Nanoinformatics Model Development & Hosting

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A place to

deploy discuss

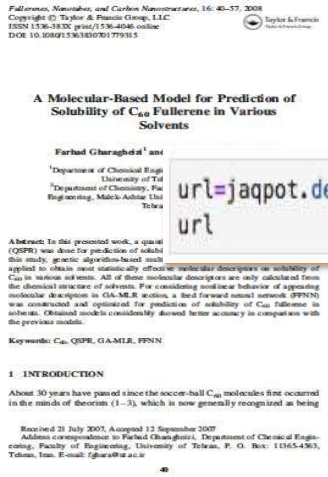
share use

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

From model to web service in 1 line



Fullerenes, Nanotubes, and Carbon Nanostructures, 16: 40–57, 2008
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ISSN 1536-383X print/1536-4046 online
DOI: 10.1080/15363830701779315

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

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University of Tel
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Engineering, Malek-Ashtar Uni
Tehra

Abstract: In this presented work, a quant
(QSPR) was done for prediction of solubil
this study, genetic algorithm-based multi
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.

Keywords: C_{60}, QSPR, GA-MLR, FFNN

1 INTRODUCTION

About 30 years have passed since the soccer-ball C_{60} molecules first occurred
in the minds of theorists (1–3), which is now generally recognized as being

Received 21 July 2007; Accepted 12 September 2007
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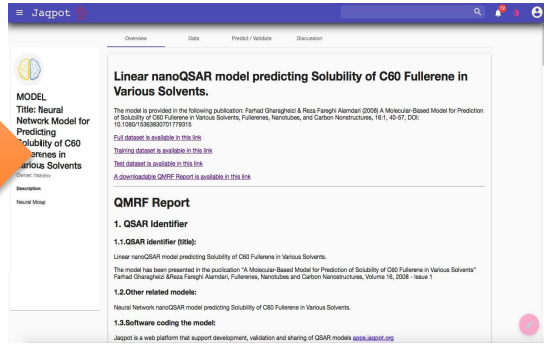
```
url=jaqpot.deploy_pipeline(clf_RFE2,XRFE3,Yall1,"ORN consensus RFE 6","Logistic Regression+RFE","linearmodel")
url
```

jaqpot.deploy_pipeline() parameters are:

- pipeline : sklearn pipeline model is a trained sklearn model
- X : pandas dataframe (X variables).
- y : pandas dataframe (y variables).
- title
- description
- algorithm



The model can be used
1. over the web page
2. in Python notebooks using the jaqpot.predict command

```
[ ]  dfJQ_RFE, predicts_RFE = jaqpot.predict(XRFE3, modelId=url)
```

and
3. over the API

The PMML description of the model is produced for PMML-enabled algorithms.


```
<?xml version="1.0" encoding="UTF-8" standalone="yes"?>
<PMML xmlns="http://www.dmg.org/PMML-4_4" xmlns:data="http://jpmml.org/jpmml-model/InlineTable" version="4.4">
    <Header>
        <Application name="JPMML-SkLearn" version="1.6.14"/>
        <Timestamp>2021-03-10T13:36:43Z</Timestamp>
    </Header>
    <MiningBuildTask>
        <Extension>PMMLPipeline(steps=[('scaler', MinMaxScaler(copy=True, feature_range=(0, 1))),
('MLR', LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None, normalize=False))])</Extension>
    </MiningBuildTask>
    <DataDictionary>
        <DataField name="logS Exp." optype="continuous" dataType="double"/>
        <DataField name="piPC03" optype="continuous" dataType="double"/>
        <DataField name="ATSie" optype="continuous" dataType="double"/>
        <DataField name="Seige" optype="continuous" dataType="double"/>
        <DataField name="MoreZe" optype="continuous" dataType="double"/>
        <DataField name="Htm" optype="continuous" dataType="double"/>
    </DataDictionary>
    <TransformationDictionary/>
    <RegressionModel functionName="regression" algorithmName="sklearn.linear_model._base.LinearRegression">
        <MiningSchema>
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            <MiningField name="piPC03"/>
            <MiningField name="ATSie"/>
            <MiningField name="Seige"/>
            <MiningField name="MoreZe"/>
            <MiningField name="Htm"/>
        </MiningSchema>
        <LocalTransformations>
            <DerivedField name="minMaxScaler(piPC03)" optype="continuous" dataType="double">
                <Apply function="*">
                    <FieldRef field="piPC03"/>
                    <Constant dataType="double">0.21612275772638864</Constant>
                </Apply>
            </DerivedField>
```
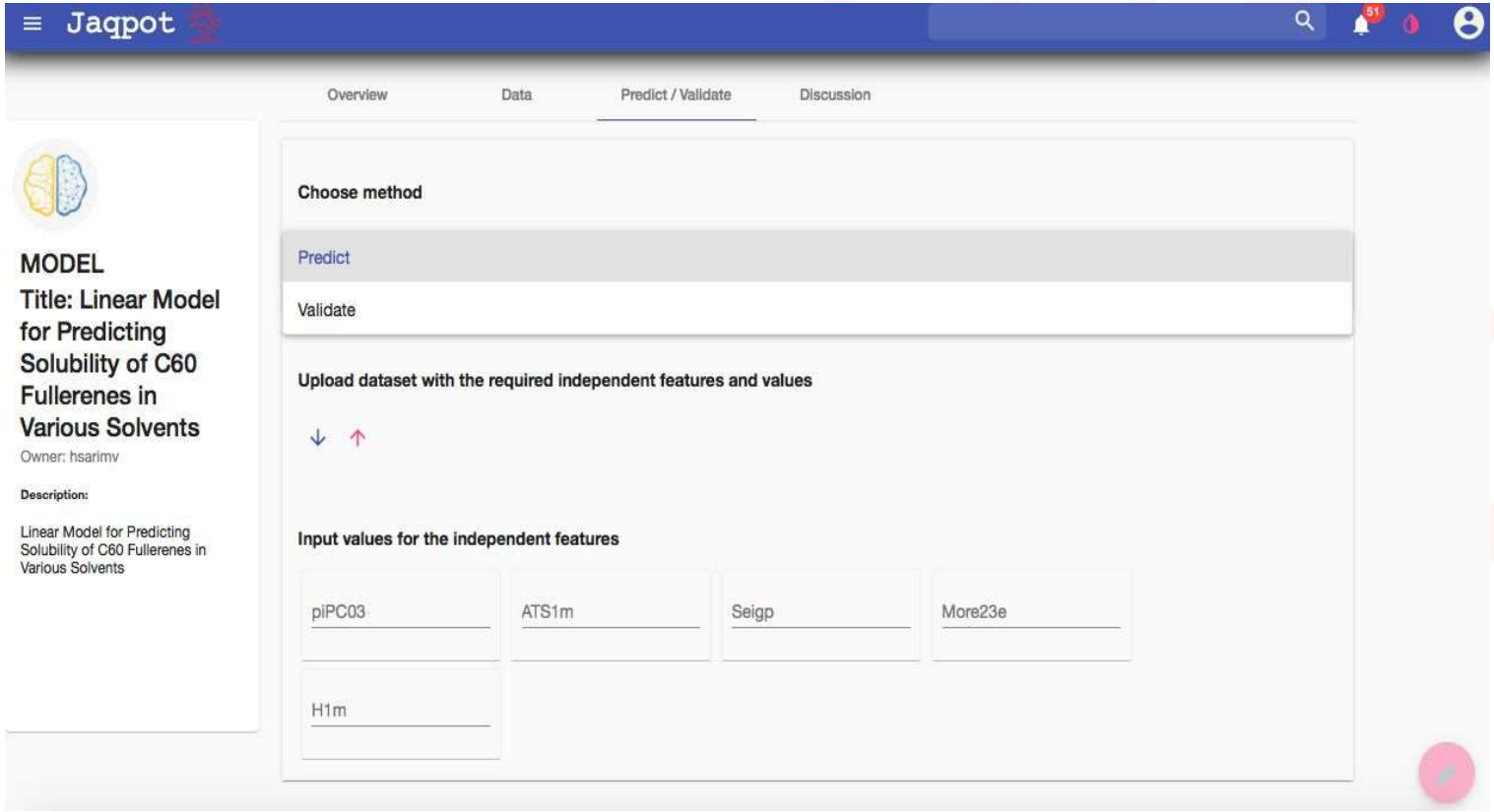

Jaqpot user interface



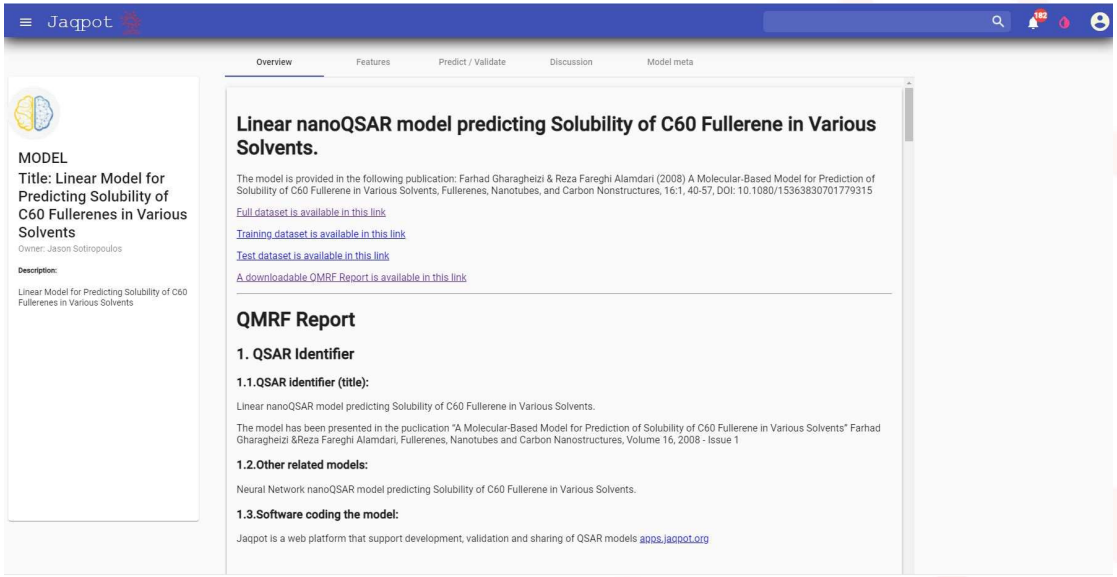
Predict-validate tab

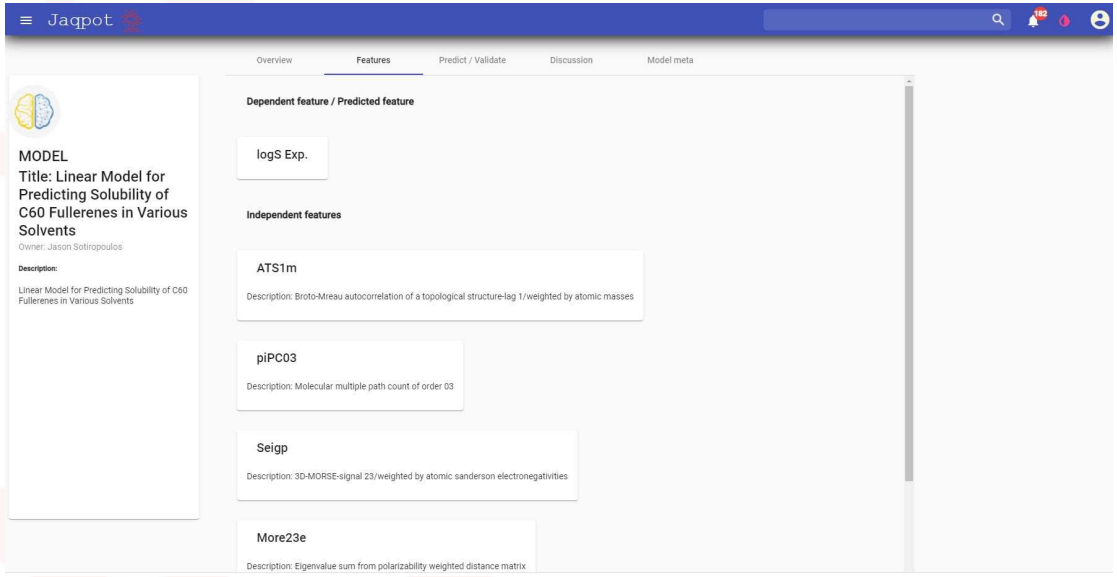
1. **Create predictions**
   a. by manually entering values
   b. CSV datasets using Jaqpot-generated template (*specific for each model*)

1. **Validate model performance:**

   using an external validation dataset as input in CSV format

Model description



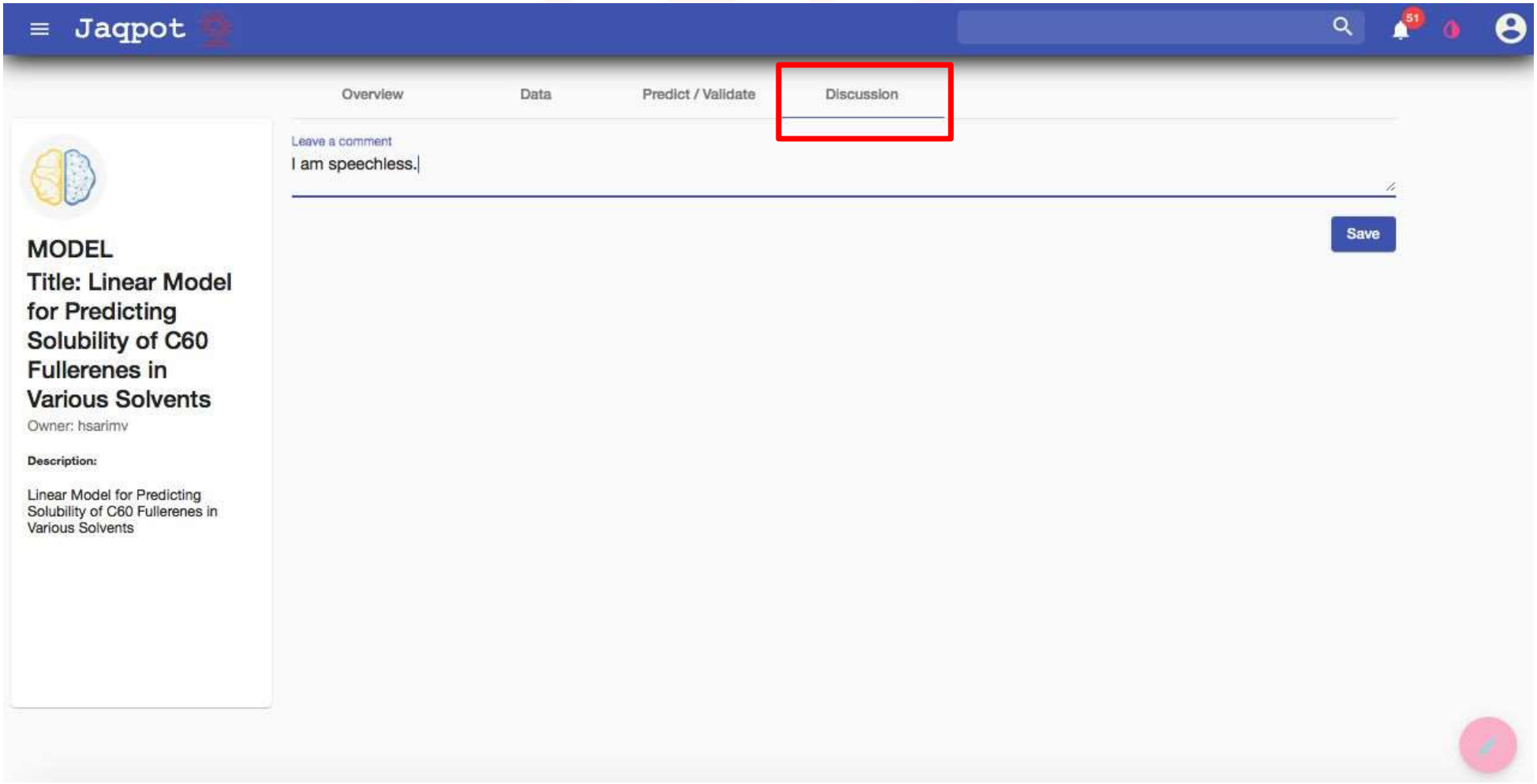


Information on the model can be provided in Markdown:
https://www.markdownguide.org/basic-syntax/

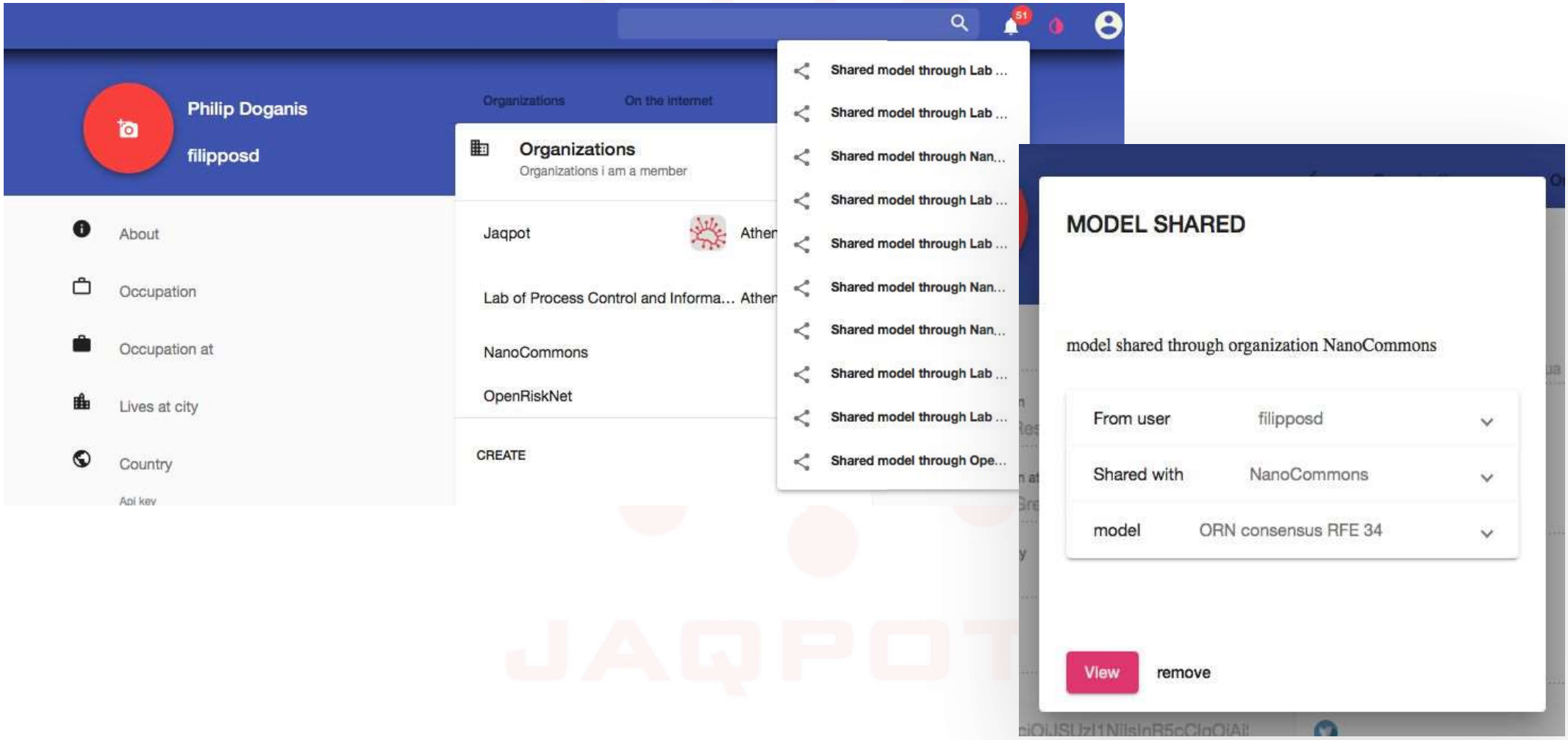
Feature documentation is a critical part of a model interpretation.
Model features can be documented with

- Description
- Units
- Ontological classes

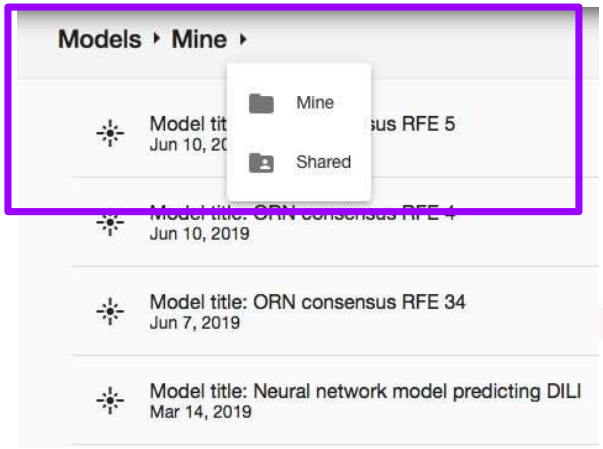
Jaqpot - Social network of models

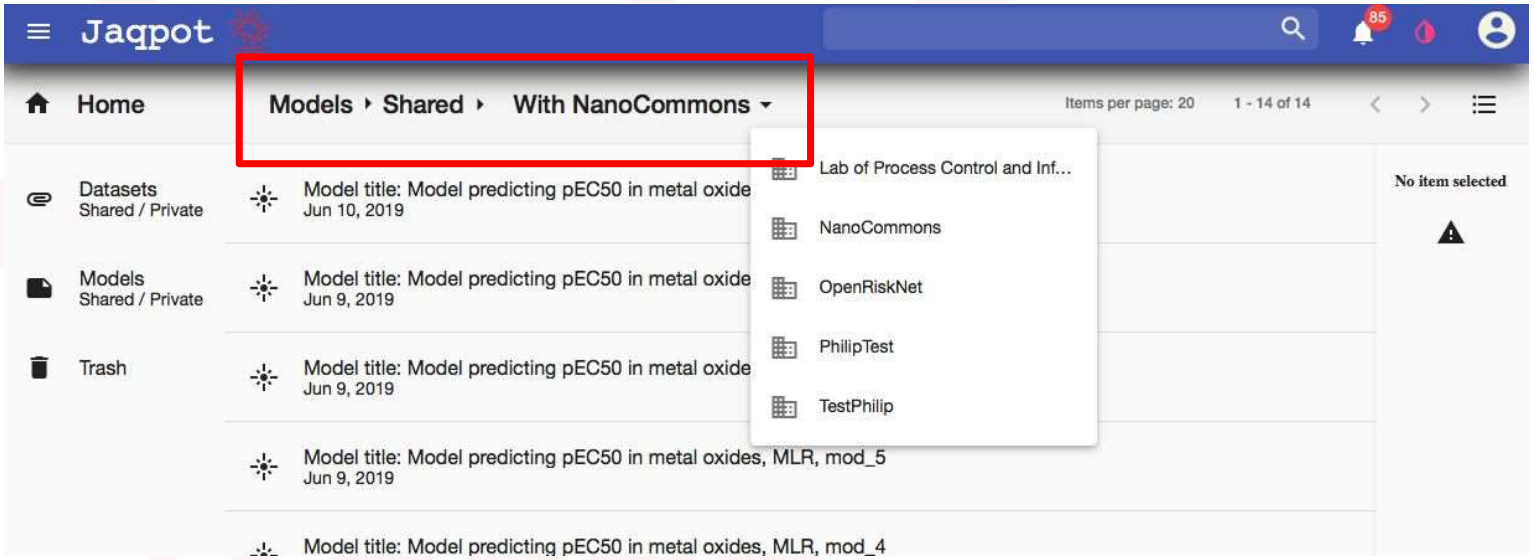


Jaqpot - Sharing of resources



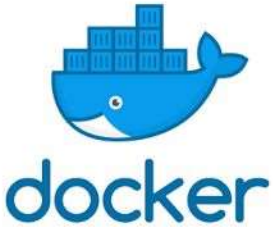
Jaqpot - Shared space - Models

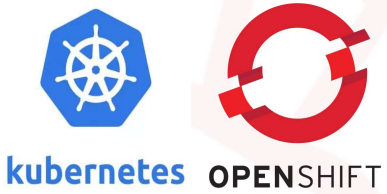




Meet the scalability requirements

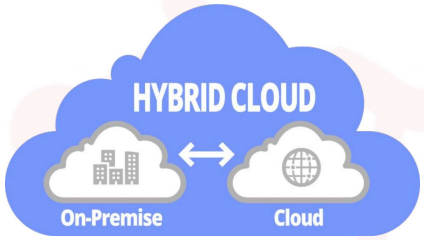
All Jaqpot services are running through containers. Consists of REST microservices that can be scaled to meet the requirements of the infrastructure.





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.

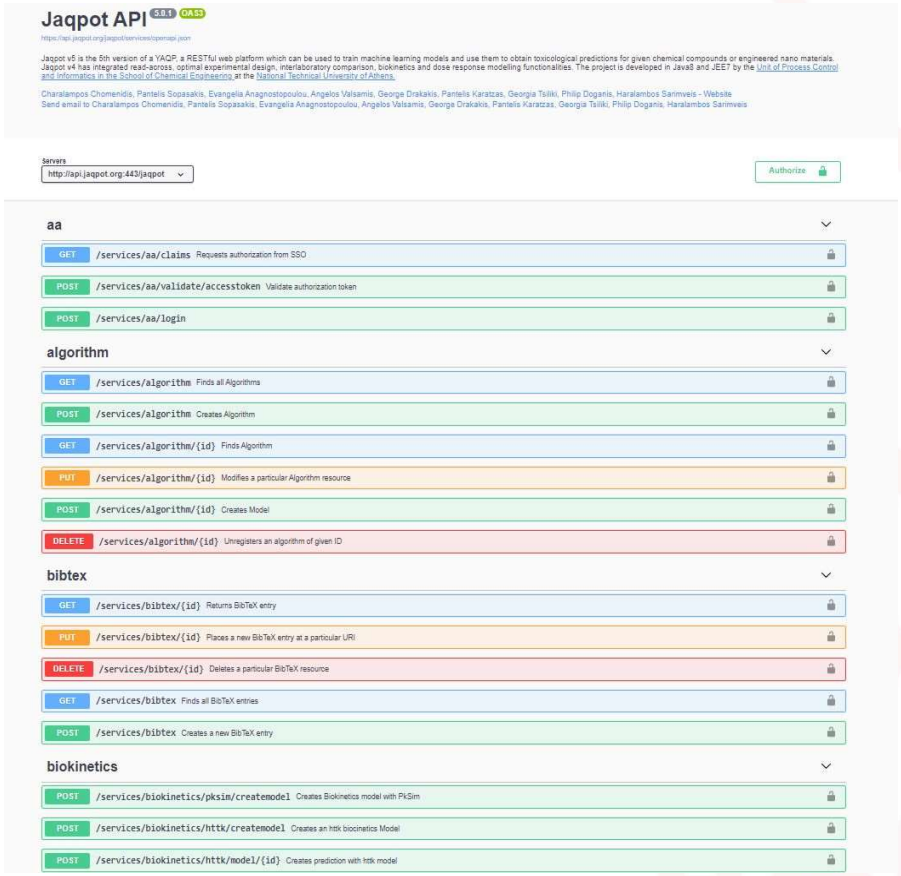


An open source software product to allow OpenID Connect single sign-on with Identity Management and Access Management aimed at modern applications and services.
Variety of user or identity providers can be integrated. From google to LDAP and Kerberos to meet the security needs of an organization

Right now integrated with

Under the stewardship of:

Integration through Application Programming Interfaces (APIs)

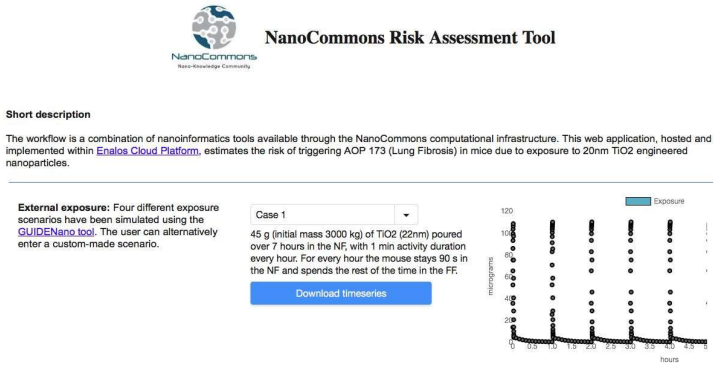


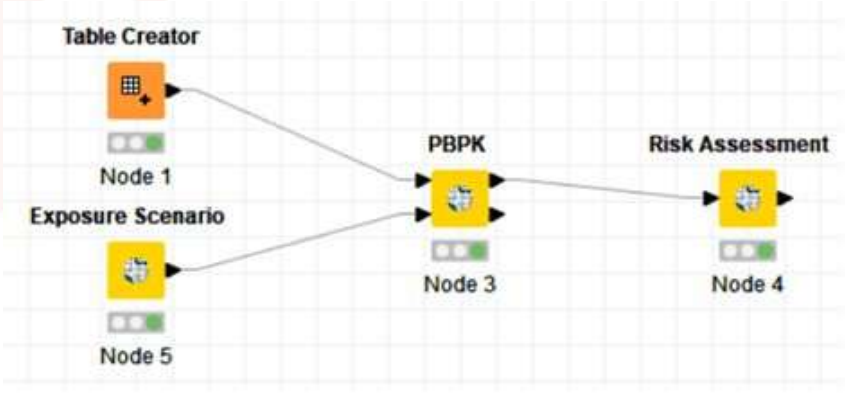
API clients

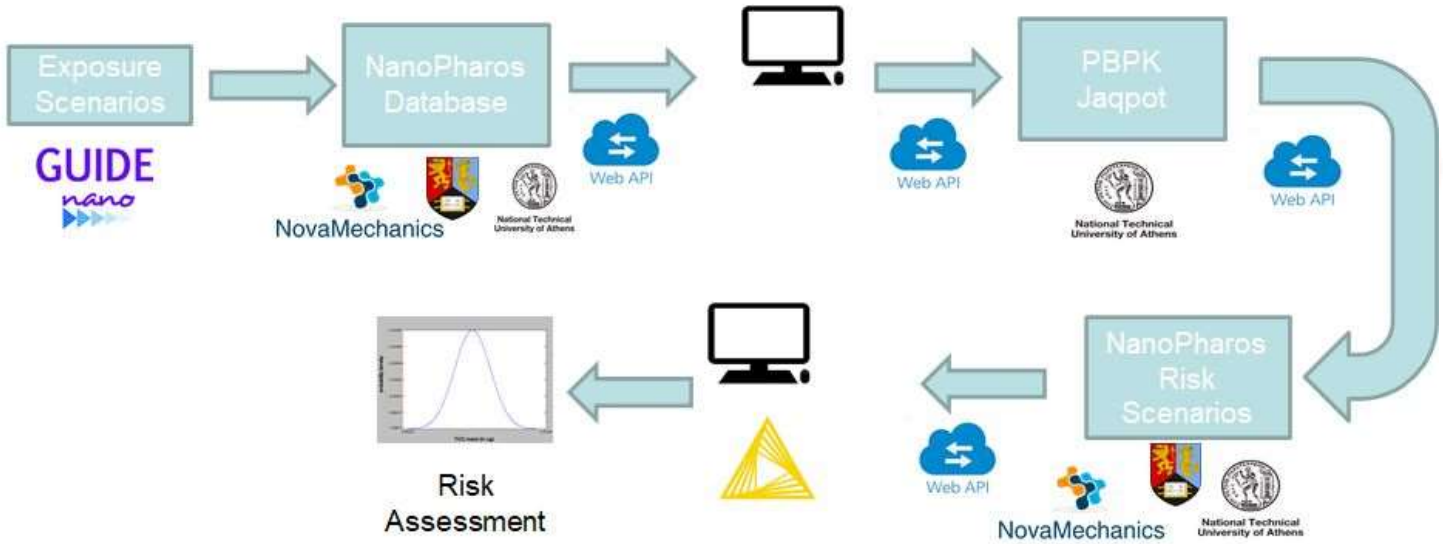
- Nuget Package (.NET): https://www.nuget.org/packages/JaqpotNet/1.0.0
- Go(lang) Package: https://github.com/euclia/gojaqpot
- Java: https://search.maven.org/artifact/xyz.euclia/jaqpotj/0.0.1/jar
- Javascript Package: https://www.npmjs.com/package/@euclia/jaqpot-client
- Python Package: https://pypi.org/project/jaqpotpy/

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

Jaqpot integrated applications and services: NanoCommons Risk Assessment Tool

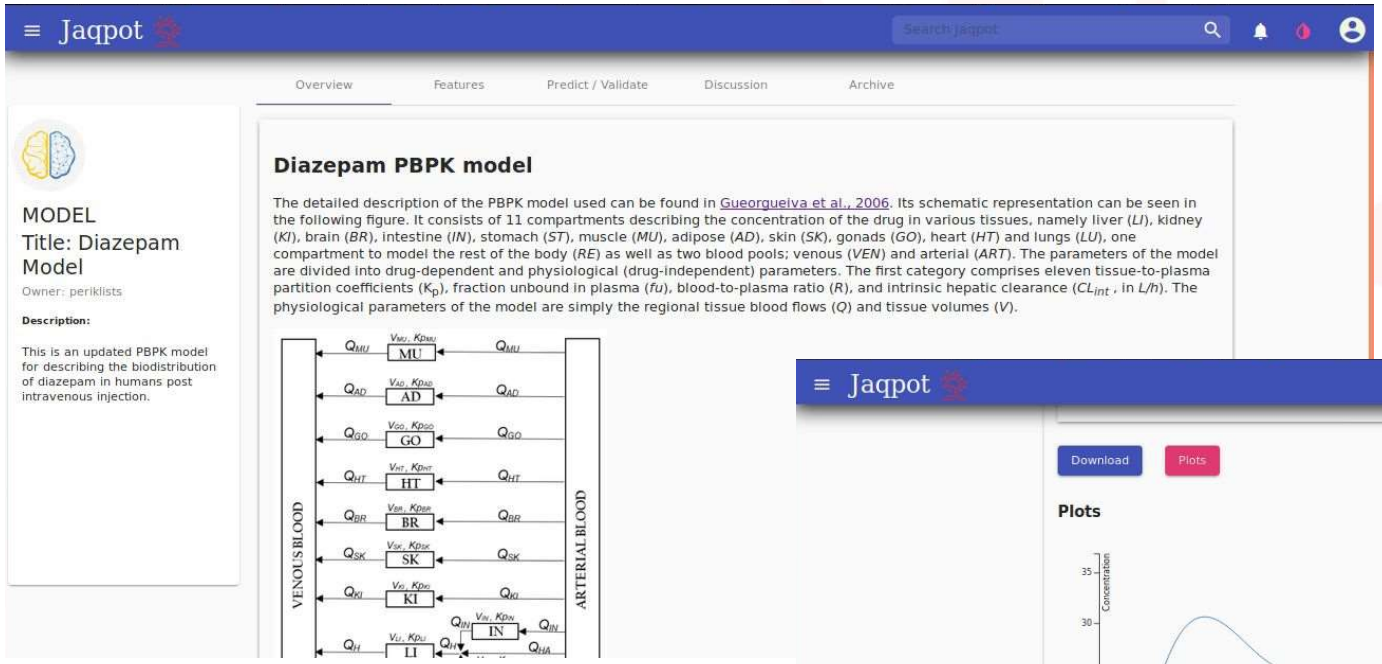


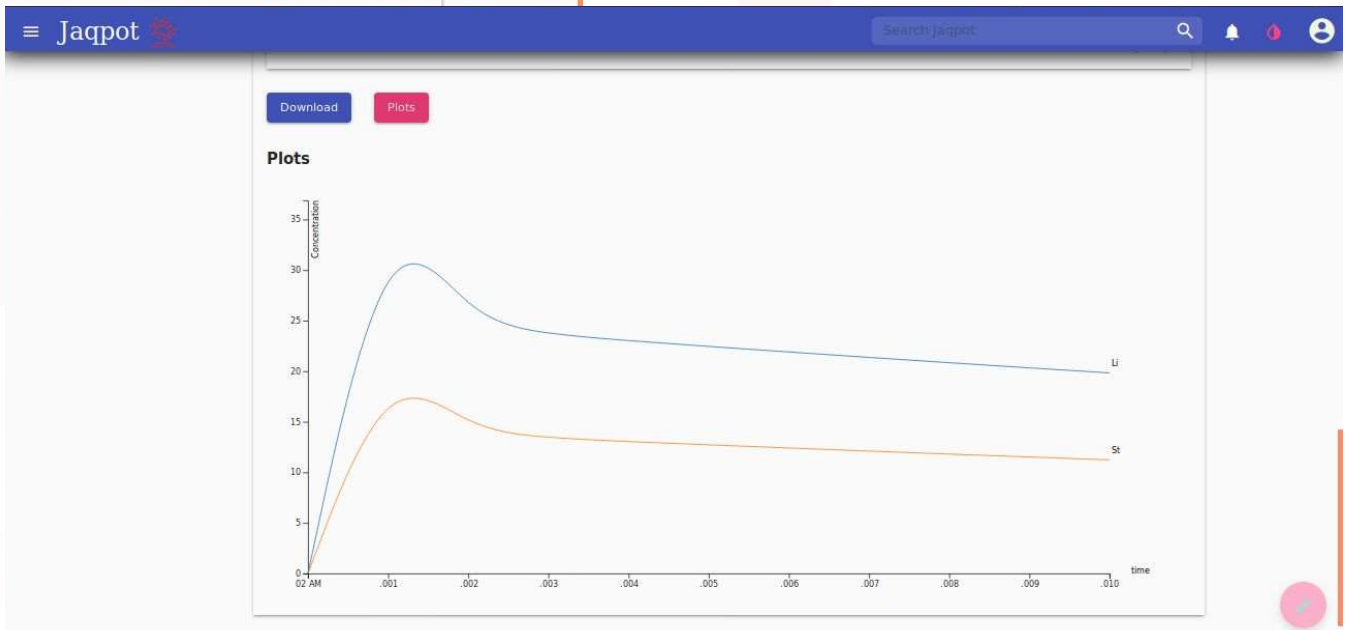




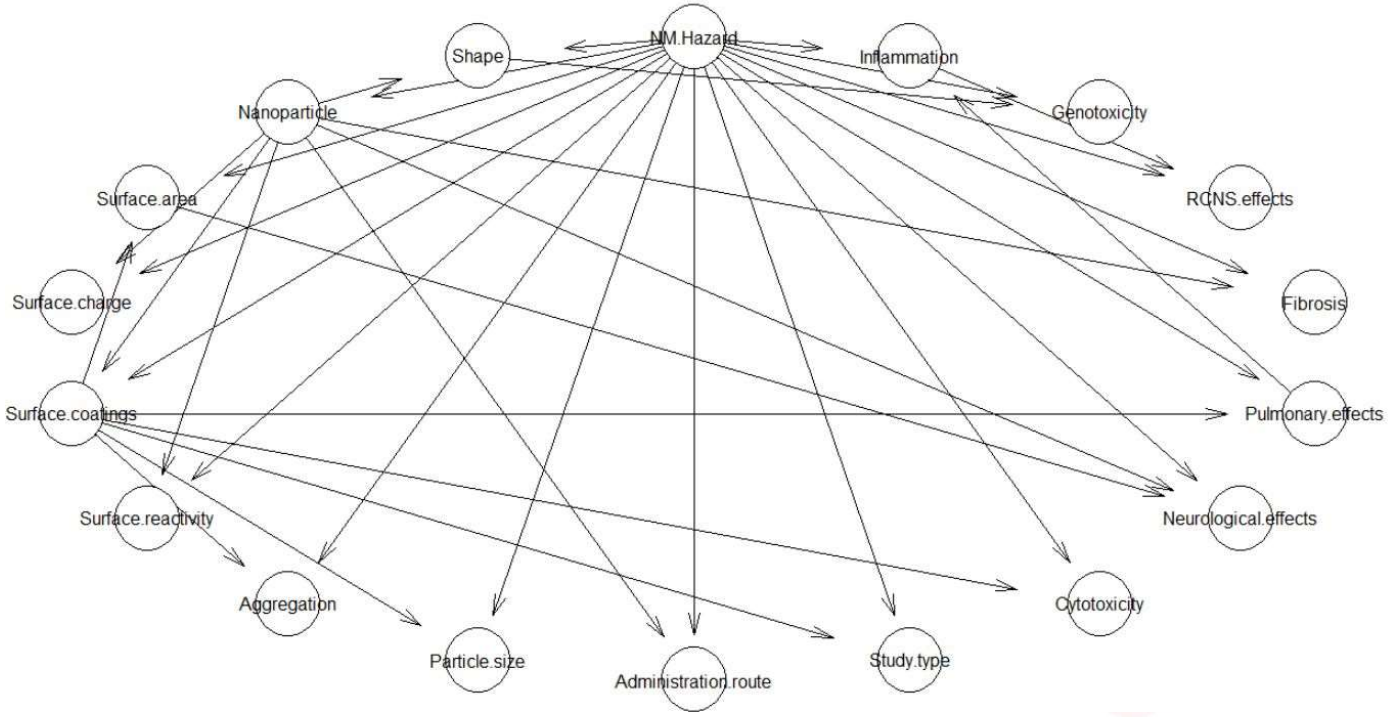
http://enaloscloud.novamechanics.com/nanocommons/exposure/

Support for PBPK models



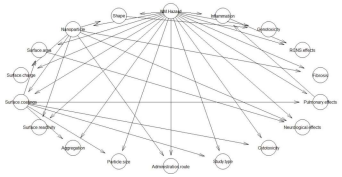


Support for safe-by-design product development strategies through integration of Bayesian network models



Conceptual diagram of properties with Bayesian networks

Support for safe-by-design product development strategies through integration of Bayesian network models



Conceptual diagram of properties with Bayesian networks

SdD use case:

Use the web service to design safe (low-hazard) NMs

Input values for the independent features

Sort

Study.type: NA (In vitro/In vivo)	Inflammation: None (None/Low/Medium/High)	Cytotoxicity: None (None/Low/Medium/High)	Genotoxicity: None (None/Low/Medium)
Neurological.effects: None (None/Low/Medium/High)	query node: Surface.coatings (One of the names of the nodes presented in the "Independent features" tab)	Pulmonary.effects: None (None/Low/Medium/High)	Administration.route: Inhalation (Inhalation/Injection /Intravenous/Oral)
NM.Hazard: None	Surface.area: 0-15	Surface.coatings: NA	Nanoparticle: TiO2

Id	probability	prediction.class	query.node
0	[0.996, 0, 0, 0, 0, 0, 0, 0, 0.004, 0, 0, 0]	[AHPP, Amine, Carbon, Carboxyl, Citrate, Hydroxyl, None, PVP, Silianes-aluminium, SO3-, Sulphate, Triethoxycapryl silane]	Surface.coatings

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Download

How Jaqpot can serve your needs

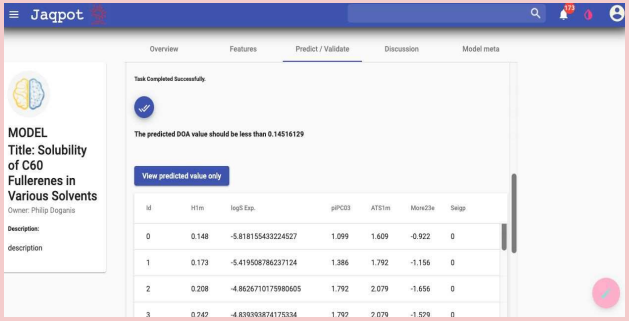
- **Publish your model** as web services
- Provide **ready-to-use implementations** of your models as supporting material to your publications
- **Collaborate** with your partners and colleagues
- **Share models** within your group, project or organisation and with the general public
- **Embed and integrate 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	Jaqpot 5 - User accounts Jaqpot 5: How to manage and use organisations Jaqpot 5: How to access and use an existing predictive model Jaqpot 5: How to deploy a predictive model using the jaqpotpy library Jaqpot 5: How to simulate biodistribution scenarios using custom PBPK models
Recent hackathons	Online QSAR Modelling Hackathon by Easy Access to Jaqpot https://zenodo.org/record/4683925#.YYIrsr1BxPM

NM dataset in Excel

No-installation
Jaqpotpy through python in Google Colab



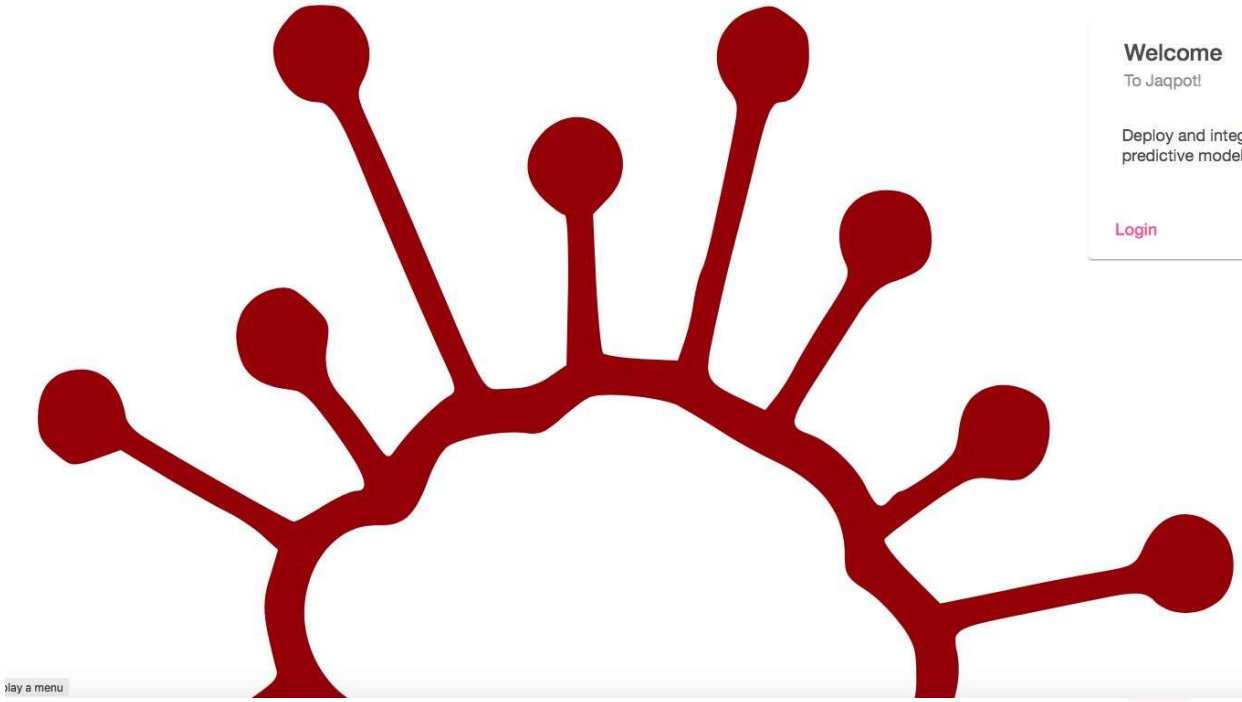
Online model and web service in Jaqpot

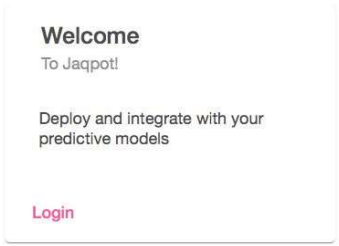
Jaqpot development team

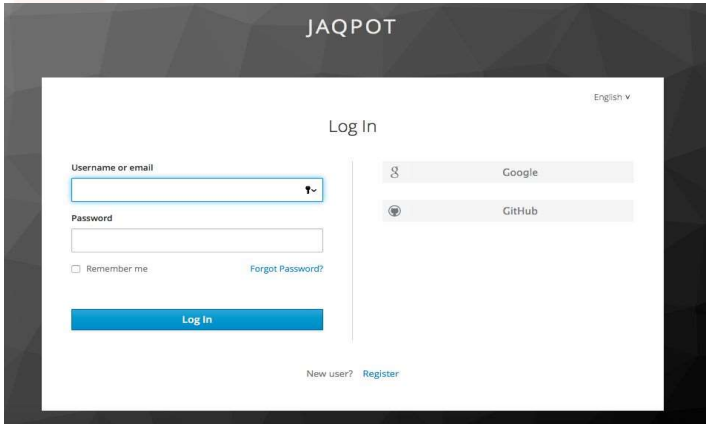
Sarimveis Haralambos	Professor, Unit of Process Control & Informatics, School of Chemical Engineering, National Technical University Of Athens, Greece
Doganis Philip	Senior Researcher, Laboratory & Teaching Staff
Karatzas Pantelis	Doctoral Researcher, Head Developer
Tsiros Periklis	Doctoral Researcher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

Thank you

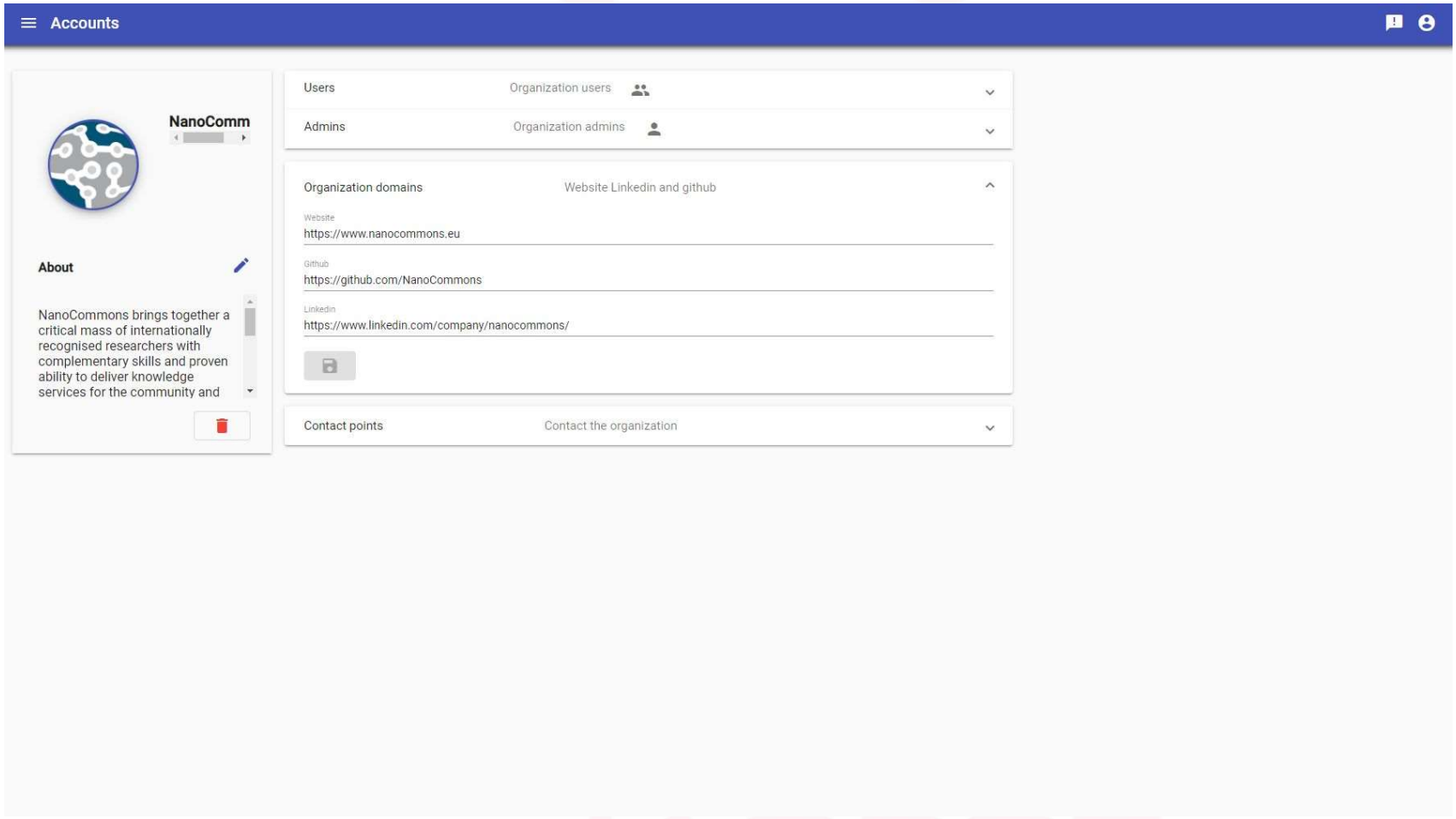
Jaqpot 5




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

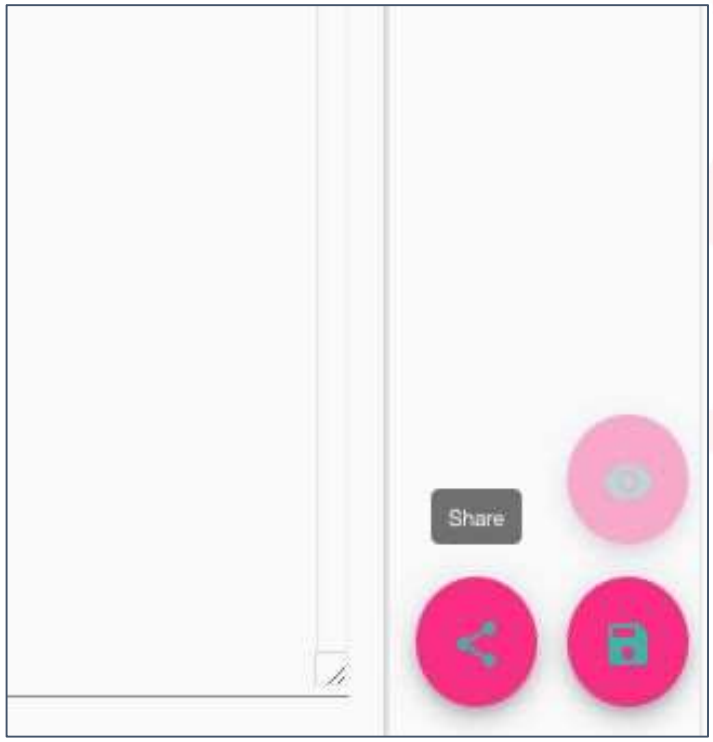
Jaqpot 5 - NanoCommons Organization page

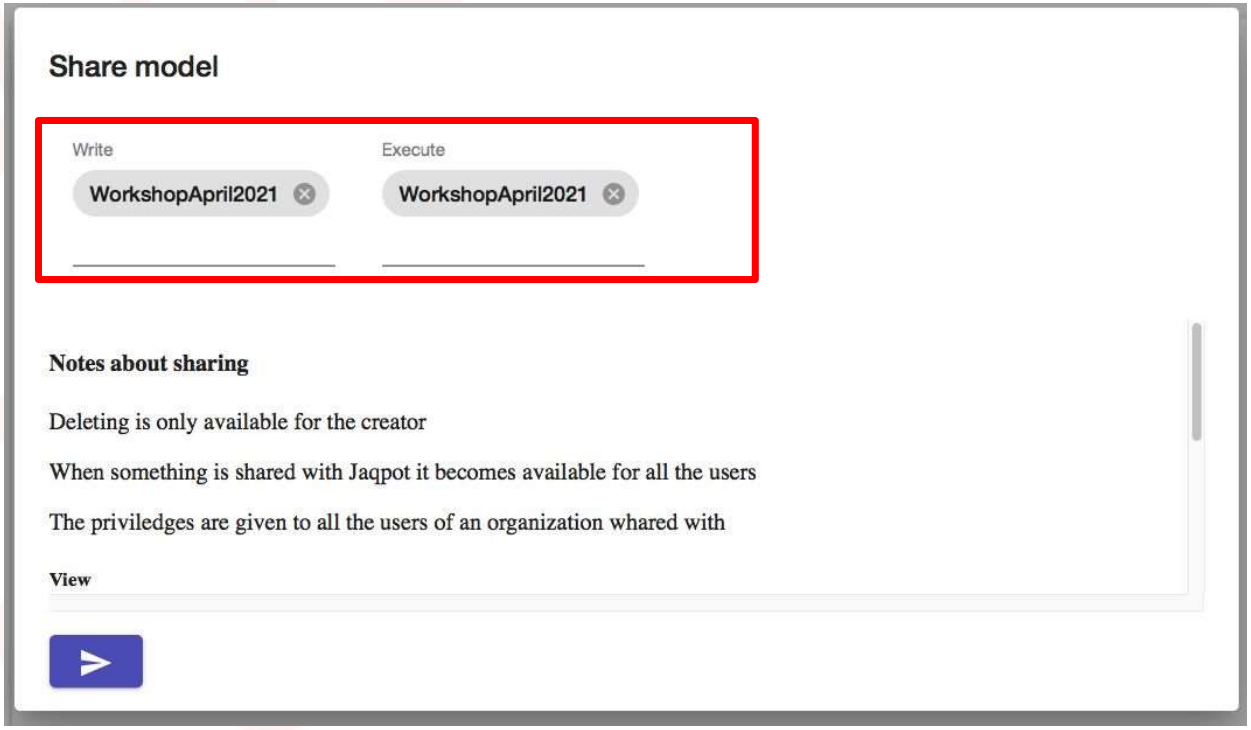


https://accounts.jaqpot.org/organization/joR8745jm3Q8AQrp

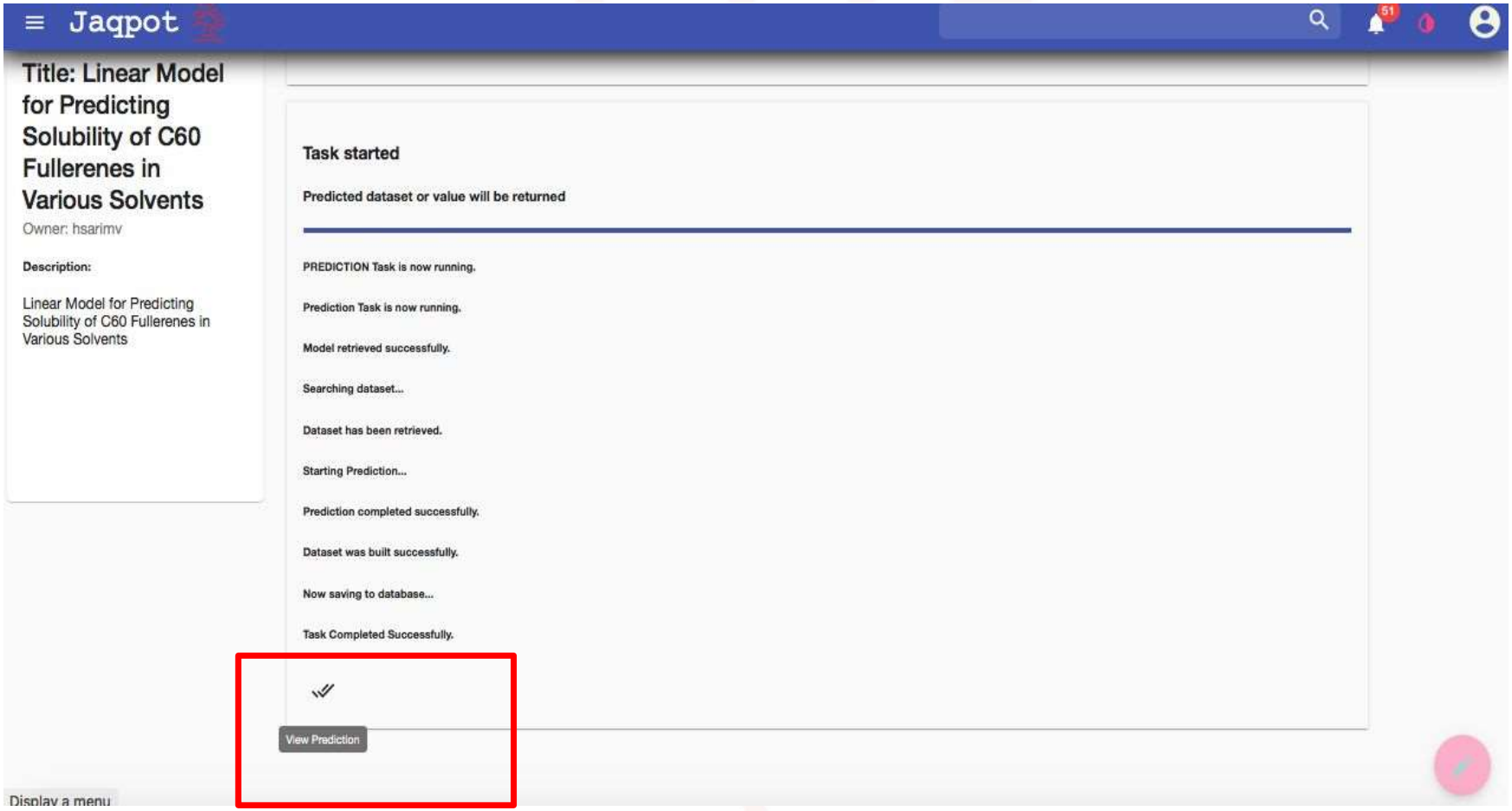
https://app.jaqpot.org/model/uxRBCMsV9lkSQT1Kw7km

Jaqpot 5 - Model page - Sharing





Jaqpot 5 - Model page - Predict tab



Jaqpot 5 - Predictions

Starting Prediction...

Prediction completed successfully.

Dataset was built successfully.

Now saving to database...

Task Completed Successfully.

View predicted value only

Id	Seigp	logS Exp.	ATS1m	More23e	H1m	piPC03
0	0	-4.186807760539802	2.197	-1.227	0.358	2.485

Items per page: 30 1 - 1 of 1

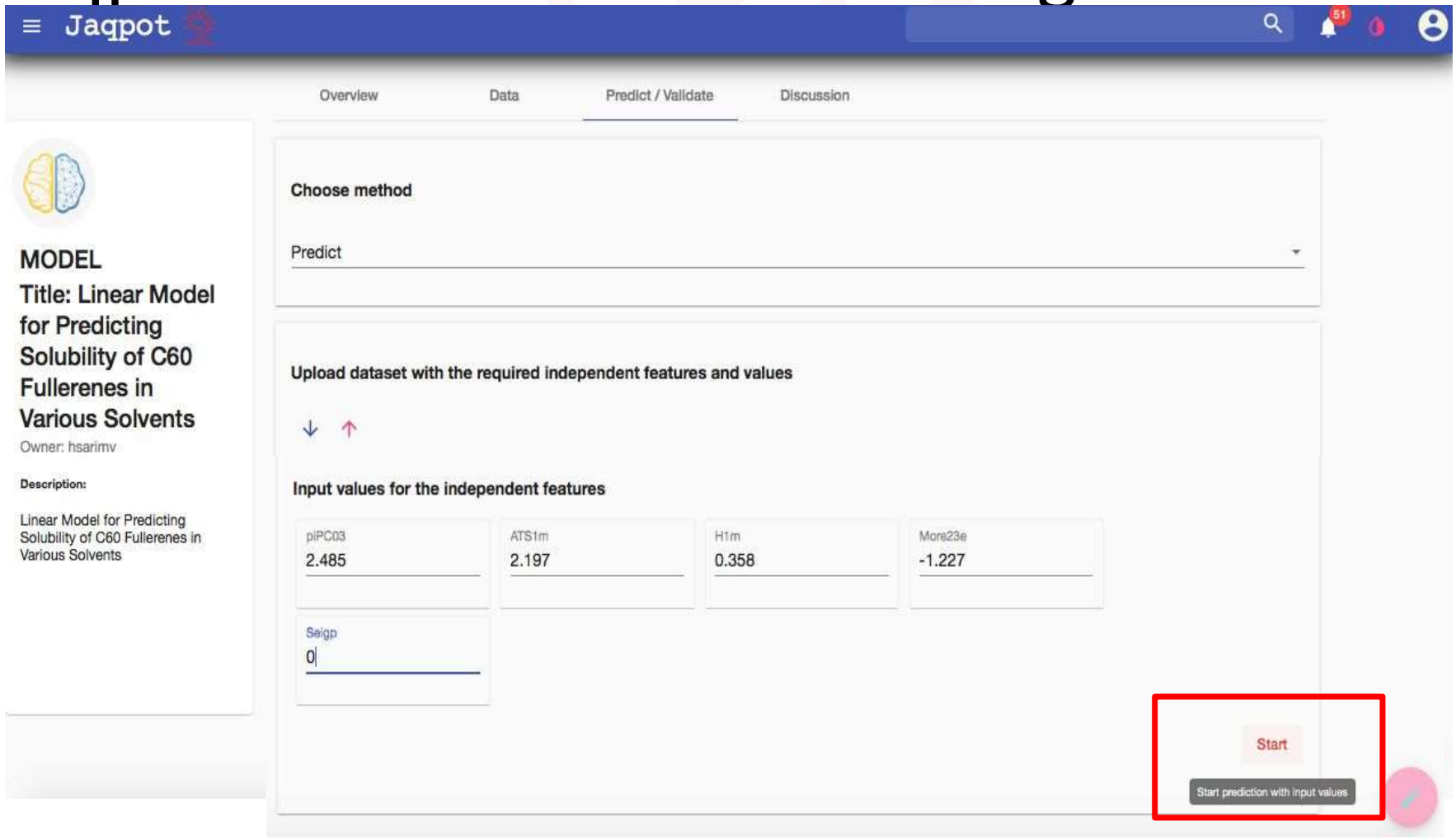
Download

Predictions can be downloaded in CSV format

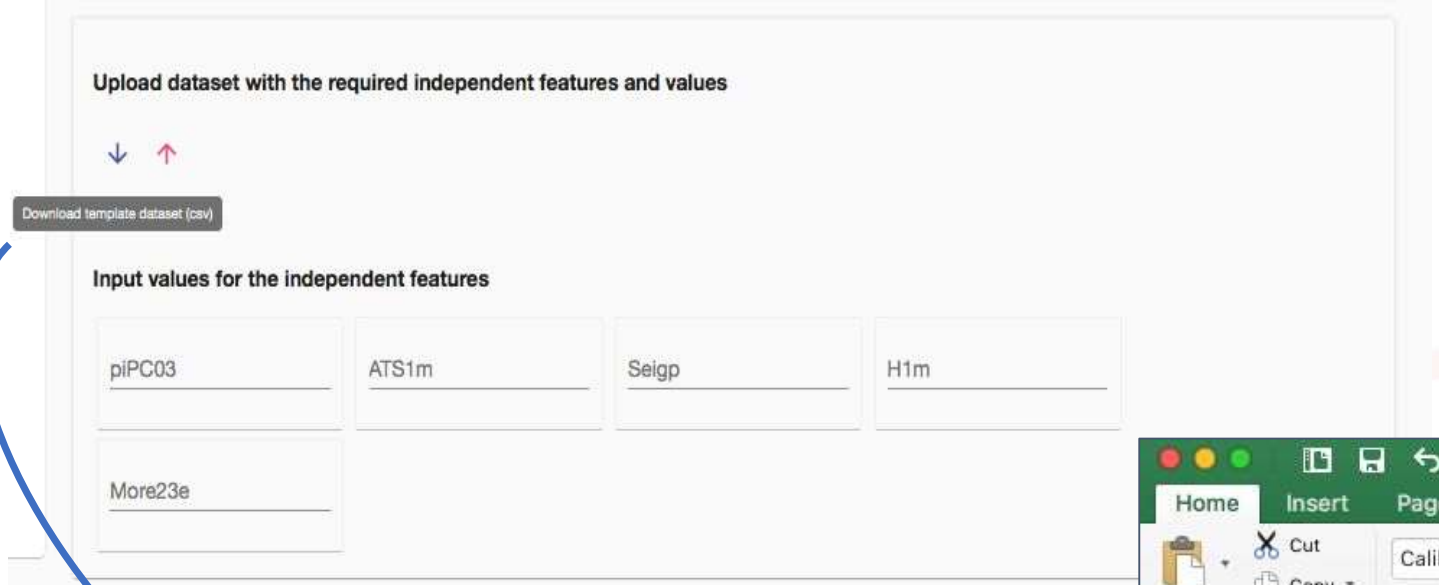
predicted_dataset

	A	B	C	D	E	F	G
1	My Report						
2							
3	**Id**	**Seigp**	**logS Exp.**	**ATS1m**	**More23e**	**H1m**	**piPC03**
4	0	0	-4,97982	1,792	-0,521	0,197	1,792
5	1	0	-3,96677	2,639	-3,047	0,263	2,485

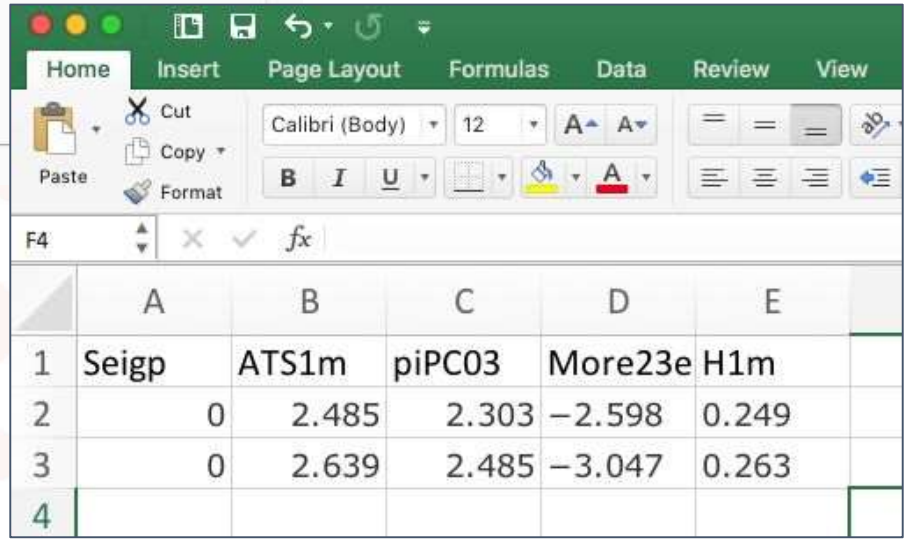
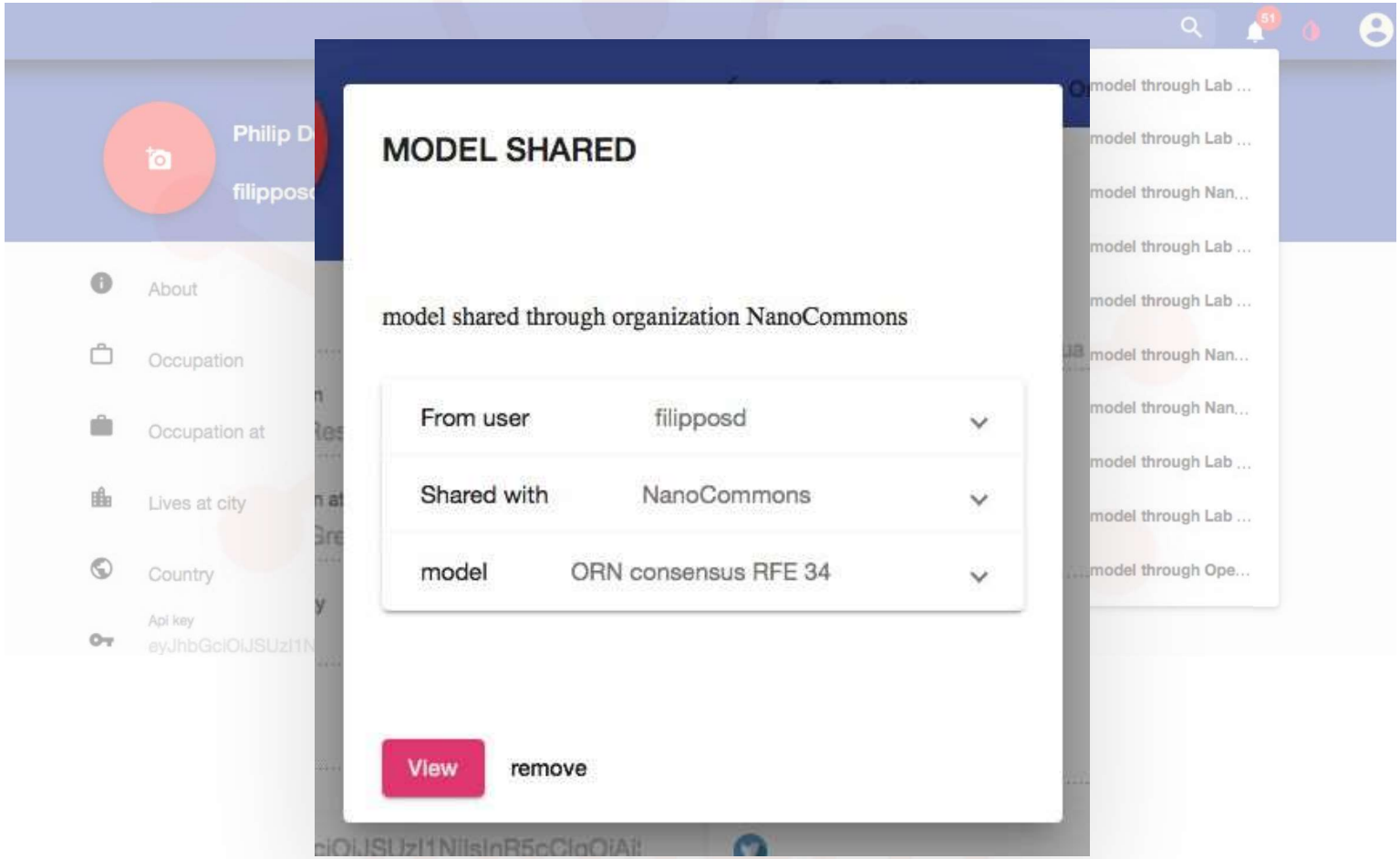
Jaqpot 5 - Predict tab - Entering values



Jaqpot 5 - Predict tab – Your data via template



Jaqpot automatically generates a template
for users to enter their data,
upload to Jaqpot
and get predictions.



Jaqpot 5 - Sharing notification