



UPCI

Unit of Process Control &
Informatics,
National Technical
University Of Athens, Greece



NanoCommons

Nano-Knowledge Community

Online Jaqpot Hackathon

*Take your research from the bench to the community
by making your models
available as a web service*

**Philip Doganis, Pantelis Karatzas, Irene Liampa, Dimitra-Danai Varsou, Periklis Tsiros,
Haralambos Sarimveis**

NanoCommons Workshop, 2020-06-03, #nanocommons

*This project has received funding from the European Union Horizon 2020 Programm (H2020)
under grant agreement no. 731032.*

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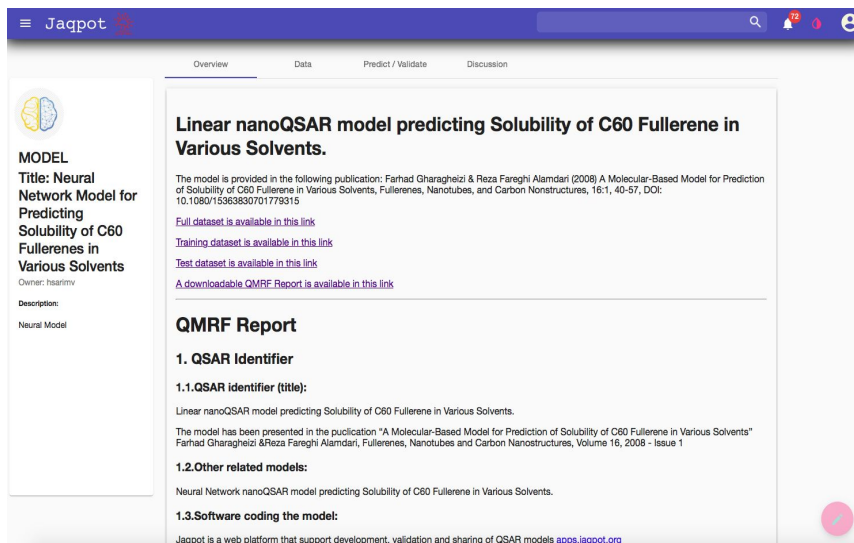
A place to

create **discuss**

share **use**

your models & datasets

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

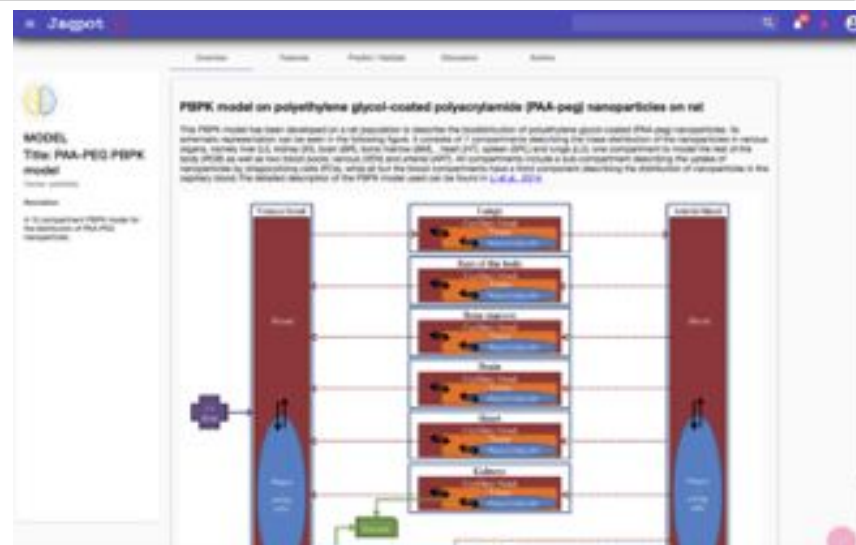


The screenshot displays the Jaqpot web application interface. The top navigation bar includes 'Overview', 'Data', 'Predict / Validate', and 'Discussion'. The main content area is titled 'Linear nanoQSAR model predicting Solubility of C60 Fullerene in Various Solvents'. It provides a description of the model, its title, and links to datasets and a QMRF report. The QMRF report section includes a '1. QSAR Identifier' and a '1.1.QSAR identifier (title):' which states the model's purpose and citation.

MODEL
Title: Neural Network Model for Predicting Solubility of C60 Fullerenes in Various Solvents
Owner: haarmiv
Description: Neural Model

Linear nanoQSAR model predicting Solubility of C60 Fullerene in Various Solvents.
The model is provided 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
[Full dataset is available in this link](#)
[Training dataset is available in this link](#)
[Test dataset is available in this link](#)
[A downloadable QMRF Report is available in this link](#)

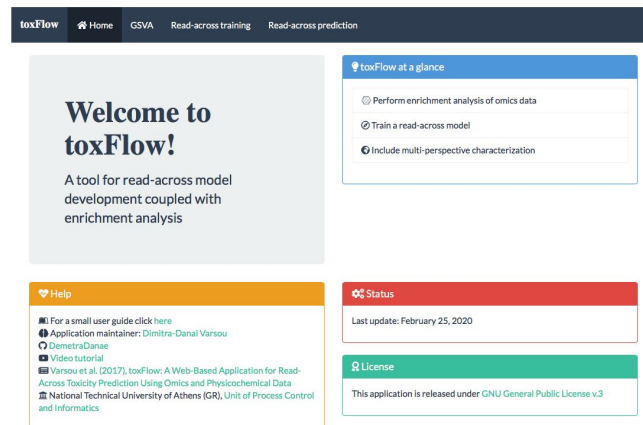
QMRF Report
1. QSAR Identifier
1.1.QSAR identifier (title):
Linear nanoQSAR model predicting Solubility of C60 Fullerene in Various Solvents.
The model has been presented in the publication "A Molecular-Based Model for Prediction of Solubility of C60 Fullerene in Various Solvents" Farhad Gharagheizi & Reza Fareghi Alamdari, Fullerenes, Nanotubes and Carbon Nanostructures, Volume 16, 2008 - Issue 1
1.2.Other related models:
Neural Network nanoQSAR model predicting Solubility of C60 Fullerene in Various Solvents.
1.3.Software coding the model:
Jaqpot is a web platform that support development, validation and sharing of QSAR models apps.jaqpot.org



<https://app.jaqpot.org/>



<https://nanoimage.jaqpot.org>



The screenshot displays the toxFlow web application interface. The top navigation bar includes 'toxFlow', 'Home', 'GSA', 'Read-across training', and 'Read-across prediction'. The main content area is titled 'Welcome to toxFlow!' and includes a description of the tool. On the right, there is a 'toxFlow at a glance' section with three bullet points: 'Perform enrichment analysis of omics data', 'Train a read-across model', and 'Include multi-perspective characterization'. At the bottom, there is a 'Help' section with links to a user guide, application maintainer, Demetrius Danie, video tutorial, and a citation. A 'Status' section shows the last update date as February 25, 2020. A 'License' section states that the application is released under GNU General Public License v3.

Welcome to toxFlow!
A tool for read-across model development coupled with enrichment analysis

toxFlow at a glance
● Perform enrichment analysis of omics data
● Train a read-across model
● Include multi-perspective characterization

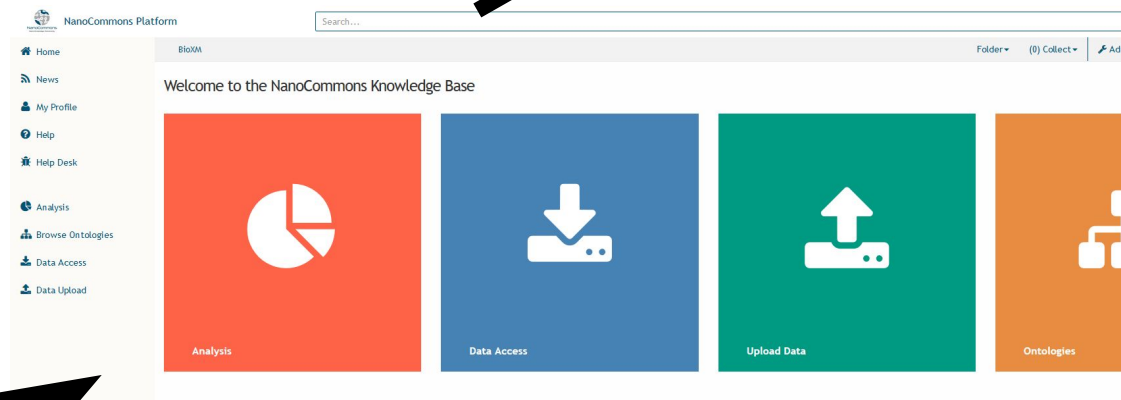
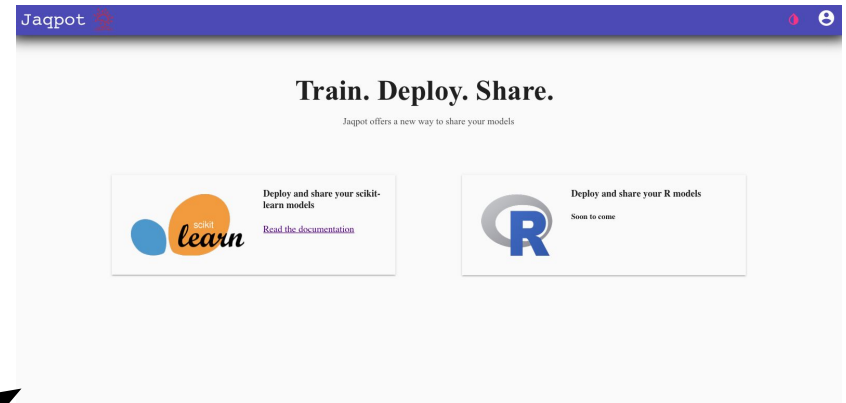
Help
● For a small user guide click [here](#)
● Application maintainer: [Dimitra-Danaï Varsou](#)
● Demetrius Danie
● Video tutorial
● Varsou et al. (2017), toxFlow: A Web-Based Application for Read-Across Toxicity Prediction Using Omics and Physicochemical Data
● National Technical University of Athens (NTUA), Unit of Process Control and Informatics

Status
Last update: February 25, 2020

License
This application is released under GNU General Public License v3

toxflow.jaqpot.org

NanoCommons KnowledgeBase & Jaqpot



Original Databases

NanoMILE/NanoFASE/NanoReg/eNanoMapper

Infrastructure

Docker is used to run software packages called "**containers**". Containers are isolated from each other and bundle their own application, tools, **libraries** and configuration files;



An open-source system for automating deployment, scaling, and management of containerized applications

OpenShift is a multifaceted, open source container application platform from Red Hat Inc. for the development, deployment and management of applications.





An open source software product to allow OpenID Connect single sign-on with Identity Management and Access Management aimed at modern applications and services.

Under the stewardship of:



Jaqpot 4


 Jaqpot [Sign in](#) [Create Account](#)



Create Dataset

Select substances, properties and descriptors.

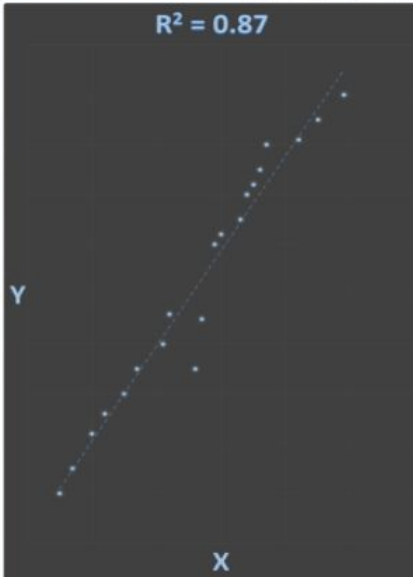
[Create Dataset](#)



NanoQSAR validation schemes

Validate model using different validation options.

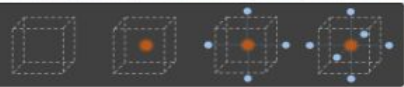
[Cross](#) [Data Split](#) [External](#)



NanoQSAR modelling

Train a model or make a prediction.


[Train](#) [Predict](#)



Optimal Experimental Design

Optimise the design of the experiments.

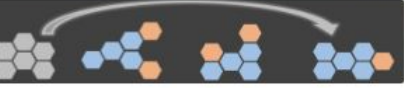
[Iterative Experimental Design](#) [Factorial Design](#)



Interlaboratory Comparison

Perform statistical laboratory quality control.

[Interlaboratory Proficiency Testing](#)



Read Across

Make a prediction based on the read across method on an existing dataset.

[Train](#) [Predict](#)



This project has received funding from the European Union's Horizon Europe Programme

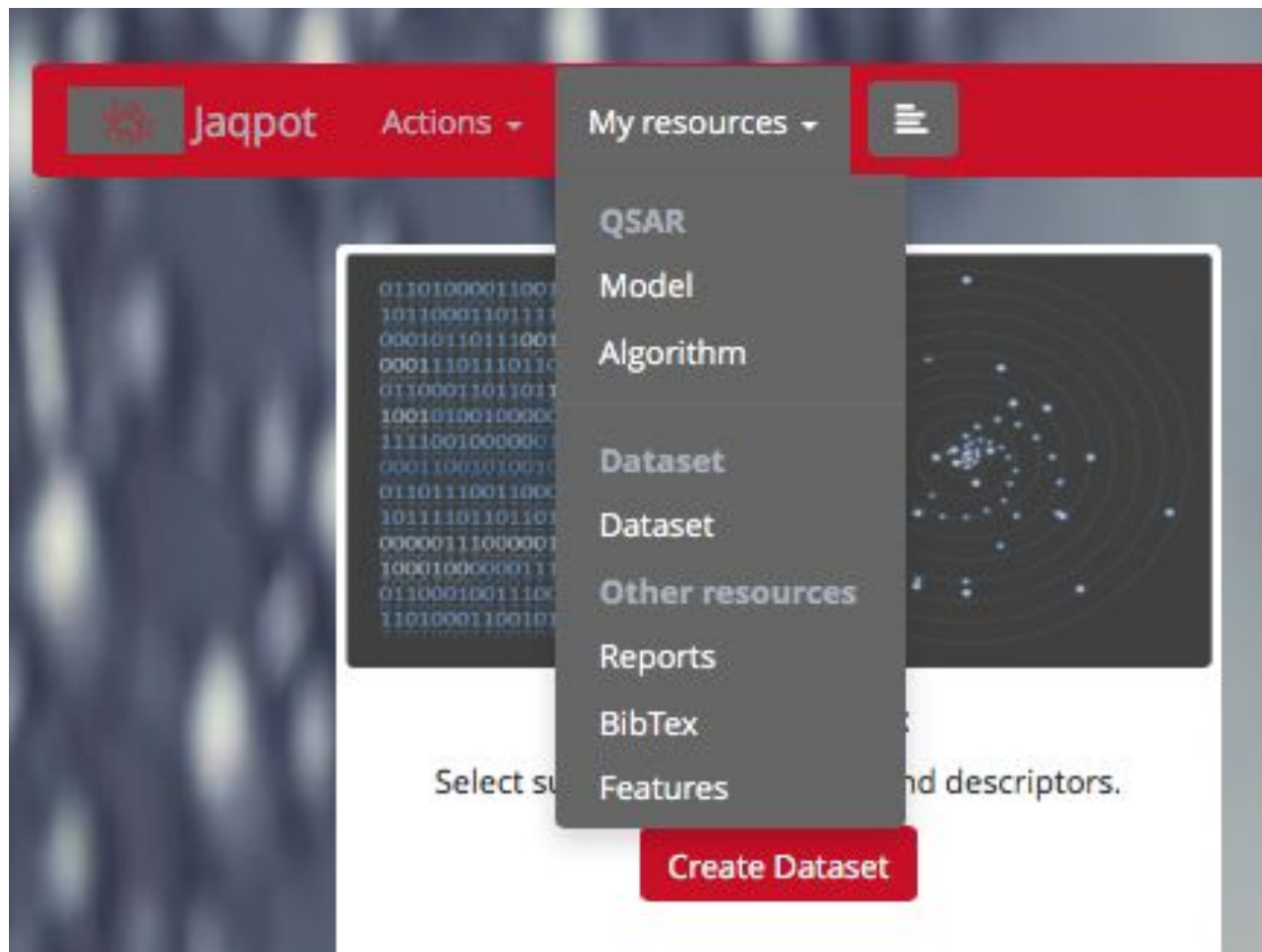
[SOURCE](#) [DOCUMENTATION](#) [ISSUES](#)





Unit of Process Control and Informatics
School of Chemical Engineering
National Technical University of Athens


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My resources



Model training - Choice of algorithm

 Jaqpot Actions ▾ My resources ▾ 

Welcome back, NanoCommons 



Train model

Choose Algorithm

Regression

- ☐ MLR - Weka (multi-response linear regression implemented in Java-WEKA)
- ☐ SVM - Weka (LibSVM, Support vector machines implemented in Java-WEKA)
- ☐ PLS - Weka (Partial Least Squares implemented in Java-WEKA)
- ☒ Linear Regression (Implemented in Python-Scikit Learn)
- ☐ Lasso Regression (Implemented in Python-Scikit Learn)
- ☐ PLS - with VIP scores (Implemented in Python)
- ☐ Readacross
- ☐ Linear Model (implemented in R - base library)
- ☐ Gradient Boosting (Implemented in Python-Scikit Learn)
- ☐ Random Forest (Implemented in Python-Scikit Learn)
- ☐ Multi-layer Perceptron (Implemented in Python-Scikit Learn)

Classification

- ☐ SVM - Weka (LibSVM) Implementation
- ☐ Id3 - with MCI (Implemented in Python-Scikit-Learn)
- ☐ ID3 Decision Tree (Implemented in Python-Scikit Learn)
- ☐ CMI Decision Tree (Implemented in Python-Scikit Learn)
- ☐ Generalised Naive Bayes (Implemented in Python-Scikit Learn)
- ☐ Multinomial Naive Bayes (Implemented in Python-Scikit Learn)
- ☐ Bernoulli Naive Bayes (Implemented in Python-Scikit Learn)
- ☐ Random Forest (Implemented in Python-Scikit Learn)
- ☐ Multi-layer Perceptron (Implemented in Python-Scikit Learn)
- ☐ Gradient Boosting (Implemented in Python-Scikit Learn)

Previous 1 Next

Next

Ontological annotation of algorithms

	Category / URI	Description	OpenTox Ontological Classes
	Preparation-additional		
1	http://iaqpot.org:8080/iaqpot/services/algorithm/scaling	Scaling	"ot:Algorithm", "ot:Scaling", "ot:Transformation"
	WEKA (Java)		
1	http://iaqpot.org:8080/iaqpot/services/algorithm/weka-mlr	MLR - Weka (multi-response linear regression implemented in Java-WEKA)	"ot:Algorithm", "ot:Regression", "ot:SupervisedLearning"
	Python		
1	http://iaqpot.org:8080/iaqpot/services/algorithm/python-id3-mci	Id3 - with MCI (Implemented in Python-Scikit-Learn)	"ot:Algorithm", "ot:Classification", "ot:SupervisedLearning"

OpenTox Algorithm Ontology <http://old.opentox.org/data/documents/development/RDF%20files/AlgorithmTypes>

Model training - Algorithm parameters

Jaqpot

Actions

My resources

Welcome back, NanoCommons

Algorithm

Title: python-lm

Title: Linear Regression (Implemented In Python-Scikit Learn)

Fill in the title and description of the produced model

Model name: Linear Model for C60 Fullerene Sol

Model description:

The model is provided 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

Select variables :

Select Input variable(s) and endpoint

Select PMML

Upload PMML file

Select endpoint only (all other variables will be used as input variables)

Select variable(s) and endpoint:

Input variable(s)

Endpoint

Select All

Seigp

Solvents

logS Exp_

H1m

More23e

ATS1m

piPC03

Seigp

Solvents

logS Exp_

H1m

More23e

ATS1m

piPC03

Select scaling method:


Scaling between zero and one

Select domain of applicability method:

Leverage method

Train

Model webpage

 Jaqpote Actions My resources

Welcome back, NanoCommons

Model: #72GEEEmGhhavY00n7O209

✓ Validate me ▶ Predict ⛔ Delete

Title: Linear Model for C60 Fullerene Solubility

Description: The model is provided 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

Transformations <http://jaqpote.org:8080/jaqpote/services/model/FqeE4mX2AC1hnXgVeUBr> <http://jaqpote.org:8080/jaqpote/services/model/4tObjaWKrls5eljTkh-y>

Doa: <http://jaqpote.org:8080/jaqpote/services/model/3id3kU4efV04Ru9puuKo>

Algorithm: python-lm

Features:

Required Features

Dependent Features

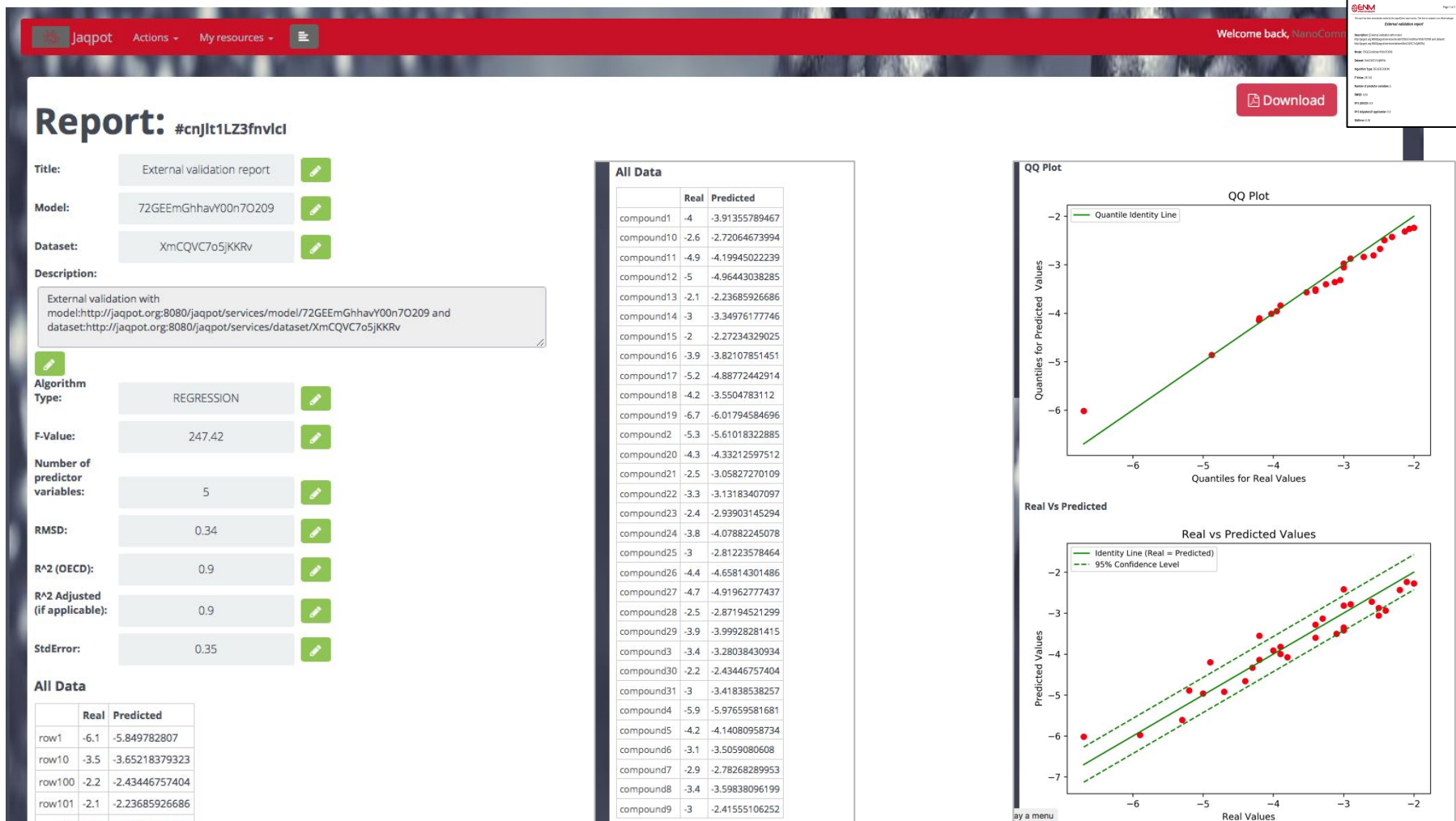
Independent Features

Predicted Features

Representation: PMML

URI of model: http://www.jaqpote.org/m_detail?name=72GEEEmGhhavY00n7O209

Validation report



<http://www.jaqpot.org/report?name=cnJlt1LZ3fnvIcl>

QPRF report

The QPRF (QSAR prediction reporting format) report generated by Jaqpot contains all the fields required by the OECD guidelines, namely:

- Substance
 - Contains information such as CAS and EC numbers, SMILES, InChi, etc.
- General
 - Information such as date and creator name and email.
- Prediction
 - Biological endpoint, variables, model used, DoA, etc
- Adequacy
 - Optional field, containing regulatory purpose, conclusion etc

Jaqpot Actions My resources

Welcome back, [UserComments](#)

[Download](#)

Report: #ND0zm2stPTRUQSu

Title:

Description:

Date:

Disclaimer and Instructions:

Time:

Title:

Version:

1. Substance

Title	Value
1.1 CAS number	Report the CAS number.
1.2 EC number	Report the EC number.
1.3 Chemical name	Report the chemical names (IUPAC and CAS names).
1.4 Structural formula	Report the structural formula.
1.5 General Structure codes	Report available structural information for the substance, including the structure code used to run the model. If you used a SMILES or InChI code, report the code in the corresponding field below. If you have used any another format (e.g. mol file), please include the corresponding structural representation as supporting information.
1.5 a. SMILES	Report the SMILES of the substance (indicate if this is the one used for the model prediction).
1.5 b. InChI	Report the InChI code of the substance (indicate if this is the one used for the model prediction).
1.5 c. Other structural representation	Indicate if another structural representation was used to generate the prediction. Indicate whether this information is included as supporting information. Example: 'mol file used and included in the supporting information'.
1.5 d. Stereochemical features	Indicate whether the substance is a stereo-isomer and consequently may have properties that depend on the orientation of its atoms in space. Identify the stereochemical features that may affect the reliability of predictions for the substance, e.g. cis-trans isomerism, chiral centres. Are these features encoded in the structural representations mentioned above?
General Instructions	This section is aimed at defining the substance for which the (Q)SAR prediction is made.

2. General information

Title	Value
Date of QPRF	14/05/2019

play a menu

PCA of Query Instance vs. Training Dataset

• Original Values • QPRF Query Values

3D Projection of Datapoints

Read Across



- Users select **distance metric** and a **threshold** between 0 and 1 (the closest to 0 the strictest) used to assess nanoparticle similarity.
- Optionally select a method to calculate the **prediction confidence level** (Currently “Nearest Neighbour Confidence”)

Predicted values of dataset #ghh5UgHv2ZuOjlsZHA

o

Search: <input type="text"/>		
Compounds	https://apps.lisacon.su.se/nanoindesl/property/TOX/UNKNOWN_TOXICITY_SECTION1.qg2Hyxstomw3BUD66CFE4925A6F400A3AD8CA731B32E049A6803e4e4291b42-387a-9965-dea3b91e0ba-mutation	https://apps.lisacon.su.se/nanoindesl/property/TOX/UNKNOWN_TOXICITY_SECTION1.qg2Hyxstomw3BUD66CFE4925A6F400A3AD8CA731B32E049A6803e4e4291b42-387a-9965-dea3b91e0ba-confidence
G15.AC_1	-5.42	0.93
G15.AHT_1	-1.01	1.0
G15.Asn-SH_1	-5.49	0.93
G15.AUT_1	-1.32	1.0
G15.CIT_1	-5.64	0.93
G15.CTAB_1	-5.86	1.0
G15.DDT@CTAB_1	-4.75	0.95

Jaqpot 5

Jaqpot 5

Train. Deploy. Share.

Jaqpot offers a new way to share your models



Deploy and share your
scikit-learn models

[Read the documentation](#)



Deploy and share your R models

Soon to come

Login!!



Jaqpot 5 - Login

JAQPOT

English ▾

Log In


Username or email


Password

☐ Remember me

[Forgot Password?](#)

Log In

 Google

 GitHub

New user? [Register](#)

Jaqpot 5 - Shared space - Models

The screenshot displays the Jaqpot 5 web interface. The top navigation bar includes the Jaqpot logo, a search bar, a notification bell with 85 alerts, and a user profile icon. The left sidebar shows navigation options: Home, Datasets (Shared / Private), Models (Shared / Private), and Trash. The main content area is titled 'Models' and shows a list of models. A red box highlights the 'Models > Shared > With NanoCommons' breadcrumb path. A dropdown menu is open, showing a list of models: 'Lab of Process Control and Inf...', 'NanoCommons', 'OpenRiskNet', 'PhilipTest', and 'TestPhilip'. A purple box highlights the 'Models > Mine' breadcrumb path. A dropdown menu is open, showing a list of models: 'Mine' and 'Shared'. The right sidebar shows 'No item selected' and a warning icon.

Jaqpot

Home

Models > Shared > With NanoCommons

Items per page: 20 1 - 14 of 14

Datasets Shared / Private

Models Shared / Private

Trash

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

Lab of Process Control and Inf...

NanoCommons

OpenRiskNet

PhilipTest

TestPhilip

No item selected

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

Jaqpote 5 - Model page


Jaqpote

Overview
Data
Predict / Validate
Discussion



MODEL
Title: Neural Network Model for Predicting Solubility of C60 Fullerenes in Various Solvents
Owner: hsarimv
Description:
Neural Model

Linear nanoQSAR model predicting Solubility of C60 Fullerene in Various Solvents.

The model is provided 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

[Full dataset is available in this link](#)

[Training dataset is available in this link](#)

[Test dataset is available in this link](#)

[A downloadable QMRF Report is available in this link](#)

QMRF Report

1. QSAR Identifier

1.1.QSAR identifier (title):

Linear nanoQSAR model predicting Solubility of C60 Fullerene in Various Solvents.


The model has been presented in the publication "A Molecular-Based Model for Prediction of Solubility of C60 Fullerene in Various Solvents" Farhad Gharagheizi & Reza Fareghi Alamdari, Fullerenes, Nanotubes and Carbon Nanostructures, Volume 16, 2008 - Issue 1

1.2.Other related models:

Neural Network nanoQSAR model predicting Solubility of C60 Fullerene in Various Solvents.

1.3.Software coding the model:

Jaqpote is a web platform that support development, validation and sharing of QSAR models apps.jaqpot.org

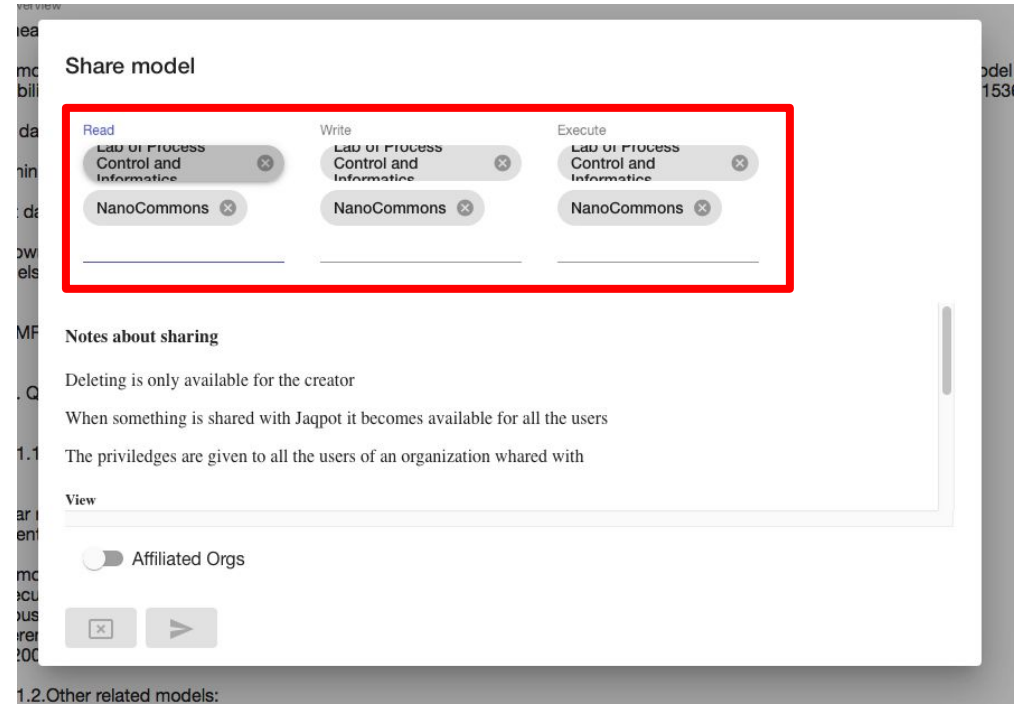
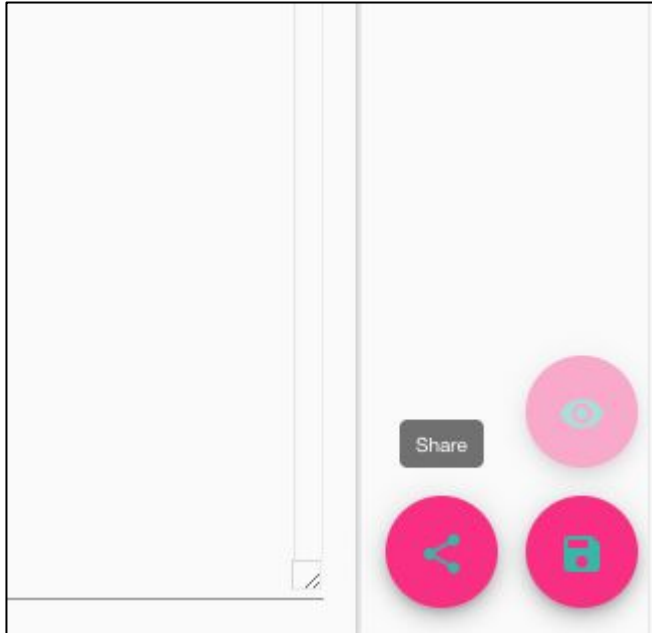


QMRF identifier (JRC Inventory): To be entered by JRC
QMRF Title: Linear nanoQSAR model predicting Solubility of C60 Fullerene in Various Solvents. The model has been presented in the publication "A Molecular-Based Model for Prediction of Solubility of C60 Fullerene in Various Solvents" Farhad Gharagheizi & Reza Fareghi Alamdari, Fullerenes, Nanotubes and Carbon Nanostructures, Volume 16, 2008 - Issue 1
Printing Date: 22-Apr-2019


1.QSAR identifier
1.1.QSAR identifier (title):
Linear nanoQSAR model predicting Solubility of C60 Fullerene in Various Solvents. The model has been presented in the publication "A Molecular-Based Model for Prediction of Solubility of C60 Fullerene in Various Solvents" Farhad Gharagheizi & Reza Fareghi Alamdari, Fullerenes, Nanotubes and Carbon Nanostructures, Volume 16, 2008 - Issue 1
1.2.Other related models:
Neural Network nanoQSAR model predicting Solubility of C60 Fullerene in Various Solvents.
1.3.Software coding the model:
Jaqpote
Jaqpote
Jaqpote
app
2.General information
2.1.Date of QMRF:
21 April 2019




QMRF report

Jaqpote 5 - Model page - Sharing




Jaqpot 5 - Model page - Data tab

 Jaqpot

Overview **Data** Predict / Validate Discussion



MODEL
Title: Neural Network Model for Predicting Solubility of C60 Fullerenes in Various Solvents
Owner: hsarimv
Description:
Neural Model

Dependent feature / Predicted feature


logS Exp.
Description: Feature created to link to independent feature of model Neural Network Model for Predicting Solubility of C60 Fullerenes in Various Solvents

Independent features

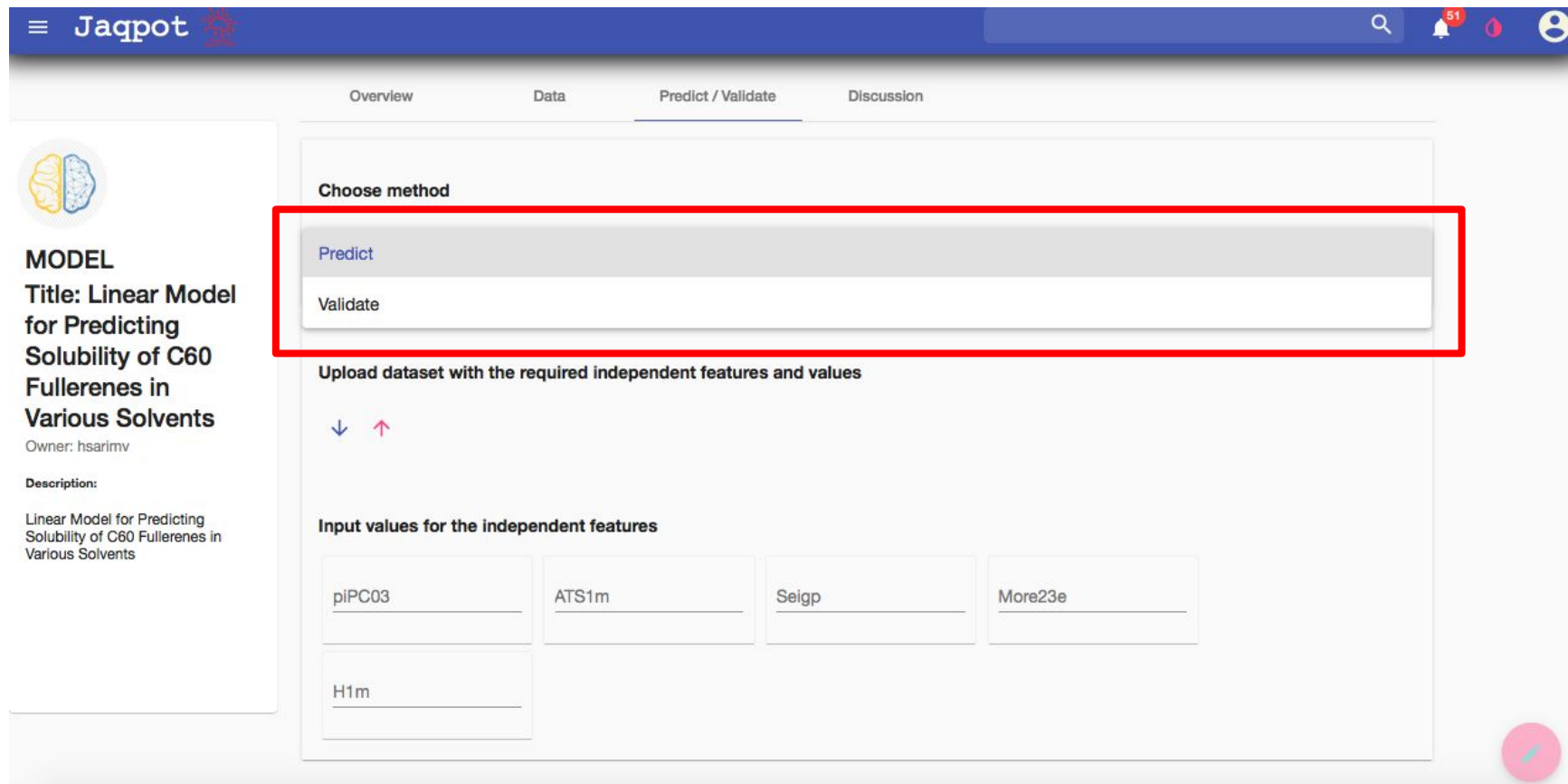
ATS1m
Description: Feature created to link to independent feature of model Neural Network Model for Predicting Solubility of C60 Fullerenes in Various Solvents

piPC03
Description: Feature created to link to independent feature of model Neural Network Model for Predicting Solubility of C60 Fullerenes in Various Solvents

Seigp
Description: Feature created to link to independent feature of model Neural Network Model for Predicting Solubility of C60 Fullerenes in Various Solvents



Jaqpot 5 - Model page - Predict tab



The image shows the Jaqpot 5 web interface, specifically the 'Predict / Validate' tab for a model. The interface has a dark blue header with the Jaqpot logo, a search bar, and notification icons. Below the header, 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, the model title 'MODEL: Linear Model for Predicting Solubility of C60 Fullerenes in Various Solvents', the owner 'hsarimv', and a description. The main content area is divided into three sections: 'Choose method', 'Upload dataset with the required independent features and values', and 'Input values for the independent features'. The 'Choose method' section has a red border around it and contains two buttons: 'Predict' (highlighted in grey) and 'Validate'. The 'Upload dataset' section has a download icon and an upload icon. The 'Input values' section has five input fields with labels: 'piPC03', 'ATS1m', 'Seigp', 'More23e', and 'H1m'. A pink circular button with a pencil icon is located in the bottom right corner.

Jaqpot

Overview Data **Predict / Validate** Discussion

MODEL
Title: Linear Model for Predicting Solubility of C60 Fullerenes in Various Solvents
Owner: hsarimv
Description:
Linear Model for Predicting Solubility of C60 Fullerenes in Various Solvents

Choose method

Predict
Validate

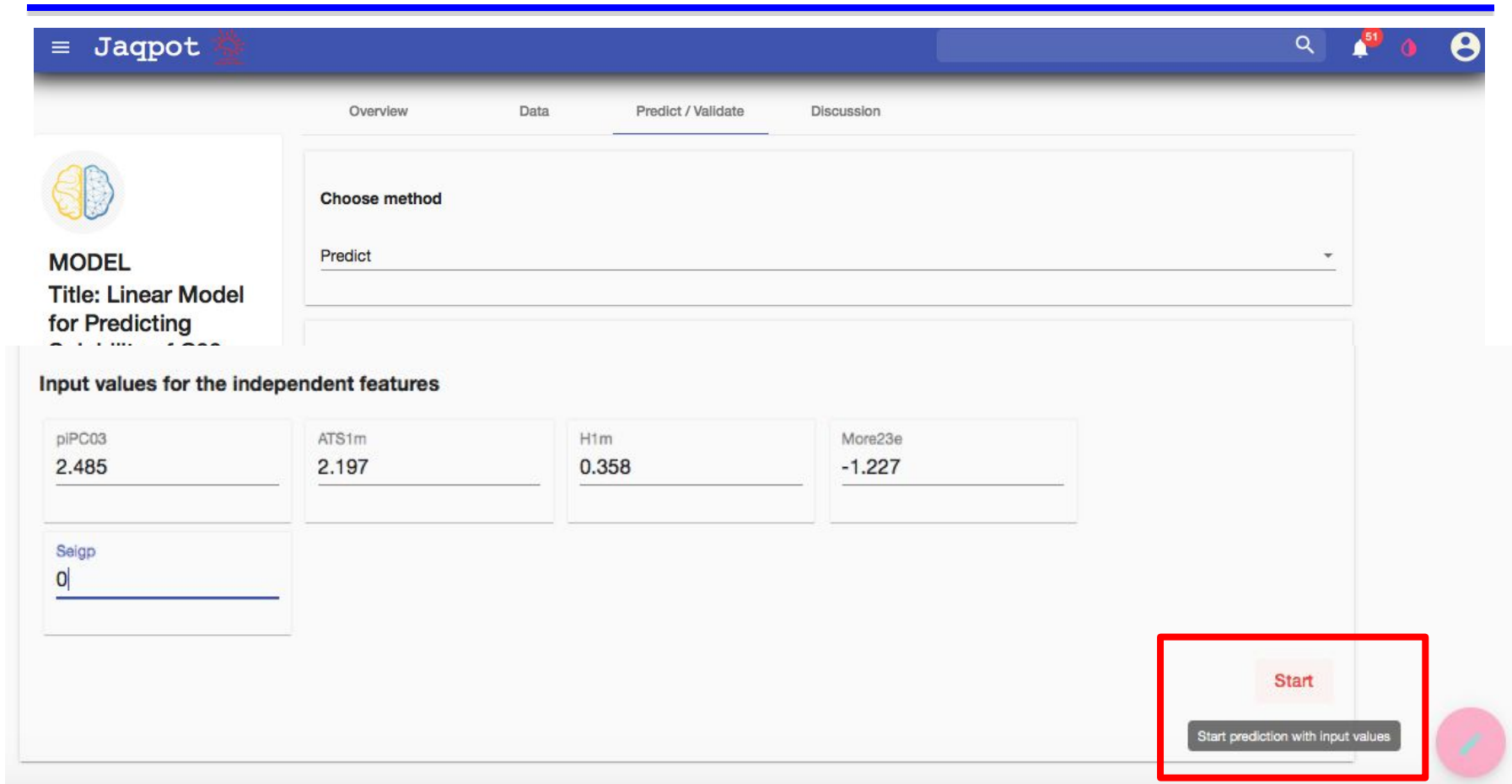
Upload dataset with the required independent features and values

↓ ↑

Input values for the independent features

piPC03 ATS1m Seigp More23e
H1m

Jaqpot 5 - Predict tab - Entering values



The image shows the Jaqpot 5 Predict tab interface. The top navigation bar is blue with the Jaqpot logo and a search icon. Below the navigation bar, there are four tabs: Overview, Data, Predict / Validate (selected), and Discussion. On the left side, there is a sidebar with a brain icon and the text "MODEL Title: Linear Model for Predicting". The main content area is divided into two sections. The top section is titled "Choose method" and contains a dropdown menu with "Predict" selected. The bottom section is titled "Input values for the independent features" and contains five input fields. The first four fields are labeled piPC03, ATS1m, H1m, and More23e, and contain the values 2.485, 2.197, 0.358, and -1.227 respectively. The fifth field is labeled Seigp and contains the value 0. At the bottom right, there is a red rectangular box containing a "Start" button and a "Start prediction with Input values" button. A pink circular icon with a pencil is located at the bottom right corner.

Jaqpot

Overview Data Predict / Validate Discussion

MODEL
Title: Linear Model for Predicting

Choose method

Predict

Input values for the independent features

Feature	Value
piPC03	2.485
ATS1m	2.197
H1m	0.358
More23e	-1.227
Seigp	0

Start

Start prediction with Input values

Jaqpot 5 - Predict tab – Your data via template

Upload dataset with the required independent features and values

↓ ↑

Download template dataset (csv)

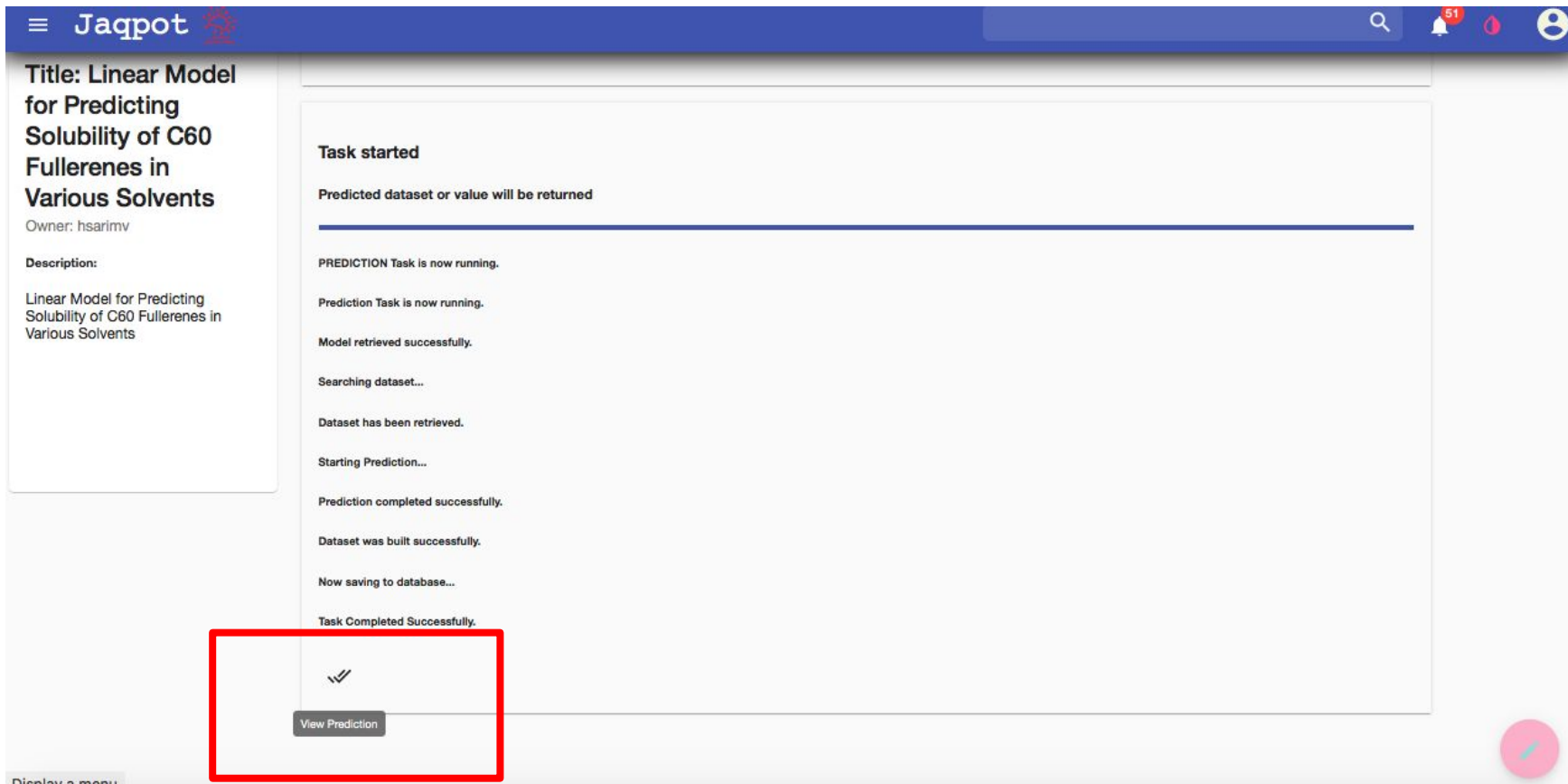
Input values for the independent features

piPC03	ATS1m	Seigp	H1m
More23e			

A template for users to enter their data, upload to Jaqpot and get predictions.

Home Insert Page Layout Formulas Data Review View						
Paste Cut Copy Format Calibri (Body) 12 A A = = =						
B I U A						
F4 x ✓ fx						
	A	B	C	D	E	
1	Seigp	ATS1m	piPC03	More23e	H1m	
2	0	2.485	2.303	-2.598	0.249	
3	0	2.639	2.485	-3.047	0.263	
4						

Jaqpot 5 - Model page - Predict tab



The screenshot shows the Jaqpot 5 web interface. The top navigation bar is blue with the Jaqpot logo on the left and search, notifications (51), and user profile icons on the right. The main content area is divided into a left sidebar and a right main panel. The sidebar contains the model title, owner, and description. The main panel displays a task log with status updates and a 'View Prediction' button at the bottom, which is highlighted by a red rectangle.

Title: Linear Model for Predicting Solubility of C60 Fullerenes in Various Solvents

Owner: hsarimv

Description:

Linear Model for Predicting Solubility of C60 Fullerenes in Various Solvents

Task started

Predicted dataset or value will be returned

PREDICTION Task is now running.

Prediction Task is now running.

Model retrieved successfully.

Searching dataset...

Dataset has been retrieved.

Starting Prediction...

Prediction completed successfully.

Dataset was built successfully.

Now saving to database...

Task Completed Successfully.

✓

[View Prediction](#)

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: 301 - 1 of 1<>

[Download](#)

Jaqpot 5 - Predictions as CSV

Starting Prediction...

Prediction completed successfully.

Dataset was built successfully.

Now saving to database...

Task Completed Successfully.

✓

[View predicted value only](#)

Id	Seigp
0	0

Download

logS Exp. ATS1m More23e H1m piPC03

predicted_dataset

Home Insert Page Layout Formulas Data Review View

Paste Cut Copy Format

Calibri (Body) 12 A A

B I U

Wrap Text

Merge & Center



General




Condit Forma

G8


	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 - Social network of models

 Jaqpot 



[Overview](#)[Data](#)[Predict / Validate](#)[Discussion](#)




MODEL
Title: Linear Model for Predicting Solubility of C60 Fullerenes in Various Solvents
Owner: hsarimv
Description:
Linear Model for Predicting Solubility of C60 Fullerenes in Various Solvents

Leave a comment

I am speechless.

Save



Jaqpot 5 - User profile

The screenshot shows the Jaqpot 5 user profile interface. At the top, a blue header bar contains the Jaqpot logo, a search bar, and notification icons. Below the header, the user's profile is displayed with a red circular profile picture, the name "Philip Doganis", and the username "filipposd". To the right of the profile, there are tabs for "Organizations", "On the internet", and "Quota". The "Organizations" tab is active, showing a list of organizations the user is a member of: NanoCommons, Jaqpot (with a red circular logo and location "Athens, Greece"), Lab of Process Control and Informa... (Athens, Greece), and OpenRiskNet. Below the list is a "CREATE" button. On the left side of the profile, there is a list of fields: "About", "Occupation", "Occupation at", "Lives at city", "Country", and "Api key" (with a value starting with "eyJhbGciOiJSUzI1NiIsInR5cCIgOiAiSldUliv"). A red circular button with a white icon is located in the bottom right corner.

Jaqpot

Philip Doganis
filipposd

Organizations On the internet Quota

Organizations
Organizations i am a member

NanoCommons

Jaqpot Athens, Greece

Lab of Process Control and Informa... Athens, Greece

OpenRiskNet

CREATE

About

Occupation


Occupation at

Lives at city


Country

Api key
eyJhbGciOiJSUzI1NiIsInR5cCIgOiAiSldUliv


Jaqpot 5 - User profile - Contact Info




Philip Doganis
filippoasd




About




Occupation
Senior Researcher, Lab&Teaching St




Occupation at
NTUA, Greece



Lives at city
Athens




Country
Greece



Api key
eyJhbGciOiJSUzI1NiIsInR5cCIgOiAi

Organizations


On the internet




WWW

People can find me on


Website url




<https://www.chemeng.ntua>




Github url







LinkedIn url

<https://www.linkedin.com/li>







Twitter url



Jaqpot 5 - Organizations




NanoCommons



Description:


community framework and infrastructure for reproducible science, and in particular for in silico workflows for nanomaterials safety assessment and beyond.

Creator:



Overview

Read-across approaches, which are currently absent for NMs, in large part as a



hsarimv

Occupation: Professor

at: National Technical University of Athens


particular for in silico workflows for nanomaterials safety assessment and beyond, by:




integration and federation of existing NMs characterisation and interaction mechanisms knowledge, protocols and data (beyond simple toxicity), along with quality assurance criteria and underpinning ontologies compilation and development of a user-friendly interface for a suite of computational tools for mechanistic and statistical modelling, read-across, grouping, safe-by-design and life cycle assessment, and bench-marking of their predictive power; and provision of (typically remote) access to its KnowledgeBase, modelling toolbox (predictive

Orga Men


<https://app.jaqpot.org/organization/NanoCommons>

Jaqpot 5 - NanoCommons Organization page

 Jaqpot




NanoCommons



Description:

NanoCommons is a H2020 infrastructure project creating a community framework and infrastructure for reproducible science, and in particular for in silico

Creator:



Overview

Read-across approaches, which are currently absent for NMs, in large part as a result of data fragmentation and inaccessibility, would reduce the cost of nanosafety research and regulation dramatically by removing the need for extensive laboratory and animal testing.

The availability of a nanosafety knowledge infrastructure, that organises and visualises data and data relationships, makes it accessible, integrates computational tools for risk assessment and decision support, enables their validation and facilitates the necessary grouping will be a critical factor in reducing regulatory costs.

The H2020 Infrastructures project, NanoCommons, addresses this gap by creating a community framework and infrastructure for reproducible science, and in particular for in silico workflows for nanomaterials safety assessment and beyond, by:

integration and federation of existing NMs characterisation and interaction mechanisms knowledge, protocols and data (beyond simple toxicity), along with quality assurance criteria and underpinning ontologies compilation and development of a user-friendly interface for a suite of computational tools for mechanistic and statistical modelling, read-across, grouping, safe-by-design and life cycle assessment, and bench-marking of their predictive power; and provision of (typically remote) access to its KnowledgeBase, modelling toolbox (predictive, grouping, risk assessment) and workflow optimisation, and the supporting expertise, to the broader user community.

Organization Members

Contact

@ hsarimv@central.ntua.gr

<https://app.jaqpot.org/organization/NanoCommons>

Jaqpot 5 - Sharing of resources

The screenshot displays the Jaqpot 5 web interface. At the top, a blue header bar contains a search icon, a notification bell with '51' alerts, and a user profile icon. Below the header, the user profile for Philip Doganis (filipposd) is shown on the left, with a red circular profile picture and a list of links: About, Occupation, Occupation at, Lives at city, Country, and an API key. The main content area is titled 'Organizations' and lists organizations the user is a member of: Jaqpot, Lab of Process Control and Informa... (Athen), NanoCommons, and OpenRiskNet. A 'CREATE' button is at the bottom of this list. A dropdown menu is open over the 'Jaqpot' entry, showing a list of shared models: 'Shared model through Lab ...', 'Shared model through Nan...', 'Shared model through Lab ...', 'Shared model through Nan...', 'Shared model through Lab ...', 'Shared model through Nan...', 'Shared model through Lab ...', 'Shared model through Lab ...', and 'Shared model through Ope...'. Each item in the dropdown is preceded by a share icon.

Philip Doganis
filipposd

About
Occupation
Occupation at
Lives at city
Country
Api key
eyJhbGciOiJSUzI1NiIsInR5cCIgOiAiSldUIiw

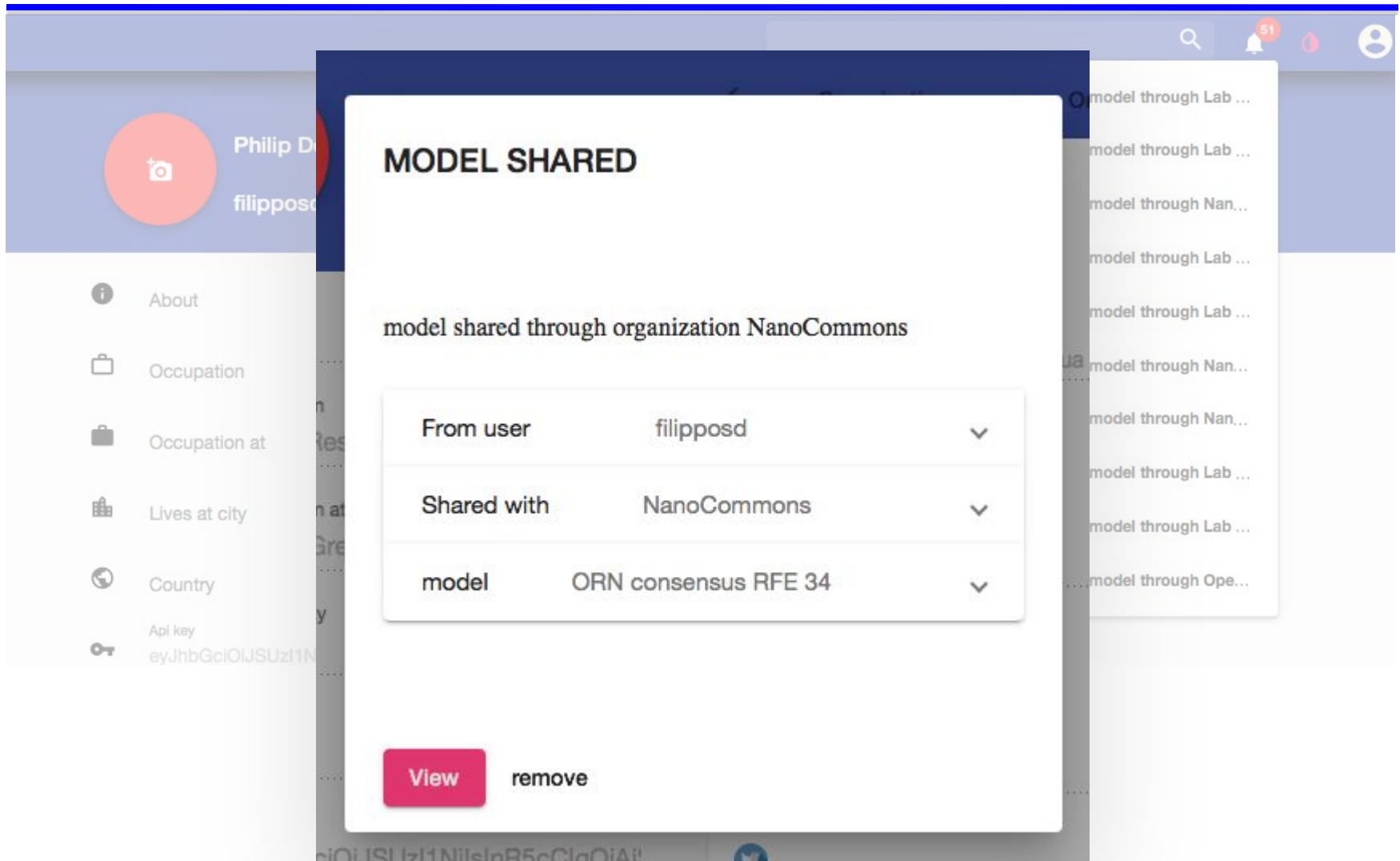
Organizations
On the Internet

Organizations
Organizations I am a member

Jaqpot
Lab of Process Control and Informa... Athen
NanoCommons
OpenRiskNet
CREATE

Shared model through Lab ...
Shared model through Lab ...
Shared model through Nan...
Shared model through Lab ...
Shared model through Nan...
Shared model through Nan...
Shared model through Lab ...
Shared model through Lab ...
Shared model through Ope...

Jaqpot 5 - Sharing notification



The image shows a user profile for Philip D. filipposc on the Jaqpot 5 platform. A modal window titled "MODEL SHARED" is displayed, showing a notification that a model was shared through the organization NanoCommons. The notification details include the user "filipposd", the organization "NanoCommons", and the model "ORN consensus RFE 34". At the bottom of the modal, there are two buttons: "View" (highlighted in pink) and "remove".





MODEL SHARED

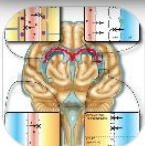
model shared through organization NanoCommons

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

[View](#) [remove](#)

Jaqpot 5 - Dataset page



DATASET
Title: Blood-Brain-Barrier Penetration
Owner: filippod
Description:
Binary Blood-Brain-Barrier Penetration Data after applying Recursive Feature Elimination (Penetrating/Non-Penetrating).


Overview

Data

Discussion

Binary Blood-Brain-Barrier Penetration Data after applying Recursive Feature Elimination (Penetrating/Non-Penetrating). Source: Effect of Selection of Molecular Descriptors on the Prediction of Blood-Brain Barrier Penetrating and Nonpenetrating Agents by Statistical Learning Methods, Hu Li, Chun Wei Yap, Choong Yong Ung, Ying Xue, Zhi Wei Cao and Yu Zong Chen, J. Chem. Inf. Model. 2005 45, 5, 1376-1384

picture by: By Stolp HB, Liddelow SA, Sá-Pereira I, Dziegielewska KM and Saunders NR - Stolp HB, Liddelow SA, Sá-Pereira I, Dziegielewska KM and Saunders NR (2013) Immune responses at brain barriers and implications for brain development and neurological function in later life. Front. Integr. Neurosci. 7:61. doi: 10.3389/fnint.2013.00061 <http://journal.frontiersin.org/article/10.3389/fnint.2013.00061/full>, CC BY-SA 3.0, <https://commons.wikimedia.org/w/index.php?curid=43530785>



Jaqpot 5 - New dataset -Dataset details

Dataset

Filename: XRFE3Yall.csv

Dataset's id

Blood-Brain-Barrier ... ▾

Dataset's id from csv: Blood-Brain-Barrier Penetration

Title *

Blood-Brain-Barrier Pene

Description *

Farhad Gharagheizi & Reza Fareghi Alamdari

Subjects

Fullerene

Audiences

Tags

Fullerene , Solubility

Submit

IdATSC3dv	ATSC6d	ATSC7i	ATSC8i	MATS2i	GATS2m	NsC
0 0.56838137	0.504558150.32772753	0.4014363	0.44868296	0.474917380		
0 0.4094099	0.570796250.33246857	0.410797420.34907413	0.5754712	0		
0 0.3725539	0.5431615	0.32753754	0.428793430.52822345	0.442805560.07		
1 0.31555578	0.4539304	0.23253489	0	0.60701066	0.460899140.07	
1 0.64531374	0.8208577	0.33246857	0.410797420.75384444	0.463907	0	
1 0.5689562	0.864756170.17511162	0.3637108	0.4746896	0.317731560.35		
1 0.5056574	0.5190517	0.29254708	0.358349140.61428285	0.437957050		
1 0.57912403	0.449200120.03931781	0.076428760.8059602	0.3211879	0.14		
1 0.4270075	0.451252070.24331617	0.430732070.5959102	0.6408699	0.14		

Features

ATSC3dv

Description

Units

Ontological Classes

ATSC6d

Description

Training a model in Python

```
[ ] from sklearn.linear_model import LogisticRegressionCV
    clf_RFE2 =LogisticRegressionCV(Cs=100, class_weight=None,
                                   cv=None, dual=False, fit_intercept=True, intercept_scaling=1.0,
                                   max_iter=100,multi_class='ovr', n_jobs=1, penalty='l2',
                                   random_state=None, refit=True, scoring=None,
                                   solver='liblinear', tol=0.0001, verbose=0).fit(XRFE3,Yall1)

    clf_RFE2.predict(XRFE3)
    clf_RFE2.score(XRFE3,Yall1)
```

Now you have a model on your computer.

Great.

From model to web service in 1 line

```
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

Fullerenes, Nanotubes, and Carbon Nanostructures, 16: 40-57, 2008.
Copyright © Taylor & Francis Group, LLC.
DOI: 10.1080/15468330701778315

A Molecular-Based Model for Prediction of Solubility of C₆₀ Fullerene in Various Solvents

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¹Department of Chemical Engineering, Faculty of Engineering,

University of Tehran, Tehran, Iran

²Department of Chemistry, Faculty of Materials and Chemical

Engineering, Mehrizadeh University of Technology, Larestan,

Tehran, Iran

Abstract: In this present 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. The resulting nonlinear behavior of appearing molecular descriptors in GA-MLR system, a feed forward neural network (FFNN) was constructed and compared for prediction of solubility of C₆₀ fullerene in various solvents. Obtained models considerably showed better accuracy in comparison with the previous models.

Keywords: C₆₀, QSPR, GA-MLR, FFNN

1. INTRODUCTION

About 30 years have passed since the second half C₆₀ molecules first occurred in the minds of theoreticians (1-3), which is now generally recognized as being

Received 20 July 2007; Accepted 12 September 2007
Address correspondence to Farhad Gharghazizadeh, Department of Chemical Engineering, Faculty of Engineering, University of Tehran, P. O. Box: 11155-4563, Tehran, Iran. E-mail: fgharghaz@ut.ac.ir

```
url=jaqpot.deploy_pipeline(clf_RFE2,XRFE3,Yall1,"ORN consensus RFE 6","Logistic Regression+RFE","linearmodel")  
url
```

The screenshot displays the Jaqpot web application interface. At the top, there is a navigation bar with tabs for Overview, Data, Predict / Validate, and Discussion. The main content area is titled "Linear nanoQSAR model predicting Solubility of C60 Fullerene in Various Solvents." Below the title, it provides the model title "Neural Network Model for Predicting Solubility of C60 Fullerenes in Various Solvents" and the owner's name "hassanv". A description section follows, detailing the model's purpose and providing links for the full dataset, training dataset, test dataset, and a downloadable QMRF report. The QMRF report section includes a "1. QSAR Identifier" and a "1.1. QSAR Identifier (title):" which is "Linear nanoQSAR model predicting Solubility of C60 Fullerene in Various Solvents." It also mentions that the model has been presented in a publication and lists other related models and software coding options.

Get predictions from a model


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

```
[ ] dfJQ_RFE
```



	NsCH3	PEOE_VSA4	ATSC7i	NdssS	ATSC3dv	JGI5	SsCH3	GATS2m	Blood-Brain-Barrier Penetration	ATSC6d
0	0.000000	0.171888	0.327728	0	0.568381	0.207983	0.000000	0.474917	1	0.504558

Jaqpot in EOSC Catalogue (through OpenRiskNet)



AboutGovernanceServices & ResourcesPolicyEOSC in practiceMediaFor Providers

Home

Jaqpot

Jaqpot

Generate, store and share predictive statistical and machine learning models

★★★★★ 5 (1) ♡ 1 👁 29

Categorization: SOFTWARE --> PLATFORM

Jaqpot is a user-friendly web-based e-infrastructure containing many data analysis and modelling microservices integrated under a common API. The Jaqpot infrastructure allows for building applications that preprocess data, compute descriptors from raw data (such as electronic images), create, validate, store and share predictive machine learning models and generate reports in standard formats.

Jaqpot user interface allows the end-user to use most Jaqpot functionalities.

Tags: CHEMICALS NANOTECHNOLOGY PREDICTIVE MODELLING BIOKINETICS
COMPUTATIONAL MODELLING PREDICTIVE TOXICOLOGY

Usage

TECHNOLOGY READINESS LEVEL

Service coverage

Countries serviced by Jaqpot =

OpenRiskNet

OPENRISKNET

SERVICE HOMEPAGE

SERVICE ORDER

CONTRACTUAL INFO

Service level agreement →

Terms of use →

<https://catalogue.eosc-portal.eu/service/openrisknet.jaqpot>

toxFlow

The screenshot shows the toxFlow web application interface. At the top is a dark navigation bar with the 'toxFlow' logo and links for 'Home', 'GSVA', 'Read-across training', and 'Read-across prediction'. The main content area is divided into several sections: a large 'Welcome to toxFlow!' section with a description of the tool; a 'toxFlow at a glance' section listing three main features; a 'Help' section with links to a user guide, maintainer information, a video tutorial, and a citation; a 'Status' section showing the last update date; and a 'License' section stating the application is under the GNU General Public License v.3.

toxFlow Home GSVA Read-across training Read-across prediction

Welcome to toxFlow!

A tool for read-across model development coupled with enrichment analysis

toxFlow at a glance

- Perform enrichment analysis of omics data
- Train a read-across model
- Include multi-perspective characterization

Help

- For a small user guide click [here](#)
- Application maintainer: [Dimitra-Danaï Varsou](#)
- [DemetraDanae](#)
- [Video tutorial](#)
- [Varsou et al. \(2017\), toxFlow: A Web-Based Application for Read-Across Toxicity Prediction Using Omics and Physicochemical Data](#)
- [National Technical University of Athens \(GR\), Unit of Process Control and Informatics](#)

Status

Last update: February 25, 2020

License

This application is released under [GNU General Public License v.3](#)

A tool for read-across model development coupled with enrichment analysis

- Perform enrichment analysis of omics data
- Train a read-across model
- Include multi-perspective characterization

toxflow.jaqpot.org

Conclusion

- Jaqpot is an **open source web infrastructure** with flexibility:
 - **generalization across disciplines**
 - **integration to 3rd-party tools** (modelling on the Cloud)
 - **easy integration** to diverse **architectures/ontologies/knowledge domains**.
- Jaqpot offers a seamless way to:
 - **take models out of the desktop or paper** and automatically make them available as web services via their URI
 - functionality is provided both through an **API and GUIs**.

Jaqpot constitutes a universal platform
that exchanges and produces semantically annotated datasets
and employs machine learning techniques to generate predictive models.



A place to

create **discuss**

share **use**

your models & datasets



NanoCommons

Nano-Knowledge Community

Thank you

Any Questions?

Jaqpot hands-on session - Meet the team



Philip
Doganis



Irini
Liampa

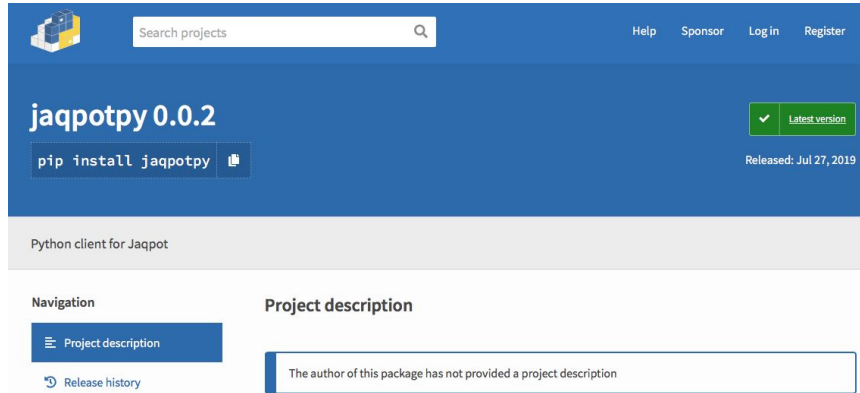


Pantelis
Karatzas

Jupyter: Setting up + brief intro

- Jupyter: Setting up + brief intro to what you need to get started in python
- After anaconda setup
- Environments
- Libraries
- import Jaqpote over pip

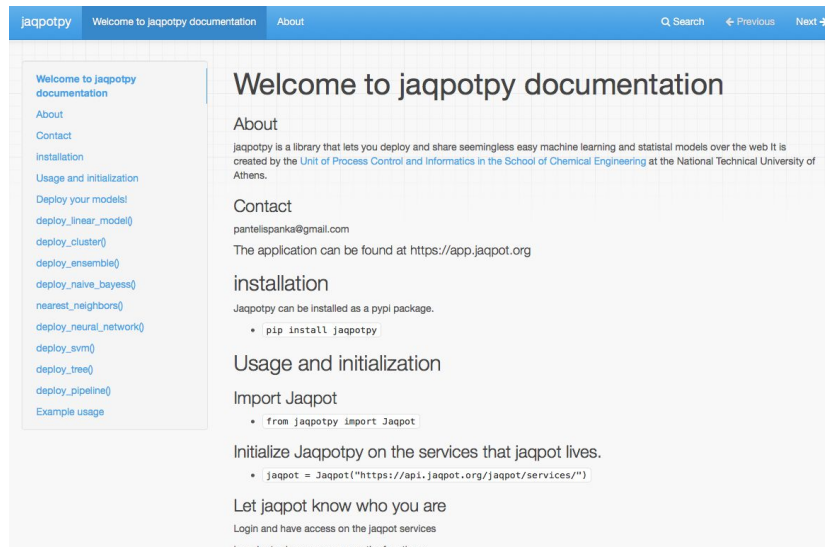
Jupyter: Setting up + brief intro



Jaqpotpy can be installed as a pypi package.

<https://pypi.org/project/jaqpotpy/>

```
pip install jaqpotpy
```



<https://jaqpotpy.readthedocs.io>

Importing and exploring the dataset

- Libraries and command for import
- Exploring the features
- Dataframes etc.

Basic preprocessing

- Basic preprocessing
- Checking the dataset
- Performing scaling

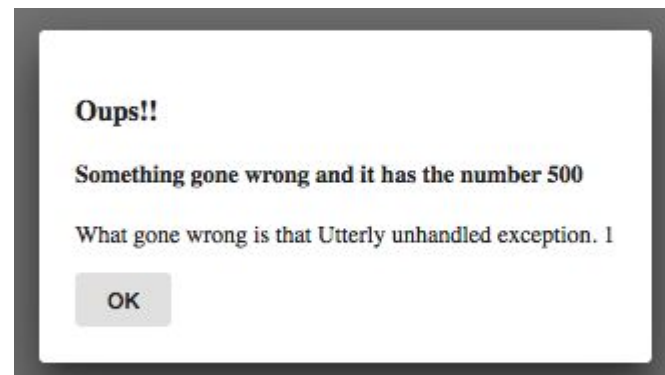
Creating a local model and its evaluation

- Creating a local model and its evaluation
- Create a model
- Evaluate performance
- Graphs and metrics

Uploading your model to Jaqpot

You now have your web service!

- Exploring your model on Jaqpot
 - adding information
 - QMRF report
 - To assist the users in adding editable versions of QMRF reports, we have created a QMRF markdown template, which can be downloaded from the following address:
<https://github.com/ntua-unit-of-control-and-informatics/QSAR-Models/blob/master/QMRF%20template.md>. The user only needs to provide the necessary information under each section and the QMRF report is generated in an easy-to-read format.
- Discussions



Using the model to get predictions on the web and in Python

- Using model on UI
- Using model over API in Python

Explore the platform, create more models and give us your ideas

- [Feedback questionnaire](#)
- [Jaqpot discussions](#)