

Easy access to QSAR modelling



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Nano-Knowledge Community



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.
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The idea – problem & solution

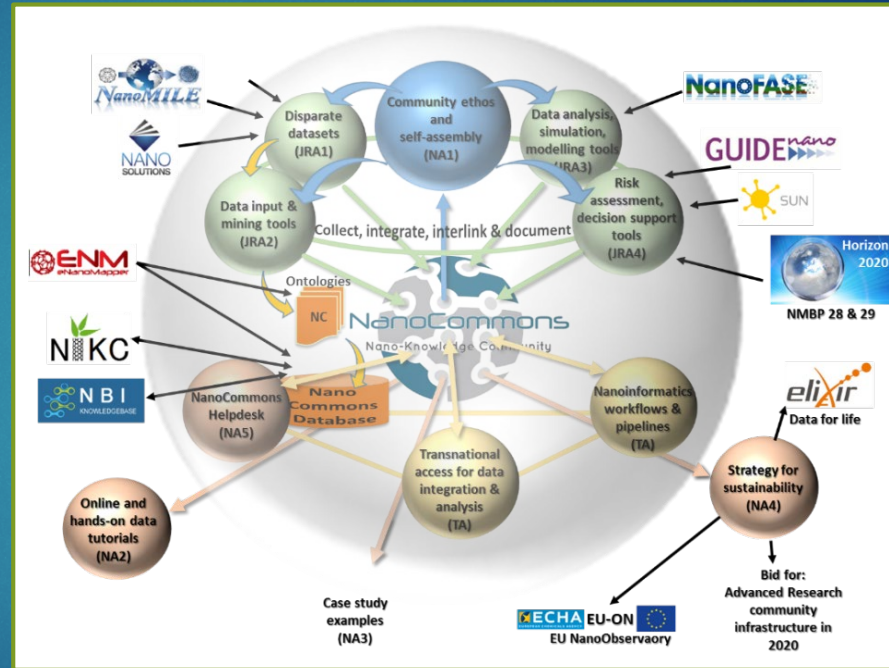
Nanotechnologies are a major area of investment & growth for the European economy

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



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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:



**Experimental Workflows
Design & Implementation**



**Data Processing
& Analysis**



**Data Visualisation
& Predictive Toxicity**



**Data Storage
& Online Accessibility**

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

 info@nanocommons.eu



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NanoCommons User Guidance Handbook

Home / e-Infrastructure / NanoCommons User Guidance Handbook



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Overview Data management Nanoinformatics Workflows Electronic lab notebooks Ontologies

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The European Nanotechnology Community Informatics Platform: Bridging data and disciplinary gaps for industry and regulators

The project has received funding from the European Union Horizon 2020 Programme (1010220) under grant agreement No. 721522

Overview

- H2020 research infrastructure project
- Call topic: NPM-NI-02-2019-2021: Integrating Activities for Advanced Communities

NanoCommons – How can we help you?

Download [2.19 MB]

US - EU
Nanotechnology Community Informatics Platform

2020 U.S.-EU NanoEHS COR Workshop: Bridging Insights and Perspectives

September 16-17, Virtual Meeting

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.

2020 U.S.-EU NanoEHS COR Workshop: Bridging Insights and Perspectives
September 16-17, Virtual Meeting

NanoCommons User Guidance Handbook

NanoCommons
Nano-Knowledge Community

For access to Services, Resources & Contacts
Go to: [www.nanocommons.eu](#)

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

zenodo

Online training tools for nanosafety assessment – NanoCommons for

www.nanocommons.eu



Events

Category Organisations involved Role

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)
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)

Tutorial ready
for download





Home / Events

Date Added

Anytime

Scientific topic

Ontology and terminology 1

Event type

Workshops and courses 6

Meetings and conferences 1

Online

Only show online events

Country

Greece 1

Organizer

www.nanocommons.eu 3

NanoCommons 2

Martin Himly, PLUS, Chair o... 1

Martin Himly, PLUS, Chair o... 1

City

Athens 1

Sponsor

EU H2020 4

EU H2020 NanoCommons 1

Target audience

Search events...

8 events found

Content provider: NanoCommons x

Ontological Annotation of Datasets: "1st NanoCommons Hackathon"
9 October 2018
Athens, Greece

Annotating Your Experimental Data workshop
28 April 2020

Online Jaqpot Hackathon
3 June 2020

EU Nanosafety Cluster Training Day @ NanoSAFE 2020 Digital Conference
23 November 2020

EU Nanosafety Cluster Education Day @ NanoSAFE 2020 Digital Conference
16 November 2020

Getting into using ELNs for experimental and computational workflows
14 July 2020

Online QSAR Modelling Hackathon by Easy Access to Jaqpot
13 April 2021

Online SPARQL Access to WikiPathways and AOP-Wiki Webinar
23 March 2021

June 3, 2020

Presentation

Open Access

Edit

New version

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

by 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

Seite: 1 von 13 Automatischer Zoom



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Iseult Lynch, UoB

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

Publication date:

June 3, 2020



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Nano-Knowledge Community

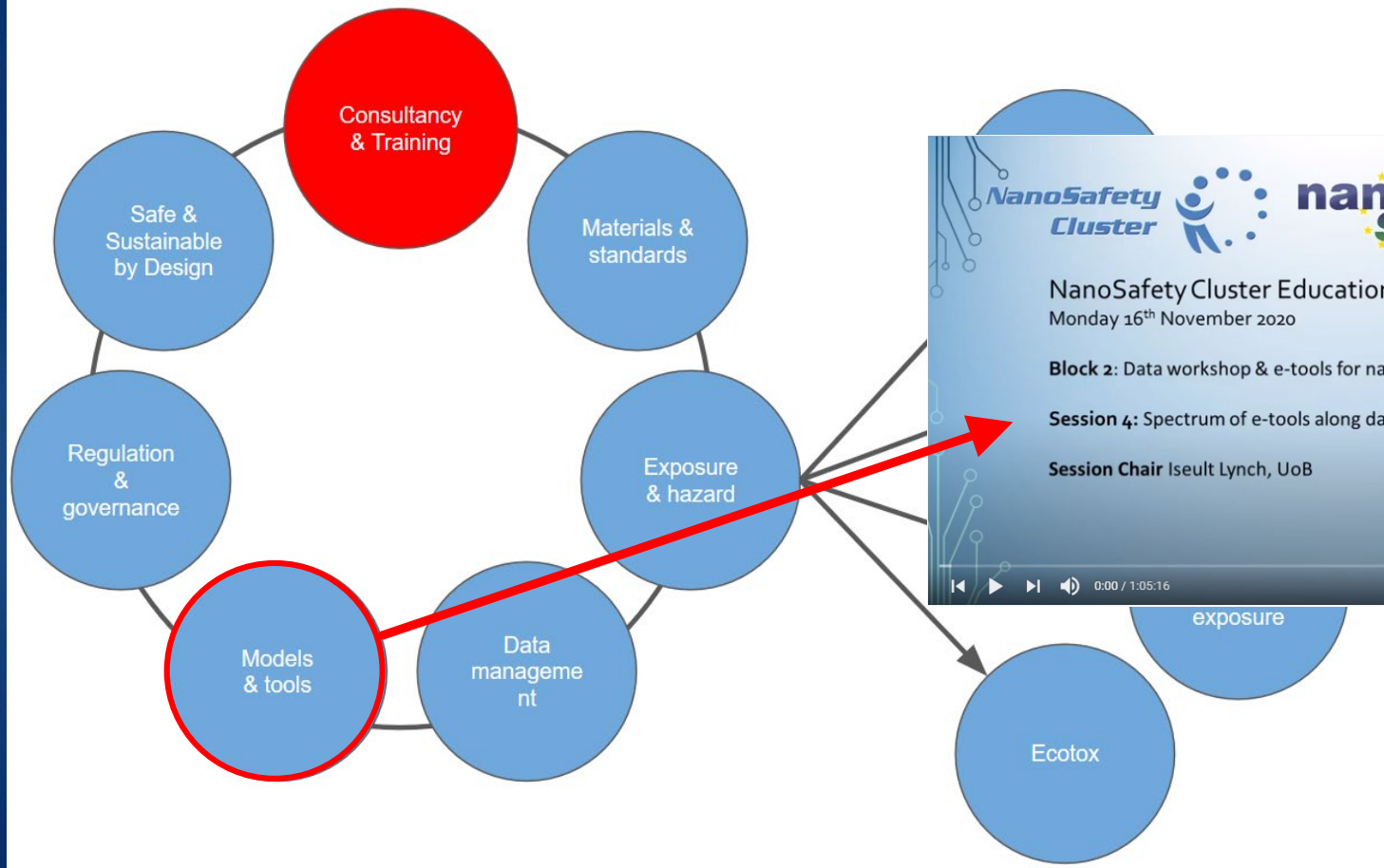


NanoSolveIT




NanoSafety
Cluster

...aligned with the EU NSC WGs



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NanoSafety Cluster  **nanoSAFE'20**

NanoSafety Cluster Education Day
Monday 16th November 2020

Block 2: Data workshop & e-tools for nano & beyond

Session 4: Spectrum of e-tools along data life cycle

Session Chair Iseult Lynch, UoB

0:00 / 1:05:16

👉 NanoCommons & NSC YouTube channels



NanoCommons
Nano-Knowledge Community



nanosafetycluster

NanoSafety Cluster

28 Abonnenten

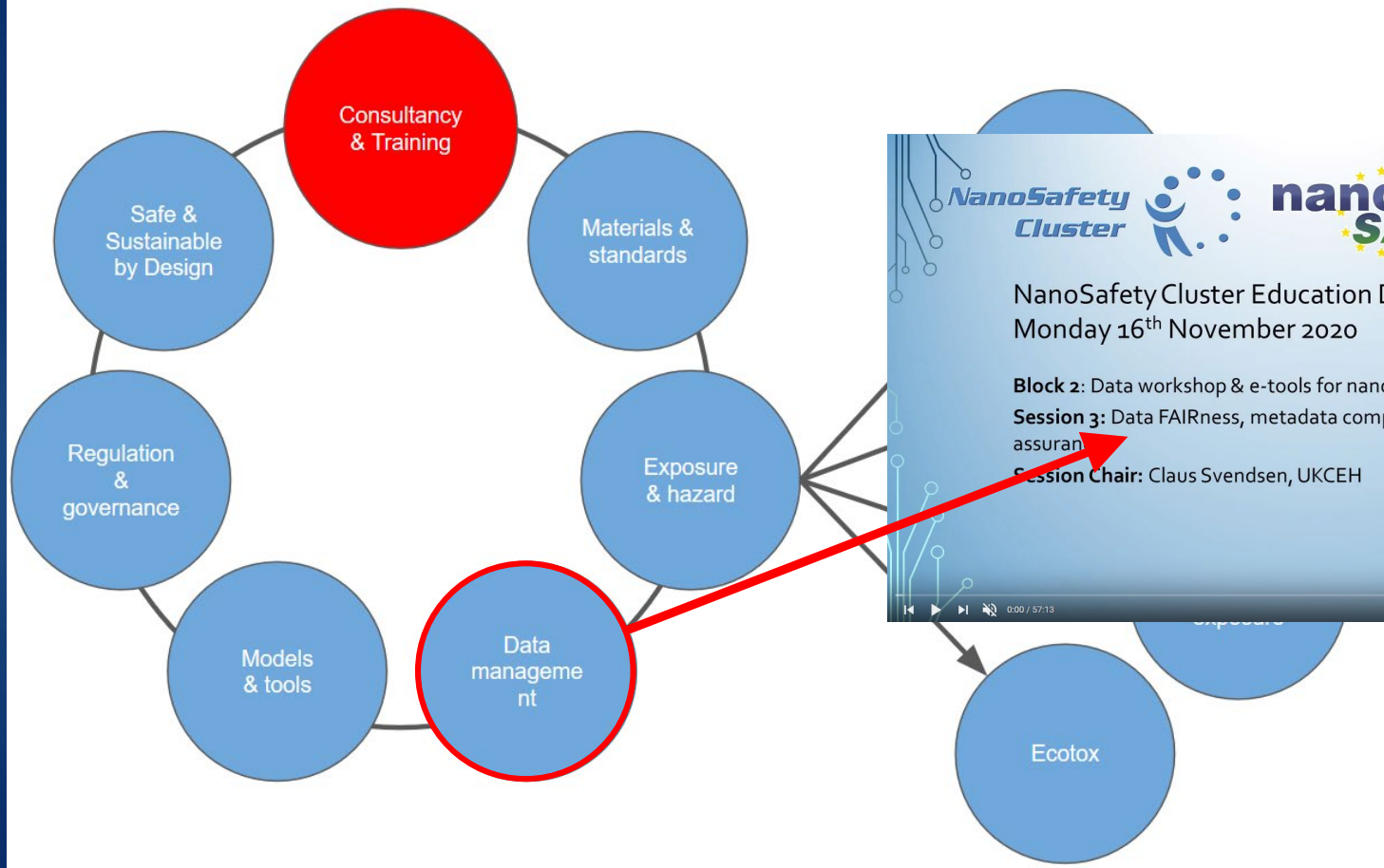
ABONNIEREN

ÜBERSICHT VIDEOS PLAYLISTS KANÄLE KANALINFO

Uploads ▶ ALLE WIEDERGEBEN


Video Title	Duration	Views
NSC Training Day: (Rm B 3) Stakeholder engagement...	2:13:34	17 Aufrufe • vor 1 Monat
NanoSafety Cluster General Assembly, 16th November...	56:08	13 Aufrufe • vor 1 Monat
NSC Education Day: Session 6 - Elements of Sbd for...	1:08:38	39 Aufrufe • vor 1 Monat
NSC Education Day: Session 5 - Features of nanoRGFs in...	1:07:01	15 Aufrufe • vor 1 Monat
nanoSAFE20 - Introduction to the NanoSafety Cluster...	6:12	11 Aufrufe • vor 1 Monat
NSC Education Day: Session 1 - New developments in...	57:15	15 Aufrufe • vor 1 Monat

...aligned with the EU NSC WGs



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Nano-Knowledge Community



NanoSafety Cluster  **nanoSAFE'20**

NanoSafety Cluster Education Day
Monday 16th November 2020

Block 2: Data workshop & e-tools for nano & beyond
Session 3: Data FAIRness, metadata completeness, scientific quality assurance
Session Chair: Claus Svendsen, UKCEH

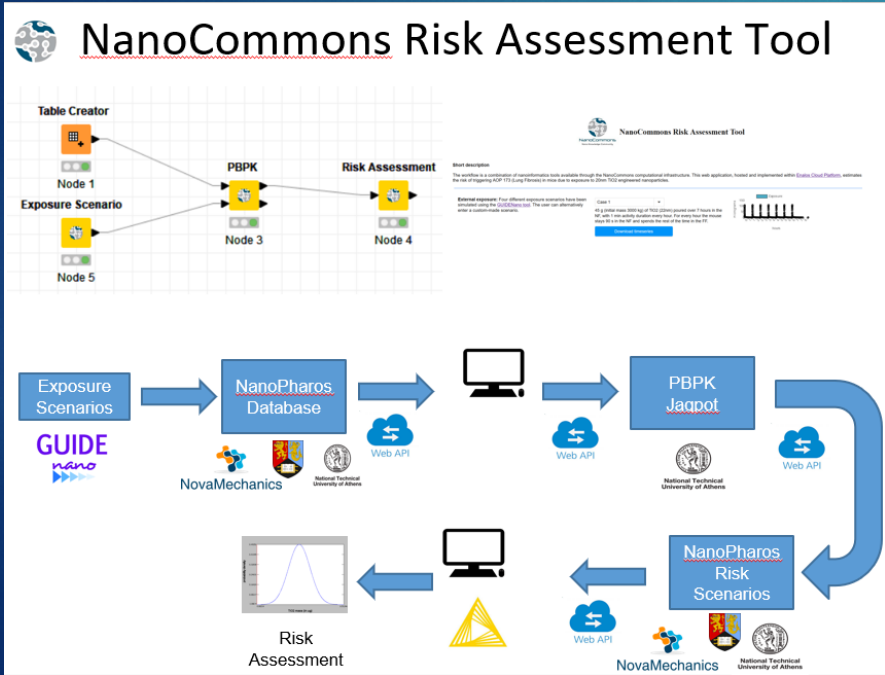
0:00 / 57:13

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**



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/UCuawpRvXNpplwyetefTctw>

mailing list of WG-A Education, Training, Communication

- ▶ www.nanosafetycluster.eu



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





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Online QSAR Modelling Hackathon by Easy Access to Jaqqpot 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

JAQPOT

models




Jaqpot in a nutshell

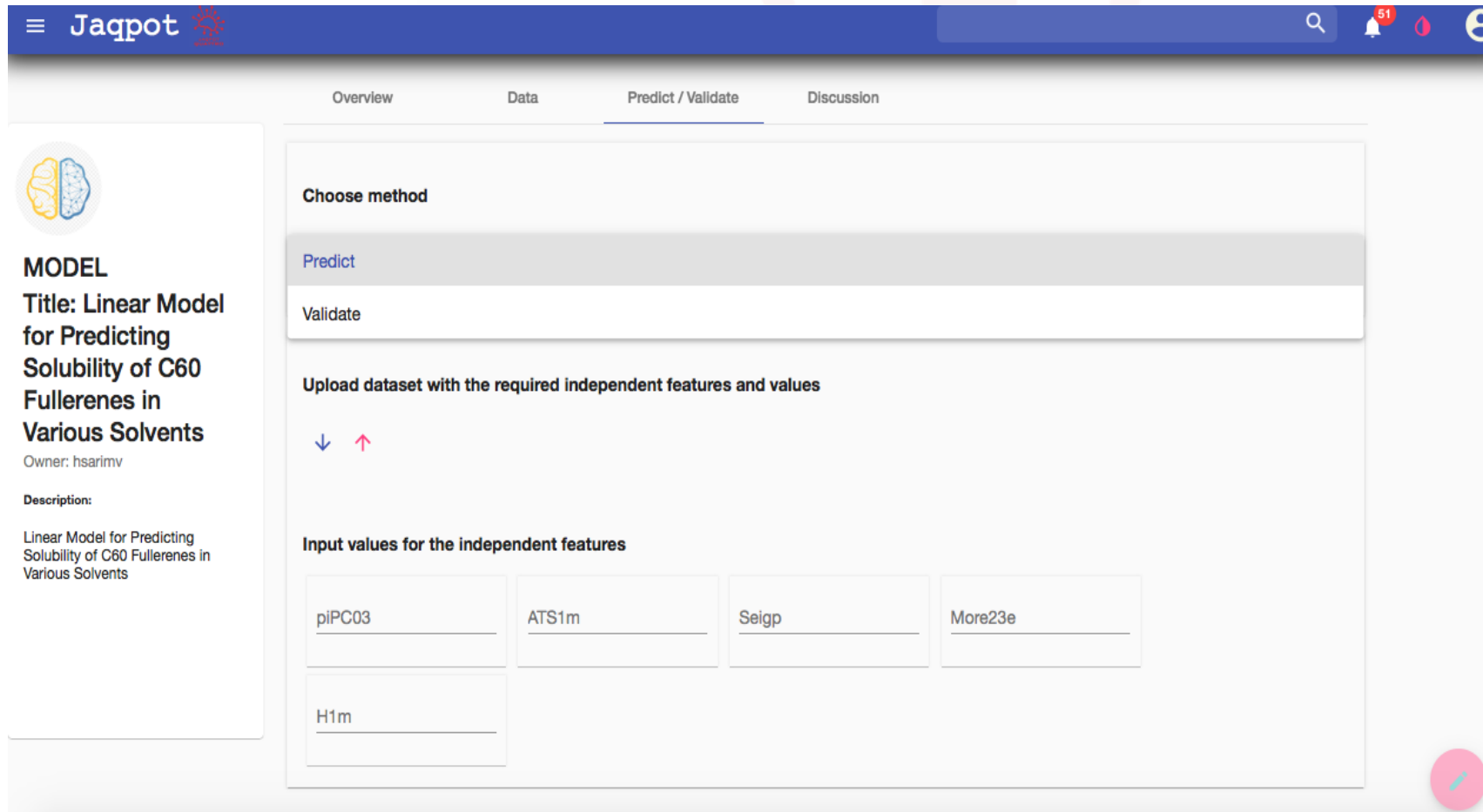


- **Develop models** on various runtimes and **deploy** them as web services in seconds
- **Validate** your models and **generate predictions** with a user friendly interface
- Make them **transparent** to the users with flexible **documentation** methods
- **Share** your models and make them **accessible**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

JAQPOT

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.



The screenshot shows the Jaqpot web application interface. At the top, there is a blue navigation bar with the Jaqpot logo and a search icon. Below the navigation bar, there are four tabs: Overview, Data, Predict / Validate (which is active), and Discussion. On the left side, there is a sidebar with a brain icon and the following text: **MODEL**, **Title: Linear Model for Predicting Solubility of C60 Fullerenes in Various Solvents**, **Owner: hsarimv**, and **Description: Linear Model for Predicting Solubility of C60 Fullerenes in Various Solvents**. The main content area is titled "Choose method" and has two options: "Predict" (highlighted) and "Validate". Below this, there is a section titled "Upload dataset with the required independent features and values" with a download and upload icon. The "Input values for the independent features" section contains five input fields: piPC03, ATS1m, Seigp, More23e, and H1m.

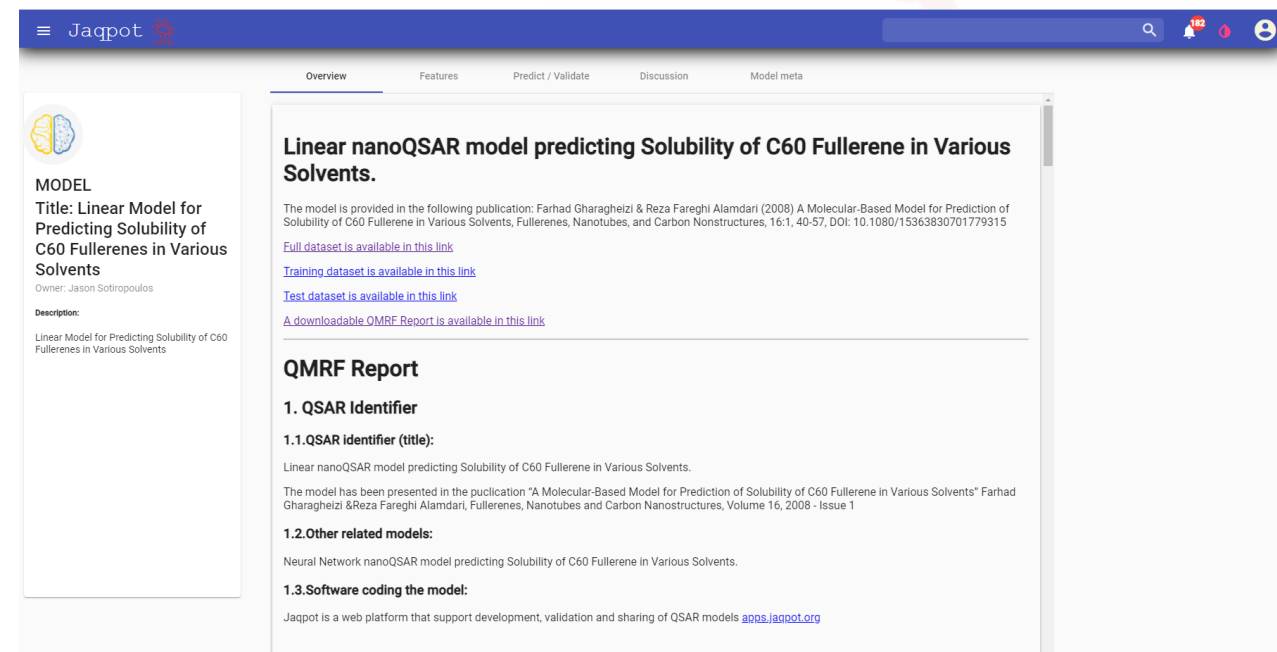
Predict-validate tab

1. Create predictions

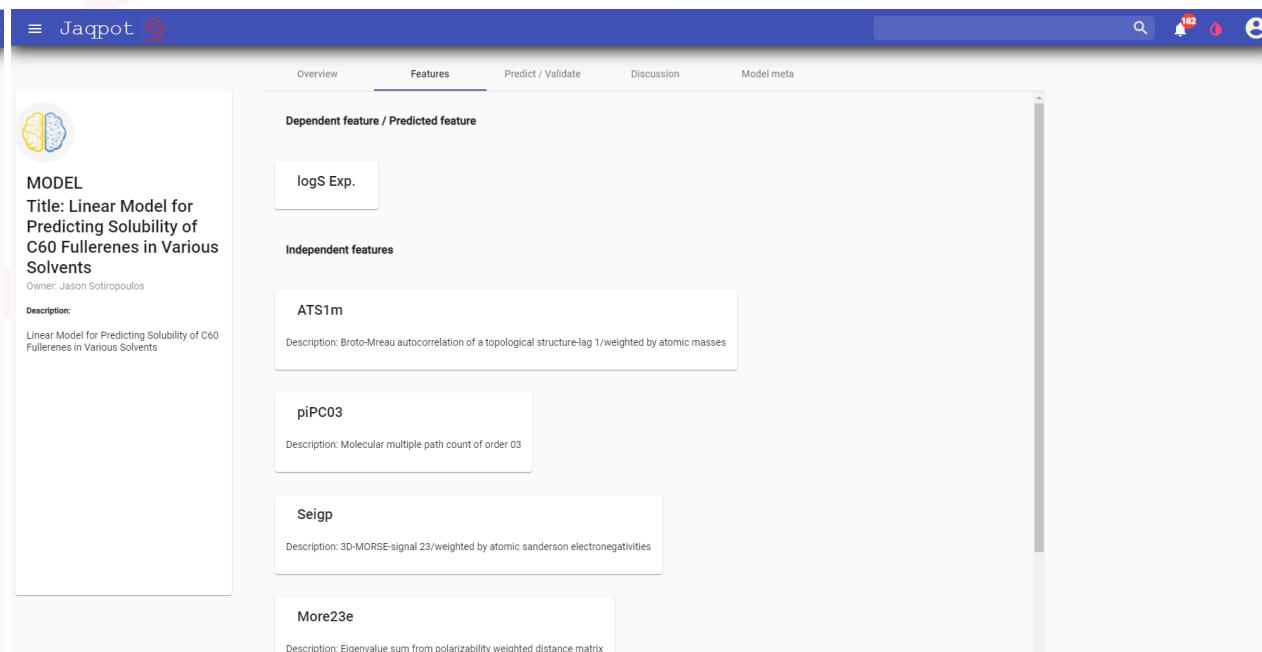
- by manually entering values
- CSV datasets using Jaqpot-generated template

1. Validate model performance:

using an external validation dataset as input in CSV format



The screenshot shows the 'Overview' tab of a model page on Jaqpot. The model title is 'Linear nanoQSAR model predicting Solubility of C60 Fullerene in Various Solvents.' The page includes a 'MODEL' section with the title, a description of the model's origin, and links to datasets and reports. Below this is a 'QMRF Report' section with three sub-sections: '1. QSAR Identifier', '1.1. QSAR Identifier (title)', '1.2. Other related models', and '1.3. Software coding the model'.



The screenshot shows the 'Features' tab of the same model page. It lists dependent and independent features with their descriptions. The dependent feature is 'logS Exp.'. The independent features are 'ATS1m', 'piPC03', 'Seigp', and 'More23e', each with a detailed 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



The screenshot shows a user profile for Philip Doganis (filipposd) with a list of organizations he is a member of: Jaqpot, Lab of Process Control and Informa..., NanoCommons, and OpenRiskNet. A sharing modal is open, displaying a list of shared models and a detailed view of one model.

Organizations
Organizations i am a member

- Jaqpot
- Lab of Process Control and Informa...
- NanoCommons
- OpenRiskNet

CREATE

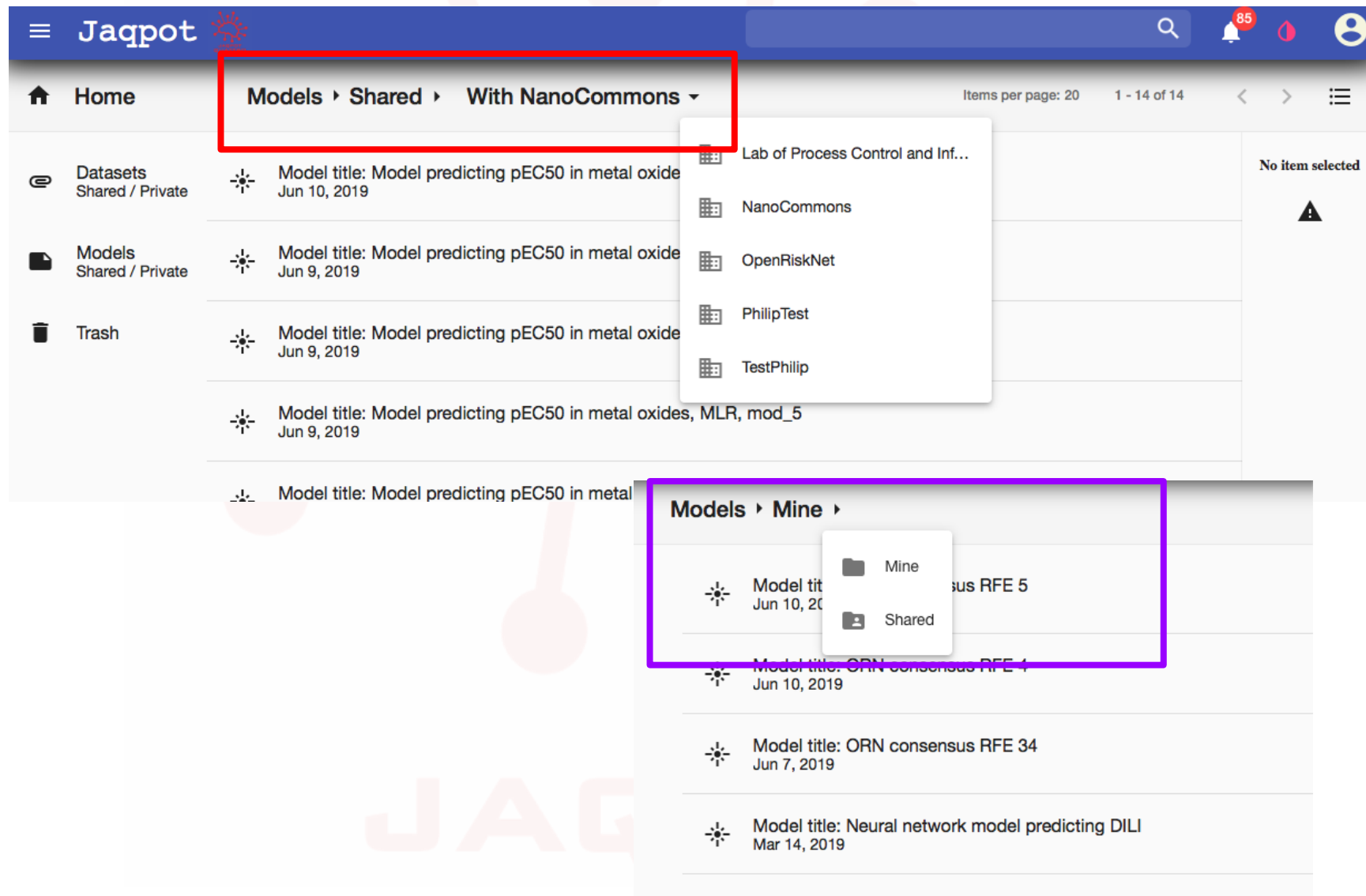
MODEL SHARED

model shared through organization NanoCommons

From user	filipposd	▼
Shared with	NanoCommons	▼
model	ORN consensus RFE 34	▼

View remove

Shared space



The screenshot shows the Jaqpot web interface. The top navigation bar includes the Jaqpot logo, a search bar, a notification bell with 85 alerts, a home icon, and a user profile icon. The main navigation menu on the left includes Home, Datasets (Shared / Private), Models (Shared / Private), and Trash. The breadcrumb path is **Models > Shared > With NanoCommons**, which is highlighted with a red box. A dropdown menu is open, showing a list of sharing options: Lab of Process Control and Inf..., NanoCommons, OpenRiskNet, PhilipTest, and TestPhilip. The main content area displays a list of models, each with a star icon, a title, and a date. The first model is titled "Model predicting pEC50 in metal oxide" and dated Jun 10, 2019. A second model is dated Jun 9, 2019. A third model is dated Jun 9, 2019. A fourth model is titled "Model predicting pEC50 in metal oxides, MLR, mod_5" and dated Jun 9, 2019. A fifth model is partially visible, titled "Model predicting pEC50 in metal". A second dropdown menu is open over the first model, showing options for "Mine" and "Shared", which is highlighted with a purple box. The right side of the interface shows "Items per page: 20" and "1 - 14 of 14" items. A "No item selected" message with a warning icon is visible on the right.

Home

Models > Shared > With NanoCommons

Items per page: 20 1 - 14 of 14

No item selected

Model title: Model predicting pEC50 in metal oxide
Jun 10, 2019

Model title: Model predicting pEC50 in metal oxide
Jun 9, 2019

Model title: Model predicting pEC50 in metal oxide
Jun 9, 2019

Model title: Model predicting pEC50 in metal oxides, MLR, mod_5
Jun 9, 2019

Model title: Model predicting pEC50 in metal

Models > Mine

Mine

Shared

Model title: ...us RFE 5
Jun 10, 20...

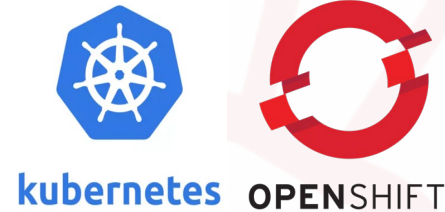
Model title: ORN consensus RFE 4
Jun 10, 2019

Model title: ORN consensus RFE 34
Jun 7, 2019

Model title: Neural network model predicting DILI
Mar 14, 2019

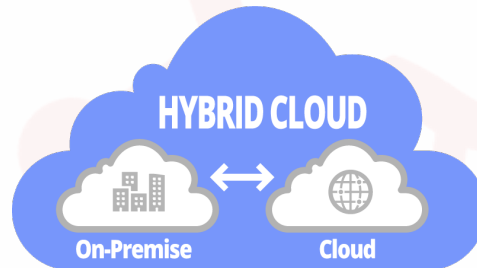
Meet the scalability requirements

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)

Jaqpot API 5.0.1 OAS3

<https://api.jaqpot.org/jaqpotservices/openapi.json>

Jaqpot v5 is the 5th version of a YACP, a RESTful web platform which can be used to train machine learning models and use them to obtain toxicological predictions for given chemical compounds or engineered nano materials. Jaqpot v4 has integrated read-across, optimal experimental design, interlaboratory comparison, biokinetics and dose response modelling functionalities. The project is developed in Java8 and JEE7 by the [Unit of Process Control and Informatics in the School of Chemical Engineers at the National Technical University of Athens](#).

Charalampos Chomenidis, Pantelis Sospasakis, Evangelia Anagnostopoulou, Angelos Valsamis, George Drakakis, Pantelis Karatzas, Georgia Tsilki, Philip Doganis, Haralambos Sarimveis - Website
Send email to Charalampos Chomenidis, Pantelis Sospasakis, Evangelia Anagnostopoulou, Angelos Valsamis, George Drakakis, Pantelis Karatzas, Georgia Tsilki, Philip Doganis, Haralambos Sarimveis

Servers

<http://api.jaqpot.org:443/jaqpot>

Authorize

aa	
GET	/services/aa/claims Requests authorization from SSO
POST	/services/aa/validate/accesstoken Validate authorization token
POST	/services/aa/login
algorithm	
GET	/services/algorithm Finds all Algorithms
POST	/services/algorithm Creates Algorithm
GET	/services/algorithm/{id} Finds Algorithm
PUT	/services/algorithm/{id} Modifies a particular Algorithm resource
POST	/services/algorithm/{id} Creates Model
DELETE	/services/algorithm/{id} Unregisters an algorithm of given ID
bibtex	
GET	/services/bibtex/{id} Returns BibTeX entry
PUT	/services/bibtex/{id} Places a new BibTeX entry at a particular URI
DELETE	/services/bibtex/{id} Deletes a particular BibTeX resource
GET	/services/bibtex Finds all BibTeX entries
POST	/services/bibtex Creates a new BibTeX entry
biokinetics	
POST	/services/biokinetics/pksim/createmodel Creates Biokinetics model with PKSim
POST	/services/biokinetics/httk/createmodel Creates an httk bioinformatics Model
POST	/services/biokinetics/httk/model/{id} Creates prediction with httk model

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



NanoCommons Risk Assessment Tool

Short description

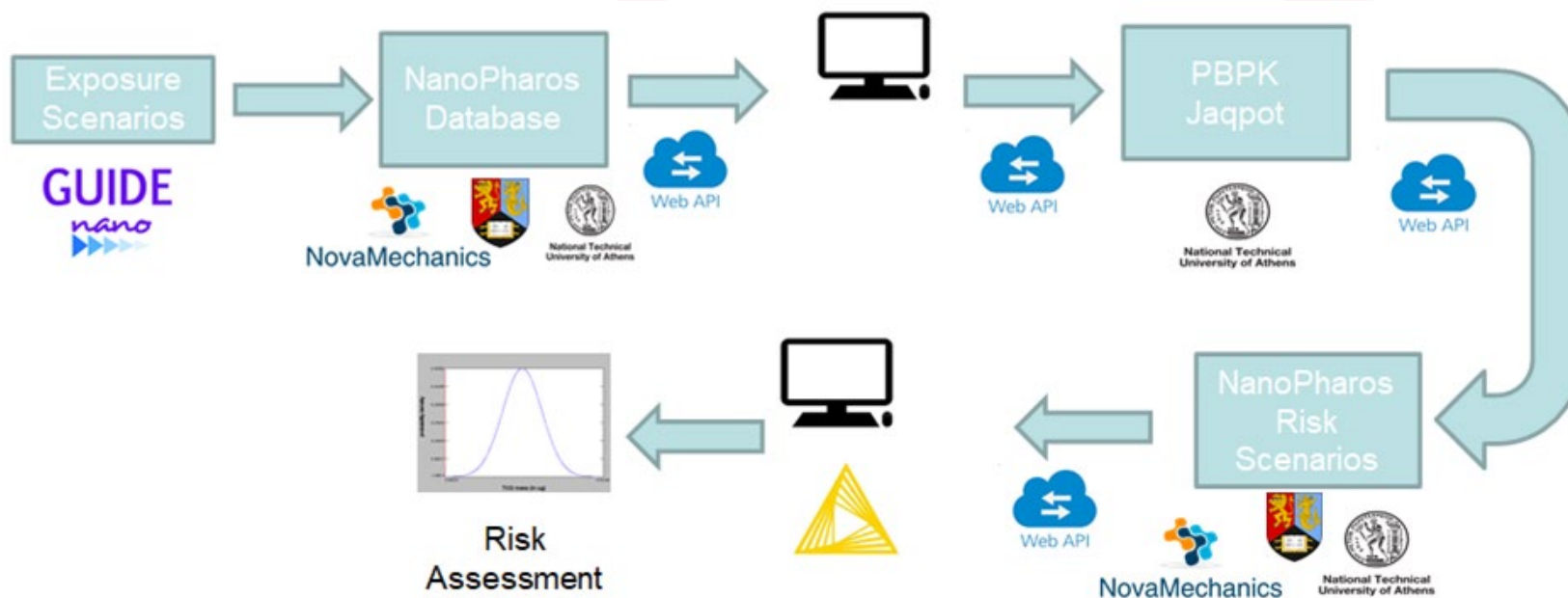
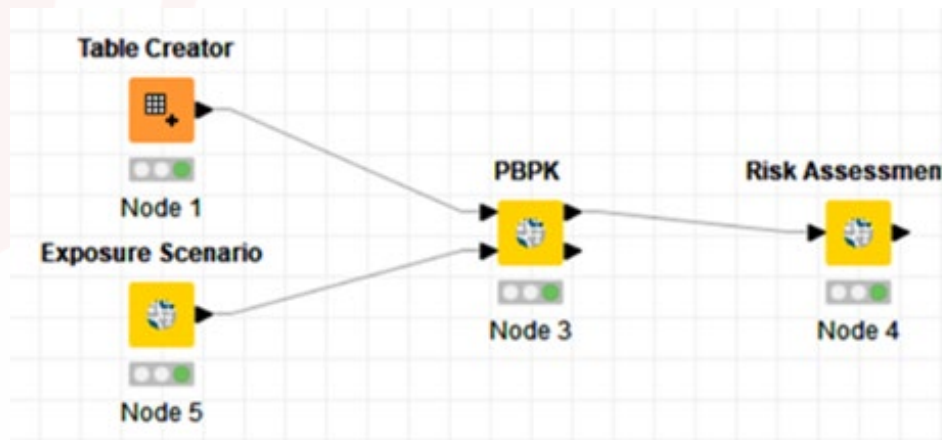
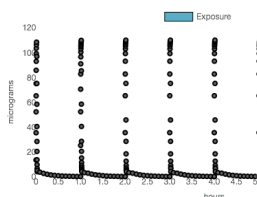
The workflow is a combination of nanoinformatics tools available through the NanoCommons computational infrastructure. This web application, hosted and implemented within [Enalos Cloud Platform](http://enaloscloud.novamechanics.com), estimates the risk of triggering AOP 173 (Lung Fibrosis) in mice due to exposure to 20nm TiO2 engineered nanoparticles.

External exposure: Four different exposure scenarios have been simulated using the GUIDENano.tool. The user can alternatively enter a custom-made scenario.

Case 1

45 g (initial mass 3000 kg) of TiO2 (22nm) poured over 7 hours in the NF, with 1 min activity duration every hour. For every hour the mouse stays 90 s in the NF and spends the rest of the time in the FF.

Download timeseries



Nanopot

Model
Predicting Zeta Potential of Gold Nanoparticles

Extra-Trees Regression Model for predicting Zeta Potential in water (mv) of Gold Nanoparticles

USE

Model
Predicting logP of Gold Nanoparticles

Extra-Trees Regression Model for predicting logP of Spherical Gold Nanoparticles

USE

Model
Predicting Cellular uptake in A549 of Gold Nanoparticles

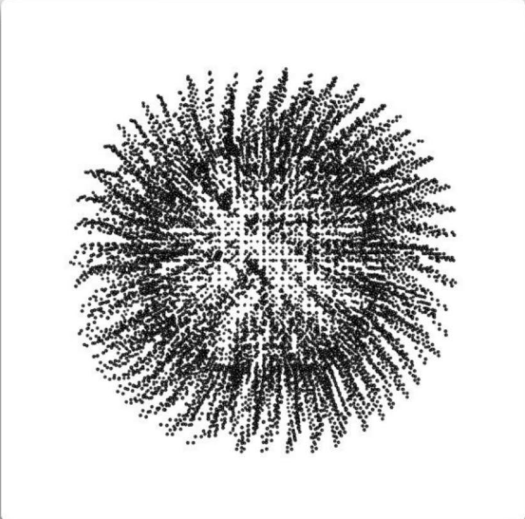
XGBoost Regression Model for predicting Cellular uptake in A549 (10-11 g Au cell-1) of Spherical Gold Nanoparticles

USE

Insert pdb file to get predictions

Zeta
-26.793512262182848

Choose pdb File (.pdb)



PDB file →

↓

Descriptors ←

↓

Modelling using Nanopot algorithms

↓

Predictions

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

Geometric
descriptors
API

Nanopot integrates the Jaqpot API to generate predictions for Engineered Nanomaterials with the use of PDB files.

<https://nanopot.cloud.nanosolveit.eu/>

Descriptors API 0.1.0 OAS3

openapi.json

default

- POST
/geomdescriptors Geom Descriptors
- POST
/xyz Xyz Coords
- POST
/tensors Tensors
- POST
/fingerprints Fingerprints
- POST
/mordred/smile Apply Descriptor To Smile
- POST
/mordred Apply Descriptor

chempot

POST
/services/chempot Creates Prediction with smiles input

Creates Prediction with smiles input

Try it out

Name	Description
Authorization	Authorization required

Request body application/json

Example Value | Schema

```

{
  "smiles": "string",
  "modelid": "string",
  "withbox": true,
  "descriptors": "string"
}

```

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

How Jaqqpot can serve your needs

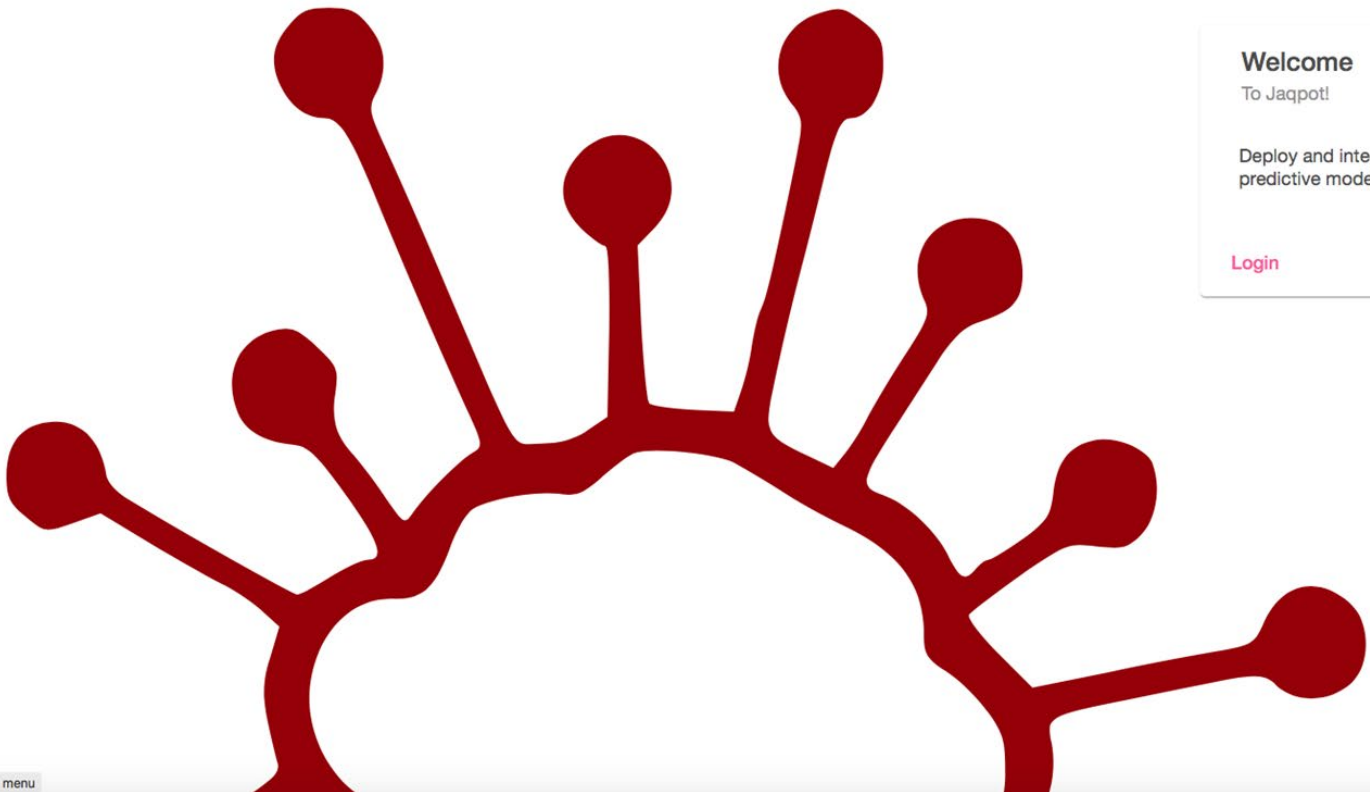
- **Publish your model** as web services
- Provide **ready-to-use implementations** of your models as supporting material to your publications
- **Collaborate** with your partners and colleagues
- **Share models** within your group, project or organisation and **disseminate** them to the community or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

Play a menu

JAQPOT

JAQPOT

English v

Log In

Username or email

Password

Remember me [Forgot Password?](#)

[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



jaqpot@jaqpot.org

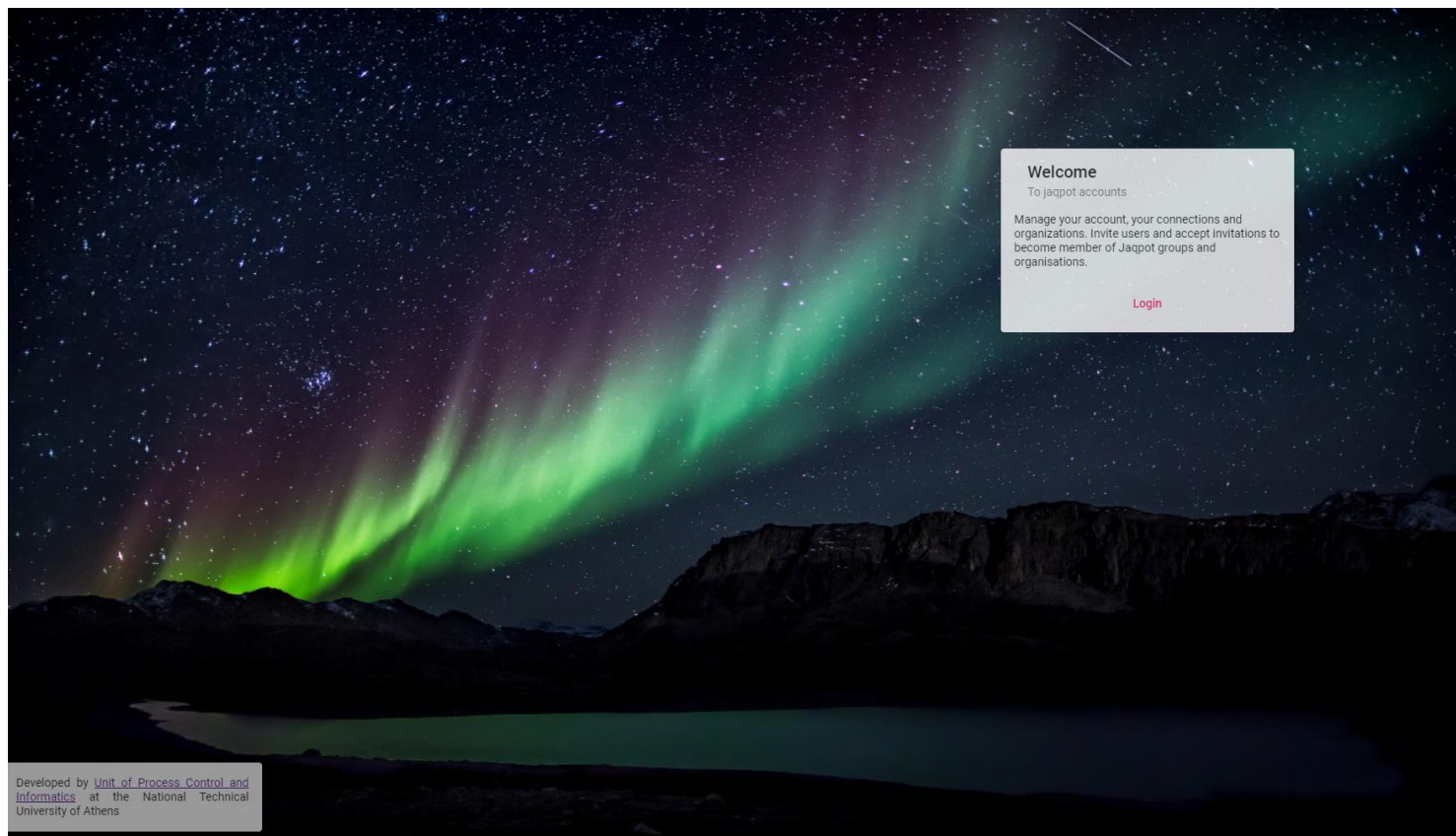
To undisclosed-recipients:

Jaqpot sent you an invitation to join WorkshopApril2021.

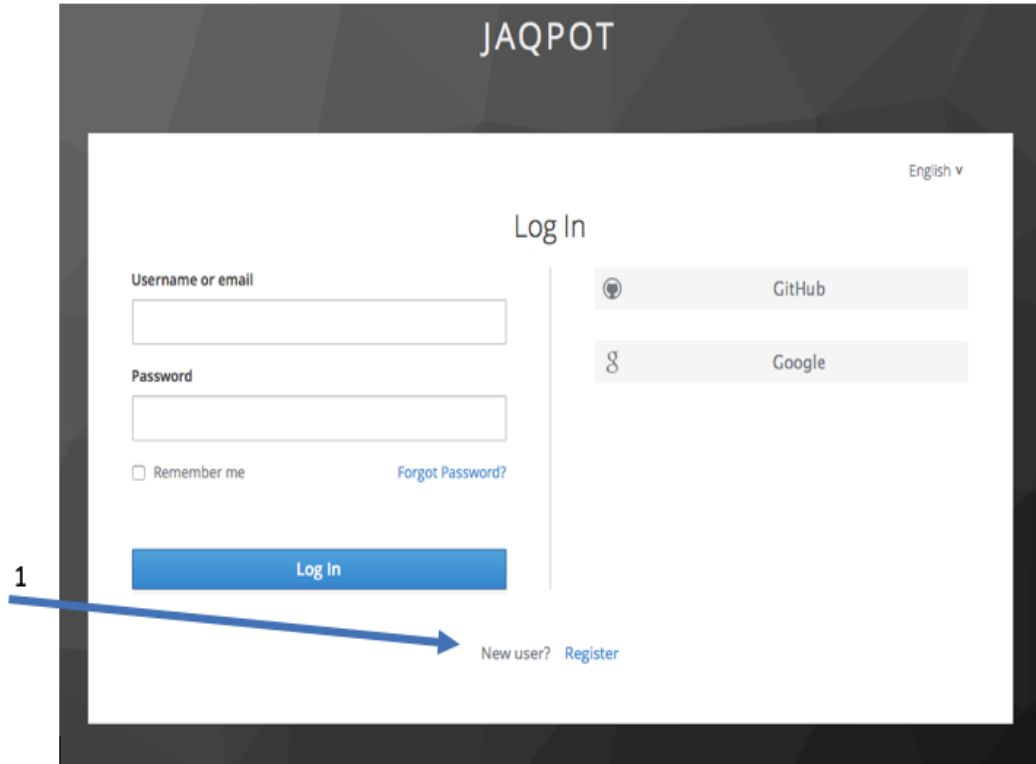
The invitation will be available on <https://accounts.jaqpot.org>

Thank you for using Jaqpot services!

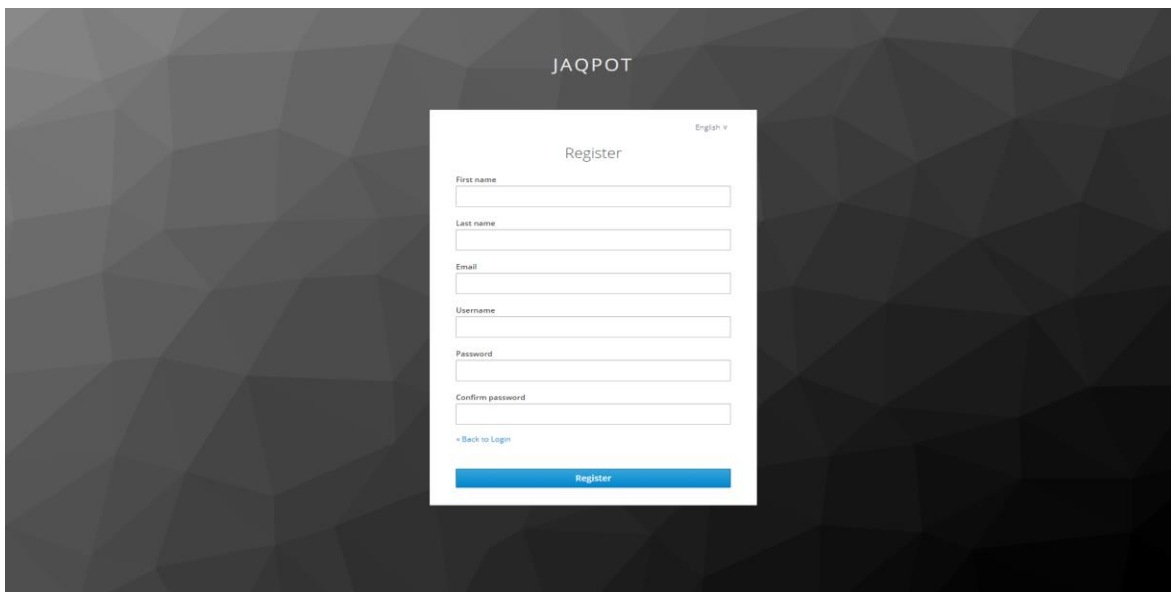
To accept the invitation, you should have a Jaqpot user account. Please create a user account by visiting the Jaqpot accounts application: <https://accounts.jaqpot.org> and clicking on "Login".



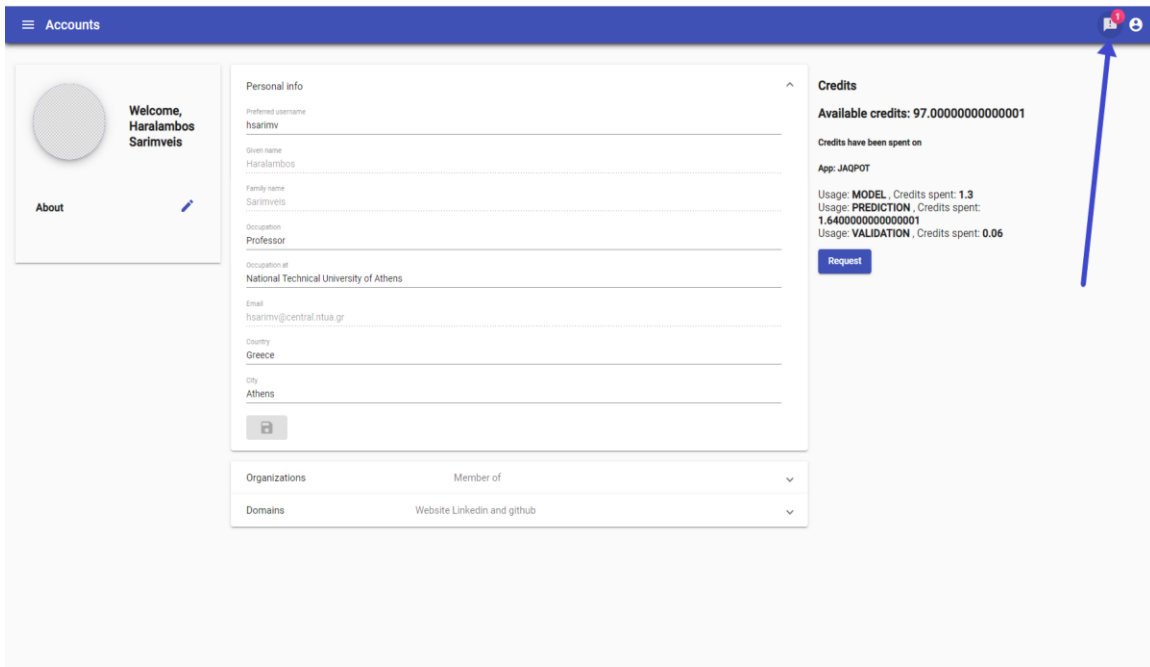
You will be redirected to the Login page. Please create your Jaqpot user account by selecting the "Register" option. For the purposes of this hackathon, please avoid using the Google/Github option, to enable a more uniform approach among participants.



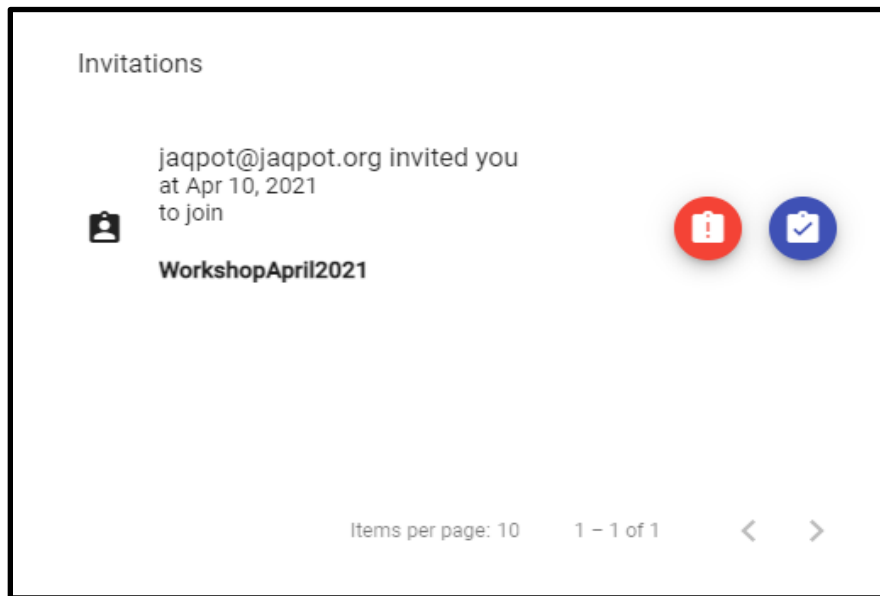
Only basic information is required for registering to Jaqpot and creating a user account. Please make sure you enter the e-mail address, where you received the invitation. If you prefer to use another email address, please inform us by sending an email to jaqpot@jaqpot.org, and we will send you a new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



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



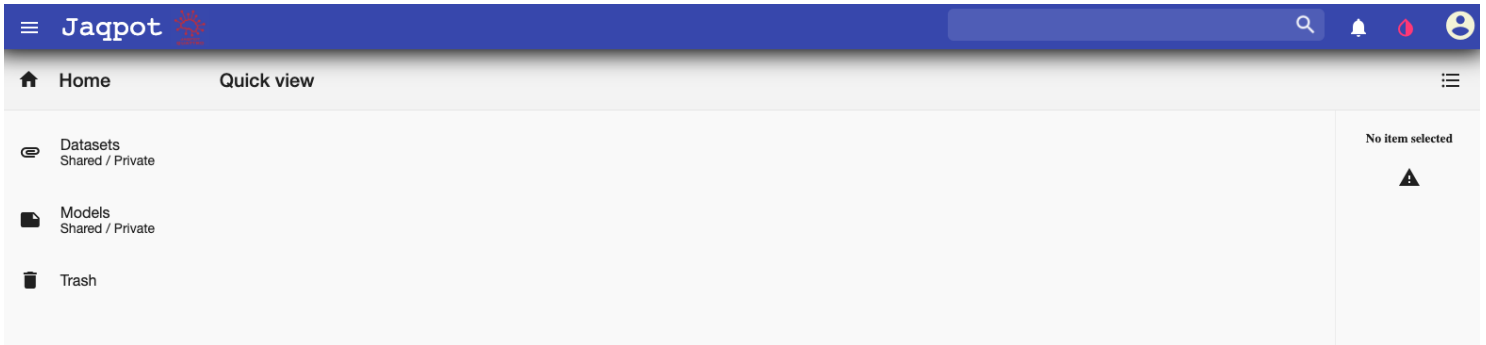
Please click on the "Invitations" icon on the top right part of the screen. This will open a window containing the invitation to the Workshop 2021 group:



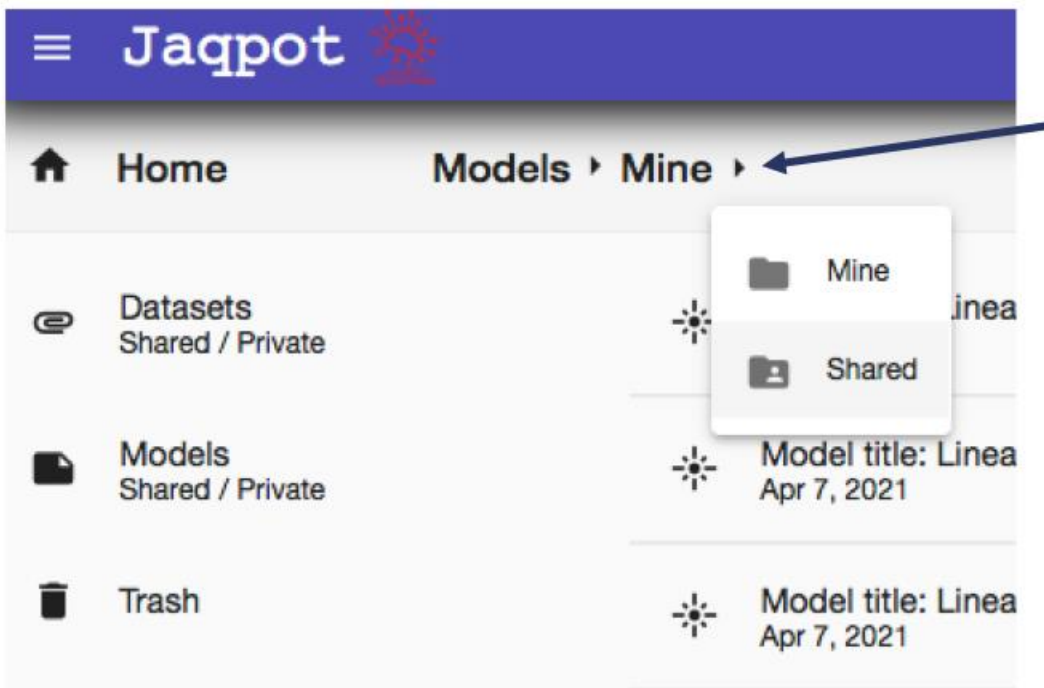
Please click on the blue icon to accept the invitation.

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

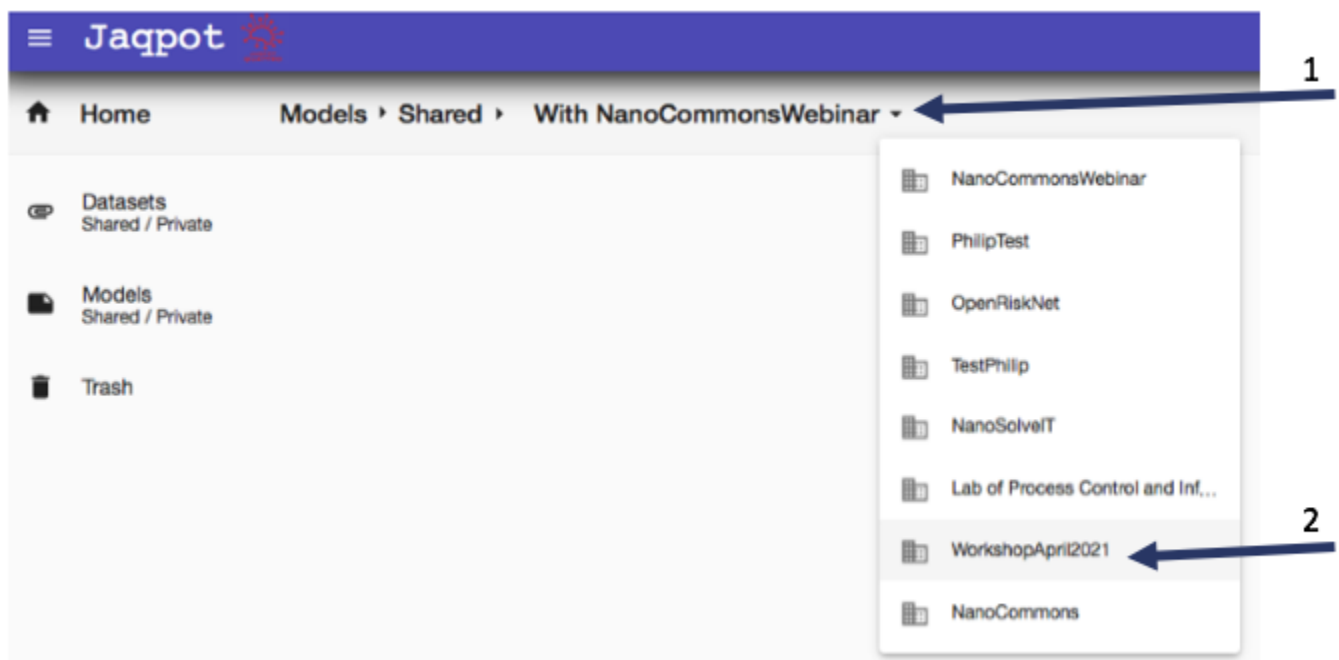
If you like to navigate through Jaqpot, you can visit the Jaqpot application: <https://app.jaqpot.org/home> with your Jaqpot username and password. Your entry page will be empty, because you have not yet created a model or dataset.



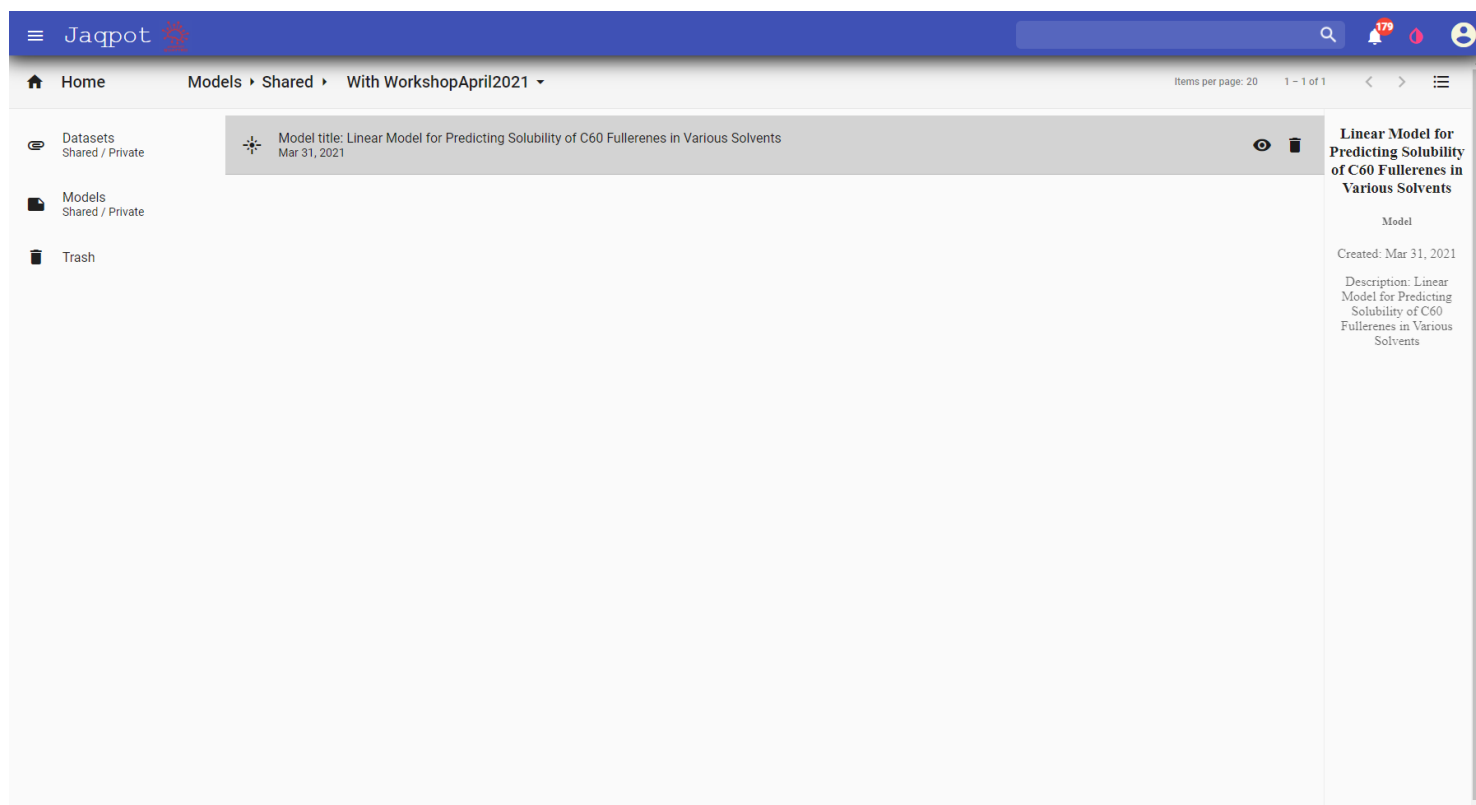
You can visit the **WorkshopApril2021** organisation by clicking the triangle icon next to **Mine**.



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!





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

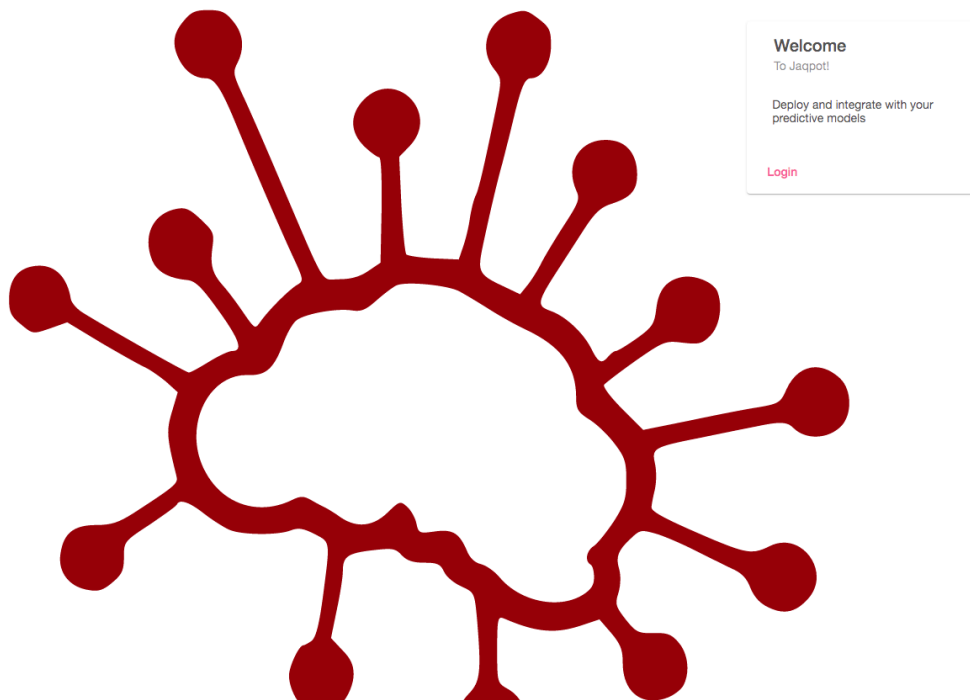
Briefly

- 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>

A Molecular-Based Model for Prediction of Solubility of C₆₀ 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 C₆₀ 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 C₆₀ 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 C₆₀ 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

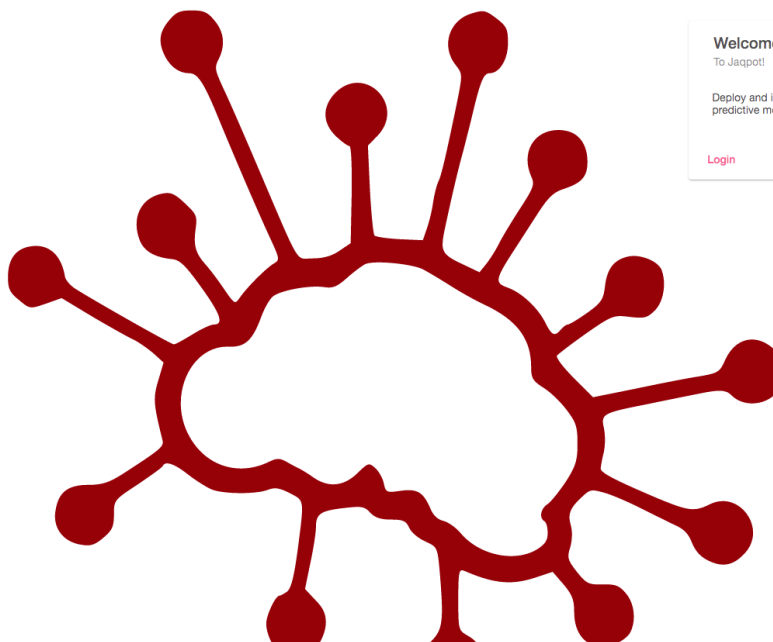
Solubility of Fullerene C₆₀ and C₇₀ in Toluene, o-Xylene and Carbon Disulfide at Various Temperatures >

Xfiroang Zhou et al.
Fullerene Science and Technology
Published online: 17 Feb 2007

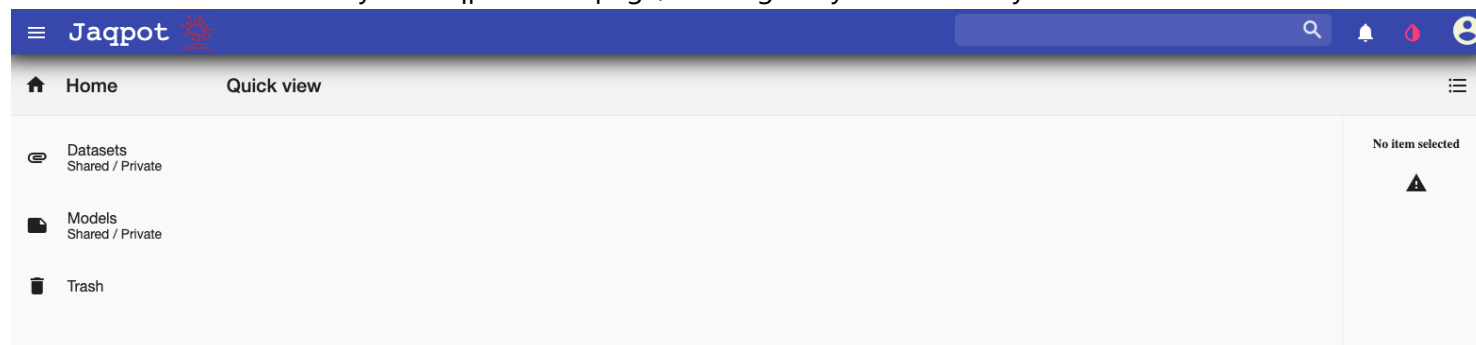
1. Accessing Jaqpot

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.

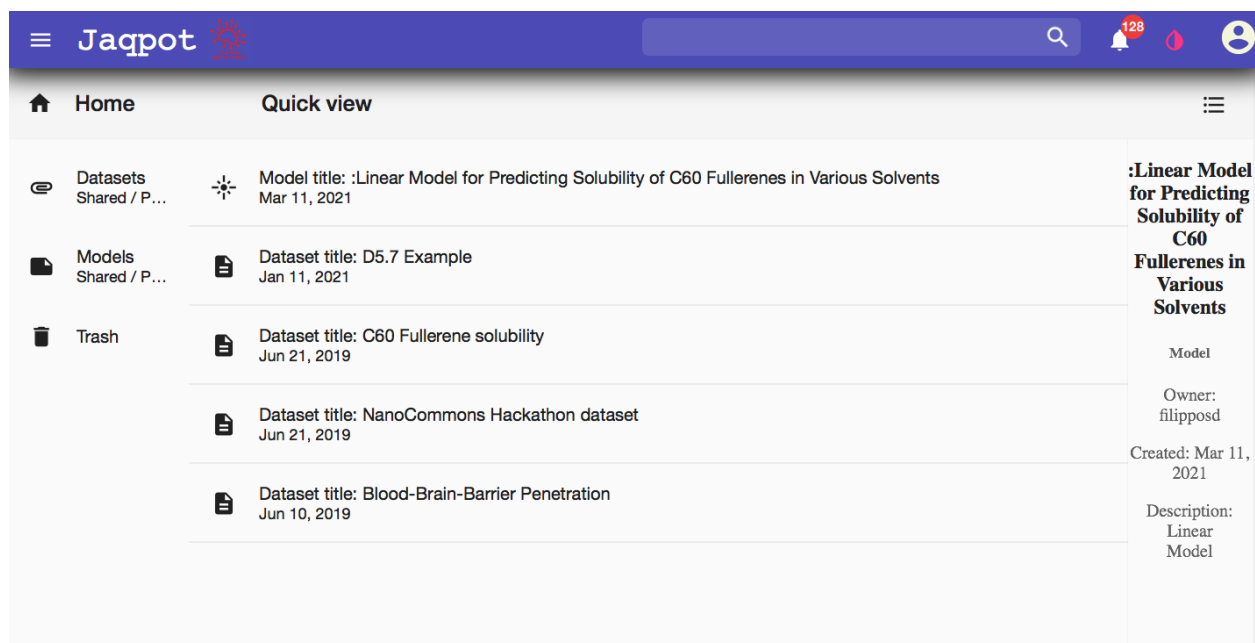
First click on **Login** on the welcome page:



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>

NanoPharos Datasets' Query

Select a dataset by name/paper	Description
Solubility of C60 Fullerene in Various Solvents	Farhad Gharagheizi & Reza Fareghi Alamdari (2008) A Molecular-Based Model for Prediction of Solubility of C60 Fullerene in Various Solvents. <i>Fullerenes, Nanotubes, and Carbon Nanostructures</i> , 16:1, 40-57, DOI: 10.1080/15363830701779315. https://www.tandfonline.com/doi/full/10.1080/15363830701779315

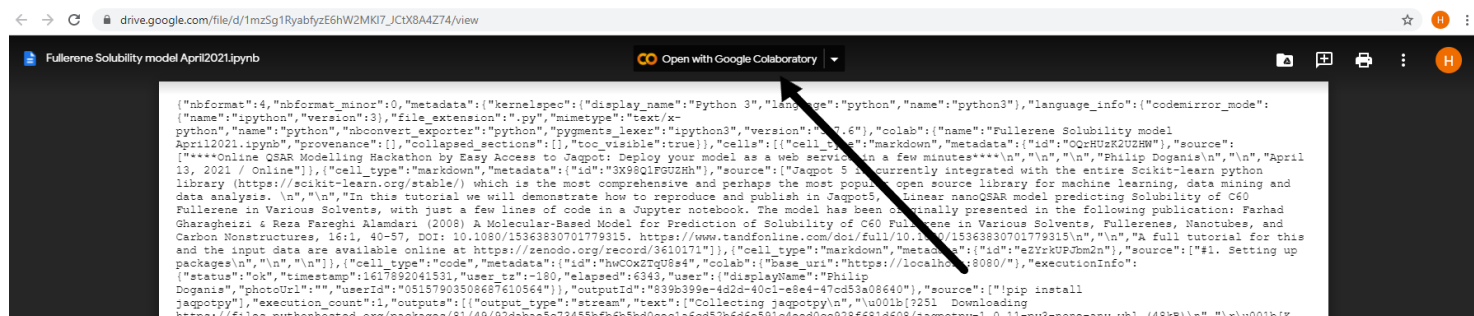
Download dataset

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

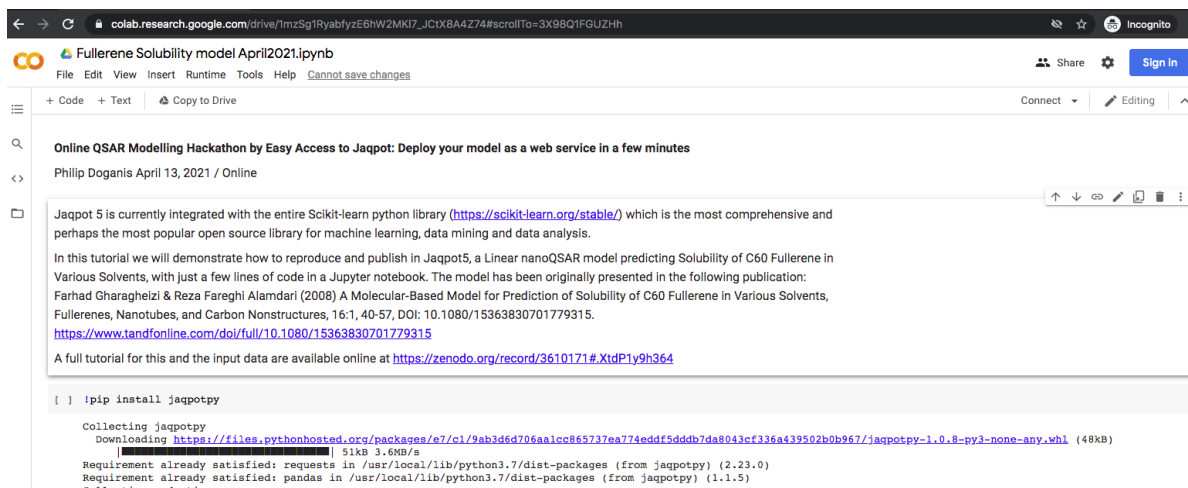
3. Accessing the Google colab notebook

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_JcT8A4Z74/view?usp=sharing

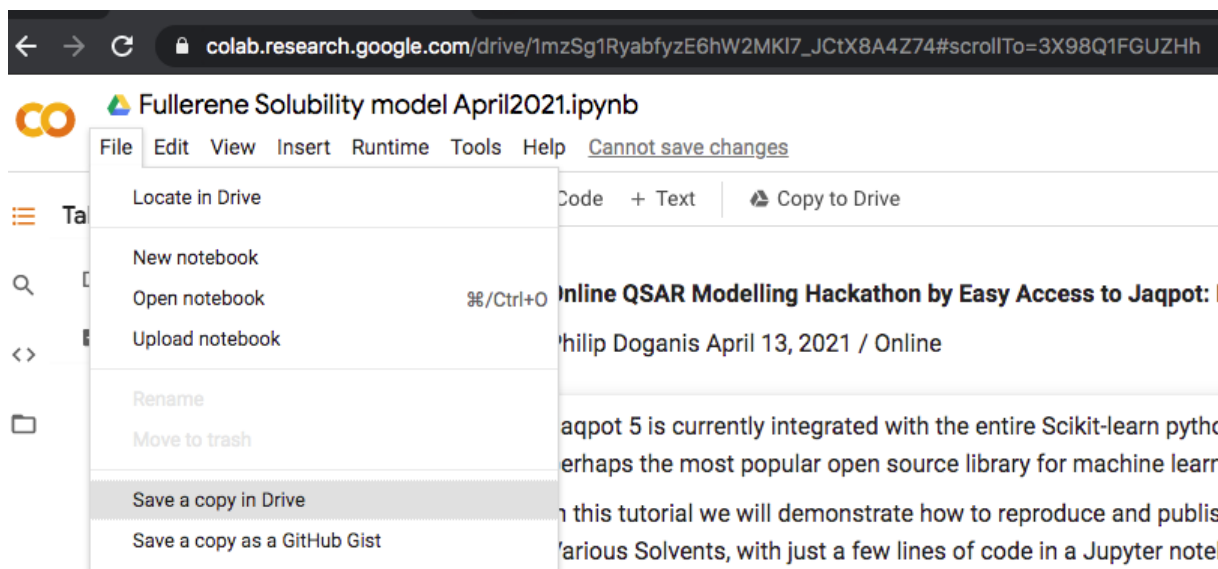
If a screen like this appears, please click on "Open with Google Colaboratory"



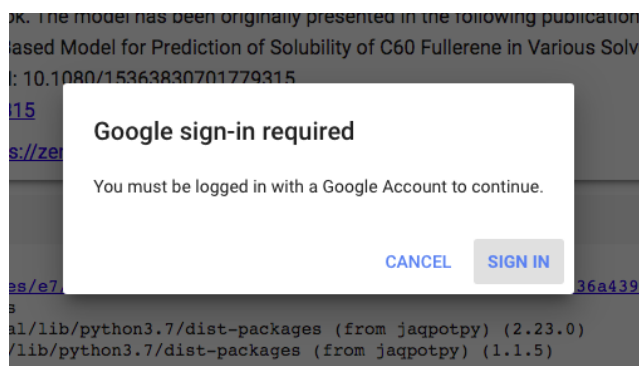
The Google colab notebook starting page looks like that:



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.

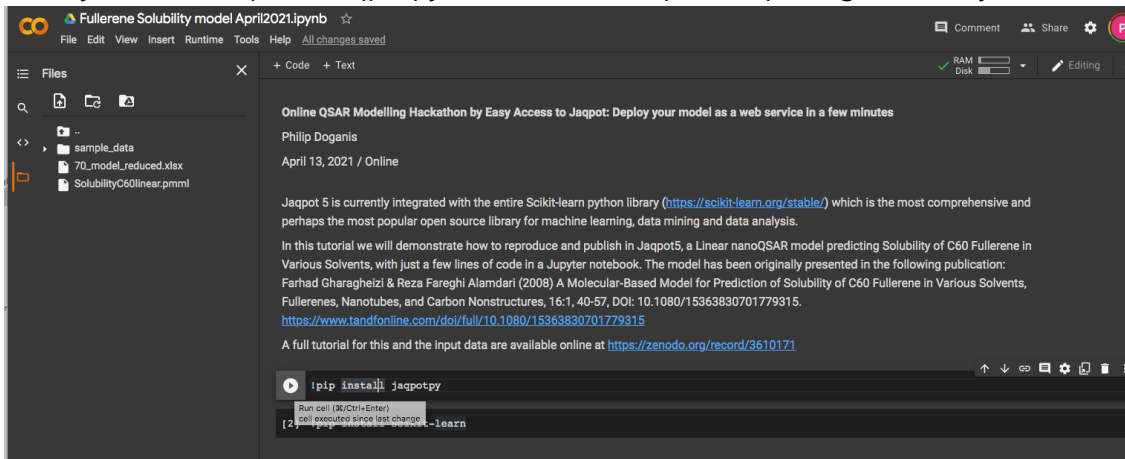
4. Running the colab notebook to create the model web service on Jaqpot

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

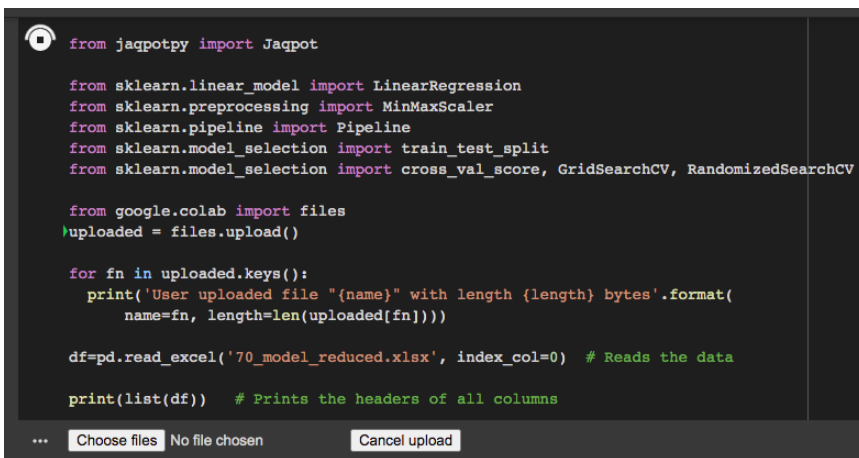
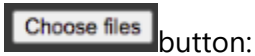
In order to execute code on the colab notebook you can go to the left of each cell and hit the  icon. You see the outcome of the cell expanding right below the cell.

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

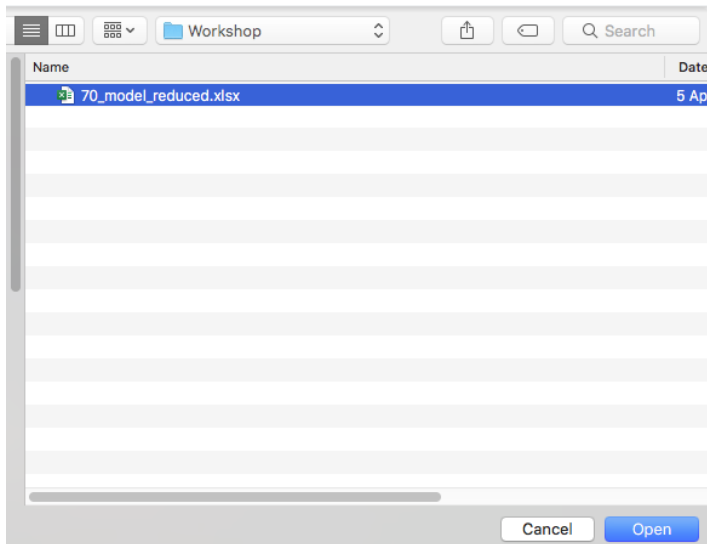


2. Uploading the data to the colab notebook

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



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

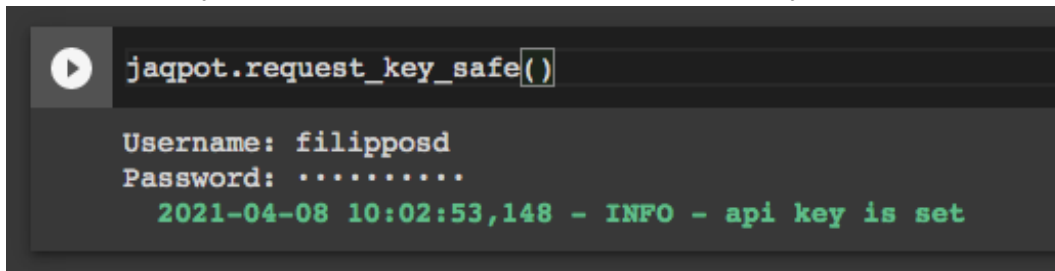
4. Training the model

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.



```
jaqpot.request_key_safe()  
Username: filippod  
Password: .....  
2021-04-08 10:02:53,148 - INFO - api key is set
```

6. Deploying the model

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

Pipeline	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)
```

```
1 command is needed to deploy the model into Jaqpot 5: https://www.jaqpot.org/docs/sklearn  
(please note some additional commands to time this procedure)  
  
[ ] import time  
    start_time = time.time()  
  
#This command deploys the model on Jaqpot  
modelId=jaqpot.deploy_sklearn(pipelineLinear, Xall, Yall, title="Solubility of C60 Fullerenes in Various Solvents-USERNAME", description:  
  
#The response is the unique Jaqpot model ID on which the model is hosted.  
  
print("---Your Jaqpot web service was created in %s seconds ---" % (time.time() - start_time))  
  
2021-04-07 21:43:42,827 - INFO - Model with id: 99vBdRvvD8NoiFA61N17 created. Storing Domain of applicability  
2021-04-07 21:43:43,413 - INFO - Stored Domain of applicability. Visit the application to proceed  
---Your Jaqpot web service was created in 1.2052156925201416 seconds ---
```

The web service has been created in Jaqpot and has a unique `modelURI` of the following form:
<https://app.jaqpot.org/model/99vBdRvvD8NoiFA61N17>.

```
[ ] modelURI='https://app.jaqpot.org/model/'+modelId  
    print("You can use your model here or over the User Interface at: %s " % modelURI)  
  
You can use your model here or over the User Interface at: https://app.jaqpot.org/model/99vBdRvvD8NoiFA61N17
```

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
```

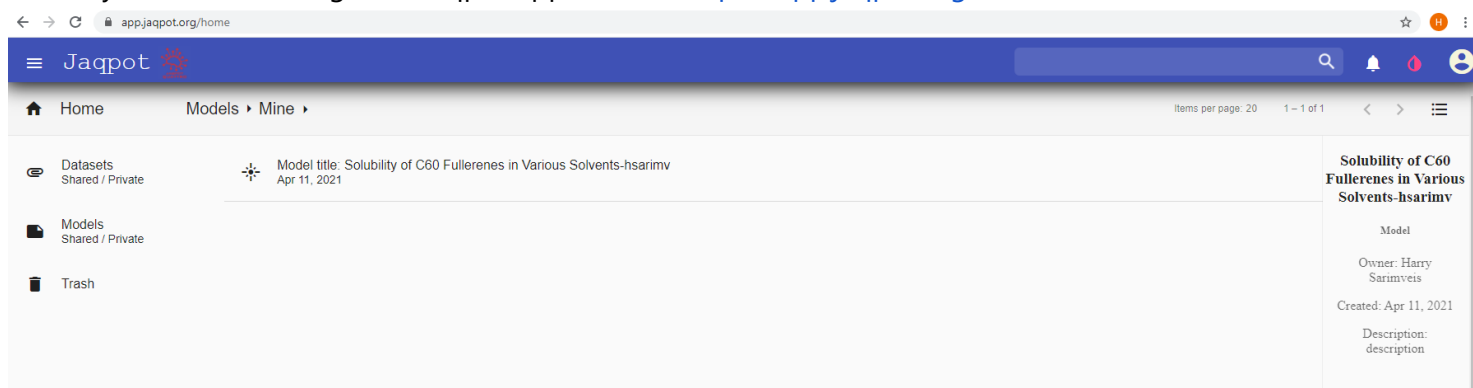
```
[ ] predictions
```

(piPC03	ATSlm	More23e	Hlm	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

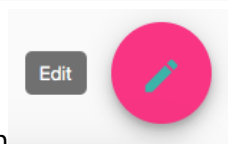
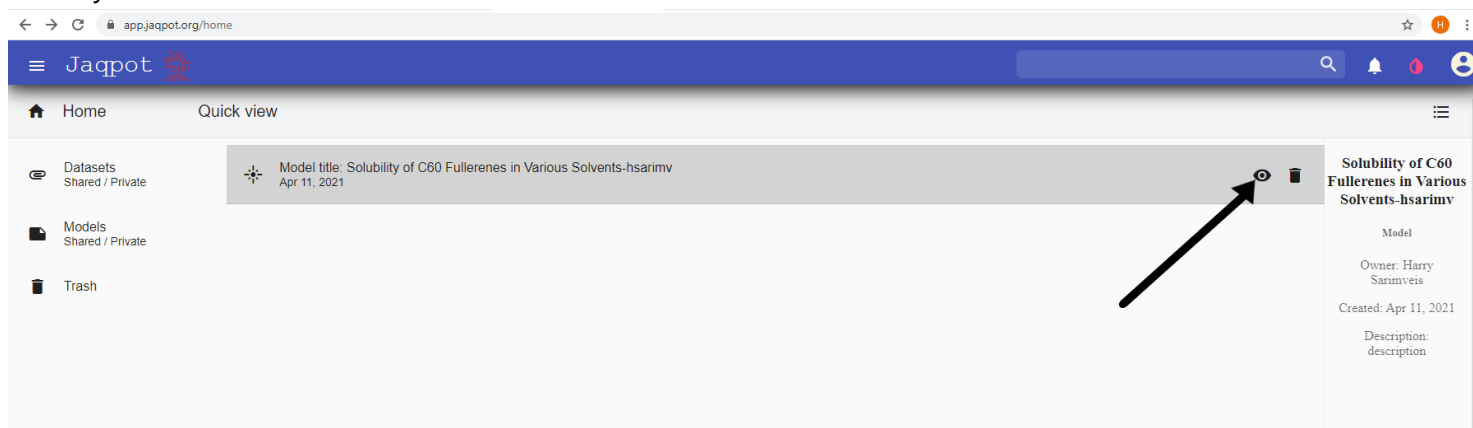
```
[124 rows x 6 columns], 'logS Exp.')
```


2. Share your model with the WorkshopApril2021 group

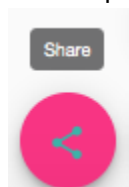
Access your model through the Jaqpot application: <https://app.jaqpot.org>:



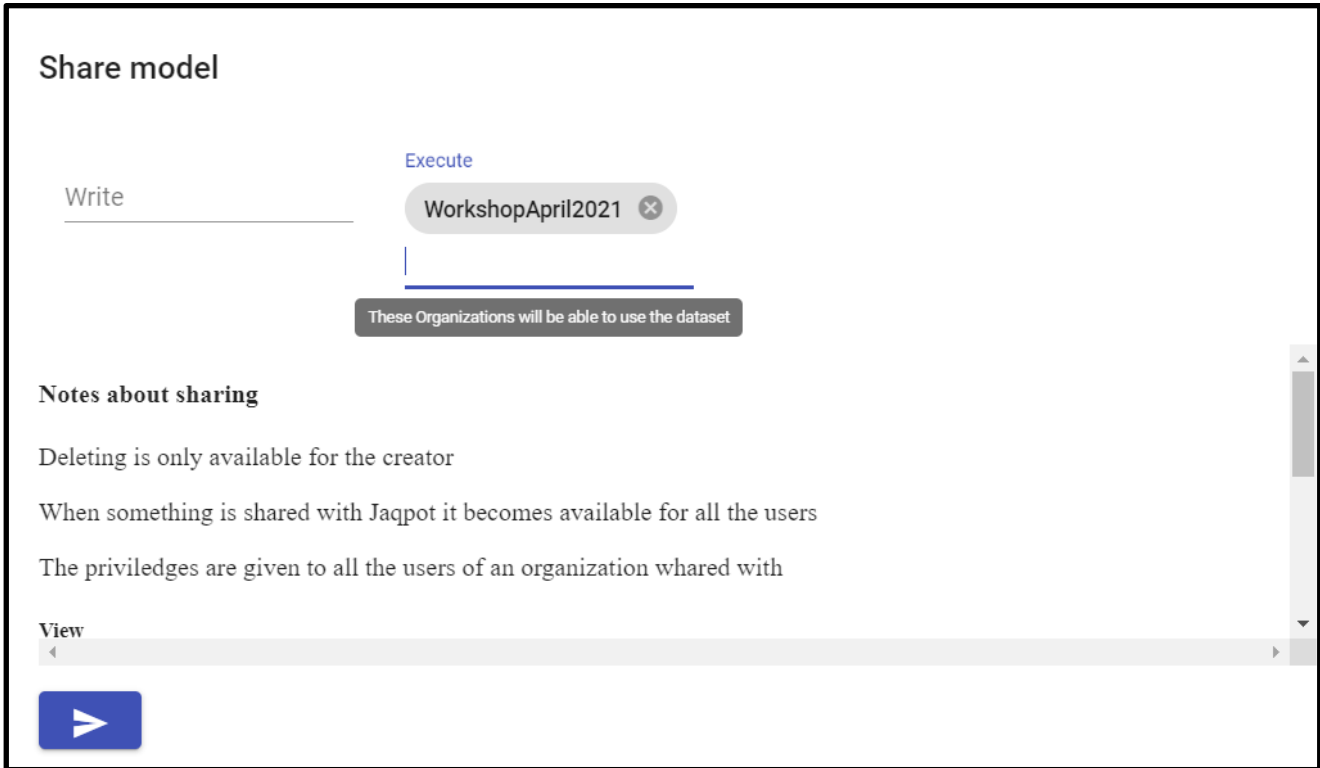
Select your model and click on the "View" icon





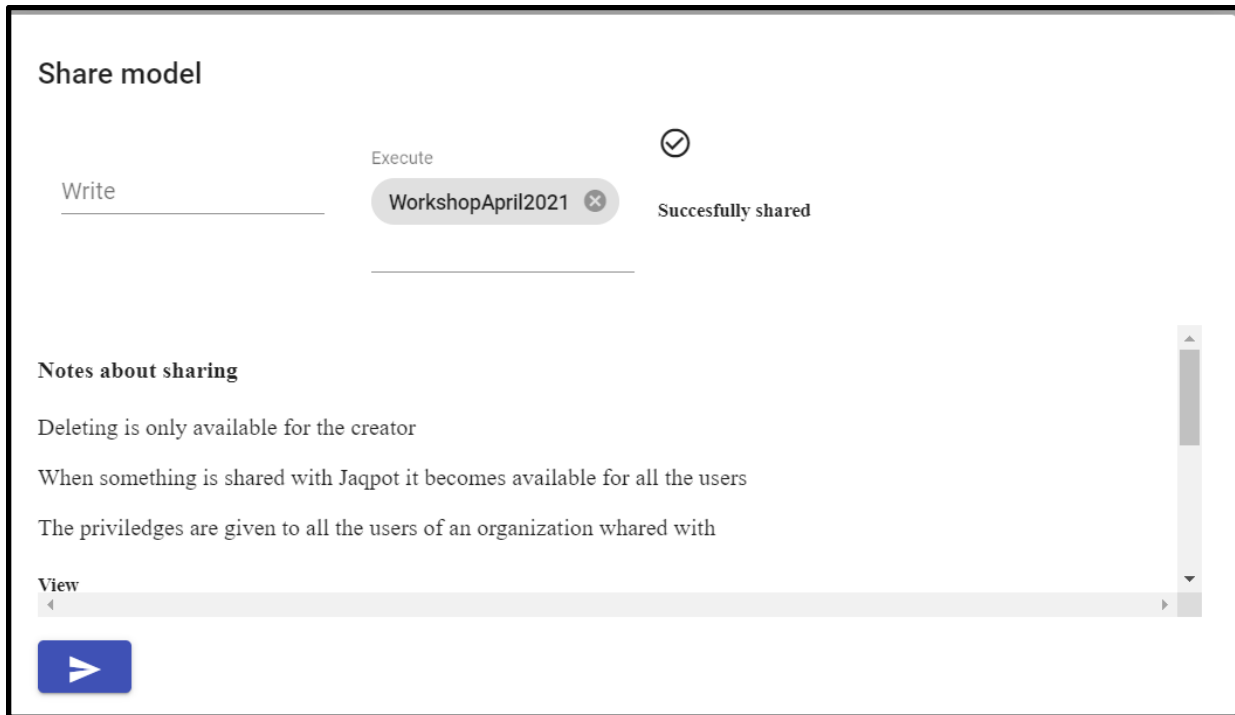
At the bottom right of the model page, click on the edit button



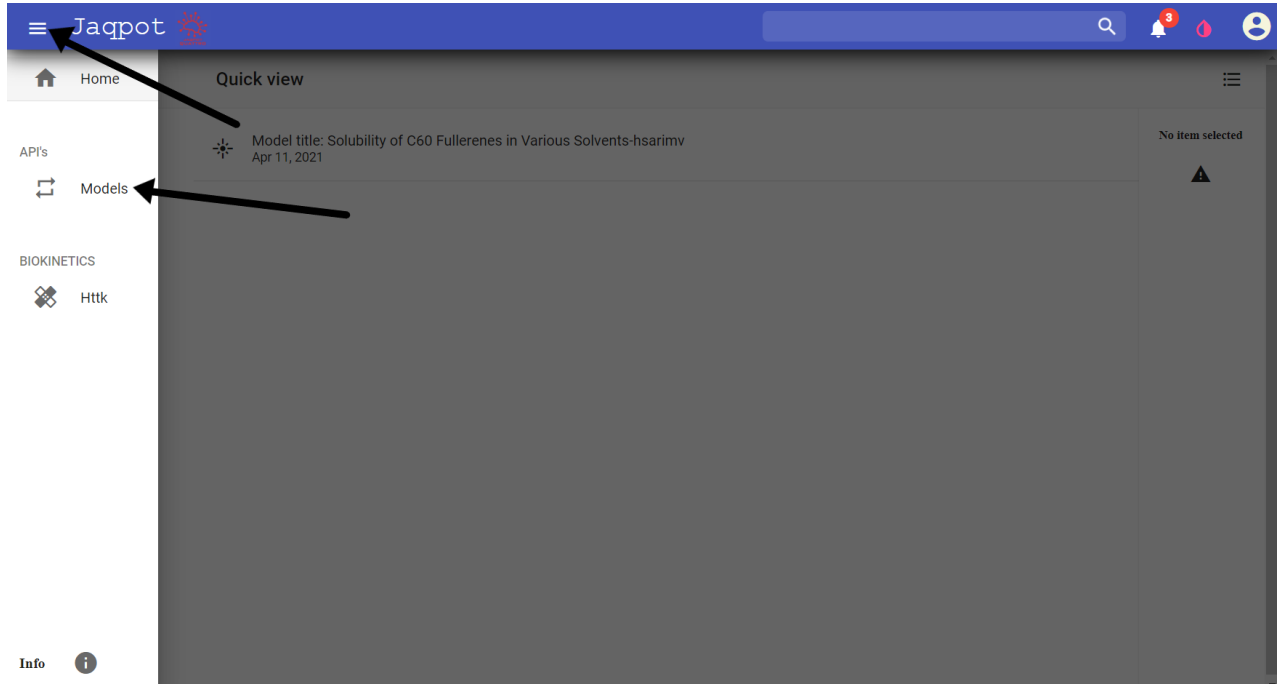
Clicking the Share button gives you the option to share the model with organisations of choice. Please select the WorkshopApril2021 group and give Execute rights only:



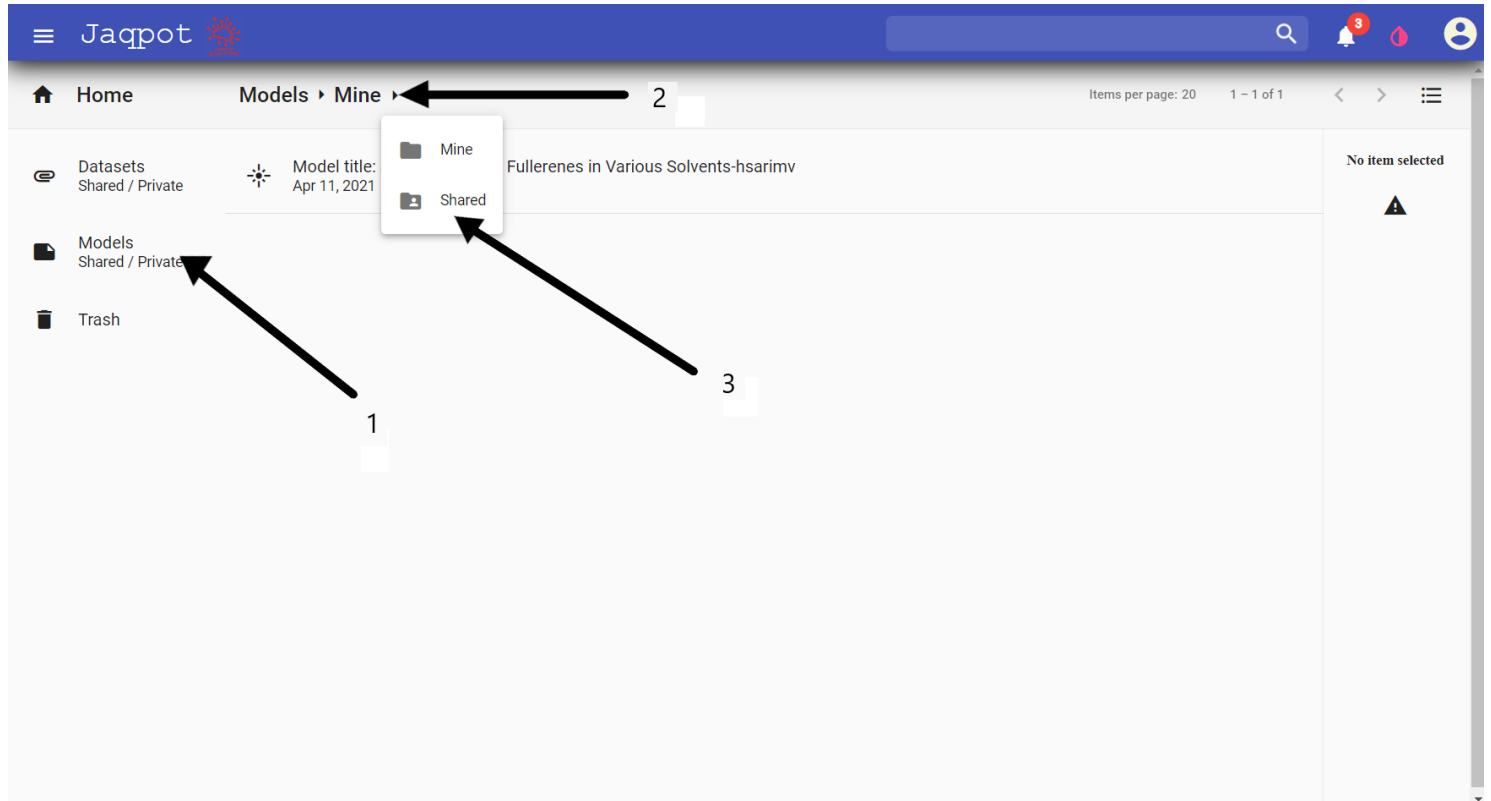
Adding an organisation to share with, activates the Share button, turning it from grey  to blue . Clicking this button causes the "Successfully shared" message to appear:



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.

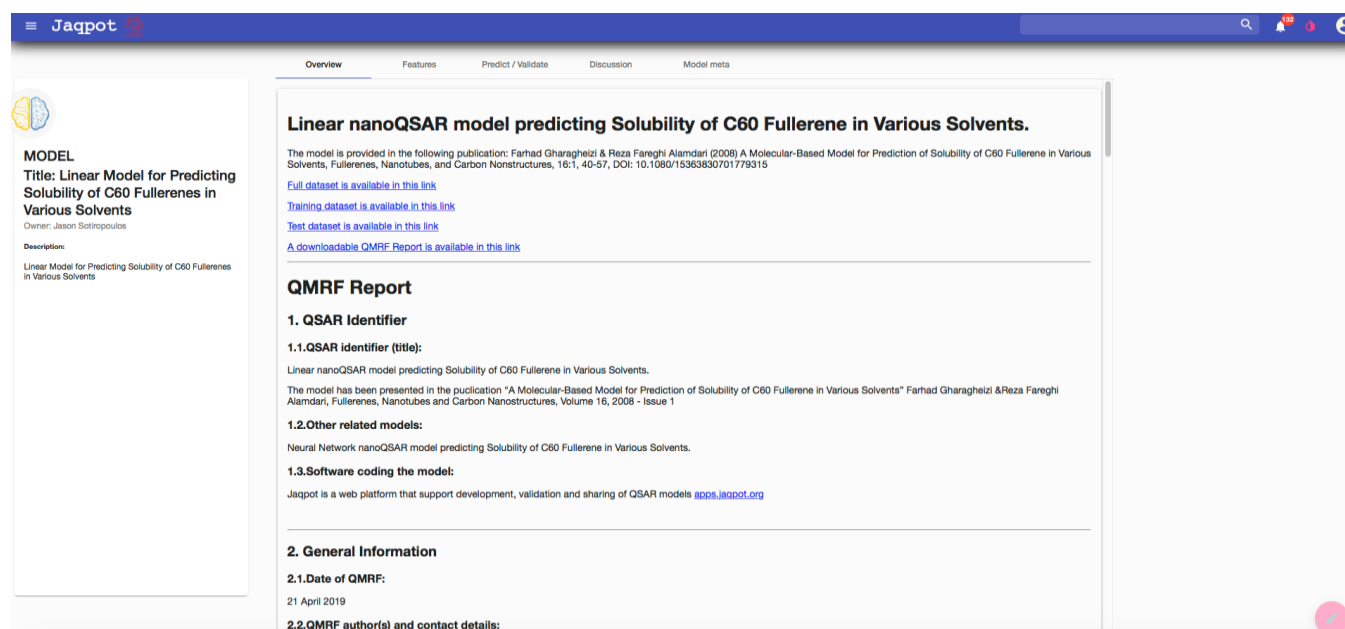
The screenshot shows the JupyterLab web interface. The top navigation bar is blue and contains the JupyterLab logo, a search bar, a notification bell with a red '3', a red flame icon, and a user profile icon. Below the navigation bar, the breadcrumb path is 'Home > Models > Shared > With WorkshopApril2021'. The main content area displays a list of items:

- Datasets** (Shared / Private): A model titled 'Solubility of C60 Fullerenes in Various Solvents-hsarimv' shared on Apr 11, 2021.
- Models** (Shared / Private): A model titled 'Linear Model for Predicting Solubility of C60 Fullerenes in Various Solvents' shared on Mar 31, 2021.
- Trash**

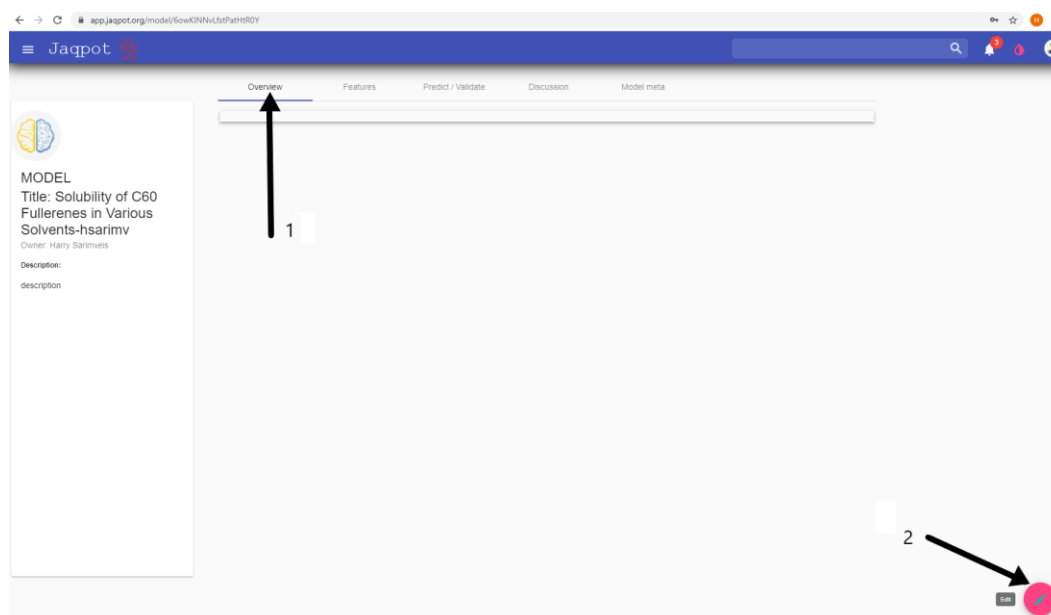
On the right side of the interface, there is a sidebar with the text 'No item selected' and a warning triangle icon.

3. Adding meta information to your model

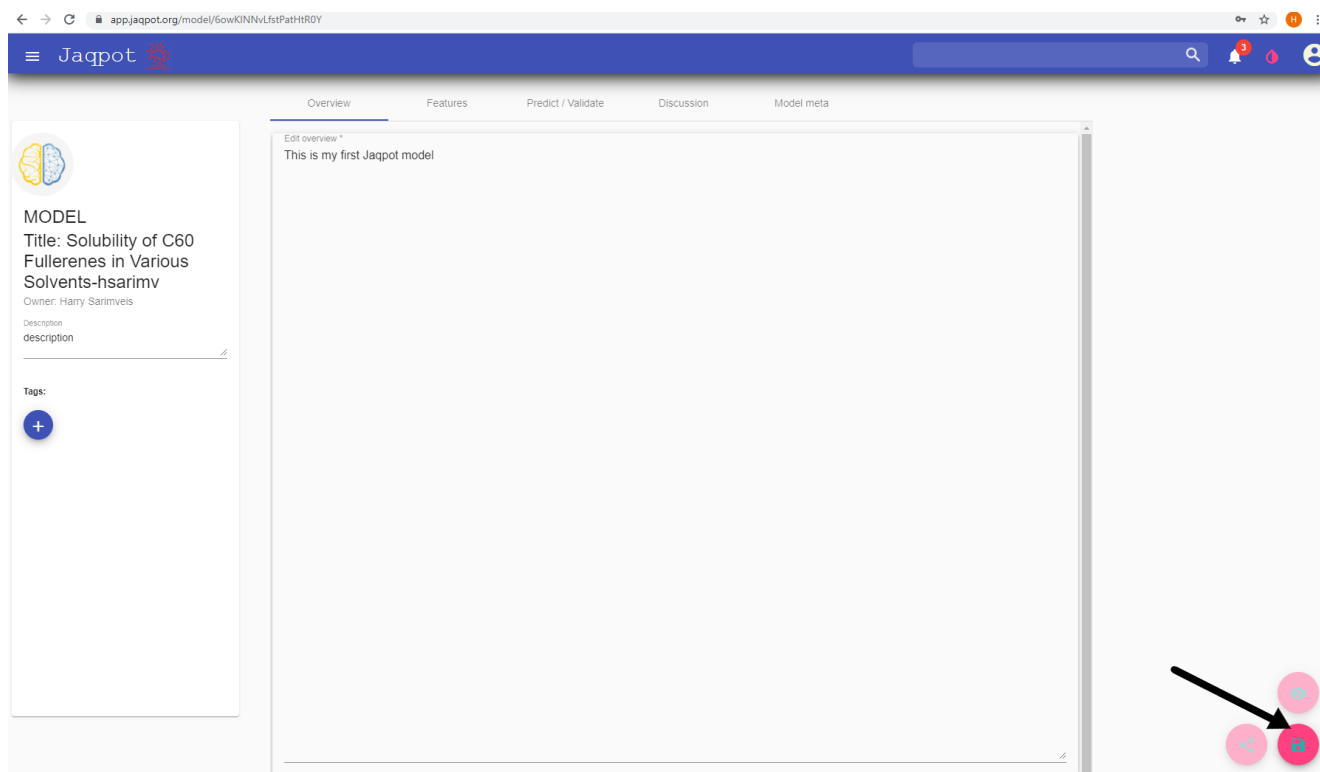
You can add any other information about the model over the user interface at <https://app.jaqpot.org/> (for example detailed description, standard reports like Quantitative Model Reporting Format (QMRF), PMML representations, ontological annotations etc., descriptions of variables, ontological classes 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/RqCRtRpY85kpbGtsiXp> and has been shared with the **WorkshopApril2021** organisation:



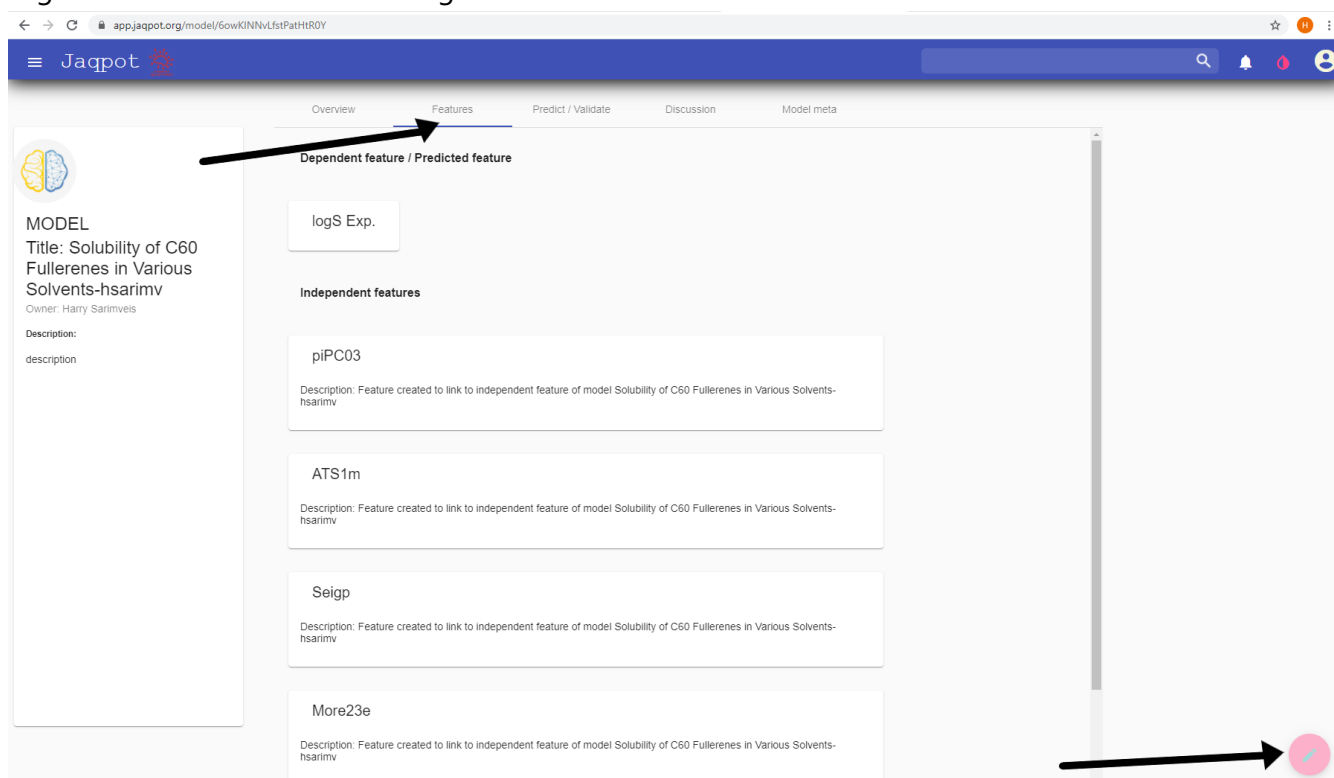
You can add information to your model by selecting the overview tab [1] and then clicking on the edit button.



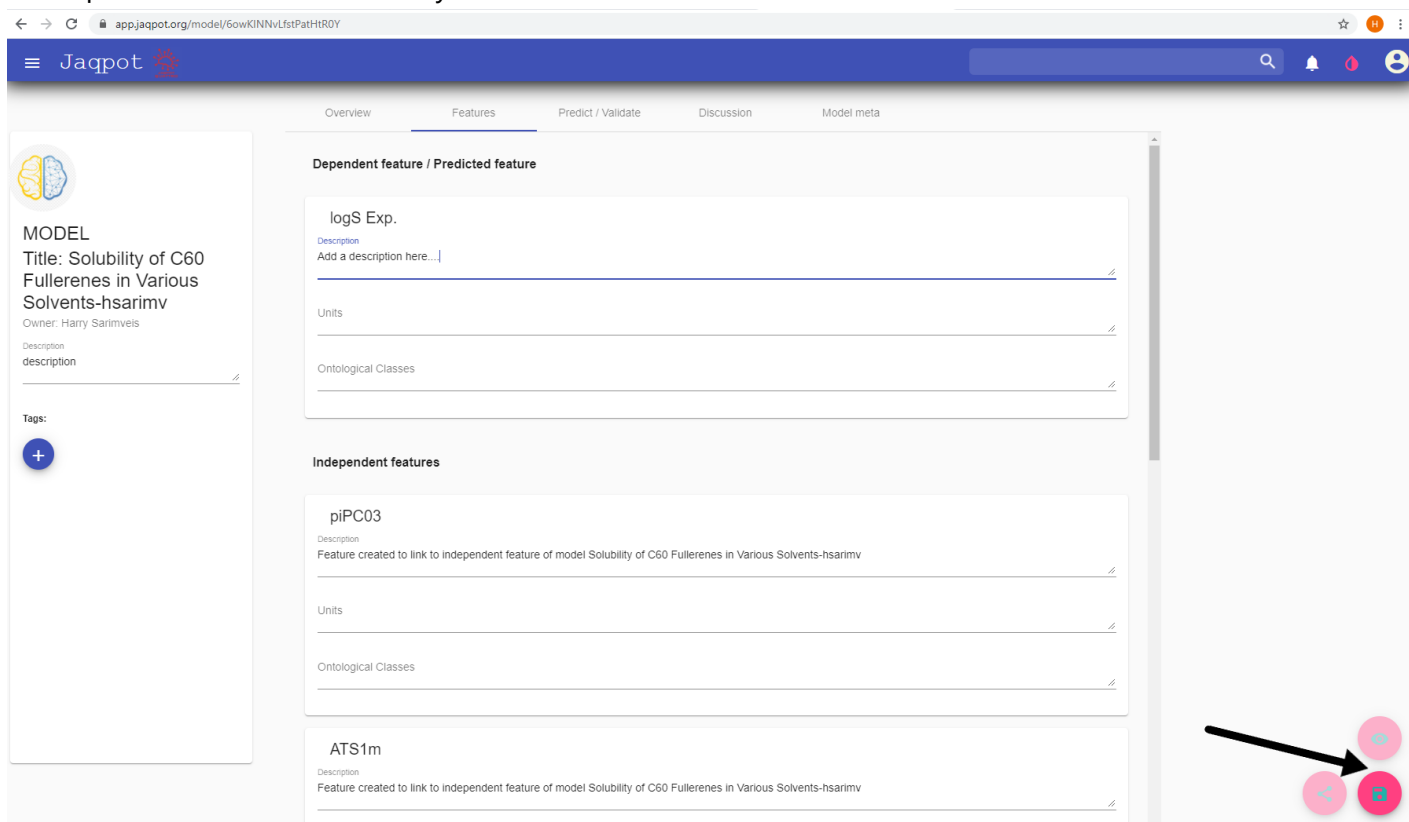
You can write any text (Markdown language is supported) and save it by clicking on the save button on the bottom right part of the page. You can return back and re-edit or extend the model description at any time.



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



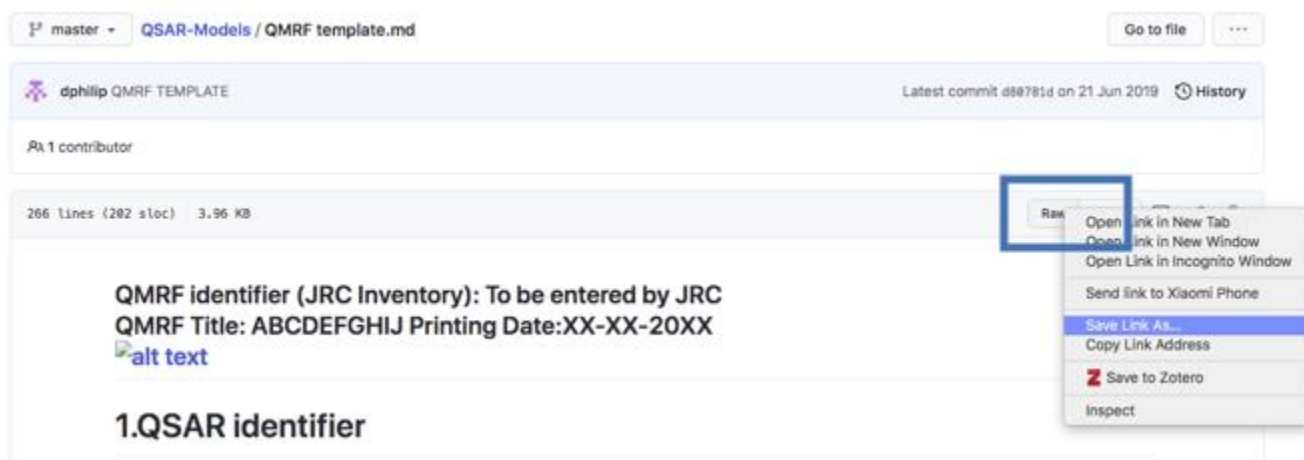
After entering the information, please click on the Save Button to store this information to the system. Descriptions can be updated and extended at any time.



To assist the users in adding editable versions of QMRF reports, we have created a QMRF markdown template, which can be downloaded at:

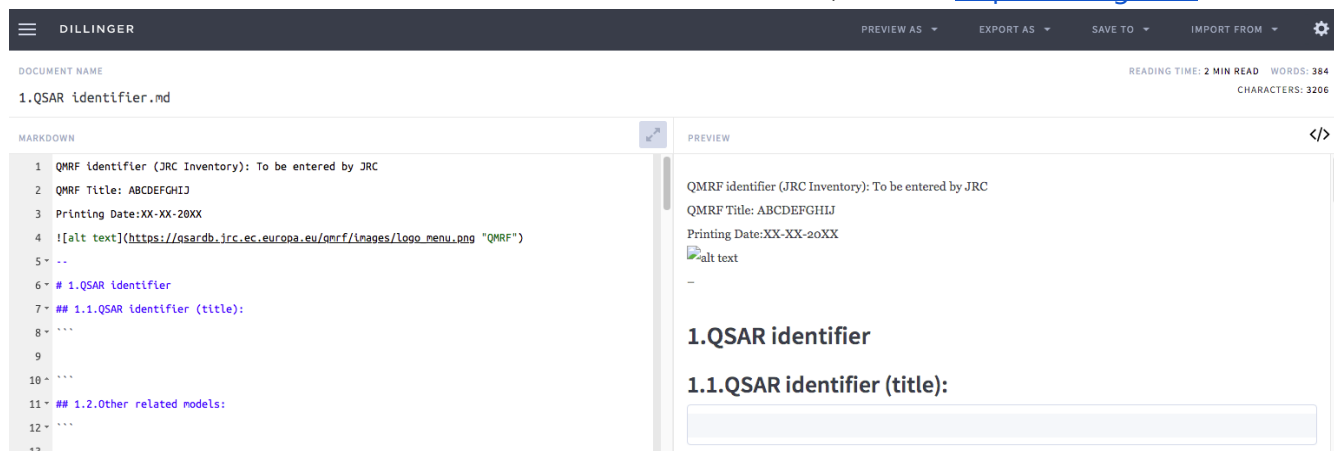
<https://github.com/ntua-unit-of-control-and-informatics/QSAR-Models/blob/master/QMRF%20template.md> .

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:


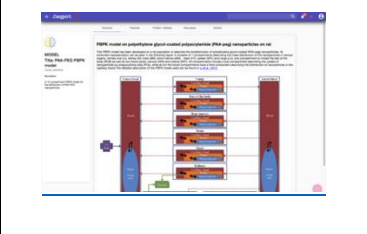
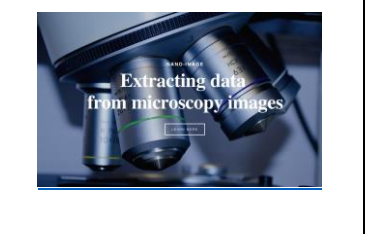
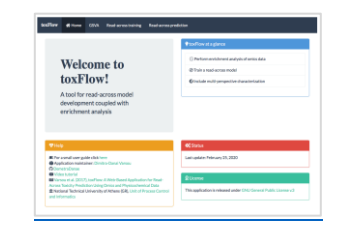
[Jaqpot 5: How to access and use an existing predictive model](#)

The data should be provided in a csv file. A sample csv file can be downloaded by clicking on the following link:

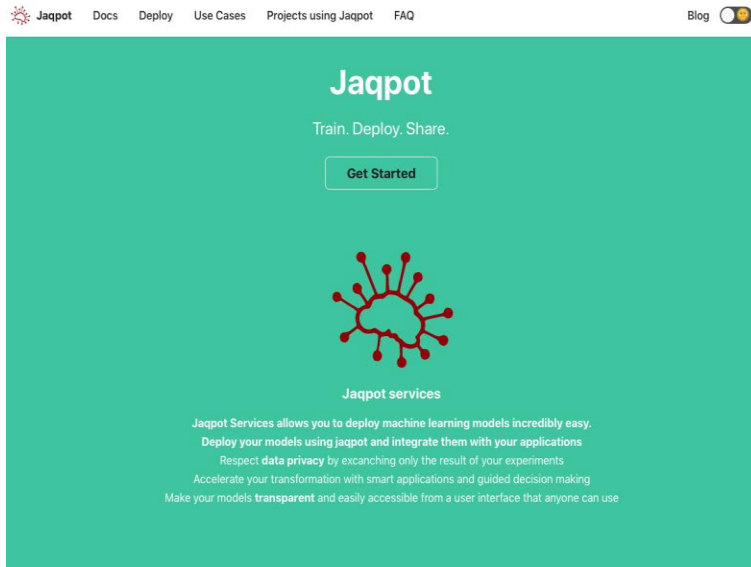
https://zenodo.org/record/4671069/files/70_model_reduced.csv?download=1

5. More information on the Jaqpot platform

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

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

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/UCuawpRvXNpglwyeltfTctw>

mailing list of WG-A Education, Training, Communication

- ▶ www.nanosafetycluster.eu



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Thank you for interest in our
training event!

