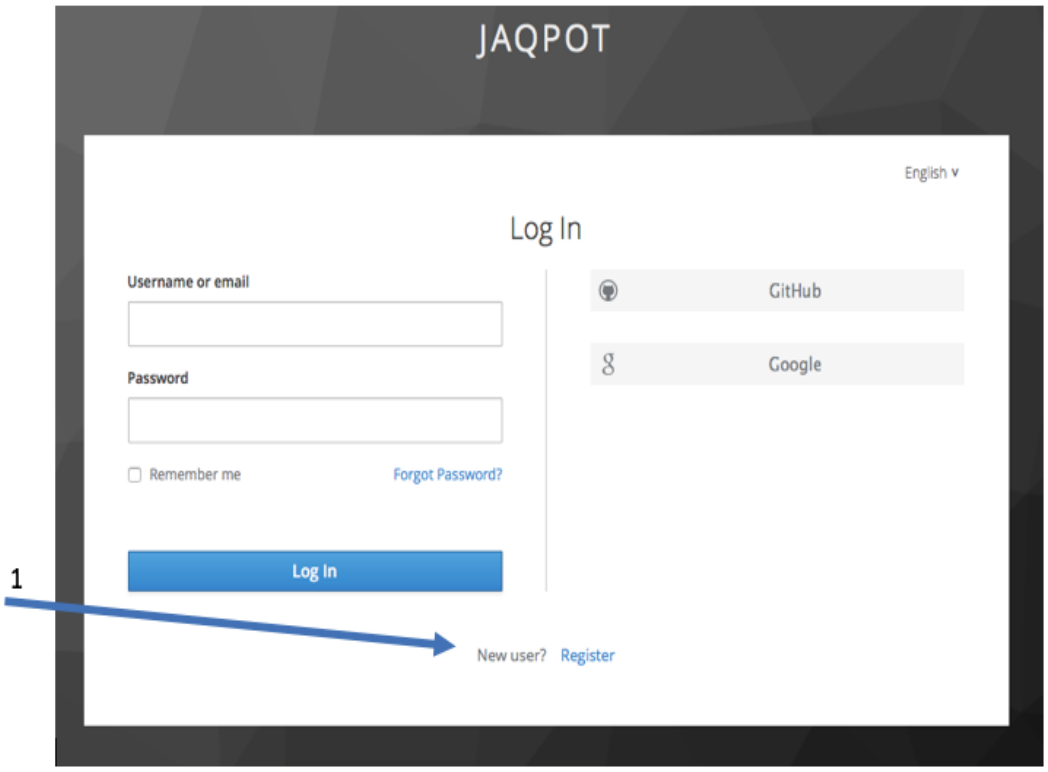
The invitation will be available on https://accounts.jaqpot.org

Thank you for using Jaqpot services!

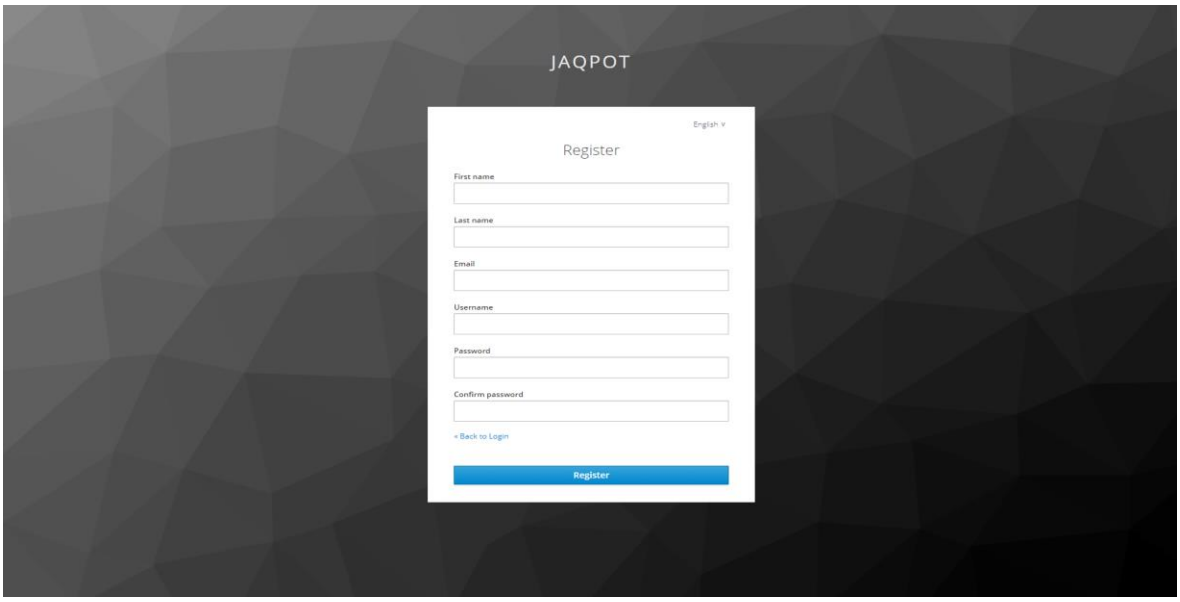
To accept the invitation, you should have a Jaqpot user account. Please create a user account by visiting the Jaqpot accounts application: https://accounts.jaqpot.org and clicking on “Login”.



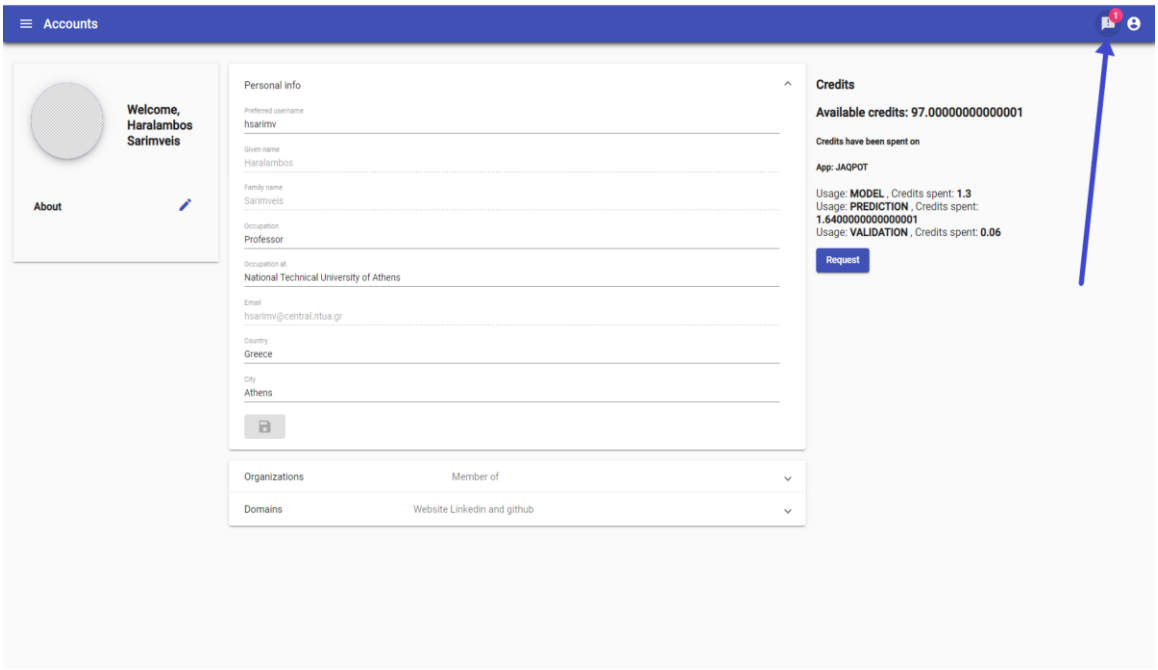
You will be redirected to the Login page. Please create your Jaqpot user account by selecting the "Register" option. For the purposes of this hackathon, please avoid using the Google/Github option, to enable a more uniform approach among participants.



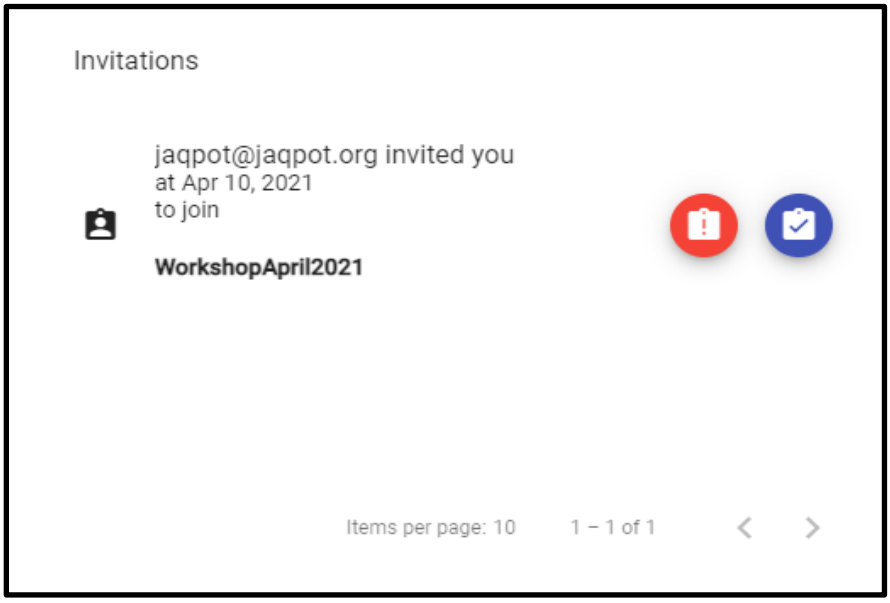
Only basic information is required for registering to Jaqpot and creating a user account. Please make sure you enter the e-mail address, where you received the invitation. If you prefer to use another email address, please inform us by sending an email to jaqpot@jaqpot.org, and we will send you a new invitation.



The entry page in the https://accounts.jaqpot.org accounts application, looks like this:



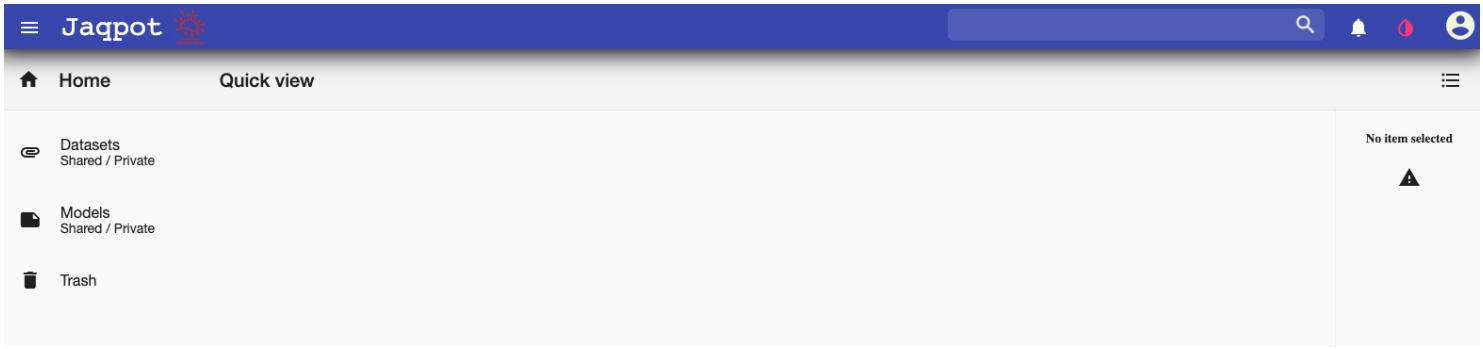
Please click on the "Invitations" icon on the top right part of the screen. This will open a window containing the invitation to the Workshop 2021 group:



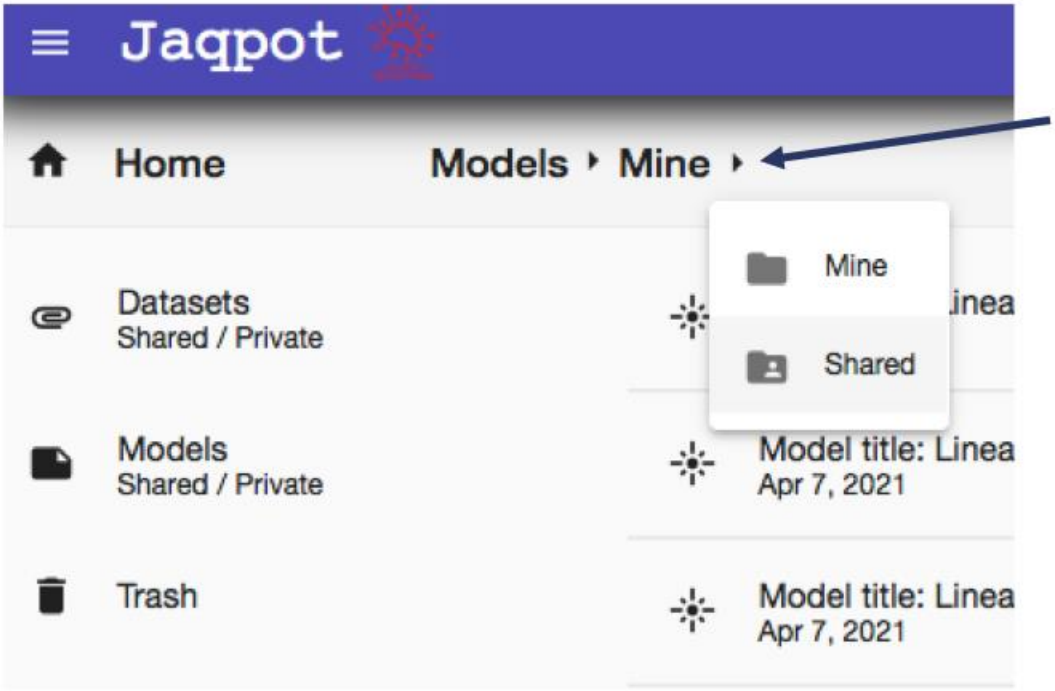
Please click on the blue icon to accept the invitation.

You now have a Jaqpot account, and you are a member of the WorkshopApril2021 group!

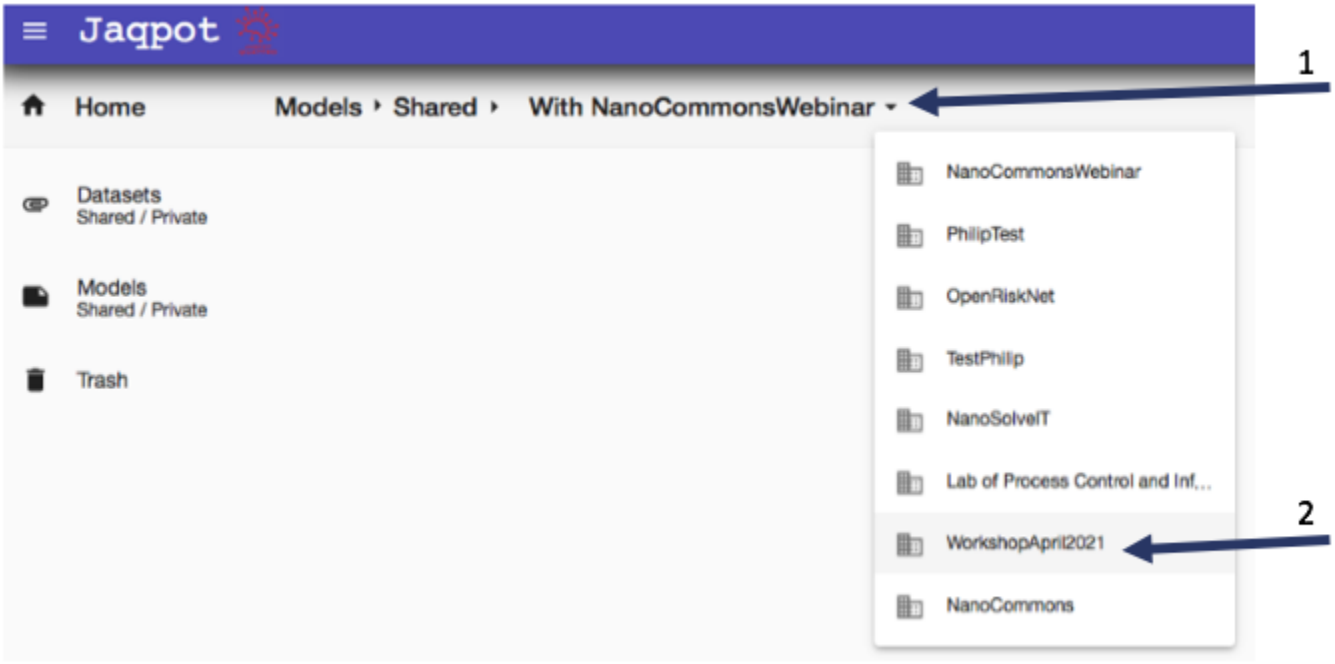
If you like to navigate through Jaqpot, you can visit the Jaqpot application: https://app.jaqpot.org/home with your Jaqpot username and password. Your entry page will be empty, because you have not yet created a model or dataset.



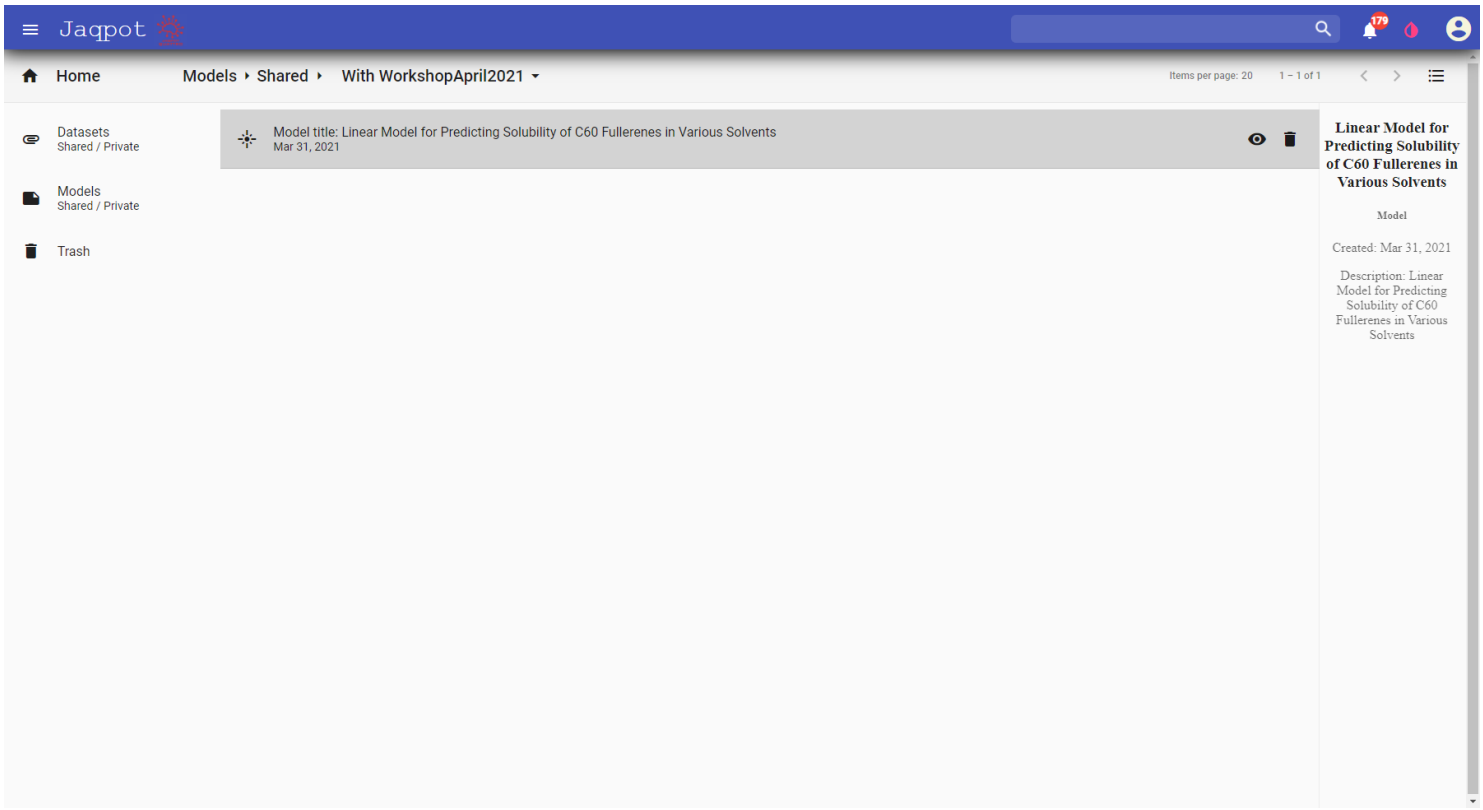
You can visit the **WorkshopApril2021** organisation by clicking the triangle icon next to **Mine**.



Please select the **shared** option and then the **WorkshopApril2021** organisation.



Now you have access to a full implementation of a Jaqpot model. The goal of the workshop will be to reproduce this web application in only a few minutes!



Online QSAR Modelling Hackathon by Easy Access to Jaqpot: Deploy your model as a web service in a few minutes

Tue, Apr 13, 2021 3:00-4:30 PM CEST

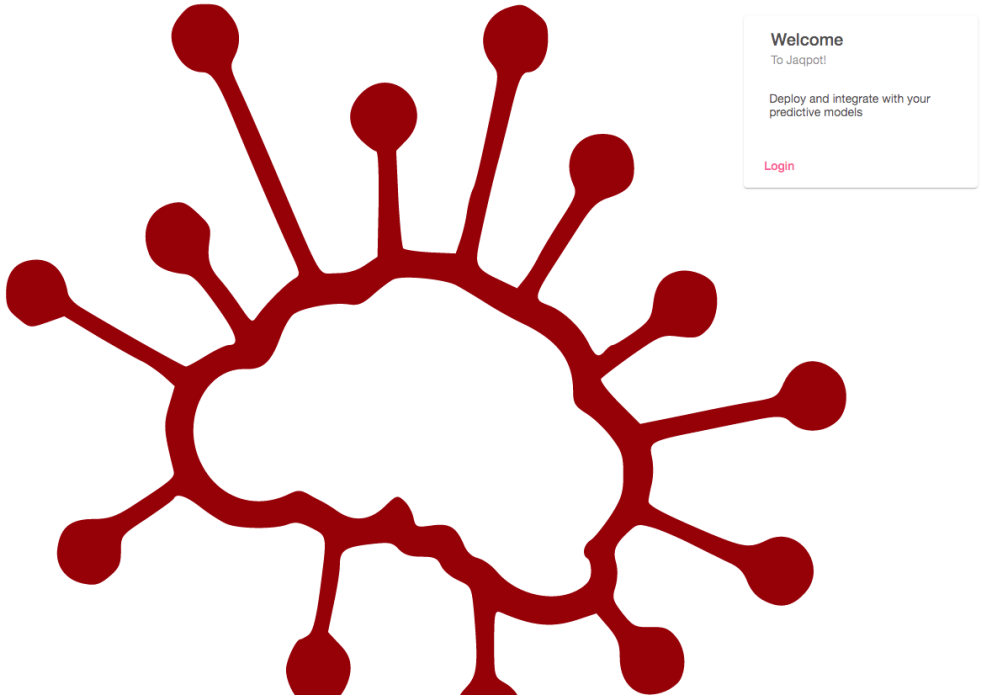
Briefly

- You will learn how a local QSAR model can be transformed to an online QSAR model web service, no installations required
- Prerequisites:
    - For access to Jaqpot, you will need a Jaqpot account
    - For access to Google colab you will need a Google account

Introduction 3
Problem studied 3
1. Accessing Jaqpot 4
2. Retrieving the dataset from NanoPharos 6
3. Accessing the Google colab notebook 6
4. Running the colab notebook to create the model web service on Jaqpot 8
1. Setting up packages 8
2. Uploading the data to the colab notebook 8
3. Viewing and Preprocessing the dataset 9
4. Training the model 9
5. Getting authentication to access Jaqpot 10
6. Deploying the model 10
ADDITIONAL STEPS 12

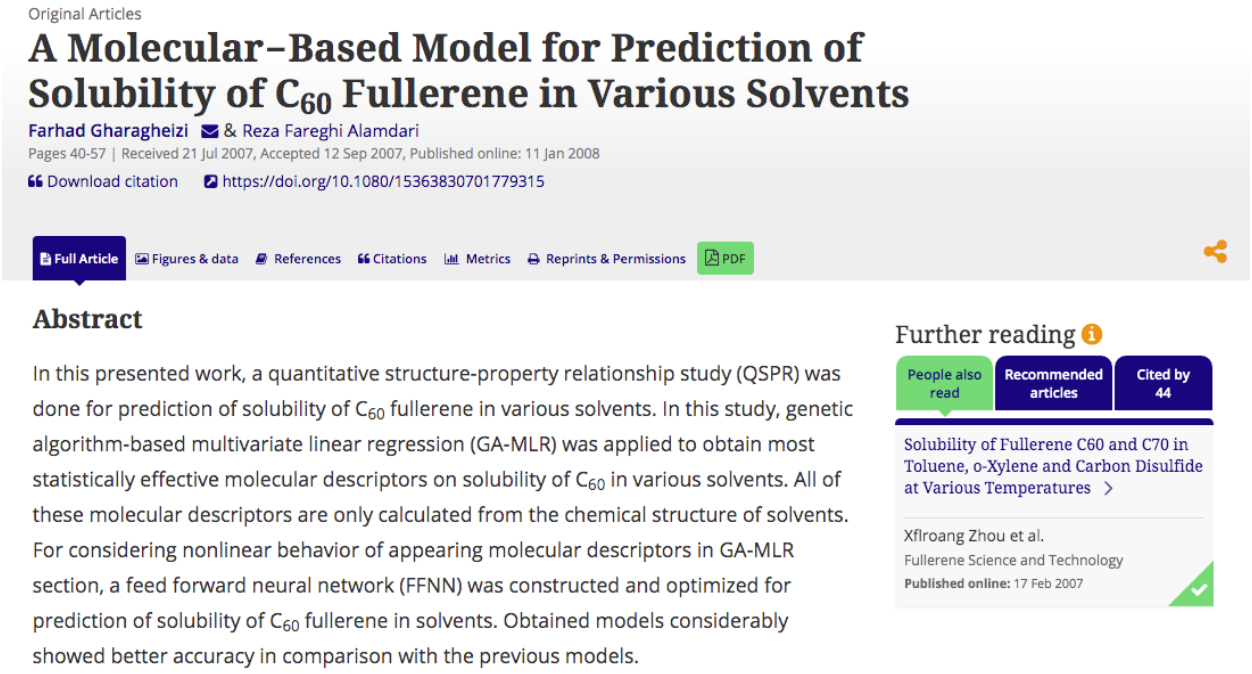
Introduction

Jaqpot 5 (https://app.jaqpot.org) is a powerful and versatile platform for toxicological in silico predictions, allowing you to deploy machine learning models incredibly easy and make them available to the community as web services.



Problem studied

In this tutorial we will demonstrate how to reproduce and publish in Jaqpot 5, a Linear nanoQSAR model predicting Solubility of C60 Fullerene in Various Solvents, with just a few lines of code in a Colab notebook. The model has been originally presented in the following publication: Farhad Gharagheizi & Reza Fareghi Alamdari (2008) *A Molecular-Based Model for Prediction of Solubility of C60 Fullerene in Various Solvents*. Fullerenes, Nanotubes and Carbon Nanostructures, 16:1, 40-57, DOI: 10.1080/15363830701779315. https://www.tandfonline.com/doi/full/10.1080/15363830701779315



Original Articles

A Molecular–Based Model for Prediction of Solubility of C_{60} Fullerene in Various Solvents

Farhad Gharagheizi & Reza Fareghi Alamdari

Pages 40-57 | Received 21 Jul 2007, Accepted 12 Sep 2007, Published online: 11 Jan 2008

Download citation https://doi.org/10.1080/15363830701779315

Full Article | Figures & data | References | Citations | Metrics | Reprints & Permissions | PDF

Abstract

In this presented work, a quantitative structure-property relationship study (QSPR) was done for prediction of solubility of C_{60} fullerene in various solvents. In this study, genetic algorithm-based multivariate linear regression (GA-MLR) was applied to obtain most statistically effective molecular descriptors on solubility of C_{60} in various solvents. All of these molecular descriptors are only calculated from the chemical structure of solvents. For considering nonlinear behavior of appearing molecular descriptors in GA-MLR section, a feed forward neural network (FFNN) was constructed and optimized for prediction of solubility of C_{60} fullerene in solvents. Obtained models considerably showed better accuracy in comparison with the previous models.

Further reading

People also read | Recommended articles | Cited by 44

Solubility of Fullerene C60 and C70 in Toluene, o-Xylene and Carbon Disulfide at Various Temperatures

Xflroang Zhou et al.

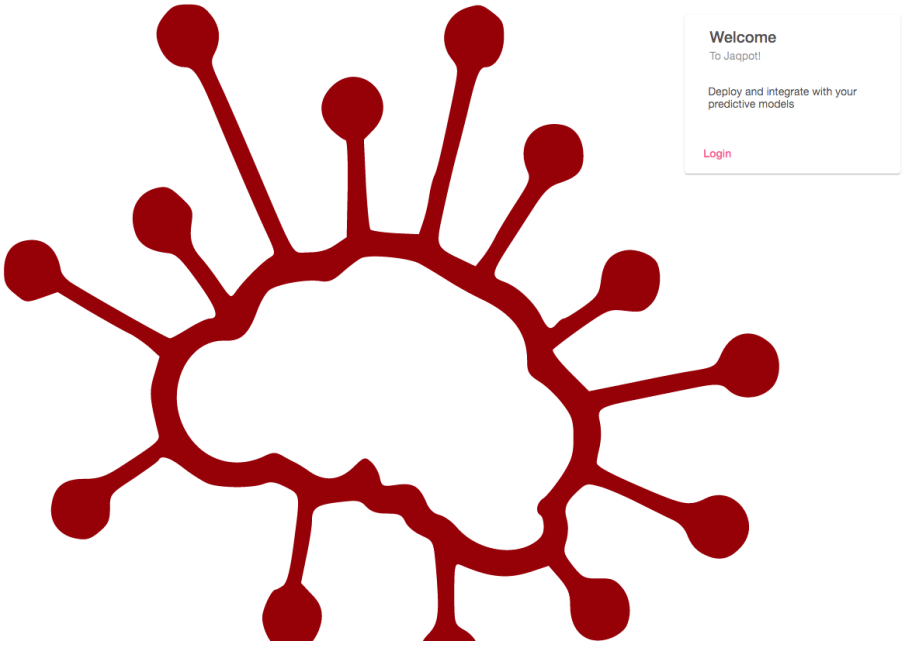
Fullerene Science and Technology

Published online: 17 Feb 2007

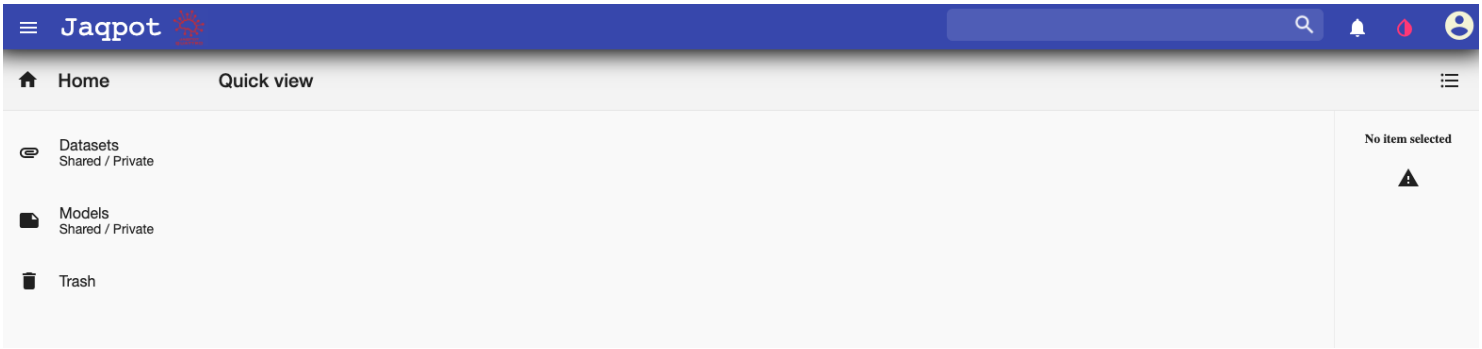
1. Accessing Jaqpot

In order to access Jaqpot, you need a Jaqpot account. For the purposes of this workshop, please avoid using the Google/Github option, to enable a more uniform approach among participants. If you are a new user, you can create a Jaqpot user account following the instructions provided in a separate document.

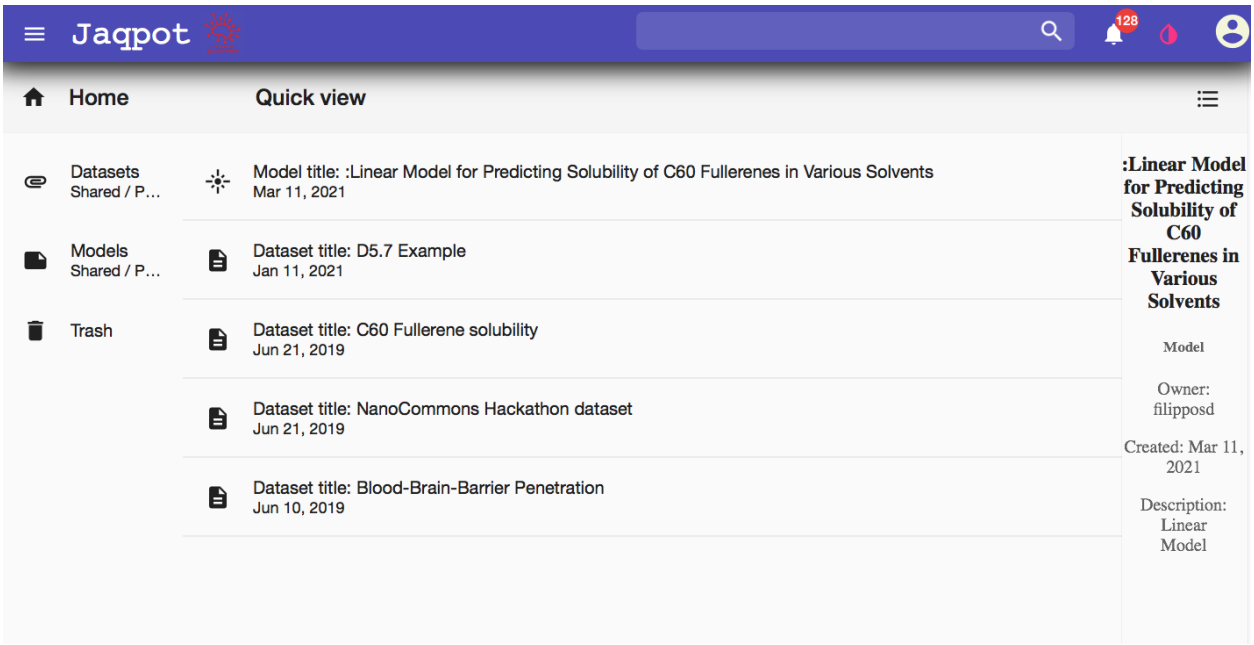
First click on **Login** on the welcome page:



You are then redirected to your Jaqpot homepage, which gives you access to your models and datasets.



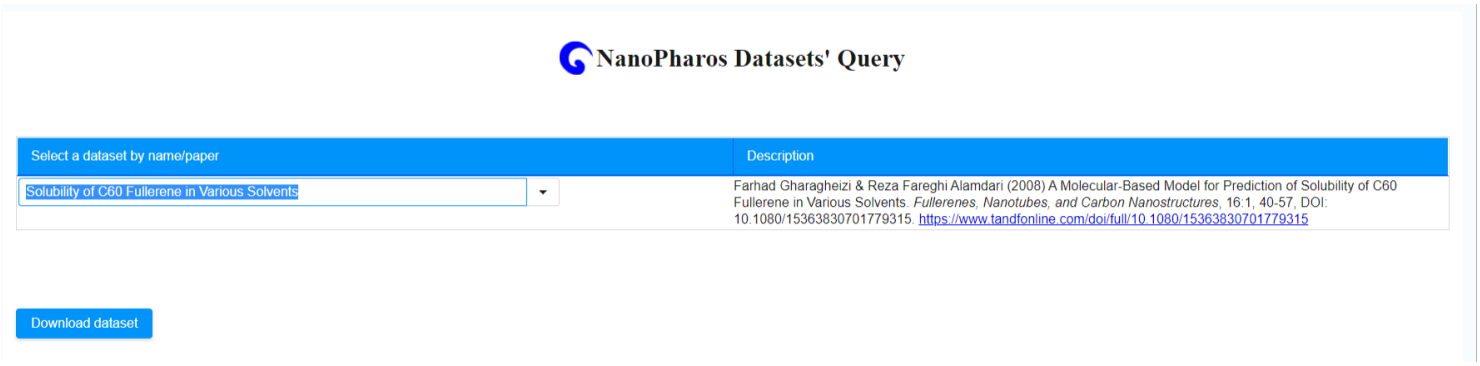
Currently you don't have any models or datasets. A populated homepage looks like this:

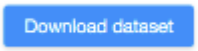


Each time you access Jaqpot on Google Colab (as we will see in a subsequent step) you need to identify yourself, in order to be granted access to your private resources by providing your username and password.

2. Retrieving the dataset from NanoPharos

The dataset can be retrieved in ready-to-model format from the NanoPharos database, which is accessible at: https://db.nanopharos.eu/Queries/Datasets.zul

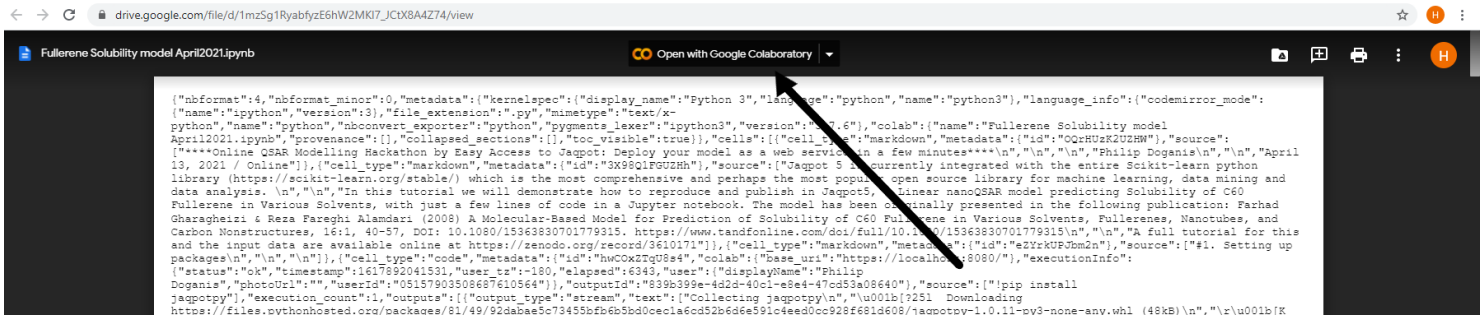


Please select the **Solubility of C60 Fullerene in Various Solvents** entry from the drop-down menu on the left and click the  button. An Excel file named '**70_model_reduced.xlsx**', will be downloaded and stored in your local computer.

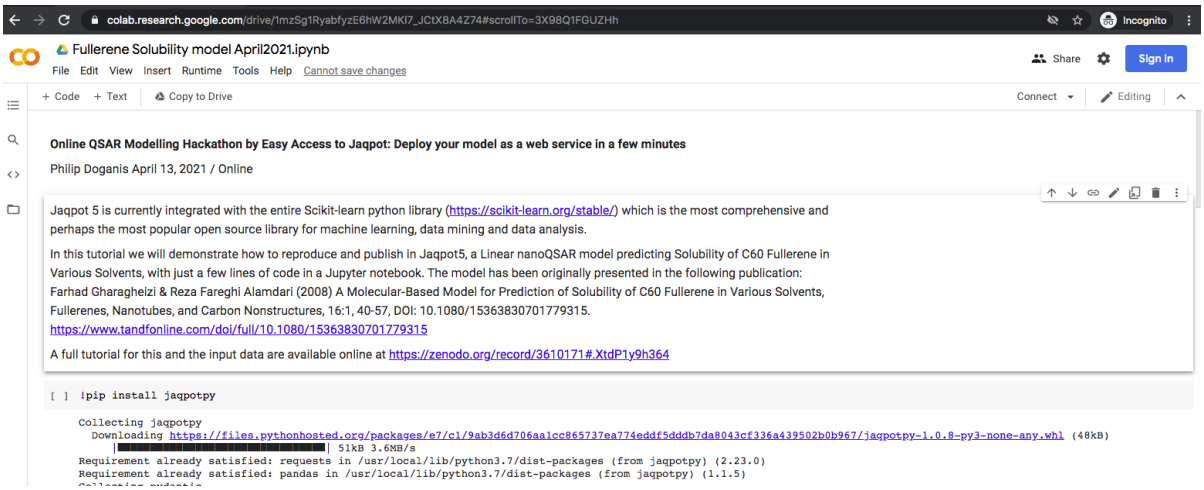
3. Accessing the Google colab notebook

The Google colab platform allows users to run code in the Python programming language without needing to perform any installation in their local machines. A Google colab notebook that performs all the calculations and contains all the commands for model creation and deployment has been prepared for you and is available at: https://drive.google.com/file/d/1mzSg1RyabfyzE6hW2MKI7_JCtX8A4Z74/view?usp=sharing

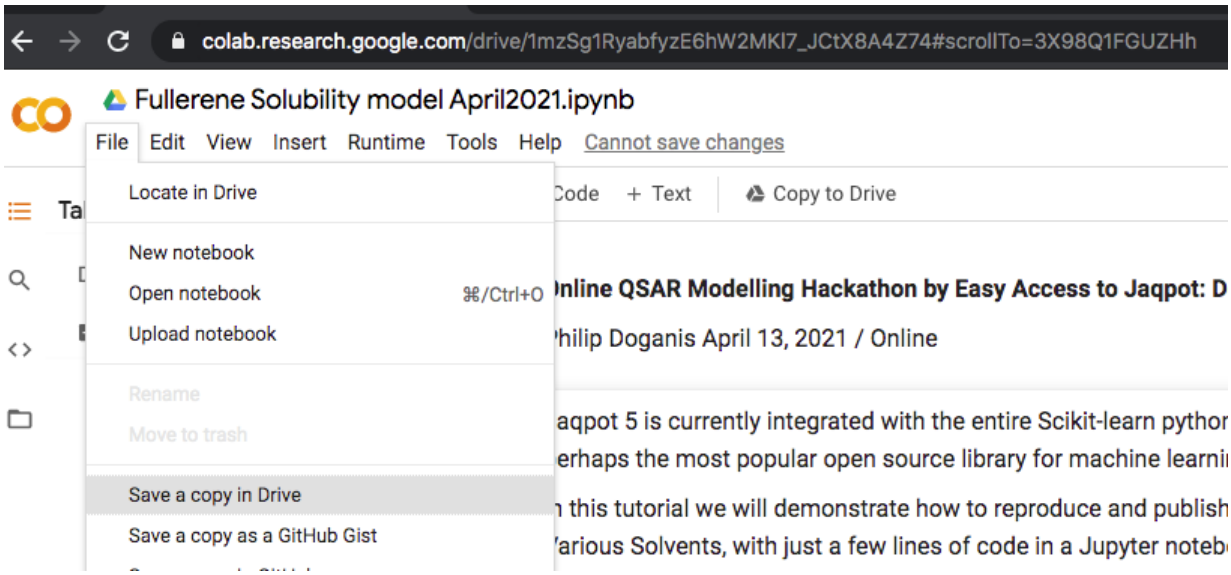
If a screen like this appears, please click on "Open with Google Colaboratory"



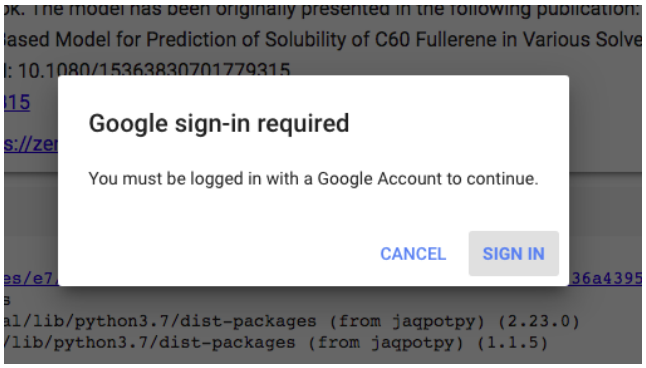
The Google colab notebook starting page looks like that:



In order to be able to use the notebook and make any changes, please save a copy of the notebook in the Drive by clicking the menu as shown below:



This can be done seamlessly when you are logged in as a Google user, if however you receive the message below you need to log in.



Now you have a local copy of the notebook that you modify and run. This is in your private space managed by Google.

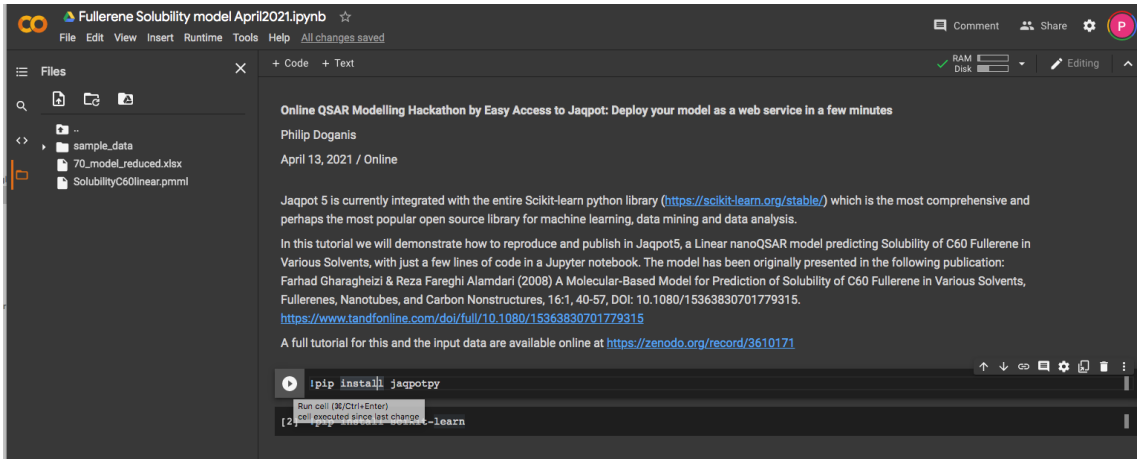
4. Running the colab notebook to create the model web service on Jaqpot

The notebook contains both text with comments, and cells containing python commands that will handle the dataset, make the necessary calculations and deploy the model as a web service. Green text in code cells are comments and are not executable.

1. Setting up packages

In order to execute code on the colab notebook you can go to the left of each cell and hit the icon. You see the outcome of the cell expanding right below the cell.

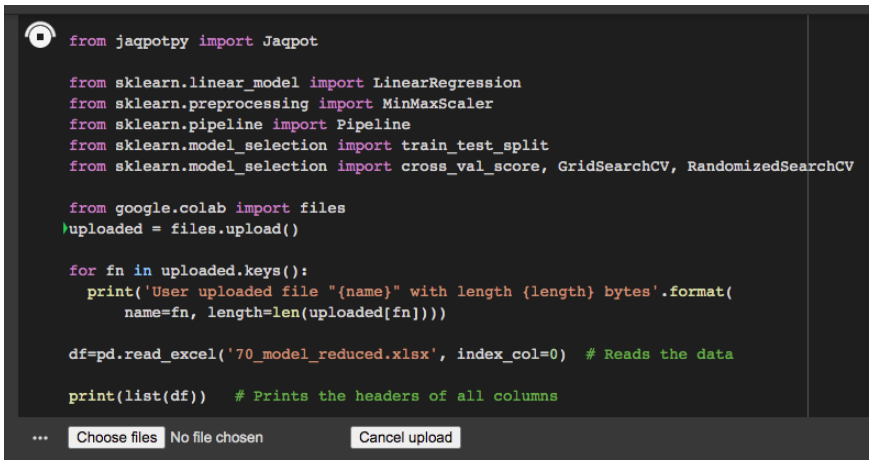
First , you will set up the Jaqpotpy, scikit-learn and pandas packages, so they can be used within the notebook:



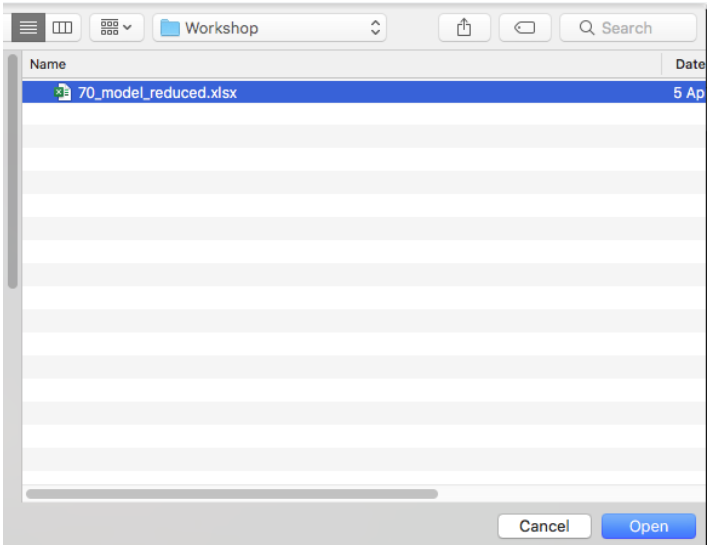
2. Uploading the data to the colab notebook

In this step, you will upload the dataset retrieved from NanoPharos. Executing the code in this cell generates a

button:



Clicking the button leads to a file browser window, where you can locate the file to be uploaded, which here is the 70_model_reduced.xlsx file.



3. Viewing and Preprocessing the dataset

In this step, you will:

- take a first look at the dataset
- generate descriptive statistics
- split the dataset randomly into training and test sets consisting of 75% and 25% of the data respectively
- generate the pipeline that will do:
    - preprocessing: transform features by scaling each feature to a given range using the MinMaxScaler function: https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.MinMaxScaler.html
    - modelling: The linear regression algorithm will be applied to the training dataset to generate the model

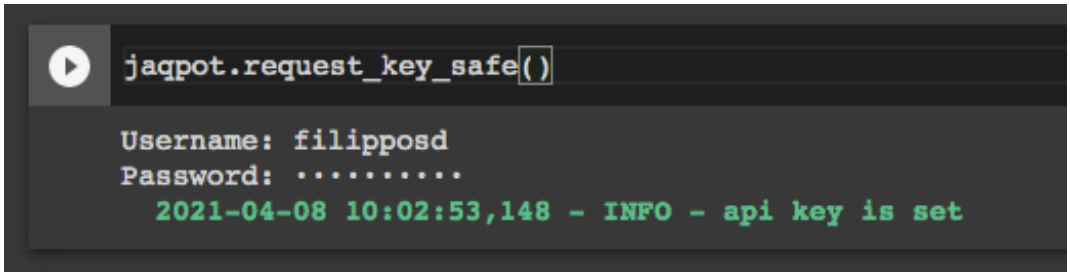
4. Training the model

Here you will:

- train the model
- print model performance metrics on the training, test dataset and on the total dataset
- perform a 5-fold cross validation test (https://scikit-learn.org/stable/modules/generated/sklearn.model_selection.cross_val_score.html).

5. Getting authentication to access Jaqpot

Please provide your username, press enter and then provide your password in the prompt that emerges.



6. Deploying the model

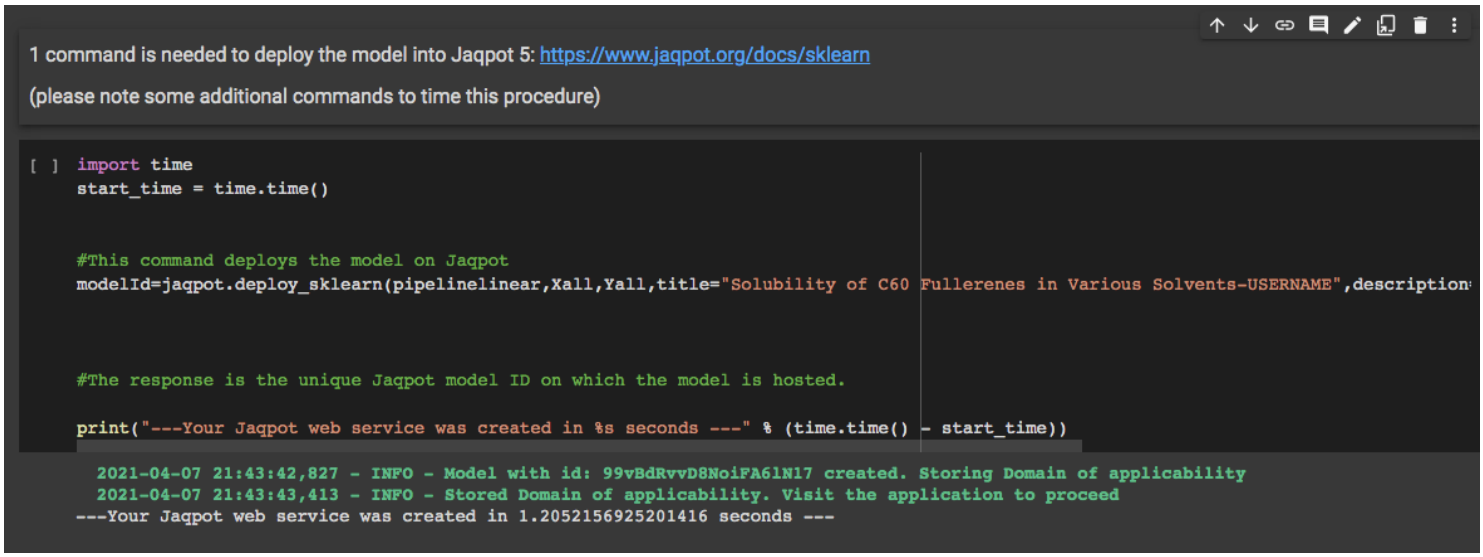
You will now deploy the model using the ***jaqpot.deploy_sklearn*** function with the following arguments:

Pipelinelinear	the pipeline to be used for preprocessing the data and the algorithm to be applied.
Xall	Dataset with the input (known) features.
Yall	Dataset with the output feature (the feature we want to predict with the model).
title="Solubility of C60 Fullerenes in Various Solvents-USERNAME"	Title of the model, as it will appear in the Jaqpot user interface. **Please change this by adding your username or any other character string that can distinguish your model and avoid multiple entries with the same model name.**
description="Description"	A short description intended to inform users about the model.
model_meta=True	By choosing True we enable listing of automatically generated model metadata (version of sklearn used, details on pipeline, preprocessing transformations and algorithm used for model). False disables this.
doa=X_train	Providing the dataset here enables Domain of Applicability calculations based on the leverage method. False disables this.

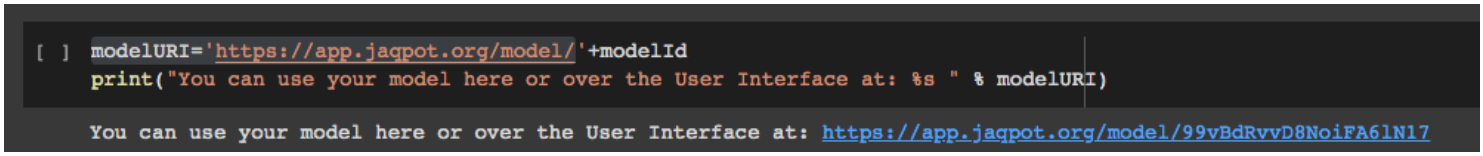
The command with the arguments listed above is:

Please change USERNAME by any string of characters that can distinguish your model.

```
modelId=jaqpot.deploy_sklearn(pipelinelinear,Xall,Yall,title="Solubility of C60
Fullerenes in Various Solvents-USERNAME",description="description",
model_meta=True,doa=X_train)
```



The web service has been created in Jaqpot and has a unique **modelURI** of the following form: https://app.jaqpot.org/model/99vBdRvvD8NoiFA6lN17 .



Now your QSAR model is a web service!

You can access your model through the Jaqpot interface

https://app.jaqpot.org

ADDITIONAL STEPS

After completing the steps above, you can take a look at the following:

1. Accessing your model through the colab notebook
2. Share the model to Organisation
3. Adding meta information to your model: QMRF report
4. Test and use your Jaqpot model
5. More information on the Jaqpot platform

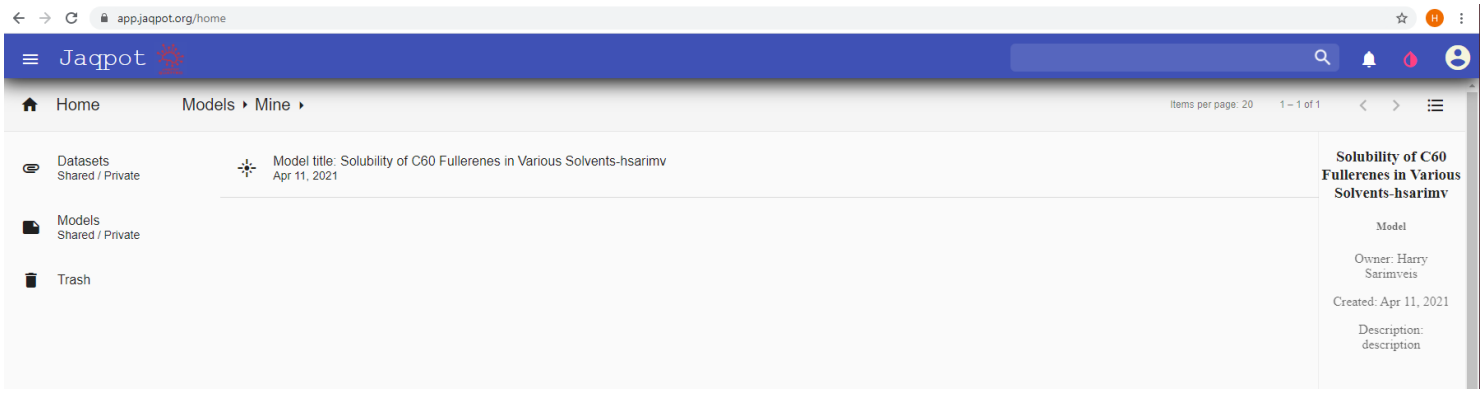
1. Access the model through the colab notebook

You can use the **jaqpot.predict** function in your colab notebook providing the dataset name (for example **Xall**) and the **`modelID`** as arguments in order to get predictions from the model, which are stored in the predictions variable:

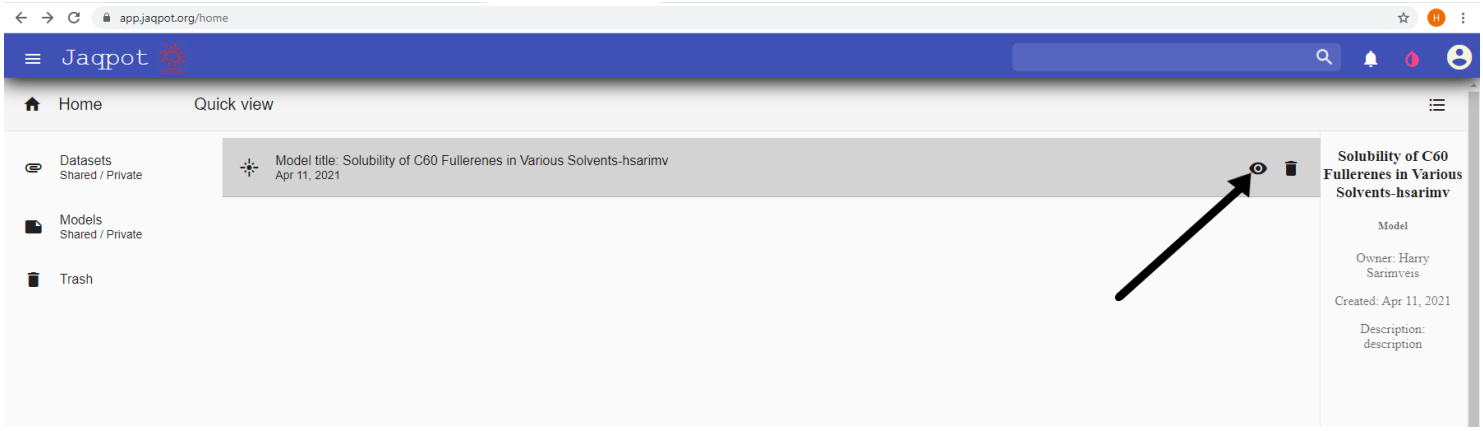
```
[ ] predictions = jaqpot.predict(Xall, modelId)

    2021-04-07 21:44:14,731 - INFO - completed 10.0
    2021-04-07 21:44:16,281 - INFO - completed 100.0

[ ] predictions

(                    piPC03  ATS1m  More23e    H1m  logS Exp.  Seigp
 pentane              1.099  1.609   -0.922  0.148  -5.818155    0.0
 hexane               1.386  1.792   -1.156  0.173  -5.419509    0.0
 octane               1.792  2.079   -1.656  0.208  -4.862671    0.0
 iso-octane           1.792  2.079   -1.529  0.242  -4.839394    0.0
 decane               2.079  2.303   -2.151  0.233  -4.479601    0.0
 ...                    ...    ...      ...    ...        ...    ...
 pyridine             3.056  1.992   -0.446  0.394  -4.148183   -0.6
 quinoline            4.123  2.512   -0.750  0.591  -2.817290   -0.6
 aniline              3.248  2.100   -0.504  0.351  -3.839706   -0.6
 N-methylaniline      3.359  2.234   -0.462  0.407  -3.556255   -0.6
 N.N-dimethylaniline  3.458  2.351   -0.435  0.399  -3.278345   -0.6

 [124 rows x 6 columns], 'logS Exp.')
```

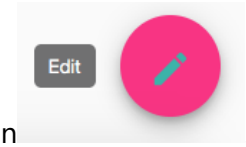
2. Share your model with the WorkshopApril2021 group

Access your model through the Jaqpot application: https://app.jaqpot.org:

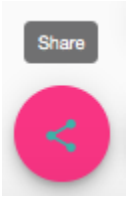


Select your model and click on the "View" icon

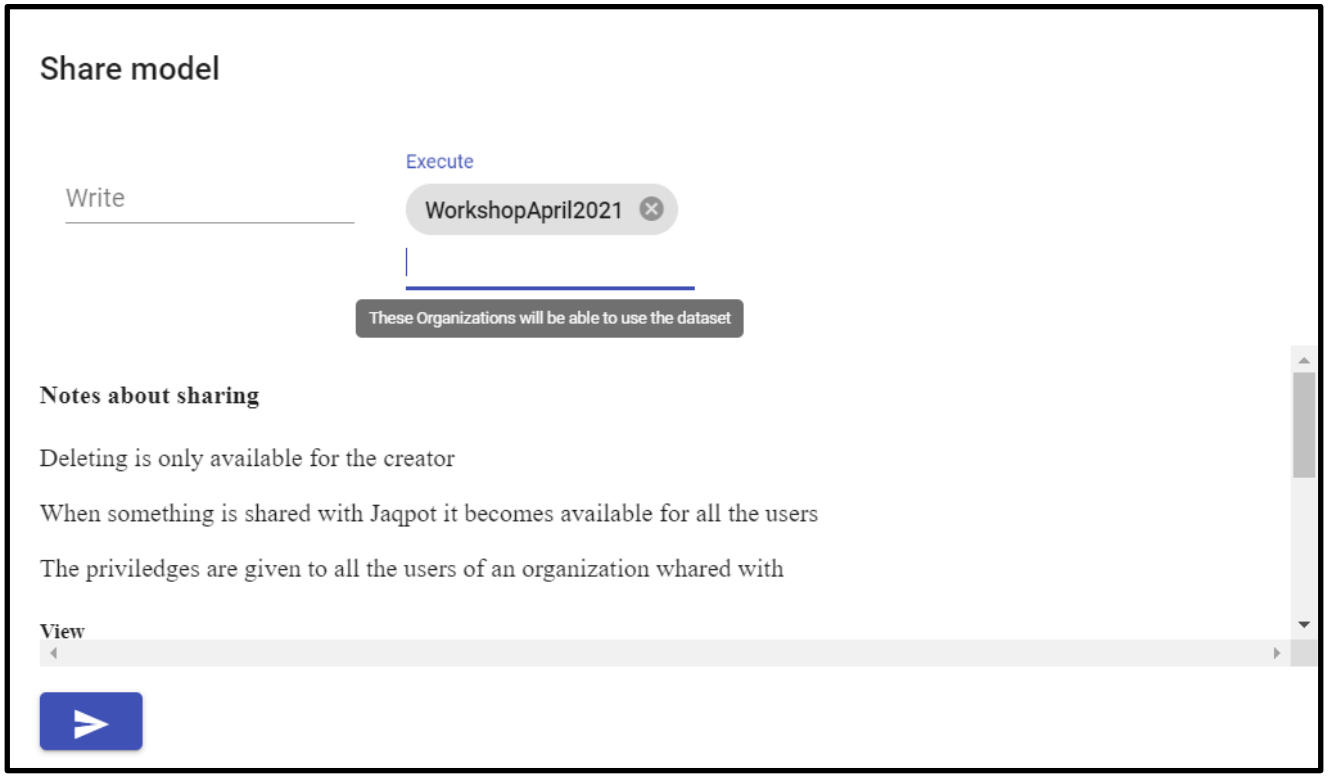


At the bottom right of the model page, click on the edit button 

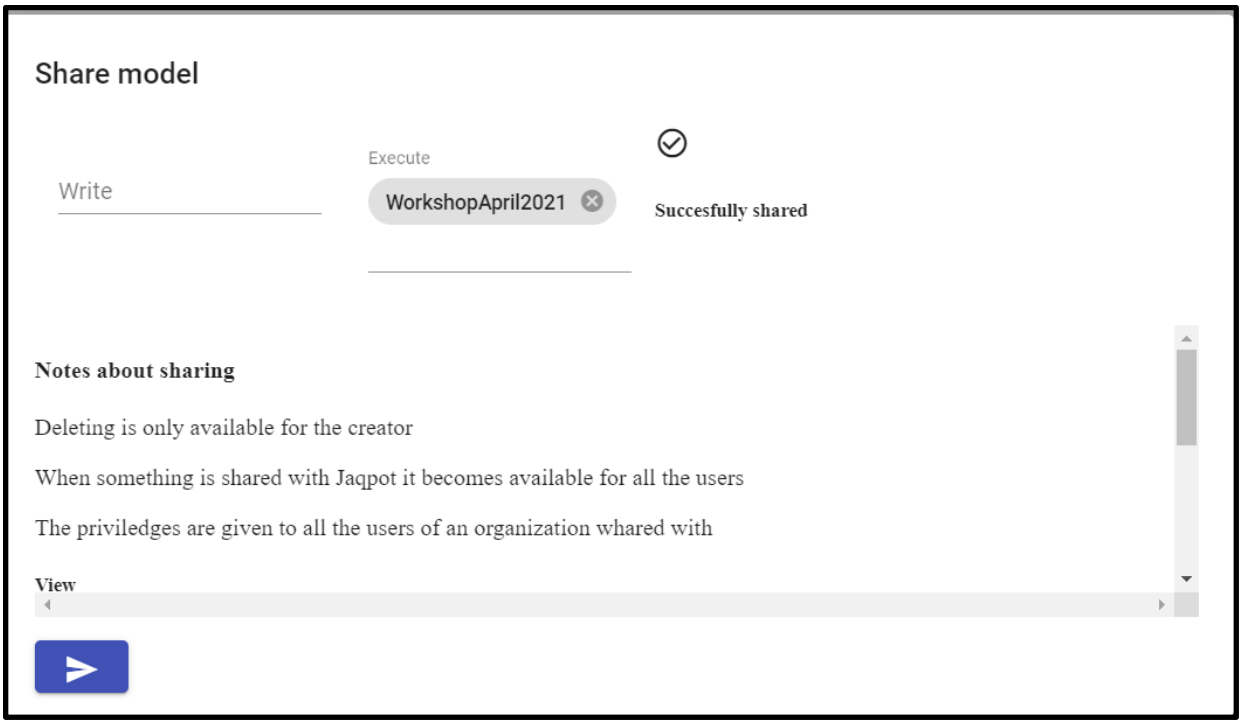
.

Clicking the Share button 

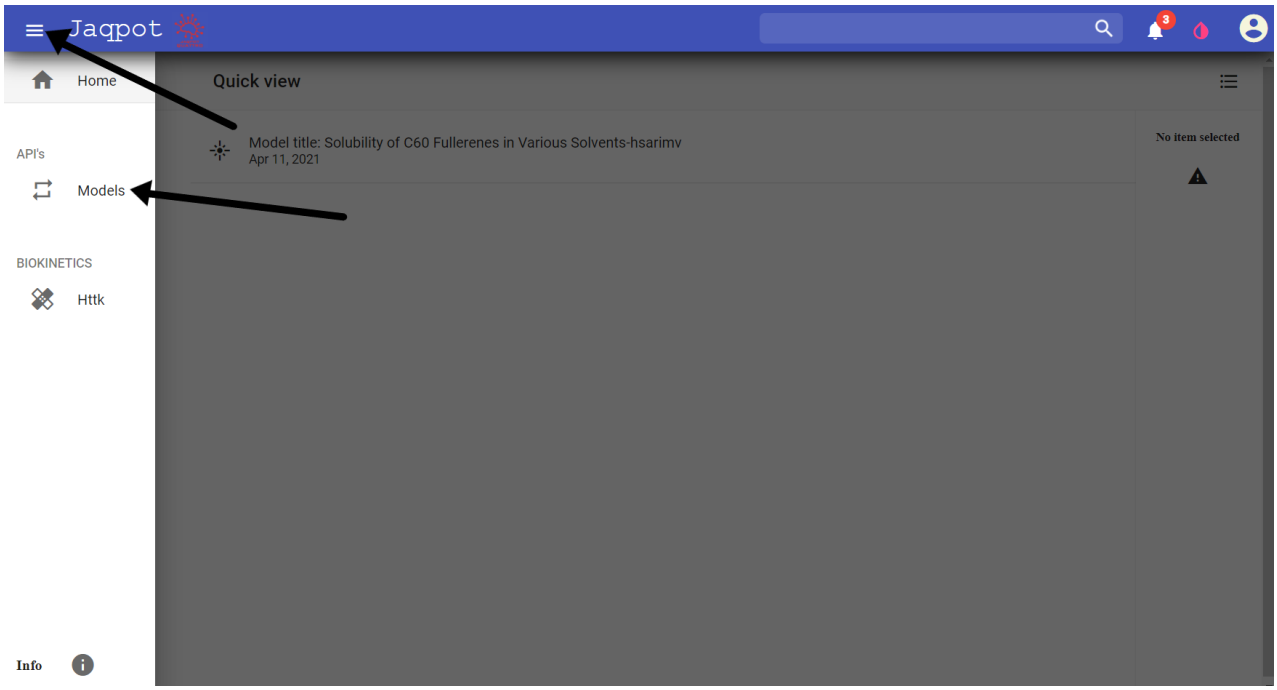
gives you the option to share the model with organisations of choice. Please select the WorkshopApril2021 group and give Execute rights only:



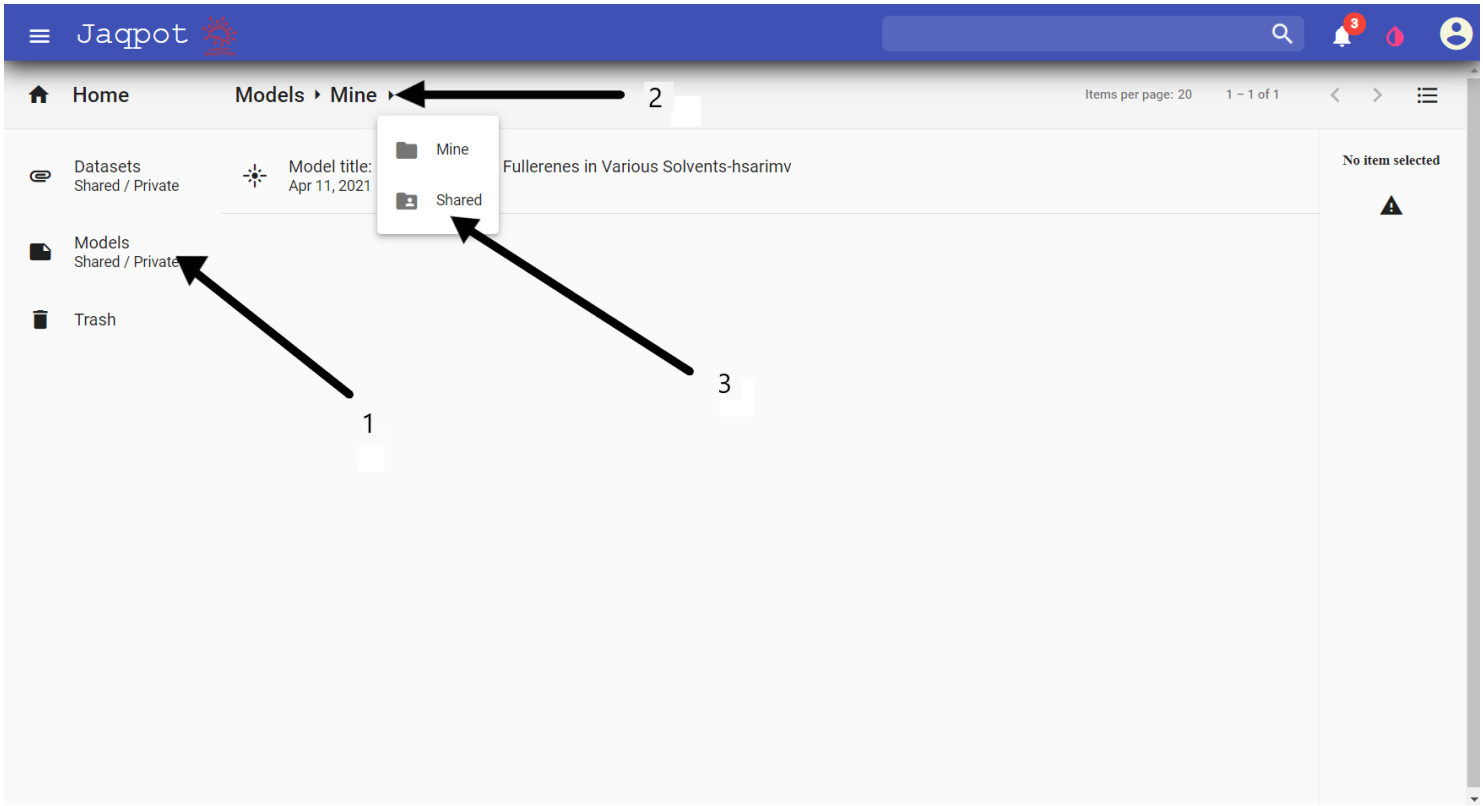
Adding an organisation to share with, activates the Share button, turning it from grey to blue .
Clicking this button causes the "Successfully shared" message to appear:



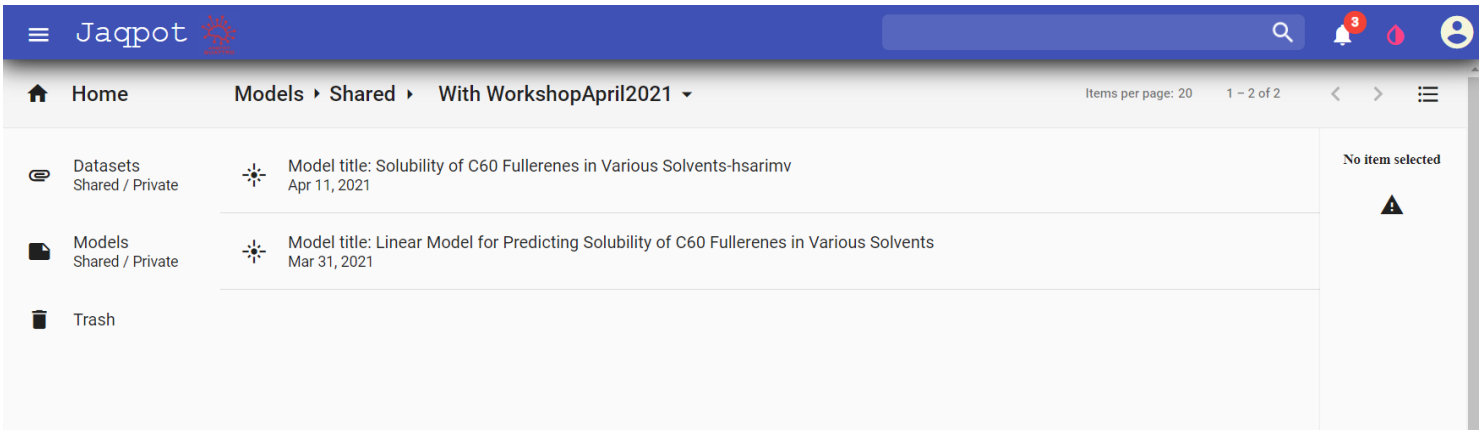
In order to view the shared models, please click on the menu button and select Models:



Select Models [1], click the triangle icon next to **Mine** [2] and select **Shared** [3]

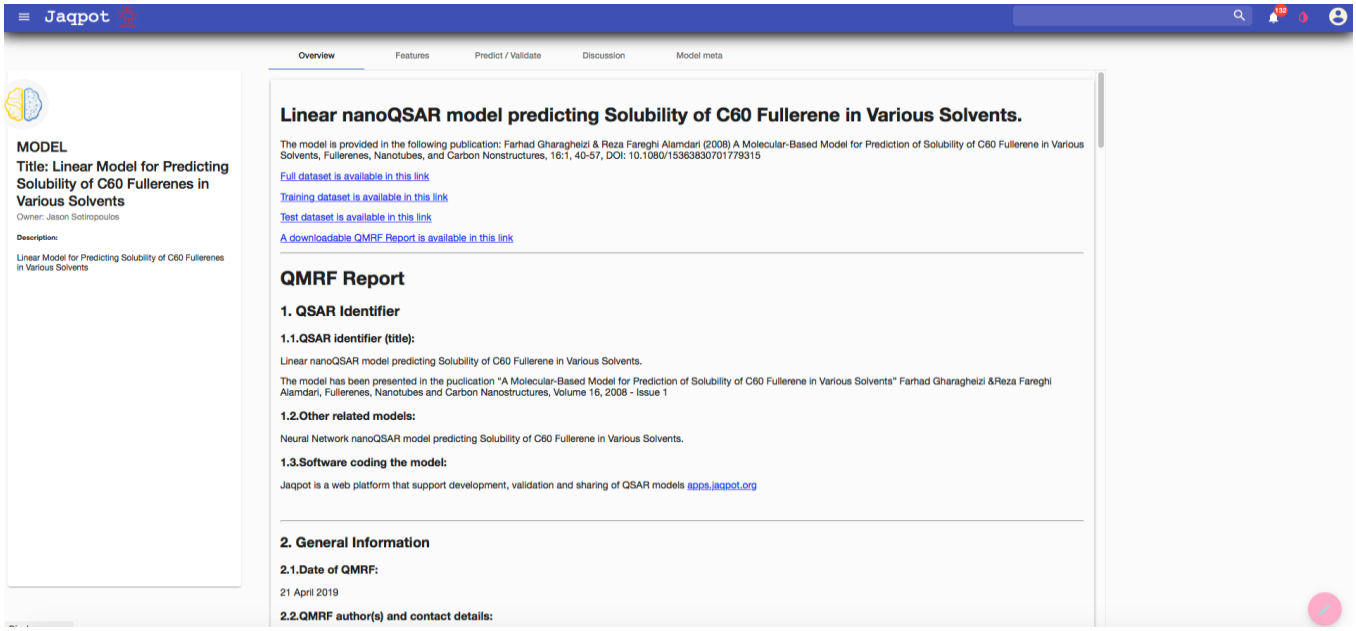


Select the **WorkshopApril2021** organisation. You are directed to a page containing all models shared through the **WorkshopApril2021** organisation.

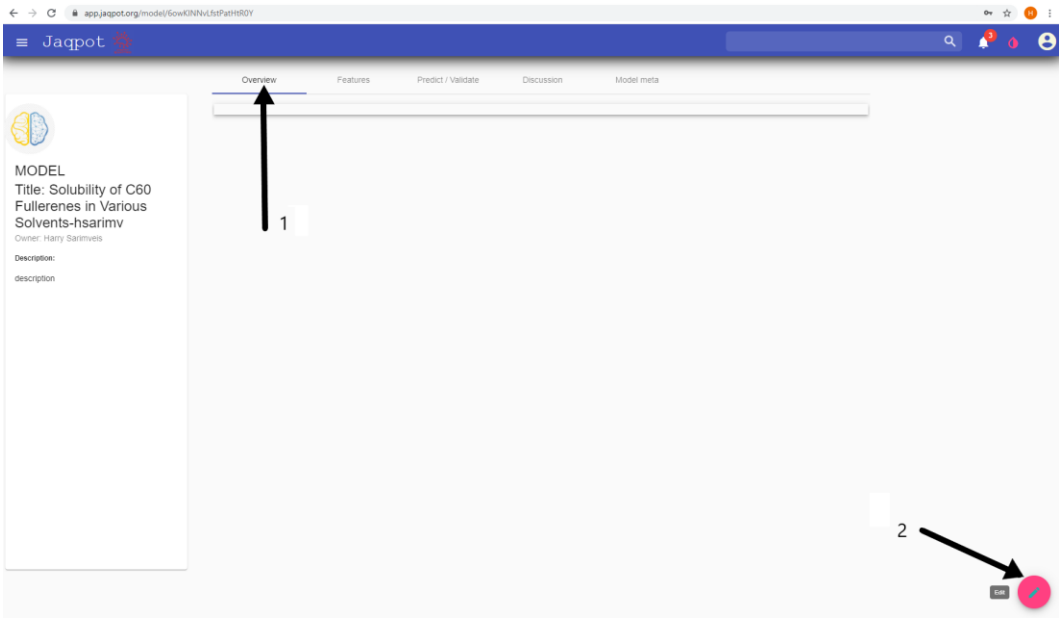


3. Adding meta information to your model

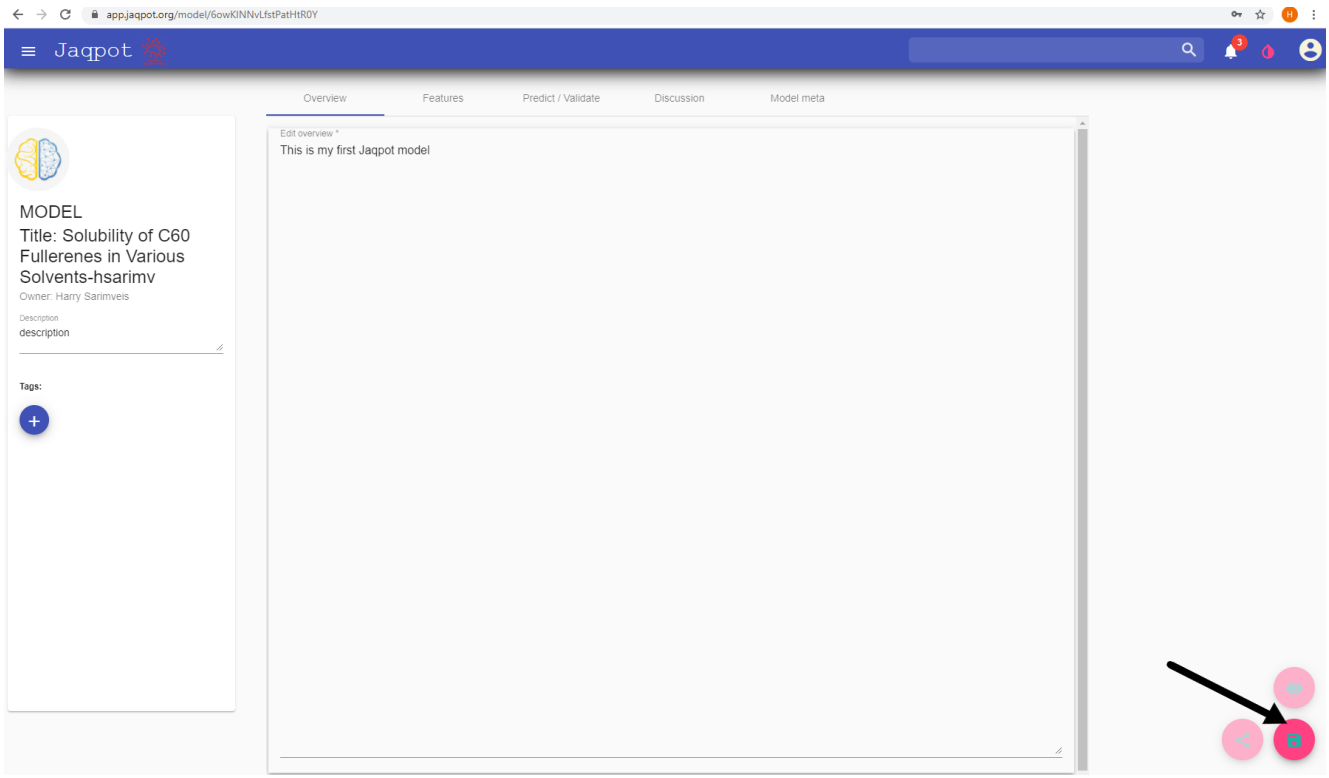
You can add any other information about the model over the user interface at https://app.jaqpot.org/ (for example detailed description, standard reports like Quantitative Model Reporting Format (QMRF), PMML representations, ontological annotations etc., descriptions of variables, ontological classes etc.). To demonstrate this, a fully documented model titled **"Linear Model for Predicting Solubility of C60 Fullerenes in Various Solvents"** is available at https://app.jaqpot.org/model/RqCRtRpY85kpbgGtsiXp and has been shared with the **WorkshopApril2021** organisation:



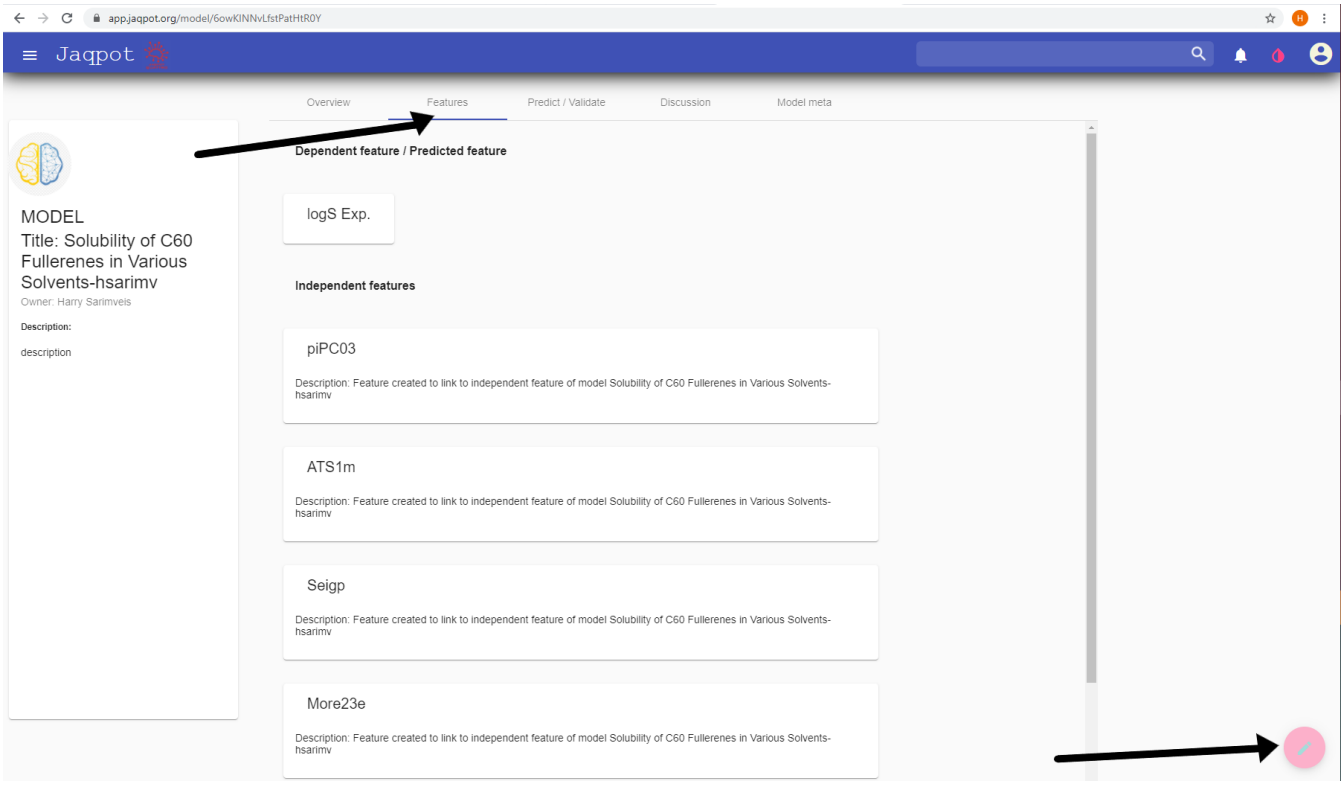
You can add information to your model by selecting the overview tab [1] and then clicking on the edit button.



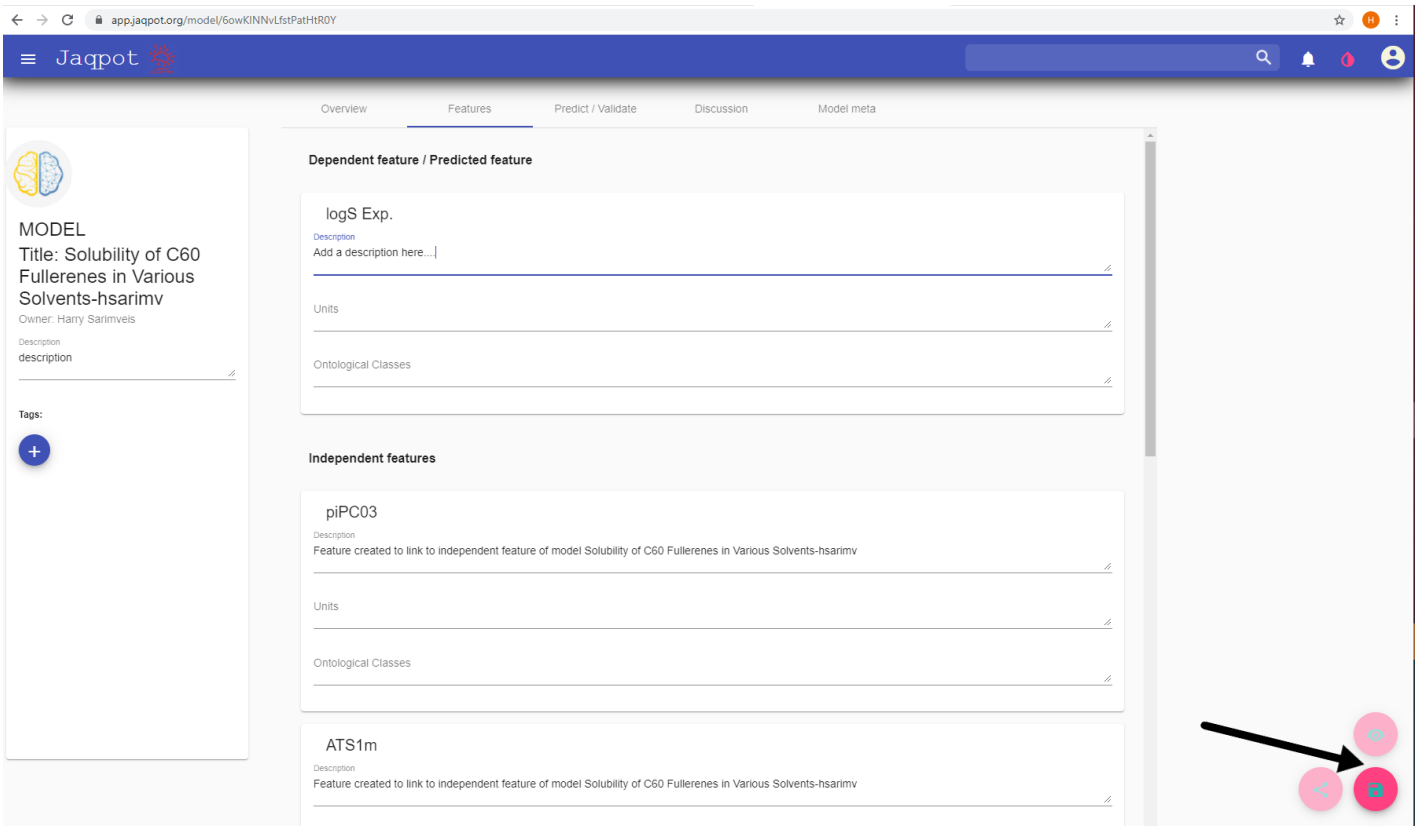
You can write any text (Markdown language is supported) and save it by clicking on the save button on the bottom right part of the page. You can return back and re-edit or extend the model description at any time.



Information about the variables used in the model (descriptions, units, ontological classes) can be added by selecting the "Features" tab and clicking on the Edit Button



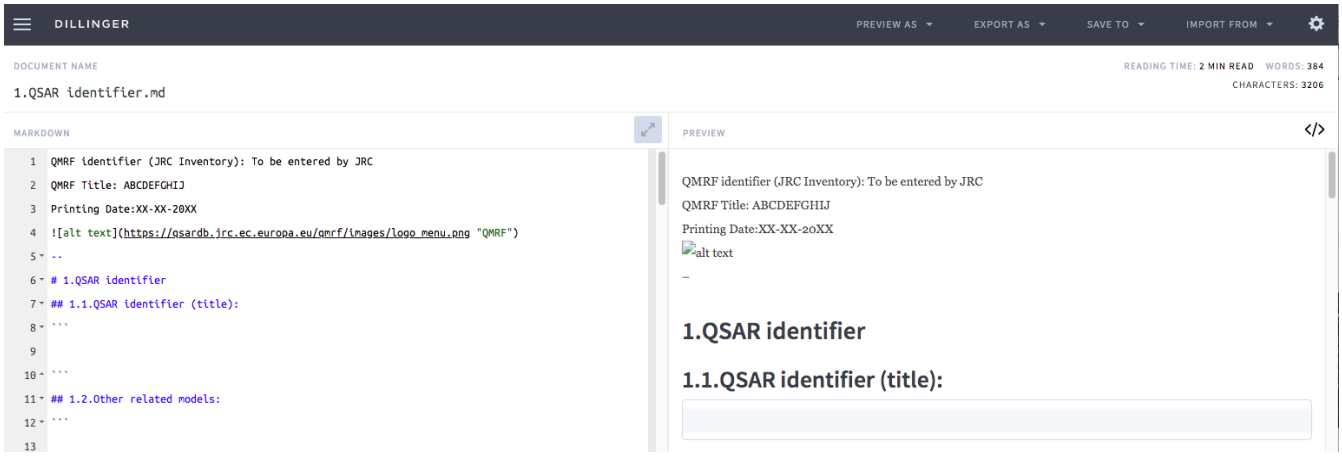
After entering the information, please click on the Save Button to store this information to the system. Descriptions can be updated and extended at any time.



To assist the users in adding editable versions of QMRF reports, we have created a QMRF markdown template, which can be downloaded at:
https://github.com/ntua-unit-of-control-and-informatics/QSAR-Models/blob/master/QMRF%20template.md .
by right clicking on the **Raw** button, as shown:

The user only needs to provide the necessary information under each section and the QMRF report is generated in an easy-to-read format.

There are online tools to edit MarkDown documents, such as: https://dillinger.io/



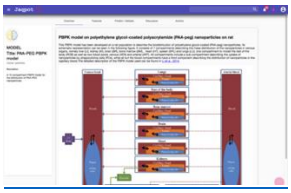
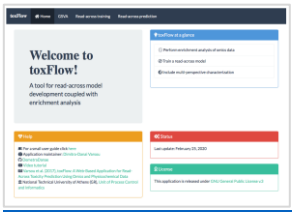
Alternatively, users can use a specialised QMRF editor for Windows at http://qmrf.sourceforge.net/.

4. Test and use your Jaqpot model

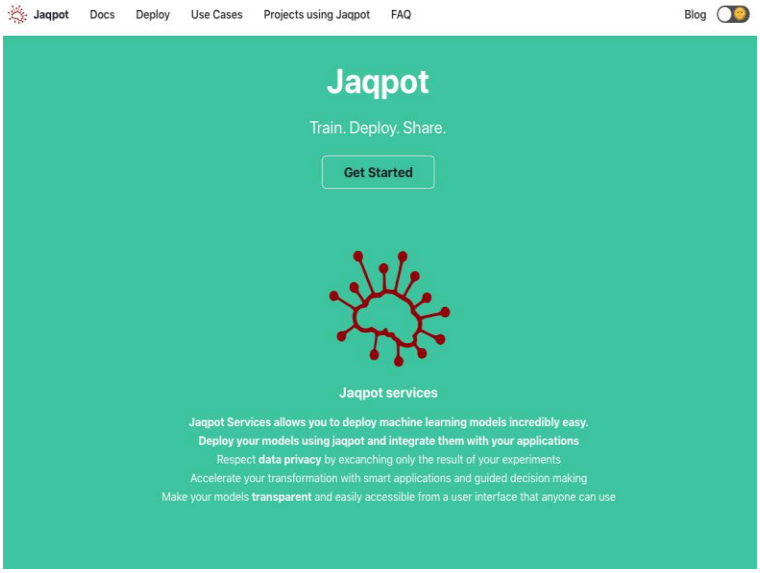
You can validate or use your model or any other Jaqpot model, by following the steps in the following tutorial:
Jaqpot 5: How to access and use an existing predictive model
The data should be provided in a csv file. A sample csv file can be downloaded by clicking on the following link:
https://zenodo.org/record/4671069/files/70_model_reduced.csv?download=1

5. More information on the Jaqpot platform

Jaqpot offers a suite of tools for QSAR, PBPK, image analysis, read-across methods:

			
https://app.jaqpot.org/ QSAR model	https://app.jaqpot.org/ PBPK model	https://nanoimage.jaqpot.org	toxflow.jaqpot.org

A comprehensive technical documentation is provided at https://www.jaqpot.org.



A collection of tutorials describing other Jaqpot functionalities is available on Zenodo:

1. Jaqpot 5 - User accounts
2. Jaqpot 5: How to manage and use organisations
3. Jaqpot 5: How to deploy a predictive model using the jaqpotpy library
4. Jaqpot 5: How to simulate biodistribution scenarios using custom PBPK models

Useful links:

User Guidance Handbook @ www.nanocommons.eu

- https://www.nanocommons.eu/e-infrastructure/user-guidance-handbook/

Training events and materials @ NanoCommons Infrastructure

- https://infrastructure.nanocommons.eu/events/

NanoCommons @ ELIXIR TeSS

- https://tess.elixir-europe.org/content_providers/nanocommons#events

NanoCommons community @ Zenodo

- https://zenodo.org/communities/nanocommons

NanoCommons Channel @ YouTube

- https://www.youtube.com/channel/UCuawpRvXNpglwyeItefTctw

mailing list of WG-A Education, Training, Communication

- www.nanosafetycluster.eu

Thank you for interest in our training event!