

Jaqqpot - An open-source web platform for creating, using, testing and sharing predictive models in nano-informatics

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Unit of Process Control and Informatics

- 1 Professor, 2 senior researchers, 3 post-docs, 6 Ph.D. students, 3 software engineers, many graduate and undergraduate students.
- Research Interests: mathematical modelling, data-driven methods, machine learning, computational intelligence, mathematical programming
- Applications: process control, production optimization, modelling in the chemical industry, **cheminformatics**, **nanoinformatics**



Outline

1. Development of Jaqpot
2. Technical Specifications
3. Predictive nanoQSAR modelling
4. Data management
5. Biokinetics – PBPK modelling
6. Image Processing
7. Other Jaqpot functionalities
8. Conclusions



Jaqpot at a glance

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:

- Preprocessing data
- Computing descriptors from raw data (such as electronic images)
- Creating, validating, storing and sharing datasets and predictive statistical and machine learning models
- Generating reports in standard formats.



Development of Jaqqpot

- Original development during the OpenTox project (2008—2011)



- Main modelling tool in the eNanoMapper project (2014-2017)



- Part of the OpenRiskNet open e-infrastructure (2017-2019)



- Major Component of the NanoCommons community framework and infrastructure (2018-2021)



- Provides infrastructure and modelling tools to the NanoSolveIT e-platform (2019-2023)



Application Programming Interfaces (Swagger Documentation)

Jaqpot API <https://api.jaqpot.org/jaqpot/services/swagger.json> [Explore](#)

Jaqpot API

Jaqpot v4 (Quattro) is the 4th version of a VAQP, 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 Java& JEE7 by the [Unit of Process Control and Informatics in the School of Chemical Engineering](#), at the [National Technical University of Athens](#).

Created by Charalambos Chomenidis, Pantelis Sopasakis, Evagelia Anagnostopoulou, Angelos Valsamis, George Drakakis, Pantelis Karatzas, Georgia Tsiliki, Philip Doganis, Haralambos Sarimveis
See more at <https://github.com/KinivDesign/jaqpot-web/issues>
[Contact the developer](#)

| | | |
|--------------|-----------|--------------|
| discussion | Show/Hide | List/Operate |
| descriptor | Show/Hide | List/Operate |
| pmml | Show/Hide | List/Operate |
| feature | Show/Hide | List/Operate |
| readacross | Show/Hide | List/Operate |
| doseresponse | Show/Hide | List/Operate |
| validation | Show/Hide | List/Operate |
| notification | Show/Hide | List/Operate |
| swaggerid | Show/Hide | List/Operate |
| report | Show/Hide | List/Operate |
| enm | Show/Hide | List/Operate |
| model | Show/Hide | List/Operate |
| dataset | Show/Hide | List/Operate |
| biokinetics | Show/Hide | List/Operate |
| openrisknet | Show/Hide | List/Operate |
| organization | Show/Hide | List/Operate |
| user | Show/Hide | List/Operate |
| interlab | Show/Hide | List/Operate |
| bibtex | Show/Hide | List/Operate |
| task | Show/Hide | List/Operate |
| aa | Show/Hide | List/Operate |
| algorithm | Show/Hide | List/Operate |

[BASE URL: /jaqpot/services , API VERSION: 4.0.3]

The screenshot displays the Swagger UI for the Jaqpot API. The browser address bar shows the URL `localhost:8080/jaqpot/swagger3/`. The main content area lists several API endpoints, each with a color-coded header indicating the HTTP method and a lock icon for security:

- doseresponse** (POST): `/services/doseresponse` - Creates Dose Response Report
- enm** (GET): `/services/enm/property/categories` - Retrieves property categories
- enm** (GET): `/services/enm/descriptor/categories` - Retrieves descriptor calculation categories
- enm** (POST): `/services/enm/dataset` - Creates Dataset By Study
- feature** (GET): `/services/feature/{id}` - Finds Feature by ID
- feature** (PUT): `/services/feature/{id}` - Places a new Feature at a particular URI
- feature** (DELETE): `/services/feature/{id}` - Deletes a particular Feature resource
- feature** (GET): `/services/feature` - Lists features
- feature** (POST): `/services/feature` - Creates a new Feature
- interlab** (POST): `/services/interlab/test` - Creates Interlab Testing Report
- model** (PUT): `/services/model/{id}/meta` - Updates meta info of a dataset
- model** (GET): `/services/model/{id}` - Finds Model by Id
- model** (POST): `/services/model/{id}` - Creates Prediction

Activate Windows
Go to Settings to activate Windows.



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.



nanoQSA(P)R

The development of a **mathematical relationship** $y=f(X)$, that predicts an end-point (property, toxicity index) as a function of one or more descriptors (phys-chem properties, computational descriptors, image descriptors, omics data)

OECD principles:

1. A defined **end-point**
2. The use of an **unambiguous algorithm**
3. A defined **domain of applicability**
4. Appropriate measures of **goodness-of-fit, robustness** and **predictive ability**
5. A **mechanistic interpretation**, if possible

Reporting formats developed by Joint Research Center (JRC):

QSAR Model Reporting Format (**QMRF**)

QSAR Prediction Reporting Format (**QPRF**)

Guidance Document on the Validation of (Quantitative) Structure-Activity Relationship [(Q)SAR] Models; OECD SERIES ON TESTING AND ASSESSMENT. (OECD, 2007), ENV/JM/MONO(2007)2



Jaqpot 4

<http://www.jaqpot.org/>

Jaqpot Sign in Create Account

011010000011001010110110001
10011000110111000100000110
00011011011001100100001000
00011101101101101101101100
011000011011011110110110101
1001100000000001110000110
11110010000011110100111010
00011000000000001100001
01101110011000010110111001
1011101101101101100001011
00000111000001100101011100
1000100000011011101100101
0110000101110011011010101
11011001110101000010110100

Create Dataset
Select substances, properties and descriptors.
Create Dataset

✓ ? ✕

NanoQSAR validation schemes
Validate model using different validation options.
Cross Data Split External

$R^2 = 0.87$

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

ENM SOURCE DOCUMENTATION ISSUES

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

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Chomenidis C, Drakakis G, Tsiliki G, Anagnostopoulou E, Valsamis A, Doganis P, Sopasakis P, Sarimveis H, (2017) Jaqpot Quattro: A Novel Computational Web Platform for Modeling and Analysis in Nanoinformatics, *Journal of Chemical Information and Modeling*, 57(9), 2161-2172.



Create new account

ENANOMAPPER JAQPOT

Log In

Username or email

Password

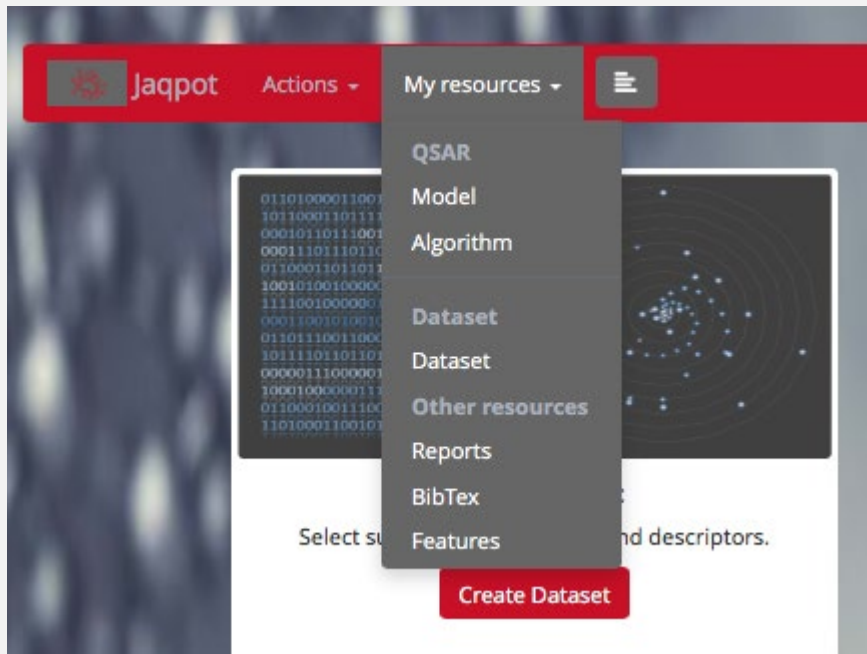
Remember me [Forgot Password?](#)

[Log In](#)

New user? [Register](#)



My resources



Algorithms

The screenshot shows the Jaqpot website interface. At the top, there is a red navigation bar with the text "Jaqpot", "Actions", "My resources", and a hamburger menu icon. On the right side of the bar, it says "Welcome back, NanoCommons". Below the navigation bar, the main content area is divided into two columns: "Regression" and "Classification". Each column contains a list of algorithm entries, each with a title and a brief description of its implementation. At the bottom of each column, there are "Previous" and "Next" navigation buttons. The "Classification" column has a "1" button between "Previous" and "Next".

| Regression | Classification |
|--|--|
| MLR - Weka (multi-response linear regression implemented in Java-WEKA) | SVM - Weka (LibSVM) Implementation |
| SVM - Weka (LibSVM, Support vector machines implemented in Java-WEKA) | Id3 - with MCI (Implemented in Python-Scikit-Learn) |
| PLS - Weka (Partial Least Squares implemented in Java-WEKA) | ID3 Decision Tree (Implemented in Python-Scikit Learn) |
| Linear Regression (Implemented in Python-Scikit Learn) | CMI Decision Tree (Implemented in Python-Scikit Learn) |
| Lasso Regression (Implemented in Python-Scikit Learn) | Generalised Naive Bayes (Implemented in Python-Scikit Learn) |
| PLS - with VIP scores (Implemented in Python) | Multinomial Naive Bayes (Implemented in Python-Scikit Learn) |
| Readacross | Bernoulli Naive Bayes (Implemented in Python-Scikit Learn) |
| Linear Model (implemented in R - base library) | Random Forest (Implemented in Python-Scikit Learn) |
| Gradient Boosting (Implemented in Python-Scikit Learn) | Multi-layer Perceptron (Implemented in Python-Scikit Learn) |
| Random Forest (Implemented in Python-Scikit Learn) | Gradient Boosting (Implemented in Python-Scikit Learn) |
| Multi-layer Perceptron (Implemented in Python-Scikit Learn) | |

Navigation buttons: Previous 1 Next



Ontological annotation of algorithms

| | Category / URI | Description | OpenTox Ontological Classes |
|---|---|--|--|
| | Preparation-additional | | |
| 1 | http://jaqpot.org:8080/jaqpot/services/algorithm/scaling | Scaling | "ot:Algorithm", "ot:Scaling", "ot:Transformation" |
| | WEKA (Java) | | |
| 1 | http://jaqpot.org:8080/jaqpot/services/algorithm/weka-mlr | MLR - Weka (multi-response linear regression implemented in Java-WEKA) | "ot:Algorithm", "ot:Regression", "ot:SupervisedLearning" |
| | Python | | |
| 1 | http://jaqpot.org:8080/jaqpot/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

Example

Modelling the Solubility of C60 fullerene in various solvents (Gharageizi et.al., 2008).

The full dataset of 124 solvents has been uploaded to Jaqpot and can be viewed in the URI

http://www.jaqpot.org/data_detail?name=nGF3G5SBo4wk5h

Training dataset of 93 solvents

http://www.jaqpot.org/data_detail?name=XmCQVC7o5jKKRv

Test dataset of 31 solvents

(http://www.jaqpot.org/data_detail?name=3UbgEPIdT2Ovs)

The screenshot displays the Jaqpot web interface. On the left, a navigation menu is open, highlighting 'Train a model'. The main content area is divided into several sections: 'Create Dataset' with a 'Create Dataset' button; 'NanoQSAR validation schemes' with 'Cross', 'Data Split', and 'External' buttons; 'NanoQSAR modelling' showing a scatter plot with a regression line and $R^2 = 0.87$, with 'Train' and 'Predict' buttons; 'Optimal Experimental Design' with 'Iterative Experimental Design' and 'Factorial Design' buttons; 'Interlaboratory Comparison' with an 'Interlaboratory Proficiency Testing' button; and 'Read Across' with 'Train' and 'Predict' buttons. The footer contains logos for ENM, SOURCE, DOCUMENTATION, ISSUES, and the Unit of Process Control and Biotechnological Engineering at the National Technical University of Athens, along with a copyright notice for 2015.

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



Model training - Dataset selection

Jaqpot Actions My resources Welcome back, NanoCommons

Select dataset:

Example datasets:

| Name | Title | Description | Date |
|----------------------|-------------------------------------|--|------------------------------|
| Gajewicz_10_29 | Gajewicz et al - 10 Metal Oxide NPs | 10 MeOx NPs with 29 descriptors, used for predicting HaCaT toxicity. | 2018-07-05T15:05:49.675+0000 |
| Gajewicz_10_29_class | Gajewicz et al - 10 Metal Oxide NPs | 10 MeOx NPs with 29 descriptors, used for predicting HaCaT toxicity. | 2018-07-05T15:05:49.959+0000 |
| Gajewicz_18_29 | Gajewicz et al - 18 Metal Oxide NPs | 18 MeOx NPs with 29 descriptors, used for predicting HaCaT toxicity. | 2018-07-05T15:05:50.083+0000 |
| Gajewicz_18_29_class | Gajewicz et al - 18 Metal Oxide NPs | 18 MeOx NPs with 29 descriptors, used for predicting HaCaT toxicity. | 2018-07-05T15:05:50.192+0000 |
| Gajewicz_8_29 | Gajewicz et al - 8 Metal Oxide NPs | 8 MeOx NPs with 29 descriptors, used for predicting HaCaT toxicity. | 2018-07-05T15:05:50.237+0000 |
| Gajewicz_8_29_class | Gajewicz et al - 8 Metal Oxide NPs | 8 MeOx NPs with 29 descriptors, used for predicting HaCaT toxicity. | 2018-07-05T15:05:50.277+0000 |

All Datasets:

| Name | Title | Description | Date |
|----------------------|---|--|------------------------------|
| XmCQVC7o5JKRv | Solubility of C60 fullerene in various solvents (training ... | The dataset includes 5 descriptors and solubility (log of molar fractions) for 93 solvents | 2019-05-14T11:11:03.244+0000 |
| nGF3G55Bo4wk5h | Solubility of C60 fullerene in various solvents | The dataset includes 5 descriptors and solubility (log of molar fractions) for 124 solvents | 2019-05-14T11:09:50.746+0000 |
| SUfms544LoBREREdx5cp | Gharagheizi et al, Fullerene C60 | Numerical values of the calculated descriptors along with solubility of C60 in solvents | 2019-05-14T10:52:15.395+0000 |
| MXw9XCFf13FzX | new dataset | | 2019-05-14T10:14:41.460+0000 |
| xYt2DM1NUct2G | Kar et al, metal oxides (training), mod_7 | Numerical values of the calculated descriptors along with cytotoxicity values for metal oxidenanoparticles | 2019-05-14T09:23:38.585+0000 |
| FZxgQrEp2RBSWN | Marcus et al, Fullerene C60, all solvents, 298_303 | Fullerene C60 Solubility (all solvents) | 2019-05-06T11:02:02.822+0000 |
| m2jbdghf107oi | Pathakoti et al, metal oxides, light (training) | Molecular properties of metal oxides | 2019-05-06T08:49:42.616+0000 |
| 4xoqetXfKMB0S | Pathakoti et al, metal oxides, light (full) | Molecular properties of metal oxides | 2019-05-06T08:49:13.215+0000 |
| r2Chi6lGaaHCrS | Pathakoti et al, metal oxides, dark (training) | Molecular properties of metal oxides | 2019-05-06T08:48:55.173+0000 |

w.jaqpot.org/dataset?dataset=XmCQVC7o5JKRv



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)
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- 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



Model training – Variable and parameters selection

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 |
|--|--|
| <input checked="" type="checkbox"/> Select All | |
| <input checked="" type="checkbox"/> Seigp | <input type="radio"/> Seigp |
| <input type="checkbox"/> Solvents | <input type="radio"/> Solvents |
| <input type="checkbox"/> logS Exp_ | <input checked="" type="radio"/> logS Exp_ |
| <input checked="" type="checkbox"/> H1m | <input type="radio"/> H1m |
| <input checked="" type="checkbox"/> More23e | <input type="radio"/> More23e |
| <input checked="" type="checkbox"/> AT51m | <input type="radio"/> AT51m |
| <input checked="" type="checkbox"/> piPC03 | <input type="radio"/> piPC03 |

Select scaling method:

Scaling between zero and one

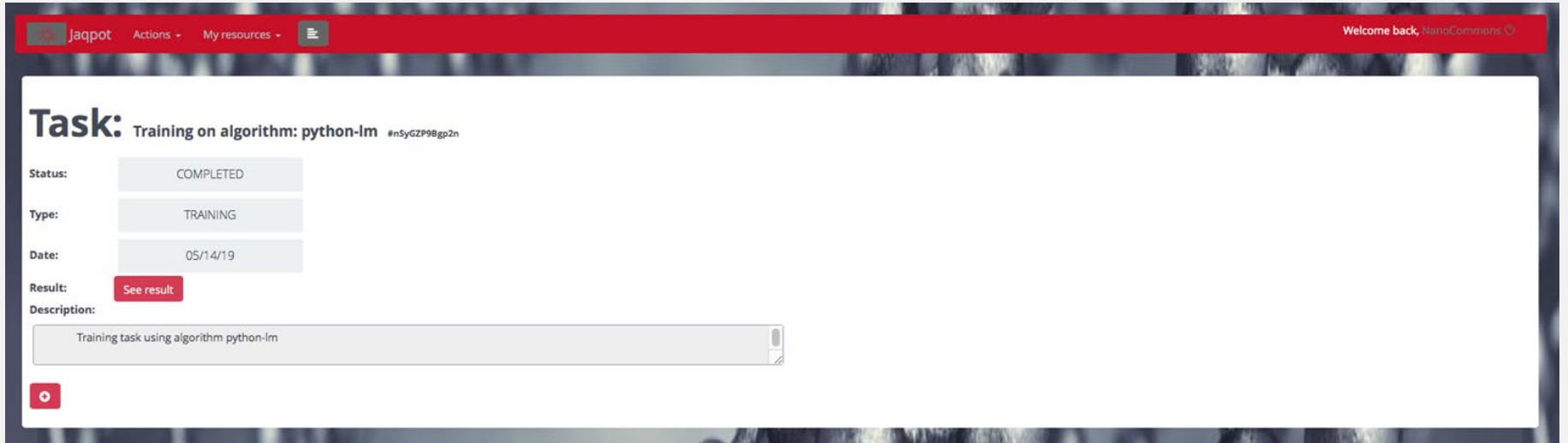
Select domain of applicability method:

Leverage method

Train



Task management



The screenshot shows a web interface for task management. At the top, a red navigation bar contains the text "Jaqpot" followed by "Actions -" and "My resources -" with a menu icon. On the right side of the bar, it says "Welcome back, NanoCommons" with a user profile icon.

The main content area is titled "Task: Training on algorithm: python-lm" with a unique ID "#nSyGZP98gp2n". Below the title, there are several fields:

- Status:** A light gray box containing the text "COMPLETED".
- Type:** A light gray box containing the text "TRAINING".
- Date:** A light gray box containing the text "05/14/19".
- Result:** A red button with the text "See result".
- Description:** A text area containing the text "Training task using algorithm python-lm".

At the bottom left of the task card, there is a small red square icon with a white play button symbol.



Model webpage

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

The screenshot shows the Jaqpot model webpage interface. At the top, there is a red navigation bar with the Jaqpot logo, "Actions", "My resources", and a menu icon. On the right side of the bar, it says "Welcome back, NanoCommons". Below the navigation bar, the main content area has a white background. At the top left of this area, it says "Model: #72GEEEmGhhavY00n7O209". To the right of this are three red buttons: "Validate me" (with a checkmark icon), "Predict" (with a play icon), and "Delete" (with a trash icon). Below the model name, there are several sections: "Title:" with a text box containing "Linear Model for C60 Fullerene Solubility"; "Description:" with a text box containing a citation: "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"; "Transformations:" with two text boxes containing URLs: "http://jaqpot.org:8080/jaqpot/services/model/FqeE4mX2AC1hnXgVeUBr" and "http://jaqpot.org:8080/jaqpot/services/model/4tObjaWKRfls5eijTKHy"; "Doa:" with a text box containing "http://jaqpot.org:8080/jaqpot/services/model/3id3kU4efV04Ru9puuKo"; "Algorithm:" with a red button labeled "python-lm"; "Features:" with four text boxes labeled "Required Features", "Dependent Features", "Independent Features", and "Predicted Features"; and "Representation:" with a red button labeled "PMML".



External validation of models

Jaqpot Actions My resources

Welcome back, NanoComments

Choose method:

Select dataset.
 Insert values.

| | piPC03 | AT51m | Seigo | More23e | H1m | logS Exp_ |
|---|--------|-------|-------|---------|-------|-----------|
| 1 | 1,609 | 2,473 | 0,578 | 0,025 | 0,927 | -4 |
| 2 | 1,609 | 1,763 | -1,8 | 0,022 | 0,328 | -5,3 |
| 3 | 3,426 | 2,398 | 0 | -1,159 | 0,449 | -3,4 |
| 4 | 1,099 | 1,674 | -1,2 | -0,449 | 0,192 | -5,9 |
| 5 | 1,099 | 2,792 | 0,846 | -0,614 | 1,495 | -4,2 |

Validate



Validation report

<http://www.jaqpot.org/report?name=cnJlt1LZ3fnvcl>

Jaqpot Actions My resources

Welcome back, [NameCommons](#)

Report: #cnJlt1LZ3fnvcl

[Download](#)

Title: External validation report

Model: 72GEEmGhhavY00n7O209

Dataset: XmCQVC7o5jKkRv

Description:
External validation with model:<http://jaqpot.org:8080/jaqpot/services/model/72GEEmGhhavY00n7O209> and dataset:<http://jaqpot.org:8080/jaqpot/services/dataset/XmCQVC7o5jKkRv>

Algorithm Type: REGRESSION

F-Value: 247.42

Number of predictor variables: 5

RMSD: 0.34

R² (OECD): 0.9

R² Adjusted (if applicable): 0.9

StdError: 0.35

All Data

| | Real | Predicted |
|--------|------|----------------|
| row1 | -6.1 | -5.849782807 |
| row10 | -3.5 | -3.65218379323 |
| row100 | -2.2 | -2.43446757404 |
| row101 | -2.1 | -2.23685926686 |



Validation report

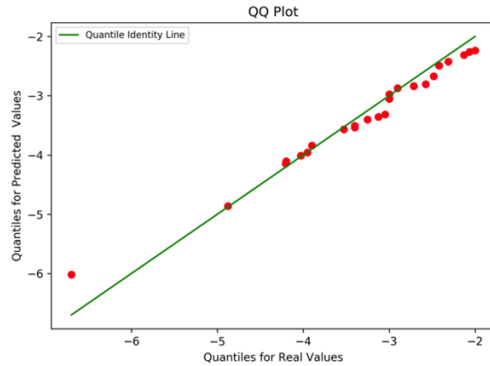
All Data

| | Real | Predicted |
|------------|------|----------------|
| compound1 | -4 | -3.91355789467 |
| compound10 | -2.6 | -2.72064673994 |
| compound11 | -4.9 | -4.19945022239 |
| compound12 | -5 | -4.96443038285 |
| compound13 | -2.1 | -2.23685926686 |
| compound14 | -3 | -3.34976177746 |
| compound15 | -2 | -2.27234329025 |
| compound16 | -3.9 | -3.82107851451 |
| compound17 | -5.2 | -4.88772442914 |
| compound18 | -4.2 | -3.5504783112 |
| compound19 | -6.7 | -6.01794584696 |
| compound2 | -5.3 | -5.61018322885 |
| compound20 | -4.3 | -4.33212597512 |
| compound21 | -2.5 | -3.05827270109 |
| compound22 | -3.3 | -3.13183407097 |
| compound23 | -2.4 | -2.93903145294 |
| compound24 | -3.8 | -4.07882245078 |
| compound25 | -3 | -2.81223578464 |
| compound26 | -4.4 | -4.65814301486 |
| compound27 | -4.7 | -4.91962777437 |
| compound28 | -2.5 | -2.87194521299 |
| compound29 | -3.9 | -3.99928281415 |
| compound3 | -3.4 | -3.28038430934 |
| compound30 | -2.2 | -2.43446757404 |
| compound31 | -3 | -3.41838538257 |
| compound4 | -5.9 | -5.97659581681 |
| compound5 | -4.2 | -4.14080958734 |
| compound6 | -3.1 | -3.5059080608 |
| compound7 | -2.9 | -2.78268289953 |
| compound8 | -3.4 | -3.59838096199 |
| compound9 | -3 | -2.41555106252 |

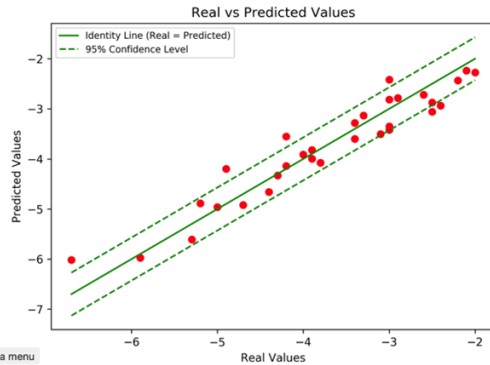


Validation report

QQ Plot



Real Vs Predicted



ay a menu



Validation report

The report is downloadable as PDF



This report has been automatically created by the JaqpotQuatro report service. [Click here to navigate to our official webpage](#)

External validation report

Description: [External validation with model:
<http://jaqpot.org:8080/jaqpot/services/model/72GEEmGhhavY00n7O209> and dataset:
<http://jaqpot.org:8080/jaqpot/services/dataset/XmCQVC7o5jKKRv>]

Model: 72GEEmGhhavY00n7O209

Dataset: XmCQVC7o5jKKRv

Algorithm Type: REGRESSION

F-Value: 247.42

Number of predictor variables: 5

RMSD: 0.34

R² (OECD): 0.9

R² Adjusted (if applicable): 0.9

StdError: 0.35



Model predictions

Welcome bar

Validate me Predict Delete

Jaqpot Actions My resources Welcome back, NanaCommens

Predicted values of dataset #72afckckagyNKRcQCRAt

Search:

| Compound | http://jaqpot.org/WWW/jaqpot.com/chem/chem/leg/leg_?word=&right= predict | Normalized Data | Report |
|------------|--|-----------------|-------------|
| compound1 | -3.91355789467 | 0.773992431967 | QPRF Report |
| compound10 | -2.72064673994 | 0.0 | QPRF Report |
| compound11 | -4.19945022239 | 0.888627058324 | QPRF Report |
| compound12 | -4.96443038285 | 0.777042094673 | QPRF Report |
| compound13 | -2.23685926686 | 0.6621450773 | QPRF Report |
| compound14 | -3.34976177746 | 0.711925639616 | QPRF Report |
| compound15 | -2.27234329025 | 0.711817089278 | QPRF Report |
| compound16 | -3.82107851451 | 0.804959215087 | QPRF Report |
| compound17 | -4.88772442914 | 0.41777676401 | QPRF Report |
| compound18 | -3.5504783112 | 0.791656797678 | QPRF Report |
| compound19 | -6.01794584696 | 0.149905815801 | QPRF Report |
| compound2 | -5.61018322885 | 0.646657429976 | QPRF Report |
| compound20 | -4.33212597512 | 0.524281783472 | QPRF Report |
| compound3 | -3.28038430934 | 0.754141037754 | QPRF Report |
| compound4 | -5.97659581681 | 0.783928066526 | QPRF Report |
| compound5 | -4.14080958734 | 0.468725564498 | QPRF Report |
| compound6 | -3.5059080608 | 0.644248422328 | QPRF Report |



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

Report: #ND0zm2stPTRUQsu [Download](#)

Title: None

Description: None

Date: 14/05/2019

Disclaimer and Instructions: Please fill in the fields of the QPRF

Time: 12:07:22

Title: QSAR Prediction Reporting Format

Version: 1

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 (QSAR) prediction is made. |

2. General information

| Title | Value |
|--------------|------------|
| Date of QPRF | 14/05/2019 |

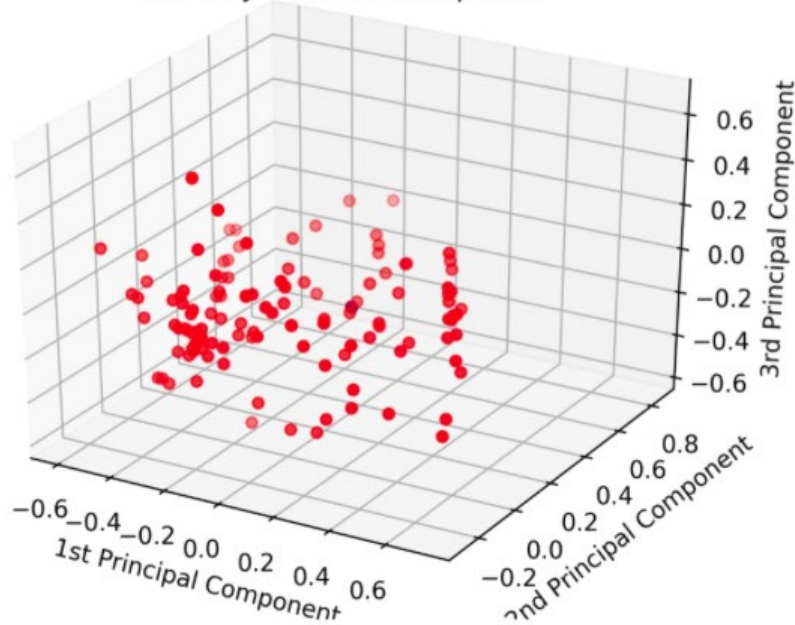


QPRF report

PCA of Query instance vs. Training Dataset

● Original Values ● QPRF Query Values

3D Projection of Datapoints



QPRF report

The report is downloadable as PDF

This report has been automatically created by the JaqpotQuatro report service. [Click here](#) to navigate to our official webpage

Report

Description: [null]

Date: 14/05/2019

Disclaimer and instructions: Please fill in the fields of the QPRF with information about the prediction and the substance for which the prediction is made. The information that you provide will be used to facilitate considerations on the adequacy of the prediction (model result) in relation to a defined regulatory purpose. The adequacy of a prediction depends on the following conditions: a) the (Q)SAR model is scientifically valid: the scientific validity is established according to the OECD principles for (Q)SAR validation; b) the (Q)SAR model is applicable to the query chemical: a (Q)SAR is applicable if the query chemical falls within the defined applicability domain of the model; c) the (Q)SAR result is reliable: a valid (Q)SAR that is applied to a chemical falling within its applicability domain provides a reliable result; d) the (Q)SAR model is relevant for the regulatory purpose: the predicted endpoint can be used directly or following an extrapolation, possibly in combination with other information, for a particular regulatory purpose. A (Q)SAR prediction (model result) may be considered adequate if it is reliable and relevant, and depending on the totality of information available in a weight-of-evidence assessment (see Section 4 of the QPRF).

Time: 12:07:22

Title: QSAR Prediction Reporting Format (QPRF)

Version: 1

Procedure completed on: Tue May 14 12:07:22 UTC 2019

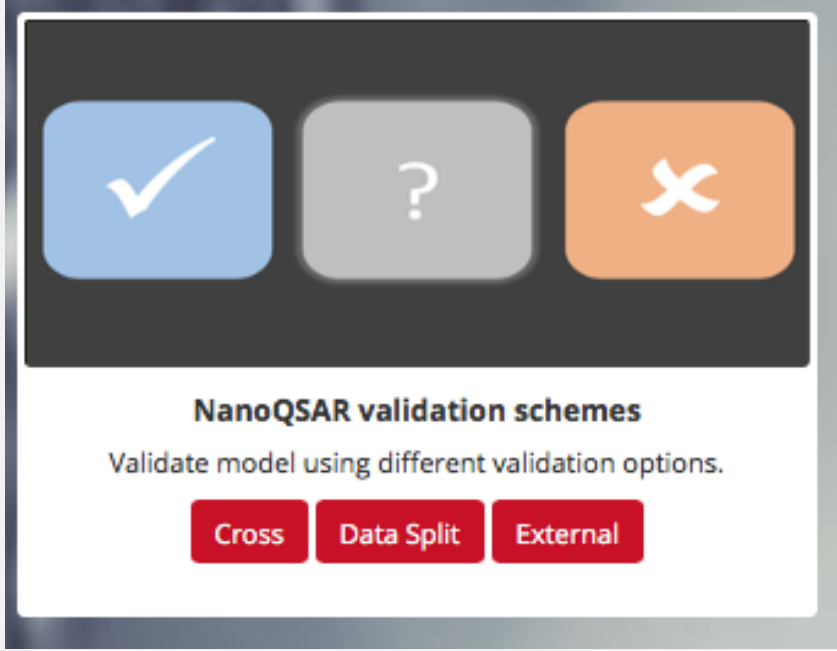
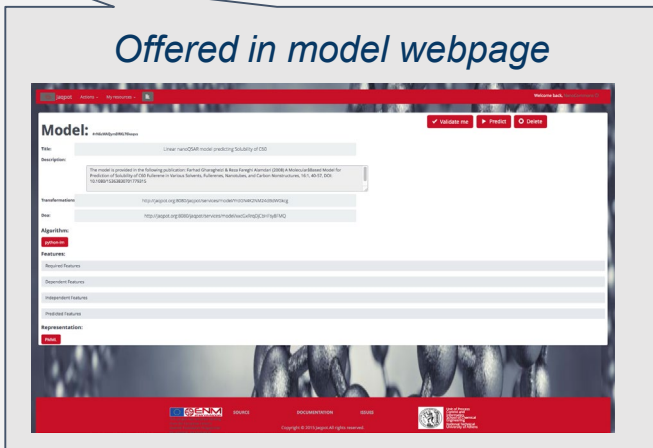


Other model validation options

Options:

- Cross Validation :performs Cross Validation
- Data Split :splits data into training and test datasets according to a split ratio
- External :validation with an external dataset

Offered in model webpage

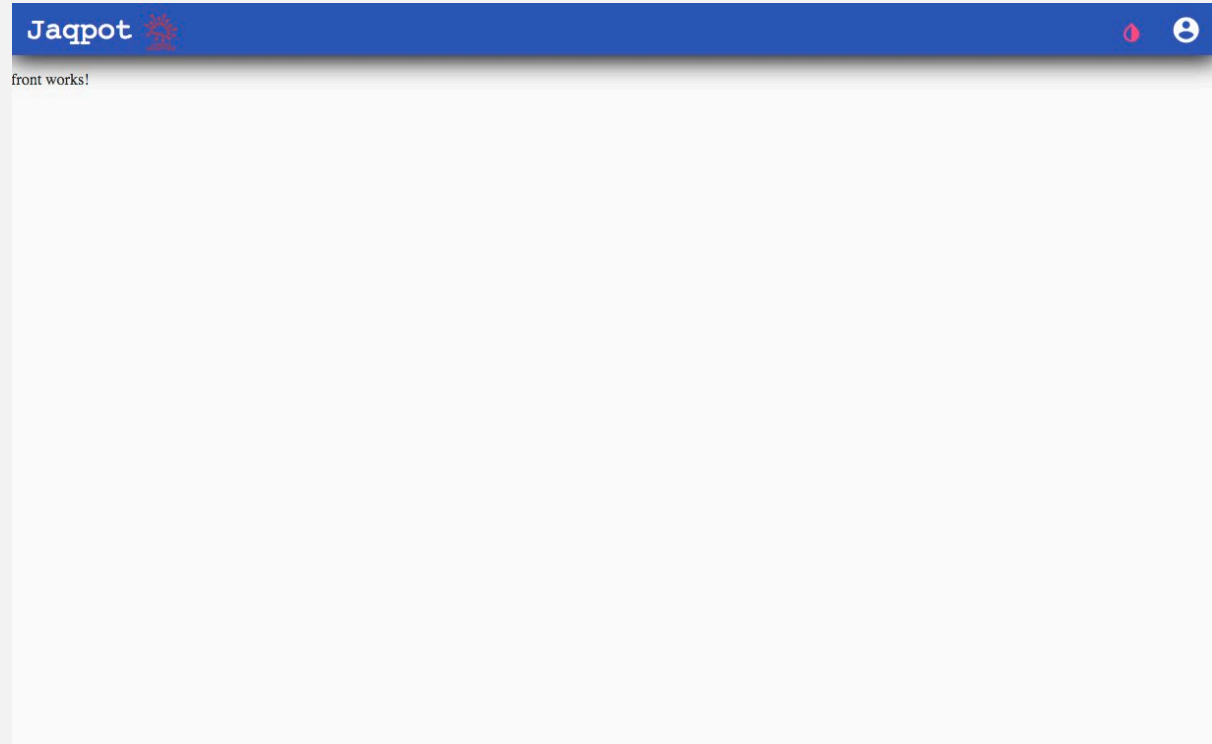


The interface features three large buttons at the top: a blue button with a white checkmark, a grey button with a white question mark, and an orange button with a white 'X'. Below these buttons, the text reads 'NanoQSAR validation schemes' and 'Validate model using different validation options.' At the bottom, there are three red buttons labeled 'Cross', 'Data Split', and 'External'.



Jaqpot 5

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



Jaqpot 5 - Login

JAQPOT

English ▾

Log In

Username or email

Password

Remember me [Forgot Password?](#)

[Log In](#)


[Google](#)

[GitHub](#)

New user? [Register](#)







Jaqpot 5 - User profile - Contact Info









Philip Doganis
filipposd

Organizations On the internet Quota

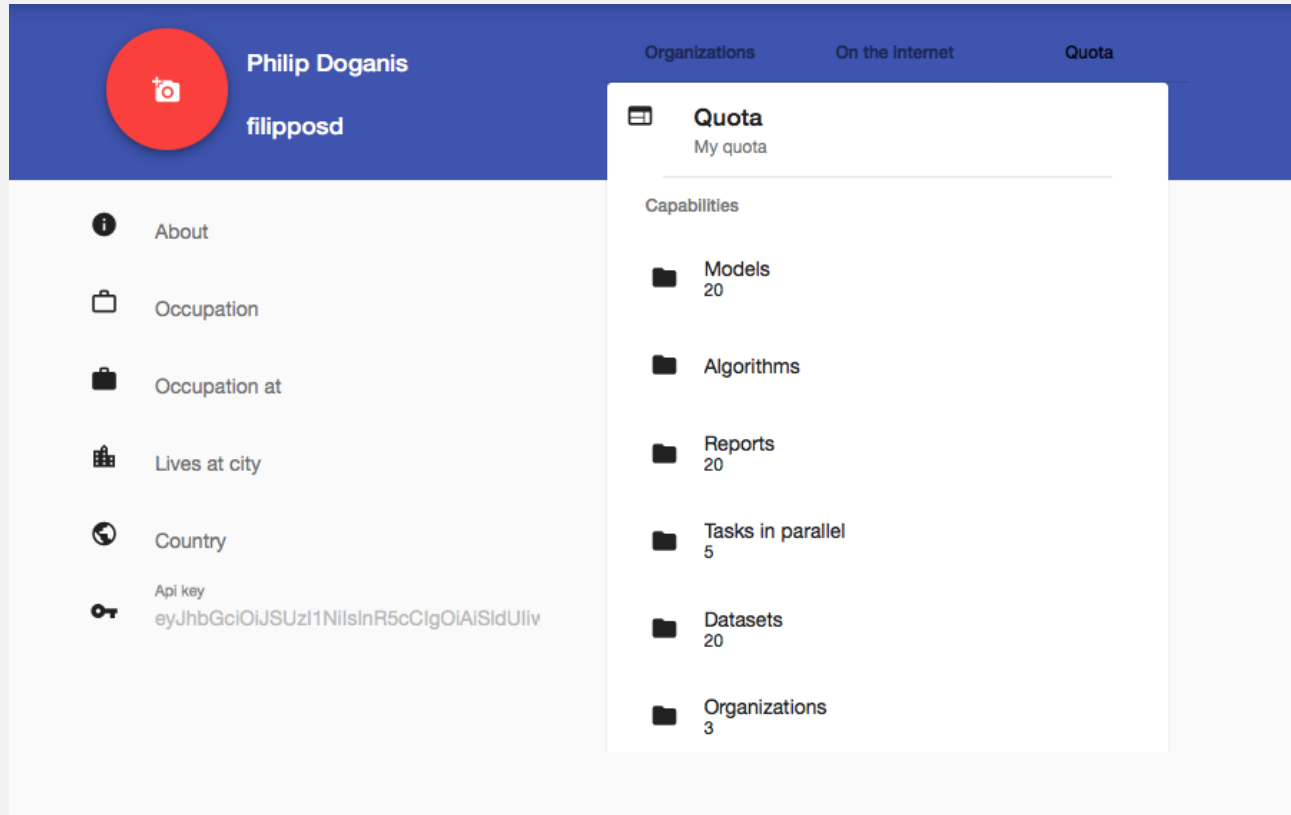
WWW
People can find me on

- Website url 
- Github url 
- Linkedin url 
- Twitter url 

-  About
-  Occupation
-  Occupation at
-  Lives at city
-  Country
-  Api key
eyJhbGciOiJSUzI1NiIsInR5cCI6IkpzZW50L3plYXQifQ.eyJ1IjoiZmliPSd0dG9uIiwiaWF0IjoiMTY1MjM0NTY3In0.



Jaqpot 5 - User profile - Quota



The screenshot displays a user profile for Philip Doganis (username: filipposd) in the Jaqpot 5 interface. The profile is shown in a blue header bar with a red profile picture icon. Below the header, there are navigation tabs for 'Organizations', 'On the internet', and 'Quota'. The 'Quota' tab is active, showing a 'My quota' section with a list of capabilities and their respective limits:

- Models: 20
- Algorithms: (no limit shown)
- Reports: 20
- Tasks in parallel: 5
- Datasets: 20
- Organizations: 3

The left sidebar contains several menu items:

- About
- Occupation
- Occupation at
- Lives at city
- Country
- Api key: eyJhbGciOiJIUzI1NiIsInR5cCIgOiAiSldUiiv



Jaqpot 5 - Organizations

The screenshot displays the Jaqpot user interface. At the top left, the Jaqpot logo and a menu icon are visible. The user's profile header shows a red circular profile picture with a camera icon, the name "Philip Doganis", and the handle "filipposd". Below the profile picture is a vertical list of profile sections: "About", "Occupation", "Occupation at", "Lives at city", "Country", and "Api key" (with a long alphanumeric string). The "Organizations" tab is selected, showing a list of organizations the user is a member of: "NanoCommons", "Jaqpot" (with the Jaqpot logo and "Athens, Greece"), "Lab of Process Control and Informa..." (with "Athens, Greece"), and "OpenRiskNet". A "CREATE" button is located at the bottom of the organizations list. The top right navigation bar includes a search icon, a notification bell with "51", a red heart icon, and a user profile icon. A red circular button with a white icon is located in the bottom right corner of the page.



Jaqpot 5 - Organizations

The screenshot displays the Jaqpot 5 user interface. At the top, the user's profile 'hsarimv' is visible. The main content area is titled 'Organizations' and shows a list of organizations the user is a member of. One organization, 'Jaqpot', is highlighted, showing its location as 'Athens, Greece'. A modal window is open over the 'Jaqpot' entry, displaying details for 'NanoCommons'. The modal includes the contact email 'hsarimv@central.ntua.gr' and an 'About' section describing it as an H2020 infrastructure project. At the bottom of the modal are 'Edit' and 'View' buttons. The background shows a sidebar with navigation icons and a 'CREATE' button at the bottom right.

hsarimv

Organizations
Organizations i am a member

About

NanoCommons

Contact: hsarimv@central.ntua.gr

About

NanoCommons is a H2020 infrastructure project creating a community framework and infrastructure for reproducible science, and in particular for in silico workflows for nanomaterials safety assessment and beyond.

Edit View

CREATE



Jaqpot 5 - NanoCommons Organization page

Description:

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

Creator:

h

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.

Members:

- h
- f
- p
- d
- g



Jaqpot 5 - Sharing of resources

The screenshot shows a user profile for Philip Doganis (filipposd). The profile includes a red circular profile picture with a white camera icon, a search bar, and navigation icons for search, notifications (51), and a user profile. The main content area is divided into two sections: 'Organizations' and 'On the internet'. The 'Organizations' section lists several organizations: Jaqpot, Lab of Process Control and Informa... Athen, NanoCommons, and OpenRiskNet. A 'CREATE' button is visible at the bottom of this list. A sharing menu is open over the 'Jaqpot' entry, displaying a list of sharing options, each with a share icon and the text 'Shared model through Lab ...' or 'Shared model through Nan...'. The left sidebar contains various profile details: About, Occupation, Occupation at, Lives at city, Country, and Api key (eyJhbGciOiJSUzI1NiIsInR5cCIgOiAiSldUliv).



Jaqpot 5 - Sharing notification

MODEL SHARED

model shared through organization OpenRiskNet

| | | |
|-------------|---|---|
| From user | hsarimv | ▼ |
| Shared with | OpenRiskNet | ▼ |
| model | Shin et al. Cytotoxicity classification Model | ▼ |

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



Jaqpot 5 - Home

The screenshot displays the Jaqpot 5 Home interface. The top navigation bar is blue and contains the Jaqpot logo, a search icon, a notification bell with a red '68' badge, a red water drop icon, and a user profile icon. Below the navigation bar, the 'Home' section is active, showing a 'Quick view' of items. The items are organized into three categories: Datasets, Models, and Trash. The Datasets category contains one item: 'Dataset title: Blood-Brain-Barrier Penetration' dated Jun 10, 2019. The Models category contains three items: 'Model title: ORN consensus RFE 5' (Jun 10, 2019), 'Model title: ORN consensus RFE 4' (Jun 10, 2019), and 'Model title: ORN consensus RFE 34' (Jun 7, 2019). The Trash category contains one item: 'Model title: Neural network model predicting DILI' (Mar 14, 2019). On the right side of the interface, a sidebar indicates 'No item selected' with a warning triangle icon.

| Category | Item Title | Date |
|----------|---|--------------|
| Datasets | Dataset title: Blood-Brain-Barrier Penetration | Jun 10, 2019 |
| Models | Model title: ORN consensus RFE 5 | Jun 10, 2019 |
| Models | Model title: ORN consensus RFE 4 | Jun 10, 2019 |
| Models | Model title: ORN consensus RFE 34 | Jun 7, 2019 |
| Trash | Model title: Neural network model predicting DILI | Mar 14, 2019 |



Jaqpot 5 - Shared space - Models

Models ▸ Mine ▸



Model title: ORN consensus RFE 5
Jun 10, 2019

Mine

Shared



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

Jaqpot

Home Models ▸ Shared ▸ With OpenRiskNet ▾

| | | | |
|------------------------------|---|-----------------------------------|----------------------|
| Datasets Shared / Private | Model title: ORN consensus RFE 5 Jun 10, 2019 | Lab of Process Control and Inf... | No item selected |
| Models Shared / Private | Model title: ORN consensus RFE 34 Jun 7, 2019 | NanoCommons | |
| Trash | Model title: Shin et al. Cytotoxicity classification Model May 10, 2019 | OpenRiskNet | |
| | Model title: Linear Model for Predicting Solubility of C60 Fullerenes in Various Solvents Apr 19, 2019 | | |



The jaqpotpy library

<https://jaqpotpy.readthedocs.io/en/latest/>

- jaqpotpy is a python library that integrates fully the python **Scikit-learn** machine learning library with Jaqpot
- Only basic python programming is required to automatically deploy a predictive model as a web service in Jaqpot. Jupyter notebooks are developed to further assist model deployment.
- Similar libraries are under development for the integration of machine learning packages from other languages, R, Julia, Java.

```
from jaqpotpy import Jaqpot
import pandas as pd
from sklearn import linear_model

df2 = pd.read_csv('/path/train.csv')
X2 = df2[['Pclass', 'SibSp', 'Parch', 'Fare']]
y2 = df2['Survived']

clf = LogisticRegression(random_state=0, solver='lbfgs', multi_class='multinomial').fit(X2, y2)

jaqpot.deploy_linear_model(clf, X2, y2, title="Sklearn 2", description="Logistic regression model from python for the tita
algorithm="logistic regression")
```



Automated machine learning

<https://jaqpotpy.readthedocs.io/en/latest/>

Automated machine learning (AutoML) is the process of automating the end-to-end process of applying machine learning methodologies with the goal of maximizing the predictive performance of their final machine learning model:

- data pre-processing
- feature extraction
- feature selection
- algorithm selection
- hyperparameter optimization

Examples of AutoML platforms

- **DataRobots**: a commercial platform for AutoML
- **Auto-sklearn**: a Bayesian hyperparameter optimization layer on top of **scikit-learn**
- **TPOT**: a genetic programming optimization layer on top of **scikit-learn** that automatically creates and optimizes full machine learning pipelines.
- **Auto-WEKA**: a Bayesian hyperparameter optimization layer on top of **WEKA**
- **RRegrs**¹: an exhaustive search layer on top of **Caret** (NTUA, University of Maastricht)

¹Tsiliki G, Munteanu CR, Seoane JA, Fernandez-Lozano C., Sarimveis H., Willighagen EL, (2015) RRegrs: an R package for computer-aided model selection with multiple regression models, Journal of Cheminformatics20157:46, <https://doi.org/10.1186/s13321-015-0094-2>



Jaqpot 5 – Create and deploy a nanoQSAR model using a Jupyter notebook

```
import pandas as pd
from jaqpotpy import Jaqpot
from sklearn.linear_model import LinearRegression
from sklearn.preprocessing import MinMaxScaler
from sklearn.pipeline import Pipeline
from sklearn.model_selection import train_test_split
from sklearn.model_selection import cross_val_score, GridSearchCV, RandomizedSearchCV
df=pd.read_csv('C:\\MyDocuments\\European-funded\\Trexonta\\NanoCommons\\Actual Project\\WP5\\NanoQSAR deliverable\\
A Molecular Based Model for Prediction of Solubility of C60 in Various Solvents\\70_model_reduced.csv') # Reads the data
```

```
Xall=df[['piPC03', 'ATS1m', 'Seigp', 'More23e', 'H1m']] # Defines the columns that will be used as independent features
Yall=df['logS Exp.1'] # Defines the end-point
X_train, X_test, Y_train, Y_test = train_test_split(Xall, Yall, train_size=0.75, test_size=0.25, random_state=1)
# Splits the data into training and test sets
stepslinear = [('scaler', MinMaxScaler()), ('MLR', LinearRegression())]
pipelinelinear = Pipeline(stepslinear) # define the pipeline object.
cross_val_score(estimator=pipelinelinear, X=X_train, y=Y_train, cv=5, n_jobs=-1) #Performs a 5-fold cross validation
```

```
pipelinelinear.fit(X_train, Y_train)
print("Training score: ", pipelinelinear.score(X_train, Y_train))
print("Testing score: ", pipelinelinear.score(X_test, Y_test))
print("Total score: ", pipelinelinear.score(Xall, Yall)) #Trains the model and prints R^2 statistics
```

```
jaqpot = Jaqpot("https://api.jaqpot.org/jaqpot/services/")
jaqpot.request_key_safe()
```

```
jaqpot.deploy_pipeline(pipelinelinear,Xall,Yall,"Linear Model for Predicting Solubility of C60 Fullerenes in Various Solvents","Linear
Model","linearmodel")
```



Jaqpot 5 - Model page

<https://app.jaqpot.org/model/uxRBCMsv9lkSGT1Kw7km>

The screenshot shows a web browser window with the Jaqpot logo and navigation tabs: Overview, Data, Predict / Validate, and Discussion. The main content area displays the following information:

- 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
- 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 app.jaqpot.org
 - 2. General Information**
 - 2.1. Date of QMRF:**



Jaqpot 5 - QMRF report



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:

Jaqpot
Jaqpot is a web platform that supports development, validation and sharing of QSAR models
Haralambos Sarimveis
apps.jaqpot.org

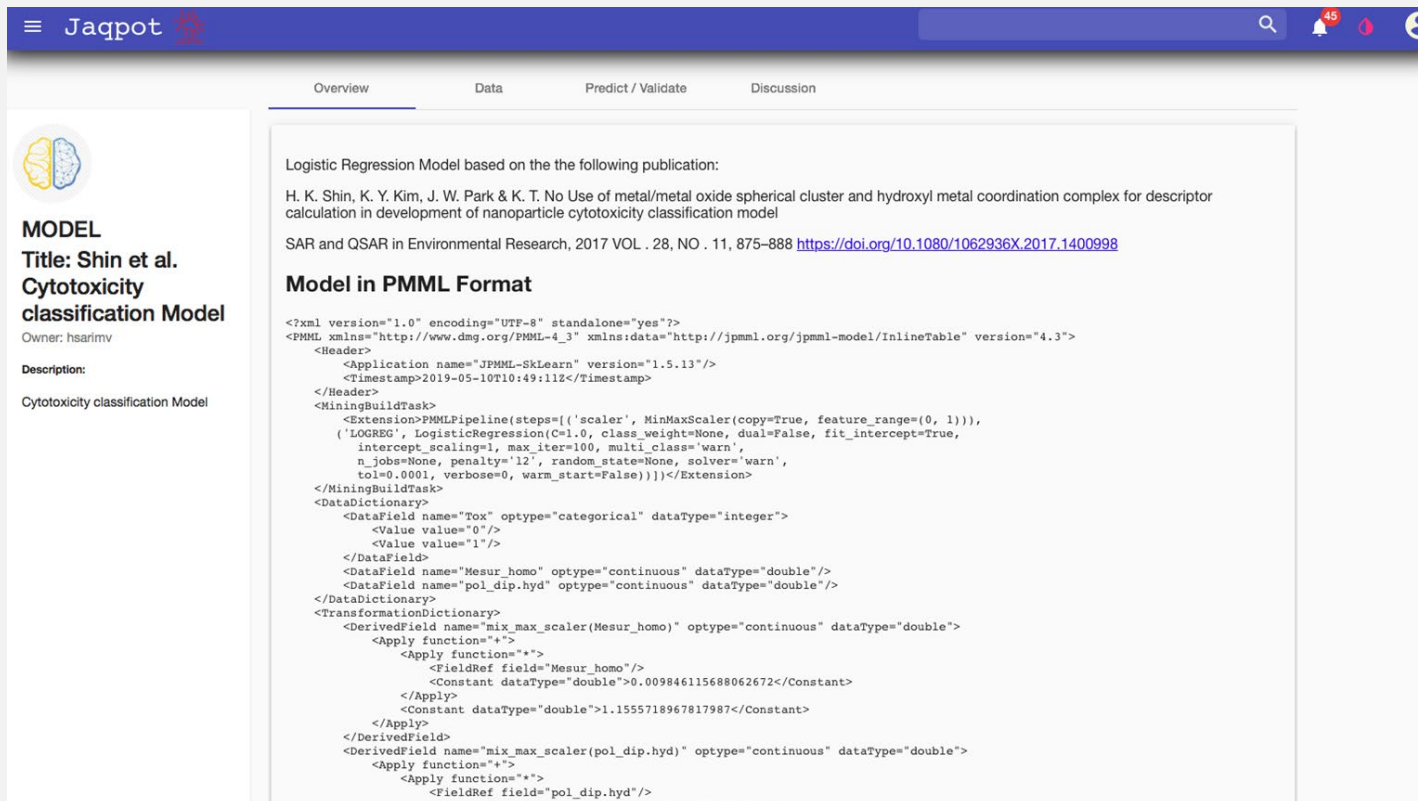
2. General information

2.1. Date of QMRF:

21 April 2019



Jaqpot 5 – PMML representation



The screenshot displays the Jaqpot 5 web interface. The top navigation bar includes a search icon, a notification bell with '45' alerts, and a user profile icon. Below the navigation bar are tabs for 'Overview', 'Data', 'Predict / Validate', and 'Discussion'. The 'Overview' tab is active, showing a model overview on the left and the PMML code on the right.

MODEL
Title: Shin et al. Cytotoxicity classification Model
Owner: hsarimv
Description: Cytotoxicity classification Model

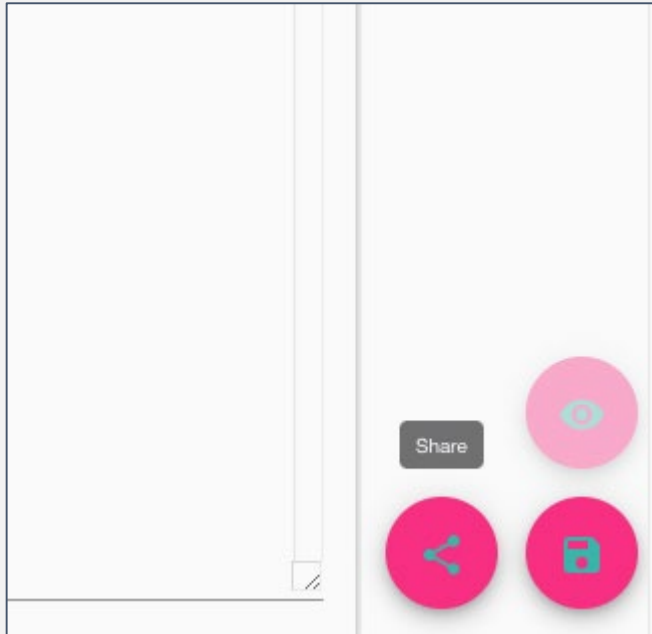
Logistic Regression Model based on the the following publication:
H. K. Shin, K. Y. Kim, J. W. Park & K. T. No Use of metal/metal oxide spherical cluster and hydroxyl metal coordination complex for descriptor calculation in development of nanoparticle cytotoxicity classification model
SAR and QSAR in Environmental Research, 2017 VOL . 28, NO . 11, 875-888 <https://doi.org/10.1080/1062936X.2017.1400998>

Model in PMML Format

```
<?xml version="1.0" encoding="UTF-8" standalone="yes"?>
<PMML xmlns="http://www.dmg.org/PMML-4_3" xmlns:data="http://jpmml.org/jpmml-model/InlineTable" version="4.3">
  <header>
    <Application name="JPMML-SkLearn" version="1.5.13"/>
    <Timestamp>2019-05-10T10:49:11Z</Timestamp>
  </header>
  <MiningBuildTask>
    <Extension>PMMLPipeline(steps=[('scaler', MinMaxScaler(copy=True, feature_range=(0, 1))),
    ('LOGREG', LogisticRegression(C=1.0, class_weight=None, dual=False, fit_intercept=True,
    intercept_scaling=1, max_iter=100, multi_class='warn',
    n_jobs=None, penalty='l2', random_state=None, solver='warn',
    tol=0.0001, verbose=0, warm_start=False))])</Extension>
  </MiningBuildTask>
  <DataDictionary>
    <DataField name="Tox" otype="categorical" dataType="integer">
      <Value value="0"/>
      <Value value="1"/>
    </DataField>
    <DataField name="Mesur_homo" otype="continuous" dataType="double"/>
    <DataField name="pol_dip_hyd" otype="continuous" dataType="double"/>
  </DataDictionary>
  <TransformationDictionary>
    <DerivedField name="mix_max_scaler(Mesur_homo)" otype="continuous" dataType="double">
      <Apply function="+">
        <Apply function="*">
          <FieldRef field="Mesur_homo"/>
          <Constant dataType="double">0.009846115688062672</Constant>
        </Apply>
        <Constant dataType="double">1.1555718967817987</Constant>
      </Apply>
    </DerivedField>
    <DerivedField name="mix_max_scaler(pol_dip_hyd)" otype="continuous" dataType="double">
      <Apply function="+">
        <Apply function="*">
          <FieldRef field="pol_dip_hyd"/>
          <Constant dataType="double">0.2425100174825472</Constant>
        </Apply>
      </Apply>
    </DerivedField>
  </TransformationDictionary>
</PMML>
```



Jaqpot 5 - Model page



Share model

| Read | Write | Execute |
|---|---|---|
| <input checked="" type="checkbox"/> Lab Of Process Control and Informatic | <input checked="" type="checkbox"/> Lab Of Process Control and Informatic | <input checked="" type="checkbox"/> Lab Of Process Control and Informatic |
| <input checked="" type="checkbox"/> NanoCommons | <input checked="" type="checkbox"/> NanoCommons | <input checked="" type="checkbox"/> NanoCommons |

Notes about sharing

Deleting is only available for the creator

When something is shared with Jaqpot it becomes available for all the users

The privileges are given to all the users of an organization whared with

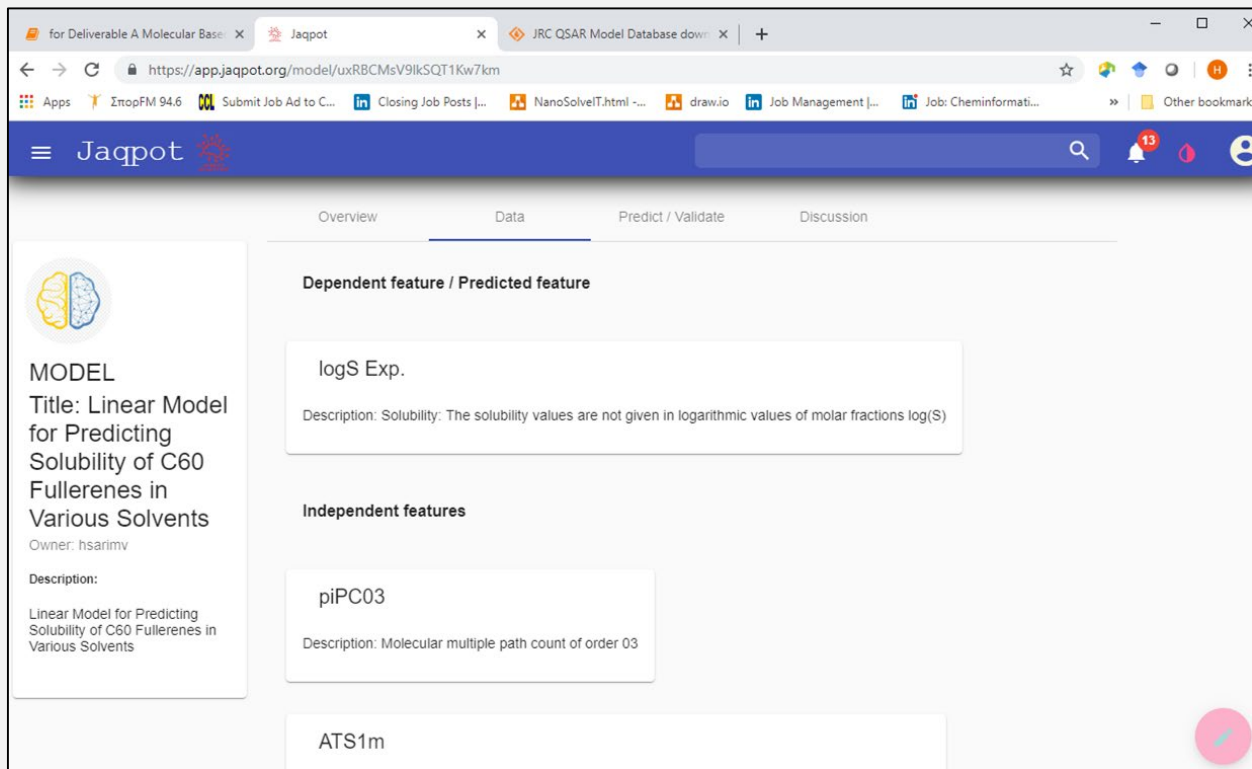
View

Affiliated Orgs

1.2.Other related models:



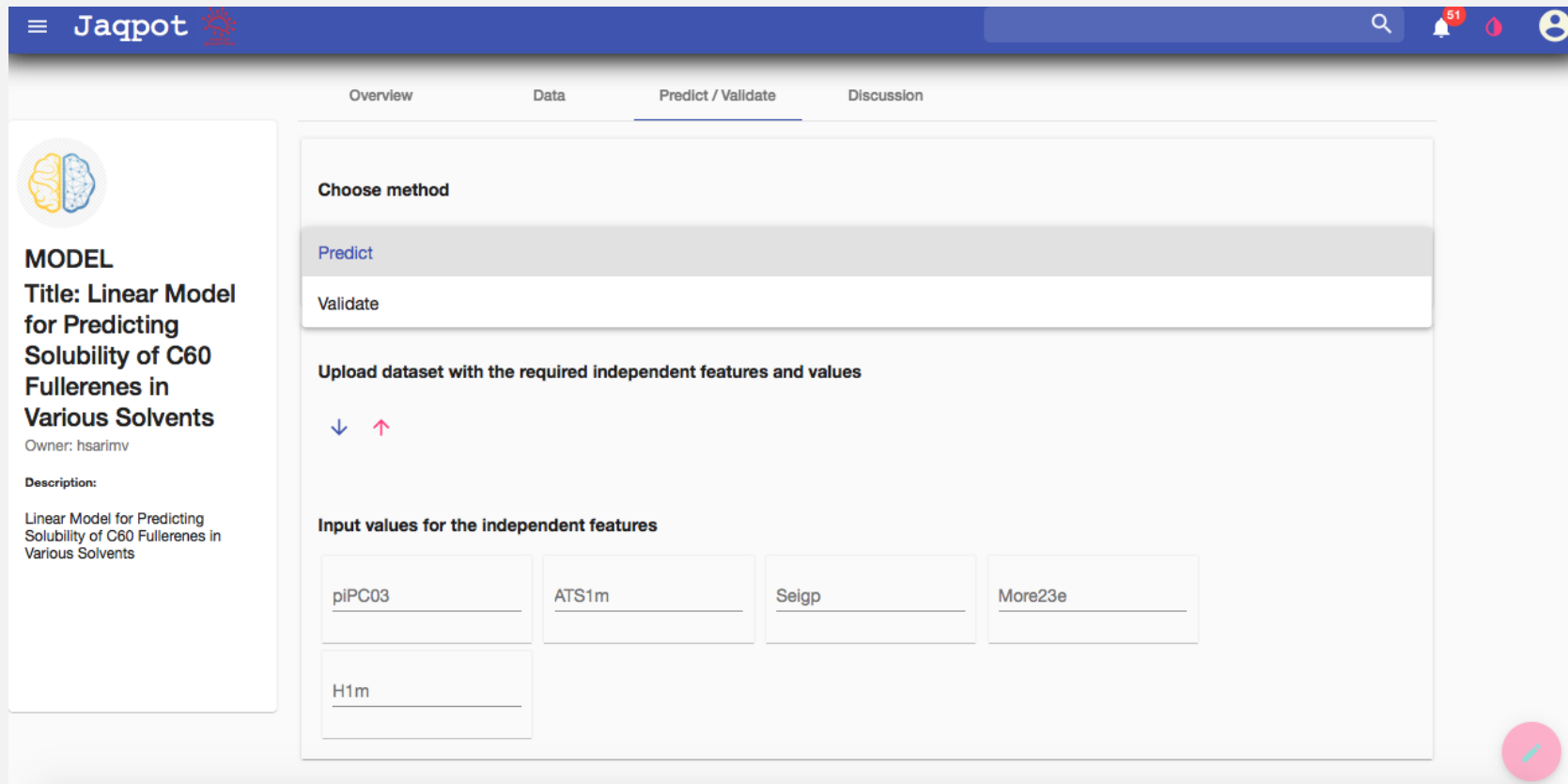
Jaqpot 5 - Model page - Data tab



The screenshot shows a web browser window displaying the Jaqpot 5 Model page for a specific model. The browser's address bar shows the URL <https://app.jaqpot.org/model/uxRBCMsv9IkSQT1Kw7km>. The page has a blue header with the Jaqpot logo and navigation tabs: Overview, Data (selected), Predict / Validate, 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 "Dependent feature / Predicted feature" and lists three features: **logS Exp.** (Description: Solubility: The solubility values are not given in logarithmic values of molar fractions log(S)), **piPC03** (Description: Molecular multiple path count of order 03), and **ATS1m**. A pink circular icon with a pencil is visible in the bottom right corner of the page.



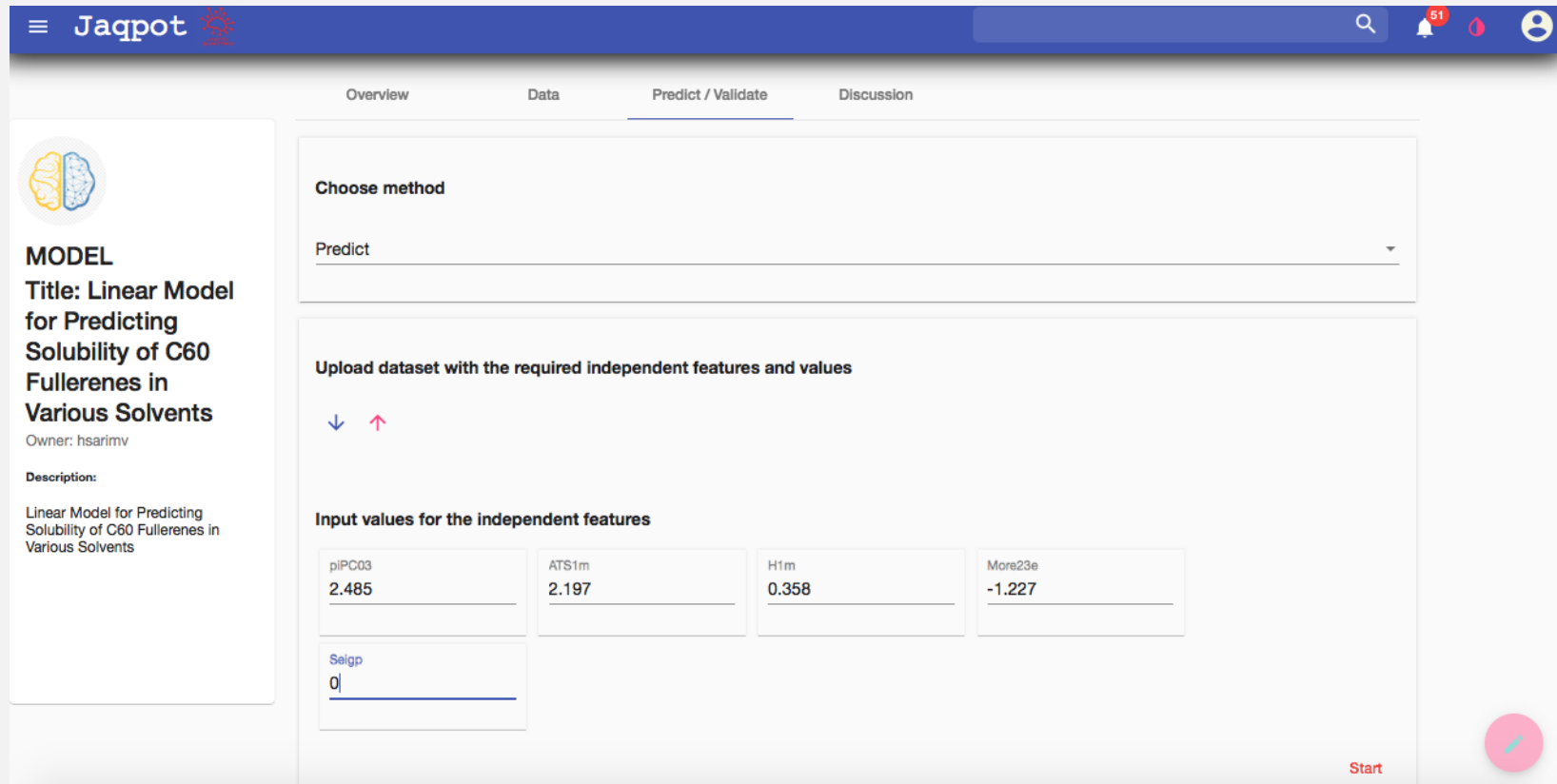
Jaqpot 5 - Model page – Predict/Validate tab



The screenshot shows the Jaqpot 5 web 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 (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 has a 'Choose method' section with two buttons: 'Predict' (highlighted) and 'Validate'. Below this is an 'Upload dataset with the required independent features and values' section with a download icon and an upload icon. The 'Input values for the independent features' section contains five input fields with the following values: piPC03, ATS1m, Seigp, More23e, and H1m. A red circular button with a pencil icon is located in the bottom right corner of the main content area.



Jaqpot 5 - Predict - Entering values

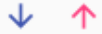


The screenshot shows the Jaqpot 5 web interface. The top navigation bar is blue with the Jaqpot logo and a search icon. Below the navigation bar, there are four tabs: Overview, Data, Predict / Validate (which is active), and Discussion. On the left side, there is a sidebar with a brain icon and the following text: **MODEL**, **Title: Linear Model for Predicting Solubility of C60 Fullerenes in Various Solvents**, and **Owner: hсарimv**. Below this, there is a **Description:** section with the text: **Linear Model for Predicting Solubility of C60 Fullerenes in Various Solvents**. The main content area is divided into three sections: **Choose method** with a dropdown menu set to 'Predict'; **Upload dataset with the required independent features and values** with a download icon and an upload icon; and **Input values for the independent features** with four input fields: 'piPC03' (2.485), 'ATS1m' (2.197), 'H1m' (0.358), and 'More23e' (-1.227). Below these fields is another input field for 'Seigp' with the value '0'. At the bottom right of the main content area, there is a red 'Start' button and a pink circular icon with a pencil.



Jaqpot 5 - Predict - Downloading 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



Jaqpot 5 - Predict - Editing template

C60 Fullerenes Test Data - Excel

File Home Insert Page Layout Formulas Data Review View Acrobat Tell me what you want to do... Sign in Share

Clipboard Font Alignment Number Styles Cells Editing

K8

| | A | B | C | D | E | F | G | H | I | J | K | L | M | N | O | P | Q |
|----|-------------------------|--------|-------|-------|---------|-------|-----------|---|---|---|---|---|---|---|---|---|---|
| 1 | Solvents | piPC03 | ATS1m | Seigp | More23e | H1m | logS Exp. | | | | | | | | | | |
| 2 | 1,2,3-trichloropropane | 1.609 | 2.473 | 0.578 | 0.025 | 0.927 | -4 | | | | | | | | | | |
| 3 | N,N-dimethylformamic | 1.609 | 1.763 | -1.8 | 0.022 | 0.328 | -5.3 | | | | | | | | | | |
| 4 | n-butylbenzene | 3.426 | 2.398 | 0 | -1.159 | 0.449 | -3.4 | | | | | | | | | | |
| 5 | 1-butanol | 1.099 | 1.674 | -1.2 | -0.449 | 0.192 | -5.9 | | | | | | | | | | |
| 6 | 1,3-dibromopropane | 1.099 | 2.792 | 0.846 | -0.614 | 1.495 | -4.2 | | | | | | | | | | |
| 7 | 1,1,2,2-tetrachloroetha | 1.609 | 2.625 | 0.771 | 0.212 | 0.925 | -3.1 | | | | | | | | | | |
| 8 | 1,2,3,4-tetramethylben | 3.778 | 2.398 | 0 | -0.549 | 0.353 | -2.9 | | | | | | | | | | |
| 9 | 1,3-diiodopropane | 1.099 | 3.184 | 1.342 | -0.322 | 2.213 | -3.4 | | | | | | | | | | |
| 10 | R,R,R-trichlorotoluene | 3.548 | 2.825 | 0.578 | -0.288 | 1.259 | -3 | | | | | | | | | | |
| 11 | 1,3-dibromobenzene | 3.409 | 3.011 | 0.846 | -0.468 | 2.212 | -2.6 | | | | | | | | | | |
| 12 | tetrahydrothiophene | 1.792 | 2.234 | 0.393 | -0.334 | 0.552 | -4.9 | | | | | | | | | | |
| 13 | 1,2-dichloroethane | 0.693 | 2.067 | 0.385 | 0.031 | 0.432 | -5 | | | | | | | | | | |
| 14 | dimethylnaphthalenes | 4.311 | 2.639 | 0 | -0.859 | 0.516 | -2.1 | | | | | | | | | | |
| 15 | 2-methylthiophene | 3.108 | 2.236 | 0.393 | -0.17 | 0.577 | -3 | | | | | | | | | | |
| 16 | 1-chloronaphthalene | 4.227 | 2.705 | 0.193 | -0.7852 | 0.836 | -2 | | | | | | | | | | |
| 17 | aniline | 3.248 | 2.1 | -0.6 | -0.504 | 0.351 | -3.9 | | | | | | | | | | |
| 18 | octane | 1.792 | 2.079 | 0 | -1.656 | 0.208 | -5.2 | | | | | | | | | | |
| 19 | benzonitrile | 3.548 | 2.216 | -0.6 | -0.437 | 0.592 | -4.2 | | | | | | | | | | |
| 20 | nitroethane | 1.609 | 1.836 | -3 | -0.029 | 0.54 | -6.7 | | | | | | | | | | |
| 21 | 1-iodo-2-methylpropan | 1.099 | 2.679 | 0.671 | -0.476 | 1.464 | -4.3 | | | | | | | | | | |
| 22 | 1,2,4-trimethylbenzene | 3.59 | 2.303 | 0 | -0.546 | 0.338 | -2.5 | | | | | | | | | | |
| 23 | bromobenzene | 3.248 | 2.614 | 0.423 | -0.552 | 1.267 | -3.3 | | | | | | | | | | |
| 24 | 1,2-dichlorobenzene | 3.458 | 2.557 | 0.385 | -0.364 | 1.084 | -2.4 | | | | | | | | | | |
| 25 | 1-methyl-1-cyclohexen | 2.565 | 2.079 | 0 | -0.597 | 0.295 | -3.8 | | | | | | | | | | |

C60 Fullerenes Test Data

Ready 100%



Jaqqot 5 - Predict - Uploading data

Upload dataset with the required independent features and values



Upload dataset (should at least contain independent features)

Input values for the independent features

piPC03

ATS1m


Seigp

H1m

More23e



Jaqpot 5 - Predict - Uploading data

Jaqpot 

Predicting Solubility of C60 Fullerenes in Various Solvents11
Owner: hсарimv
Description: Neural Model


Upload dataset with the required independent features and values

↓ ↑

Dataset formed

| Id | piPC03 | More23e | Seigp | ATS1m | H1m |
|------------------------|--------|---------|-------|-------|-------|
| 1,3-Br-Cl-benzene | 3.409 | -0.421 | 0.616 | 2.81 | 1.669 |
| 2-iodo-2-methylpropane | 0 | -0.375 | 0.671 | 2.679 | 0.96 |
| 1,1,1-trichloroethane | 0 | 0.109 | 0.578 | 2.385 | 0.761 |
| tetralin | 3.707 | -0.869 | 0 | 2.485 | 0.493 |
| nitrobenzene | 3.631 | -0.422 | -3 | 2.423 | 0.747 |
| 1-methylnaphthalene | 4.227 | -0.863 | 0 | 2.565 | 0.535 |
| chlorobenzene | 3.248 | -0.476 | 0.193 | 2.298 | 0.721 |

Erase dataset Start procedure



Jaqpot 5 – Calculating predictions

The screenshot displays the Jaqpot 5 web interface. The top navigation bar is blue and contains the Jaqpot logo, a search icon, a notification bell with a red '51' badge, a red drop icon, and a user profile icon. On the left side, there is a sidebar with the following information:

- Title:** Linear Model for Predicting Solubility of C60 Fullerenes in Various Solvents
- Owner:** hсарimv
- Description:** Linear Model for Predicting Solubility of C60 Fullerenes in Various Solvents

The main content area shows a log of a prediction task:


- 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.**

At the bottom of the log, there is a checkmark icon and a button labeled "View Prediction".

At the bottom left of the interface, there is a button labeled "Display a menu". At the bottom right, there is a pink circular button with a pencil icon.



Jaqpot 5 – Displaying predictions

Jaqpot 


86

View predicted value only

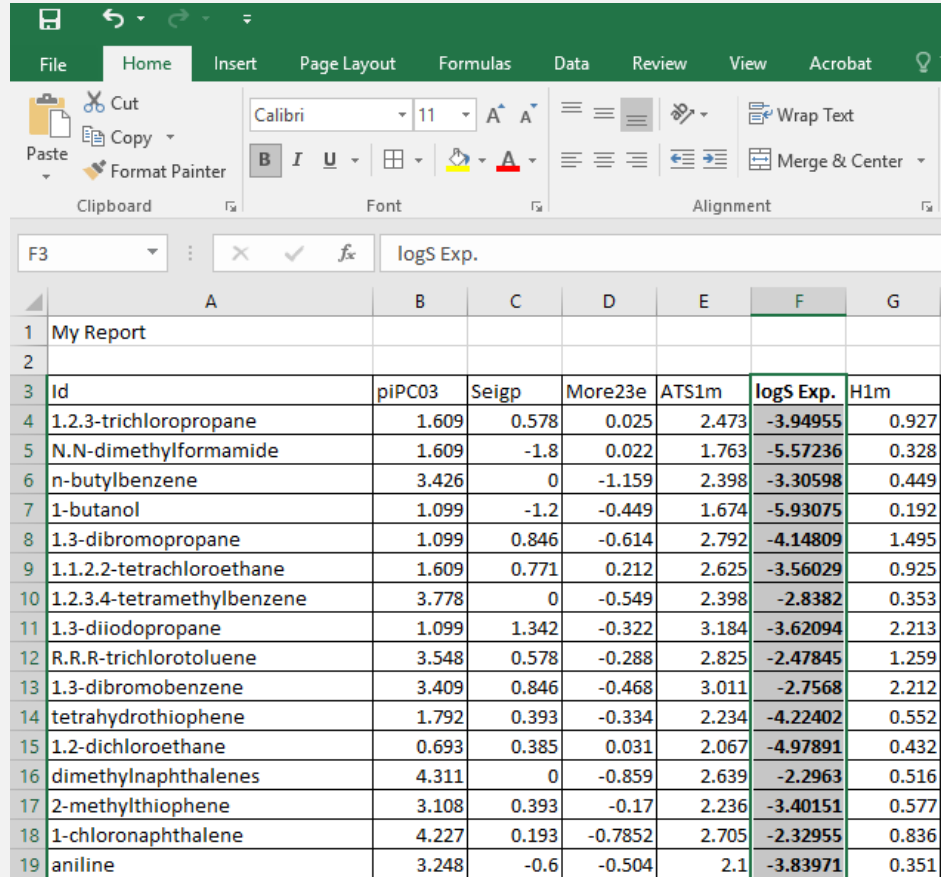
| Id | piPC03 | Seigp | More23e | ATS1m | logS Exp. | H1m |
|------------------------|--------|-------|---------|-------|---------------------|-------|
| benzonitrile | 3.548 | -0.6 | -0.437 | 2.216 | -3.573224659989597 | 0.592 |
| nitroethane | 1.609 | -3 | -0.029 | 1.836 | -5.942685616120331 | 0.54 |
| 1-iodo-2-methylpropane | 1.099 | 0.671 | -0.476 | 2.679 | -4.335365062673921 | 1.464 |
| 1.2.4-trimethylbenzene | 3.59 | 0 | -0.546 | 2.303 | -3.106857374005953 | 0.338 |
| bromobenzene | 3.248 | 0.423 | -0.552 | 2.614 | -3.1667103426568666 | 1.267 |
| 1.2-dichlorobenzene | 3.458 | 0.385 | -0.364 | 2.557 | -2.986707060947116 | 1.084 |
| 1-methyl-1-cyclohexene | 2.565 | 0 | -0.597 | 2.079 | -4.0994582410835925 | 0.295 |

Items per page: 30 1 - 30 of 31

[Download](#)



Jaqpot 5 - Predictions as CSV

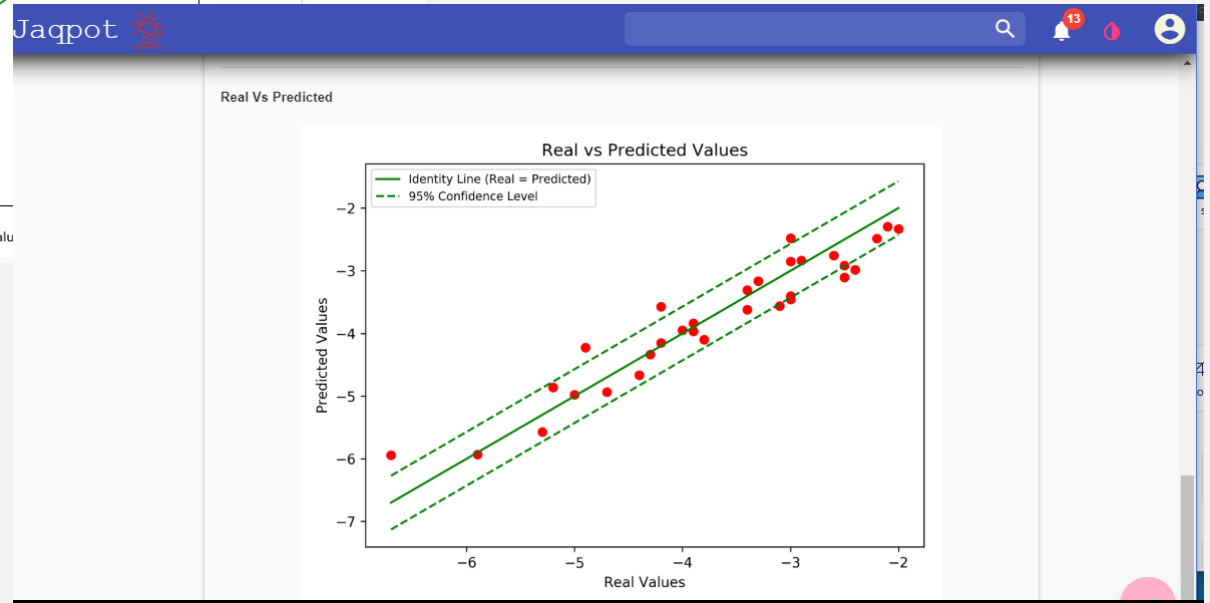
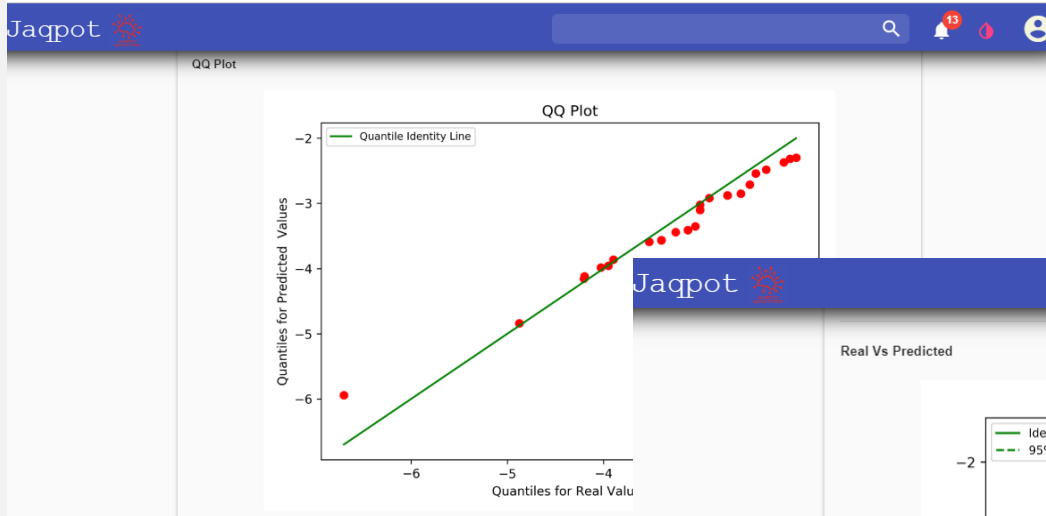


The screenshot shows an Excel spreadsheet with the following data:

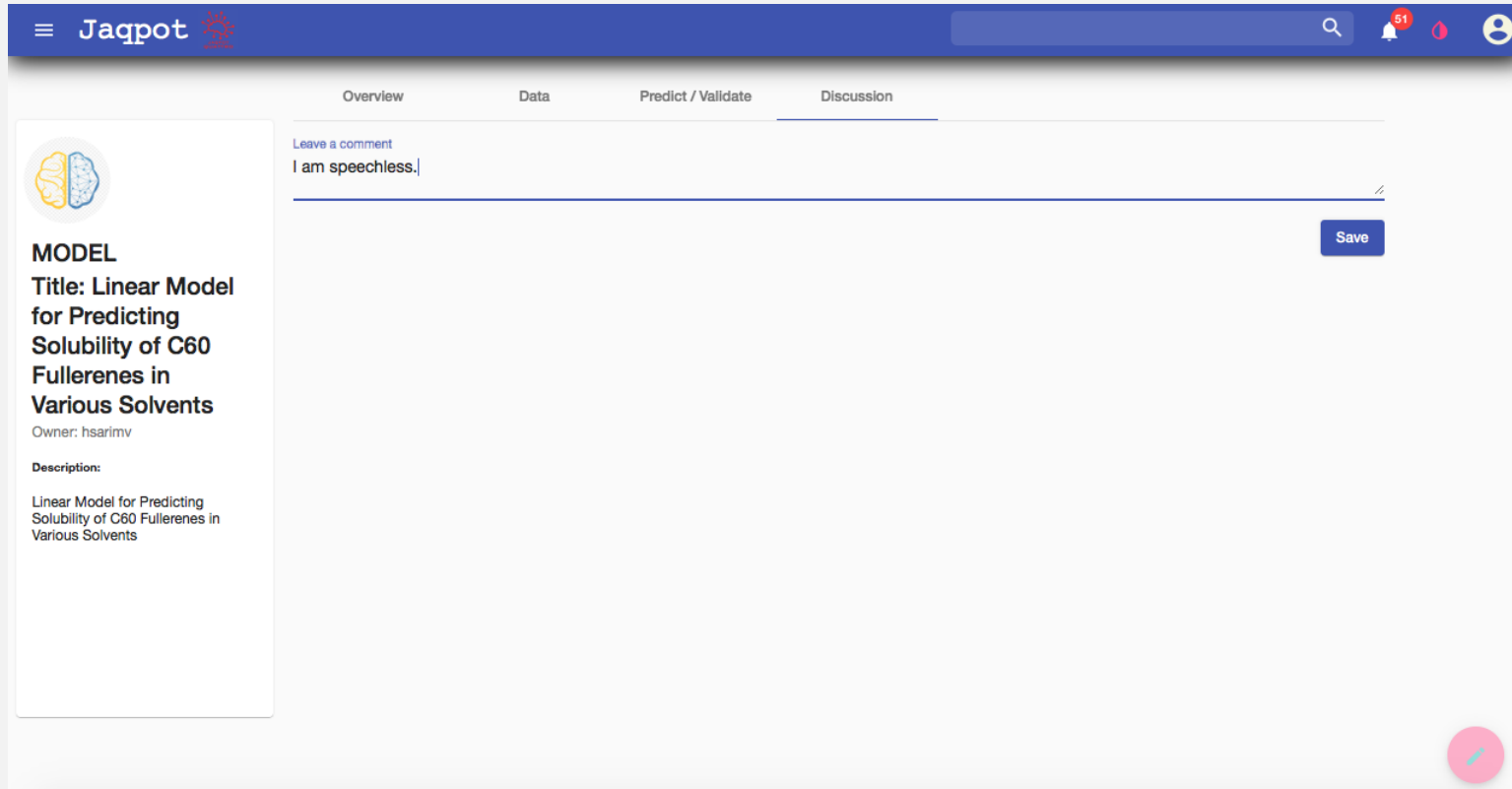
| | A | B | C | D | E | F | G |
|----|----------------------------|--------|-------|---------|-------|-----------|-------|
| 1 | My Report | | | | | | |
| 2 | | | | | | | |
| 3 | Id | piPC03 | Seigp | More23e | ATS1m | logS Exp. | H1m |
| 4 | 1.2.3-trichloropropane | 1.609 | 0.578 | 0.025 | 2.473 | -3.94955 | 0.927 |
| 5 | N,N-dimethylformamide | 1.609 | -1.8 | 0.022 | 1.763 | -5.57236 | 0.328 |
| 6 | n-butylbenzene | 3.426 | 0 | -1.159 | 2.398 | -3.30598 | 0.449 |
| 7 | 1-butanol | 1.099 | -1.2 | -0.449 | 1.674 | -5.93075 | 0.192 |
| 8 | 1.3-dibromopropane | 1.099 | 0.846 | -0.614 | 2.792 | -4.14809 | 1.495 |
| 9 | 1.1.2.2-tetrachloroethane | 1.609 | 0.771 | 0.212 | 2.625 | -3.56029 | 0.925 |
| 10 | 1.2.3.4-tetramethylbenzene | 3.778 | 0 | -0.549 | 2.398 | -2.8382 | 0.353 |
| 11 | 1.3-diiodopropane | 1.099 | 1.342 | -0.322 | 3.184 | -3.62094 | 2.213 |
| 12 | R,R,R-trichlorotoluene | 3.548 | 0.578 | -0.288 | 2.825 | -2.47845 | 1.259 |
| 13 | 1.3-dibromobenzene | 3.409 | 0.846 | -0.468 | 3.011 | -2.7568 | 2.212 |
| 14 | tetrahydrothiophene | 1.792 | 0.393 | -0.334 | 2.234 | -4.22402 | 0.552 |
| 15 | 1.2-dichloroethane | 0.693 | 0.385 | 0.031 | 2.067 | -4.97891 | 0.432 |
| 16 | dimethylnaphthalenes | 4.311 | 0 | -0.859 | 2.639 | -2.2963 | 0.516 |
| 17 | 2-methylthiophene | 3.108 | 0.393 | -0.17 | 2.236 | -3.40151 | 0.577 |
| 18 | 1-chloronaphthalene | 4.227 | 0.193 | -0.7852 | 2.705 | -2.32955 | 0.836 |
| 19 | aniline | 3.248 | -0.6 | -0.504 | 2.1 | -3.83971 | 0.351 |



Jaqpot 5 – Model validation



Jaqpot 5 - Social network of models



The screenshot displays the Jaqpot 5 web interface. At the top, there is a blue navigation bar with the Jaqpot logo and a search bar. Below the navigation bar, there are four tabs: Overview, Data, Predict / Validate, and Discussion. The Discussion tab is currently selected. On the left side, there is a model card with a brain icon. The model title is "Linear Model for Predicting Solubility of C60 Fullerenes in Various Solvents" and the owner is "hsarimv". The description is "Linear Model for Predicting Solubility of C60 Fullerenes in Various Solvents". In the center, there is a comment input field with the text "I am speechless." and a "Save" button. A pink circular button with a pencil icon is visible in the bottom right corner.

Jaqpot

Overview Data Predict / Validate Discussion

Leave a comment

I am speechless.

Save

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



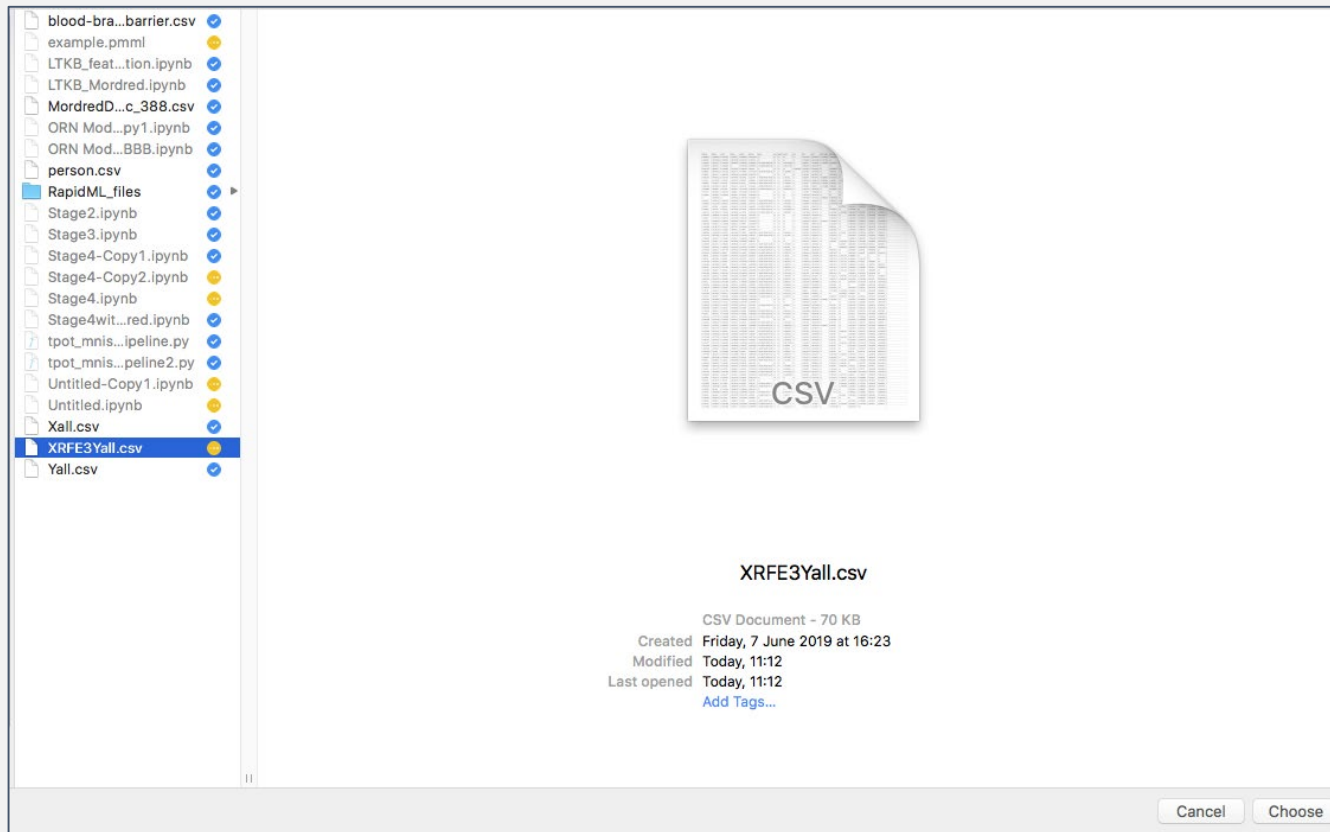
Jaqpote library of nanoQSAR models

Jaqpote 4/NanoCommons account, Jaqpote 5/ Nanocommons organization

| | Model description | Endpoint | Model URIs |
|----|--|---|--|
| 1 | Methodology for developing structure-activity evaluation to identify combinations of physical features of nanomaterial that influence potential cell damage by MLR/LDA (TiO ₂ case) Sayes & Ivanov (2010) | In vitro - Cytotoxicity - membrane damage measured as lactate dehydrogenase (LDH) release [units/L] | Jaqpote 4: http://jaqpote.org/m_detail?name=2KoKHcigMjloSeWuZ03a Jaqpote 5: https://app.jaqpote.org/model/izMnmcn5LMbgC6o7Fkj8 |
| 2 | Methodology for developing structure-activity evaluation to identify combinations of physical features of nanomaterial that influence potential cell damage by MLR/LDA (ZnO case) Sayes & Ivanov (2010) | In vitro - Cytotoxicity - membrane damage measured as lactate dehydrogenase (LDH) release [units/L] | Jaqpote 4: http://jaqpote.org/m_detail?name=cm49kGhUjkMw6wyntKQF Jaqpote 5: https://app.jaqpote.org/model/fvAe4KniOOiNgGf7Ve1p |
| 3 | Regression model to understand the aggregated ZVCN against E.Coli by MLR (Placket-Burman design) Rispoli et al. (2010) | In vitro - Cytotoxicity - measured as percentage of dead E. Coli population | Jaqpote 4: http://jaqpote.org/m_detail?name=48JYATzOKFTkzJGd8AFs Jaqpote 5: https://app.jaqpote.org/model/8su6n4cfcjzZD2NDZGN |
| 4 | Prediction of the Biological surface adsorption index (BSAI) on different NPs by MLR Xia et al. (2011) | log(k) k: adsorption coefficient | Jaqpote 4: http://jaqpote.org/m_detail?name=DjRQk8AqG42nckg5KoxZ Jaqpote 5: https://app.jaqpote.org/model/gSvjUz17EEAV5OWL7Uls |
| 5 | Predictive model of TiO ₂ NPs damage on membrane cell by SMILES-based optimal descriptor and Monte Carlo technique (CORAL software) Toropova & Toropov (2013) | In vitro - Cytotoxicity - membrane damage measured as lactate dehydrogenase (LDH) release [units/L] | Jaqpote 4: http://jaqpote.org/m_detail?name=4oxlwXBZMJ4suYFTS14d Jaqpote 5: https://app.jaqpote.org/model/nTjgb4Ss3zHIYZEcgb78 |
| 6 | Cytotoxicity of metal oxide to bacteria E.Coli models by Periodic table-based descriptors and stepwise-MLR Kar et al. (2014) | In vitro - Cytotoxicity - measured as pEC50 | Jaqpote 4: http://jaqpote.org/m_detail?name=EFfilLYKMlUg3qNYBw Jaqpote 5: https://app.jaqpote.org/model/QgRRwyU8r7e0NubEuDdX |
| 7 | Photo-induced toxicity of metal oxide NPs to E. Coli by MLR (dark condition case) Pathakoti et al. (2014) | In vitro - Cytotoxicity - measured as -log(LC50) | Jaqpote 4: http://jaqpote.org/m_detail?name=KIWUeelVM8x7x1iC7cXi Jaqpote 5: https://app.jaqpote.org/model/hygpzrH71X51Wr8IGS69 |
| 8 | Photo-induced toxicity of metal oxide NPs to E. Coli by MLR (Photo-induced (light) case) Pathakoti et al. (2014) | In vitro - Cytotoxicity - measured as -log(LC50) | Jaqpote 4: http://jaqpote.org/m_detail?name=o6Jr81BfQtUddgmwqae Jaqpote 5: https://app.jaqpote.org/model/5gCY316DzDh1Fdw4aigo |
| 9 | Predicting metal oxide Nps toxicity to E. Coli cell line by MLR Toropov et al. (2018) | In vitro - Cytotoxicity - measured as log(1/EC50) | Jaqpote 4: http://jaqpote.org/m_detail?name=qul6HILHSypXWX8zvMQ3 Jaqpote 5: https://app.jaqpote.org/model/OAiBYuee5PLU7F580f2J |
| 10 | Predicting C60 solubility in organic solvents by SMILES-based optimal descriptor and Monte Carlo technique Gharagheizi & Alamdari (2008) | Solubility in organic solvents | Jaqpote 4: http://jaqpote.org/m_detail?name=sCoqY3D3xCpSuyS6RdoQ Jaqpote 5: https://app.jaqpote.org/model/VRp8f6A4Dujc8fsavvpB |



Jaqqot 5 - Datasets - Uploading new dataset



Jaqqot 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 |
|-------------|----------------------|----------------------|----------------------|----------------|----------------|-----|
| 0.56838137 | 0.504558150.32772753 | 0.4014363 | 0.44868296 | 0.474917380 | | |
| 0.4094099 | 0.570796250.33246857 | 0.410797420.34907413 | 0.5754712 | 0 | | |
| 0.3725539 | 0.5431615 | 0.32753754 | 0.428793430.52822345 | 0.442805560.07 | | |
| 1.031555578 | 0.4539304 | 0.23253489 | 0 | 0.60701066 | 0.460899140.07 | |
| 1.064531374 | 0.8208577 | 0.33246857 | 0.410797420.75384444 | 0.463907 | 0 | |
| 1.05689562 | 0.864756170.17511162 | 0.3637108 | 0.4746896 | 0.317731560.35 | | |
| 1.05056574 | 0.5190517 | 0.29254708 | 0.358349140.61428285 | 0.437957050 | | |
| 1.057912403 | 0.449200120.03931781 | 0.076428760.8059602 | 0.3211879 | 0.14 | | |
| 1.04270075 | 0.451252070.24331617 | 0.430732070.5959102 | 0.6408699 | 0.14 | | |

Features

ATSC3dv

Description

Units

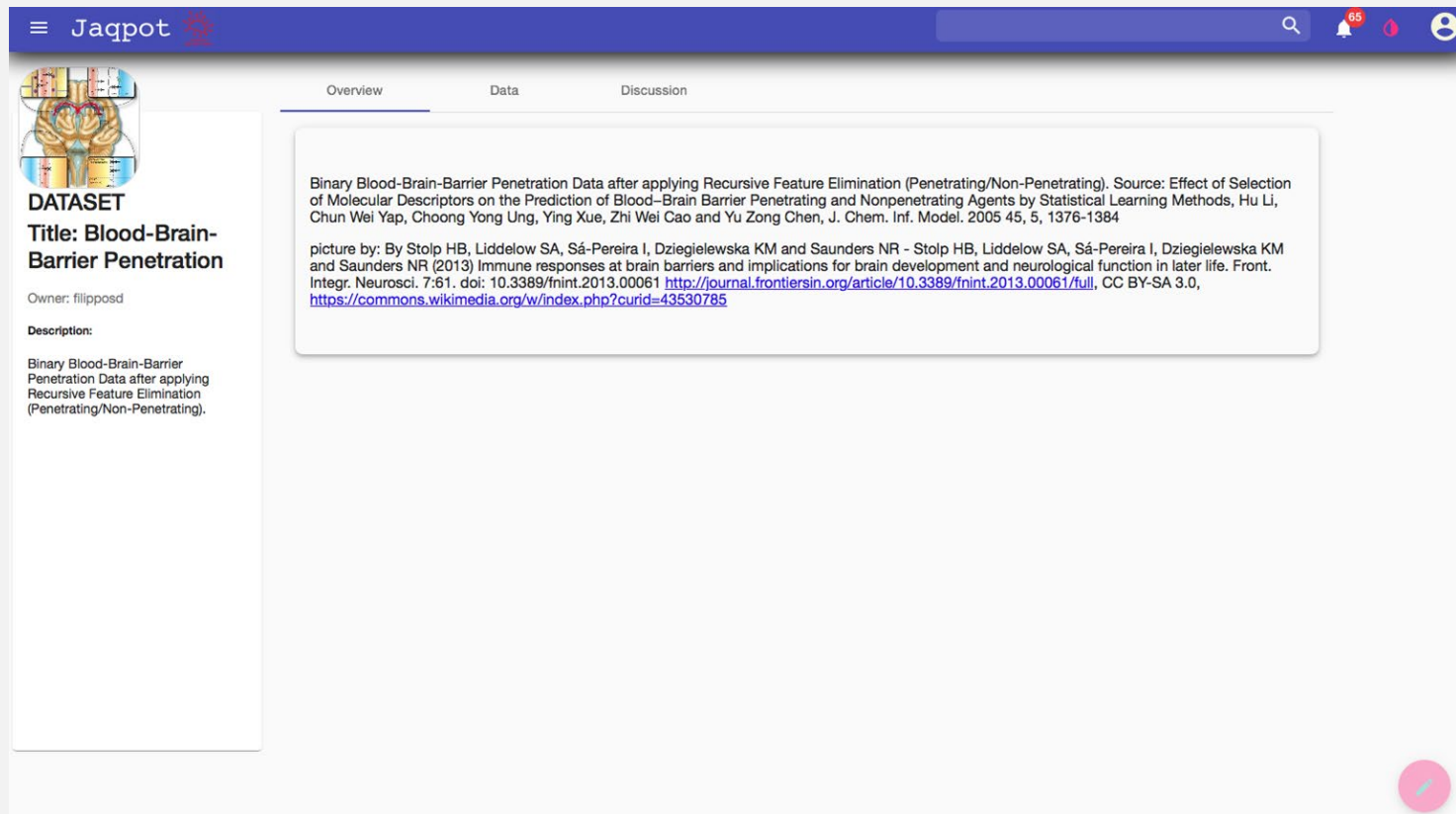
Ontological Classes

ATSC6d

Description



Jaqpot 5 - Dataset page



Jaqpot

Overview Data Discussion

DATASET

Title: Blood-Brain-Barrier Penetration

Owner: filliposd

Description:

Binary Blood-Brain-Barrier Penetration Data after applying Recursive Feature Elimination (Penetrating/Non-Penetrating).

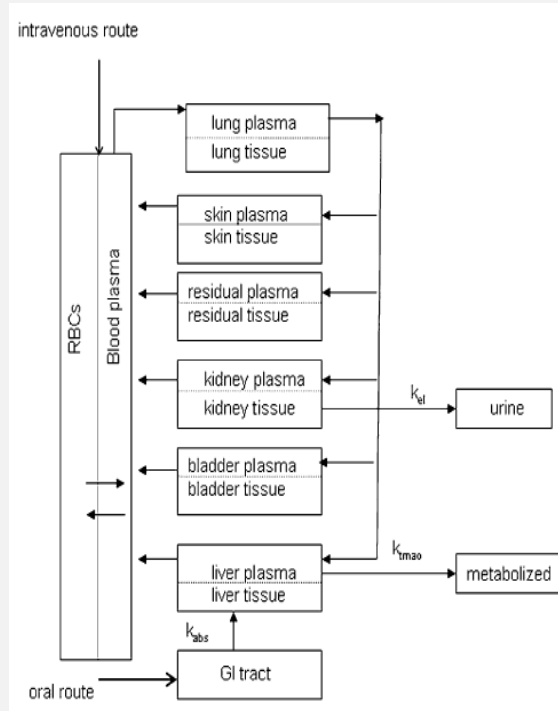
Binary Blood-Brain-Barrier Penetration Data after applying Recursive Feature Elimination (Penetrating/Non-Penetrating). Source: Effect of Selection of Molecular Descriptors on the Prediction of Blood-Brain Barrier Penetrating and Nonpenetrating Agents by Statistical Learning Methods, Hu Li, Chun Wei 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, Liddelw SA, Sá-Pereira I, Dziegielewska KM and Saunders NR - Stolp HB, Liddelw 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>



PBPK model: Multi-compartment model (System of Ordinary Differential Equations, ODEs)

- Mechanistic models that incorporate species' physiology
- Provide information about the concentration-time profile
- Advantage: can conduct meaningful extrapolation
- Two types of parameters: physiological and drug-related



Non-metabolizing compartments:

$$V_{bl}^i \frac{dC_v^i(t)}{dt} = Q_i (C_{art}(t) - C_v^i(t)) - \pi_i \left(C_v^i(t) - \frac{C^i(t)}{P_i} \right)$$

$$V^i \frac{dC^i(t)}{dt} = \pi_i \left(C_v^i(t) - \frac{C^i(t)}{P_i} \right)$$

Metabolizing compartments:

$$V_{bl}^i \frac{dC_v^i(t)}{dt} = Q_i (C_{art}(t) - C_v^i(t)) - \pi_i \left(C_v^i(t) - \frac{C^i(t)}{P_i} \right) - r_{ex}^i (C_v^i(t)) V_{bl}^i$$

$$V^i \frac{dC^i(t)}{dt} = \pi_i \left(C_v^i(t) - \frac{C^i(t)}{P_i} \right) - r_{met}^i (C^i(t)) V^i$$

Blood:

$$V^{pl} \frac{dC^{pl}(t)}{dt} = u(t) + \sum_{i \in I_0 \cup I_1} Q_i C_v^i(t) + \pi_{rbc} C^{rbc}(t) - \pi_{pl} C^{pl}(t) - Q_{pl} C^{pl}(t)$$

$$V^{rbc} \frac{dC^{rbc}(t)}{dt} = \pi_{pl} C^{pl}(t) - \pi_{rbc} C^{rbc}(t)$$

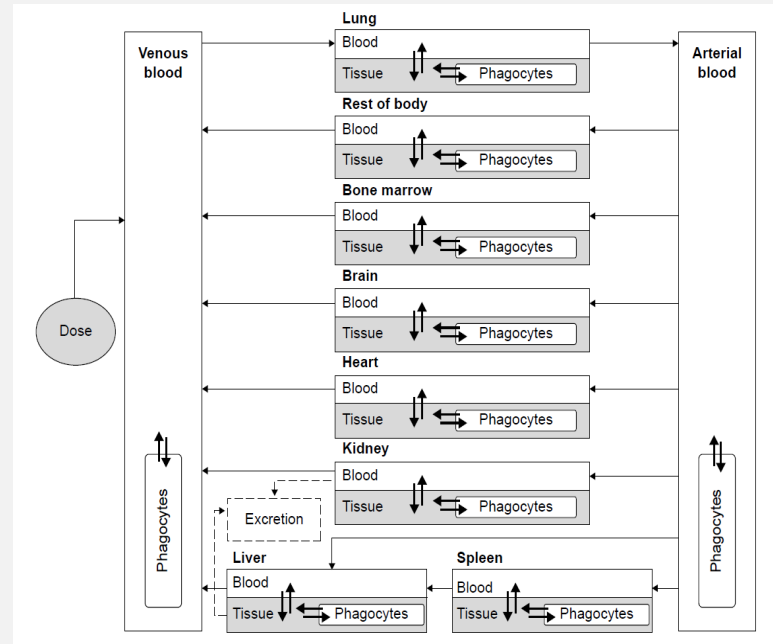
Lung:

$$V_{bl}^{lu} \frac{dC_{art}(t)}{dt} = Q_{lu} (C^{pl}(t) - C_{art}(t)) - \pi_{lu} \left(C_{art}(t) - \frac{C^{lu}(t)}{P_{lu}} \right)$$

$$V^{lu} \frac{dC^{lu}(t)}{dt} = \pi_{lu} \left(C_{art}(t) - \frac{C^{lu}(t)}{P_{lu}} \right)$$



Physiologically based pharmacokinetics (PBPK) models for nanomaterials



Carlander U., Li D., Joliet O., Emond C., Johanson G., Toward a general physiologically-based pharmacokinetic model for intravenously injected nanoparticles, *International Journal of Nanomedicine*, 2016



The Jaqpotr library: Uploading a model to Jaqpot through R

- Define a dataset containing the dose, infusion time, initial concentrations and other covariates used as model input
- Define a system of differential equations as a function (according to the deSolve package)
- Define a function that generates covariates, whose output will be parsed to the differential equations
- Define the compartment names and declare the input compartment

```
#####
# User input #
#####

weight <- 70 #in kg
gender <- 0 #0 for male | 1 for female
dose <- 10 # in mg
infusion_time <- 5/60 #infusion time in hours
CO_MU <- 0
CO_AD <- 0
CO_G0 <- 0
CO_SK <- 0
CO_HT <- 0
CO_BR <- 0
CO_KI <- 0
CO_RE <- 0
CO_ST <- 0
CO_IN <- 0
CO_LU <- 0
CO_LI <- 0
CO_ART <- 0
CO_VEN <- 0

user_input <- data.frame(weight, gender, dose, infusion_time, CO_MU, CO_AD, CO_G0, CO_SK, CO_HT, CO_BR, CO_KI,
                        CO_RE, CO_ST, CO_IN, CO_LU, CO_LI, CO_ART, CO_VEN)

#####
# compartment names #
#####

comp_names <- c("MU", "AD", "G0", "SK", "HT", "BR", "KI", "RE", "ST", "IN", "LU", "LI", "ART", "VEN")
```

```
#####
# Covariate model for calculation of organ flows and volumes #
#####

covariates <- function(w,gender){
  density <- rep(1,14)
  flow_frac <- c(0.17,0.05,0.001,0.05,0.04,0.12,0.19,0.0,0.01,0.14,1,0.065)

  const <- list(k1,k2,k3,k4,k5,k6,k7,k8,k9,k10,k11,k12,k13,k14)
  const_w <- list(k1_w,k2_w,k3_w,k4_w,k5_w,k6_w,k7_w,k8_w,k9_w,k10_w,k11_w,k12_w,k13_w,k14_w)
  vol <- rep(0,14)
  flow <- rep(0,12)
  TF <- (187*(w^0.81))^60/1000 #Total flow
  weight <- w

  if (gender==0){
    if (w<75){
      w <- 75*1000
    }
    else{
      w <- w*1000
    }
    co <- const
    for (i in 1:14){
      vol[i] <- (co[[i]][1]+co[[i]][2]*w+co[[i]][3]*w^2+co[[i]][4]*w^3+co[[i]][5]*w^4+co[[i][6]*w^5)
      vol[i] <- vol[i]*weight/density[i]
    }
  }
  else if (gender==1){
    if (w<65){
      w <- 65*1000
    }
    else{
      w <- w*1000
    }
    co <- const_w
    for (i in 1:14){
      vol[i] <- (co[[i]][1]+co[[i]][2]*w+co[[i]][3]*w^2+co[[i]][4]*w^3+co[[i]][5]*w^4+co[[i][6]*w^5)
      vol[i] <- vol[i]*weight/density[i]
    }
  }
  vol[8] <- weight - sum(vol)
  combine <- c(flow,vol)
  return(combine)
}
```

```
#####
# ODES Function #
#####

odes <- function(time,c,params){
  dcdt <- rep(0,14)

  Q_MU <- params[1]
  Q_AD <- params[2]
  Q_G0 <- params[3]
  Q_SK <- params[4]
  Q_HT <- params[5]
  Q_BR <- params[6]
  Q_KI <- params[7]
  Q_RE <- params[8]
  Q_ST <- params[9]
  Q_SPL <- params[10]
  Q_LU <- params[11]
  Q_LI <- params[12]
  Q_ART <- params[13]
  Q_VEN <- params[14]

  dcdt[1] <- -Q_MU*c[1]/(KP_MU*V_MU)+(Q_MU*c[13]/V_MU)
  dcdt[2] <- -Q_AD*c[2]/(KP_AD*V_AD)+(Q_AD*c[13]/V_AD)
  dcdt[3] <- -Q_G0*c[3]/(KP_G0*V_G0)+(Q_G0*c[13]/V_G0)
  dcdt[4] <- -Q_SK*c[4]/(KP_SK*V_SK)+(Q_SK*c[13]/V_SK)
  dcdt[5] <- -Q_HT*c[5]/(KP_HT*V_HT)+(Q_HT*c[13]/V_HT)
  dcdt[6] <- -Q_BR*c[6]/(KP_BR*V_BR)+(Q_BR*c[13]/V_BR)
  dcdt[7] <- -Q_KI*c[7]/(KP_KI*V_KI)+(Q_KI*c[13]/V_KI)
  dcdt[8] <- -Q_RE*c[8]/(KP_RE*V_RE)+(Q_RE*c[13]/V_RE)
  dcdt[9] <- -Q_ST*c[9]/(KP_ST*V_ST)+(Q_ST*c[13]/V_ST)
  dcdt[10] <- -Q_SPL*c[10]/(KP_SPL*V_SPL)+(Q_SPL*c[13]/V_SPL)
  dcdt[11] <- -Q_LU*c[11]/(KP_LU*V_LU)+(Q_LU*c[13]/V_LU)
  dcdt[12] <- -Q_LI*c[12]/(KP_LI*V_LI)+(Q_LI*c[13]/V_LI)
  dcdt[13] <- -Q_ART*c[13]/(KP_ART*V_ART)+(Q_ART*c[13]/V_ART)

  if (time==T_inf){
    dcdt[14] <- -Q_LU*c[14]/V_VEN+(Q_H*c[12]/(KP_LI*V_VEN)+(Q_KI*c[7]/(KP_KI*V_VEN)+
      Q_MU*c[1]/(KP_MU*V_VEN)+(Q_AD*c[2]/(KP_AD*V_VEN)+(Q_SK*c[4]/(KP_SK*V_VEN)+
      Q_G0*c[3]/(KP_G0*V_VEN)+(Q_HT*c[5]/(KP_HT*V_VEN)+(Q_BR*c[6]/(KP_BR*V_VEN)+
      Q_RE*c[8]/(KP_RE*V_VEN)+(Q_ST*c[9]/(KP_ST*V_VEN)+(Q_SPL*c[10]/(KP_SPL*V_VEN)+
      Q_LU*c[11]/(KP_LU*V_VEN)+(Q_LI*c[12]/(KP_LI*V_VEN)+
      Q_ART*c[13]/(KP_ART*V_VEN)) #units are in mg/ml
    }
  } else {
    dcdt[14] <- -Q_LU*c[14]/V_VEN+(Q_H*c[12]/(KP_LI*V_VEN)+(Q_KI*c[7]/(KP_KI*V_VEN)+
      Q_MU*c[1]/(KP_MU*V_VEN)+(Q_AD*c[2]/(KP_AD*V_VEN)+(Q_SK*c[4]/(KP_SK*V_VEN)+
      Q_G0*c[3]/(KP_G0*V_VEN)+(Q_HT*c[5]/(KP_HT*V_VEN)+(Q_BR*c[6]/(KP_BR*V_VEN)+
      Q_RE*c[8]/(KP_RE*V_VEN))
    }
  }
  list(dcdt)
}
```

Calling `deploy.pbpk()`

- Load `jaqpotr`
- Call `deploy.pbpk()` and provide the dataset, covariate model, differential equations, compartment names and input
- Give Jaqpot base path (<https://api.jaqpot.org/>) and choose the authentication method (Api key or Jaqpot credentials, i.e. username and password)
- Add a model title (cannot be edited) and a short description (editable)
- The PBPK model is generated and the model id is provided.
- The user can further refine the model description and information through the Jaqpot UI

```
> deploy.pbpk(data=user_input, odes=odes, comp.names=comp_names, comp.in='VEN', cov.model=covariates )
Base path of jaqpot *e.g.: https://api.jaqpot.org/ : https://api.jaqpot.org/
Please choose authentication method ([1]=login / [2]=Provide Api Key): 1
Username: PeriklisTs
Title of the model: upload test
Short description of the model:this is a short description
[1] "Model created. The id is: DLGxOzkvGkU9ctHi4wRW . Please visit the application to further document your
model."
> |
```

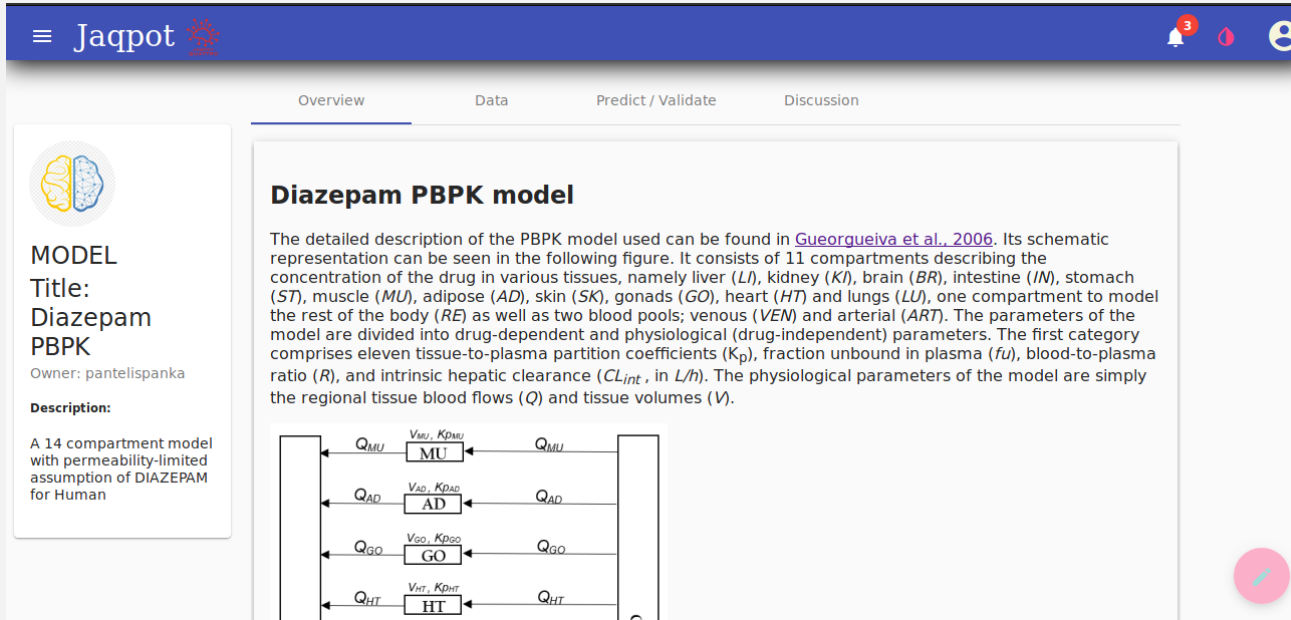


Accessing the model

The screenshot displays the Jaqpot web interface. At the top, there is a blue header with the Jaqpot logo and navigation icons. Below the header, the breadcrumb path is "Home > Models > Shared > With Lab of Process Control and Informatics". The main content area shows a list of items, with one item selected: "Model title: Diazepam PBPK" with a date of "Feb 22, 2019". To the right of this item, there are icons for "View" (a magnifying glass) and "Delete" (a trash can). A black arrow points to the "View" icon. On the right side of the interface, there is a panel that says "No item selected" and a warning triangle icon. The left sidebar contains navigation options: "Datasets Shared / Priv...", "Models Shared / Priv...", and "Trash".



Entering model information through Jaqpot UI

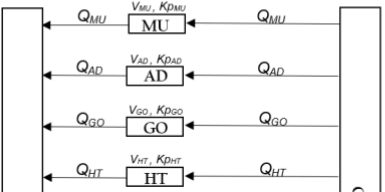


The screenshot displays the Jaqpot web interface. The top navigation bar includes a menu icon, the text 'Jaqpot', and user profile icons. Below the navigation bar are tabs for 'Overview', 'Data', 'Predict / Validate', and 'Discussion'. The 'Overview' tab is active, showing a sidebar with a model icon and a main content area with a title and description.

MODEL
Title: Diazepam PBPK
Owner: pantelispanka
Description: A 14 compartment model with permeability-limited assumption of DIAZEPAM for Human

Diazepam PBPK model

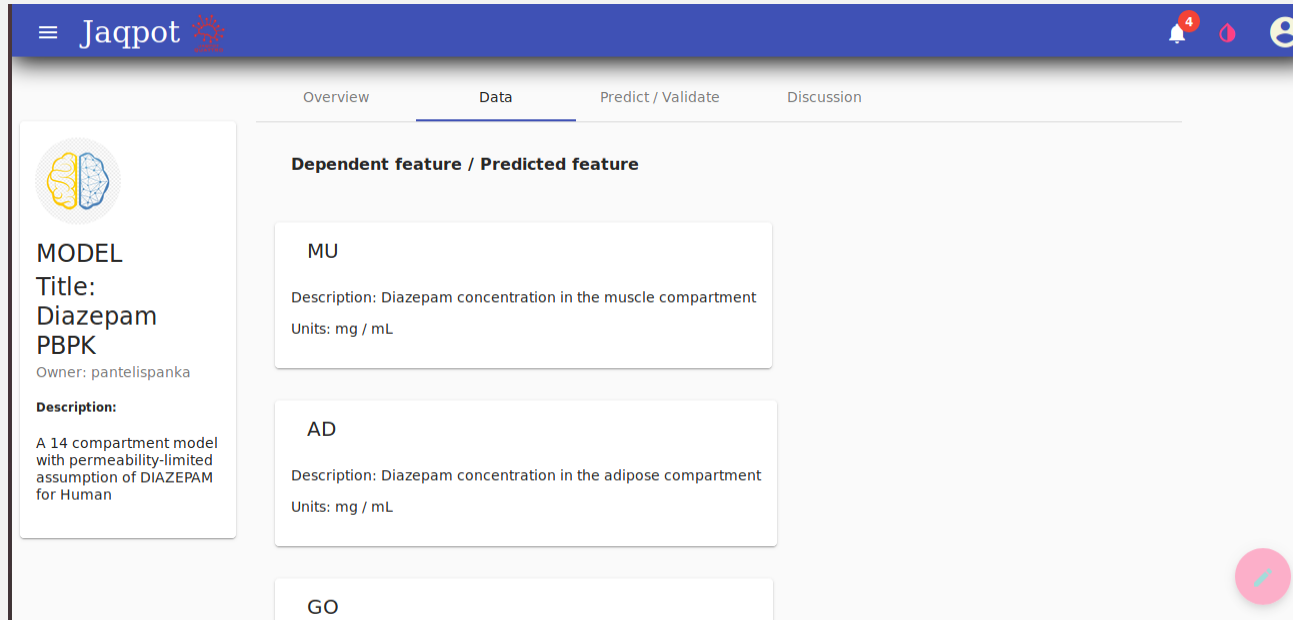
The detailed description of the PBPK model used can be found in [Gueorgueiva et al., 2006](#). Its schematic representation can be seen in the following figure. It consists of 11 compartments describing the concentration of the drug in various tissues, namely liver (*LI*), kidney (*KI*), brain (*BR*), intestine (*IN*), stomach (*ST*), muscle (*MU*), adipose (*AD*), skin (*SK*), gonads (*GO*), heart (*HT*) and lungs (*LU*), one compartment to model the rest of the body (*RE*) as well as two blood pools; venous (*VEN*) and arterial (*ART*). The parameters of the model are divided into drug-dependent and physiological (drug-independent) parameters. The first category comprises eleven tissue-to-plasma partition coefficients (K_p), fraction unbound in plasma (f_u), blood-to-plasma ratio (R), and intrinsic hepatic clearance (CL_{int} , in L/h). The physiological parameters of the model are simply the regional tissue blood flows (Q) and tissue volumes (V).



```
graph LR
    MU[MU] -- "Q_MU" --> Blood
    Blood -- "Q_MU" --> MU
    AD[AD] -- "Q_AD" --> Blood
    Blood -- "Q_AD" --> AD
    GO[GO] -- "Q_GO" --> Blood
    Blood -- "Q_GO" --> GO
    HT[HT] -- "Q_HT" --> Blood
    Blood -- "Q_HT" --> HT
```



Add description and units to the model variables



The screenshot shows the Jaqpot web application interface. The top navigation bar is blue and contains the Jaqpot logo, a notification bell with a red '4', a red flame icon, and a user profile icon. Below the navigation bar, there are four tabs: 'Overview', 'Data', 'Predict / Validate', and 'Discussion'. The 'Data' tab is currently selected.

On the left side, there is a sidebar with a brain icon. The sidebar contains the following information:

- MODEL**
- Title:** Diazepam PBPK
- Owner:** pantelispanka
- Description:** A 14 compartment model with permeability-limited assumption of DIAZEPAM for Human

The main content area displays a list of model variables under the heading 'Dependent feature / Predicted feature':

- MU**
Description: Diazepam concentration in the muscle compartment
Units: mg / mL
- AD**
Description: Diazepam concentration in the adipose compartment
Units: mg / mL
- GO**

A pink circular edit button is visible in the bottom right corner of the main content area.



Perform PBPK simulations

- Users can enter dose and physiological characteristics and get predictions
- Upload dataset or manually fill in values

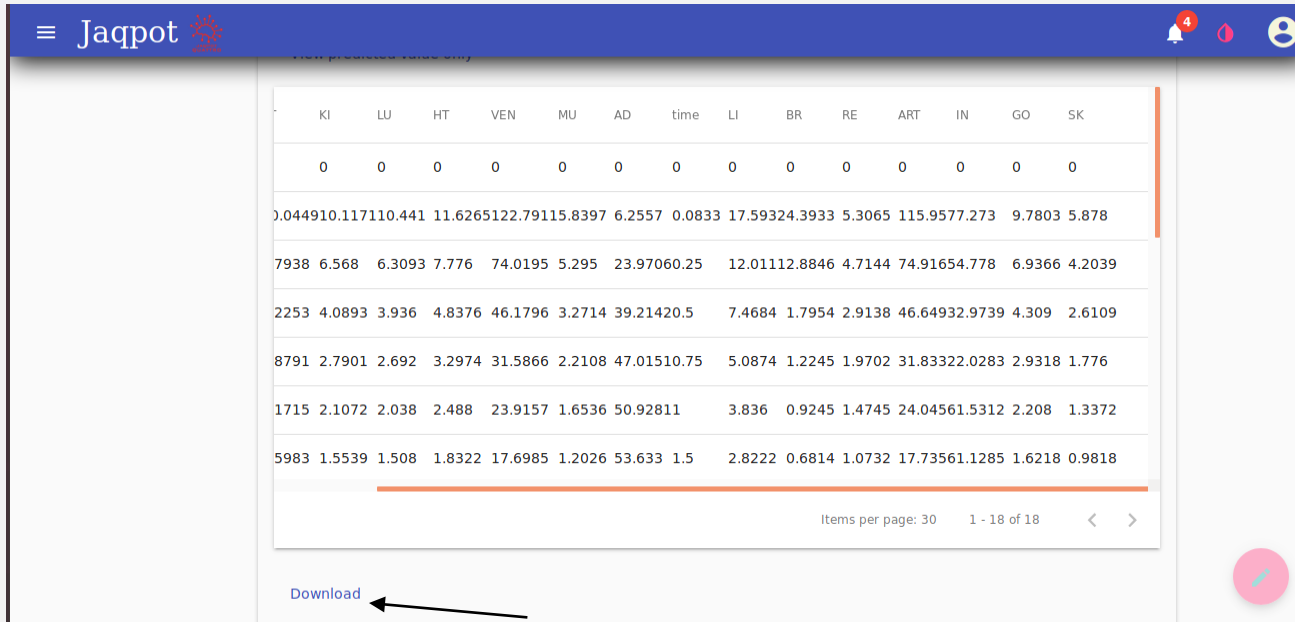
The screenshot shows the Jaqpot web application interface. The header is blue with the Jaqpot logo and a notification bell with a red '3'. Below the header, there is a section for 'for Human' and a main area titled 'Input values for the independent features'. This area contains 16 input fields arranged in a grid, each with a label, a value, and a unit. The inputs are: weight (70 kg), gender (0: male, 1: female), dose (10 mg), infusion_time (0.08 hours), C0_MU (0 mg/mL), C0_AD (0 mg/mL), C0_HT (0 mg/mL), C0_BR (0 mg/mL), C0_TE (0 mg/mL), C0_SK (0 mg/mL), C0_RE (0 mg/mL), C0_KI (0 mg/mL), C0_ST (0 mg/mL), C0_LU (0 mg/mL), C0_LI (0 mg/mL), and C0_SPL (0 mg/mL). A 'Start' button is located at the bottom right, and a pink circular icon with a pencil is also visible.

| Parameter | Value | Unit |
|---------------|-------|--------------------|
| weight | 70 | kg |
| gender | 0 | 0: male, 1: female |
| dose | 10 | mg |
| infusion_time | 0.08 | hours |
| C0_MU | 0 | mg/mL |
| C0_AD | 0 | mg/mL |
| C0_HT | 0 | mg/mL |
| C0_BR | 0 | mg/mL |
| C0_TE | 0 | mg/mL |
| C0_SK | 0 | mg/mL |
| C0_RE | 0 | mg/mL |
| C0_KI | 0 | mg/mL |
| C0_ST | 0 | mg/mL |
| C0_LU | 0 | mg/mL |
| C0_LI | 0 | mg/mL |
| C0_SPL | 0 | mg/mL |
| C0_ART | 0 | mg/mL |
| C0_VEN | 0 | mg/mL |



Getting predictions

- Predictions are generated in a table form and can be downloaded as a csv file and be further processed offline



The screenshot shows the Jaqpot web application interface. The header includes the Jaqpot logo and navigation icons. The main content area displays a table of predictions with 14 columns: KI, LU, HT, VEN, MU, AD, time, LI, BR, RE, ART, IN, GO, and SK. The table contains 7 rows of data. Below the table, there is a 'Download' button with an arrow pointing to it. The footer of the table indicates 'Items per page: 30' and '1 - 18 of 18'.

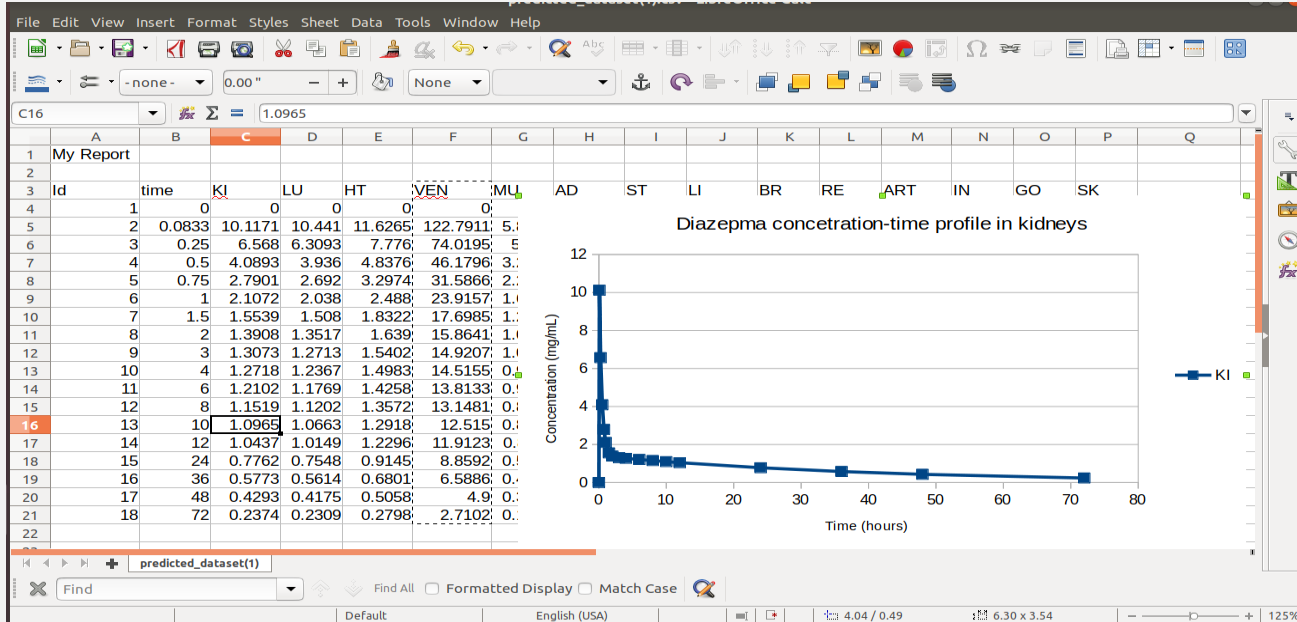
| KI | LU | HT | VEN | MU | AD | time | LI | BR | RE | ART | IN | GO | SK | |
|----------|------------|------------|--------|---------|----------|----------|--------|----------|--------|--------|----------|-------|--------|--------|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 0.044910 | 11.6265122 | 79115.8397 | 6.2557 | 0.0833 | 17.59324 | 3.933 | 5.3065 | 115.9577 | 2.73 | 9.7803 | 5.878 | | | |
| 7938 | 6.568 | 6.3093 | 7.776 | 74.0195 | 5.295 | 23.97060 | 25 | 12.01112 | 8.846 | 4.7144 | 74.91654 | 7.78 | 6.9366 | 4.2039 |
| 2253 | 4.0893 | 3.936 | 4.8376 | 46.1796 | 3.2714 | 39.21420 | 5 | 7.4684 | 1.7954 | 2.9138 | 46.64932 | 9.739 | 4.309 | 2.6109 |
| 8791 | 2.7901 | 2.692 | 3.2974 | 31.5866 | 2.2108 | 47.01510 | 7.5 | 5.0874 | 1.2245 | 1.9702 | 31.83322 | 0.283 | 2.9318 | 1.776 |
| 1715 | 2.1072 | 2.038 | 2.488 | 23.9157 | 1.6536 | 50.92811 | | 3.836 | 0.9245 | 1.4745 | 24.04561 | 5.312 | 2.208 | 1.3372 |
| 5983 | 1.5539 | 1.508 | 1.8322 | 17.6985 | 1.2026 | 53.633 | 1.5 | 2.8222 | 0.6814 | 1.0732 | 17.73561 | 1.285 | 1.6218 | 0.9818 |

Items per page: 30 1 - 18 of 18 < >

[Download](#)

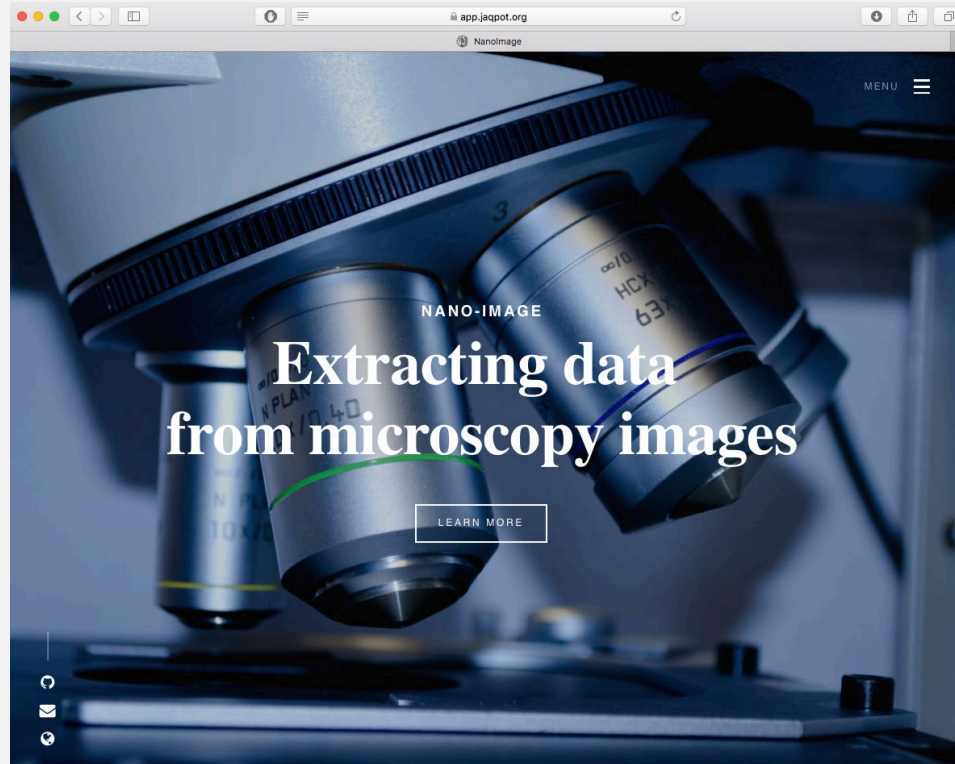


Predictions in a csv file




Jaqpot Image Analysis

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



Calculating image descriptors for spherical nanomaterials



Spherical Particles

MENU

Image Preview

Parameters

Select filter type:

Select function type:

pixel/nm:

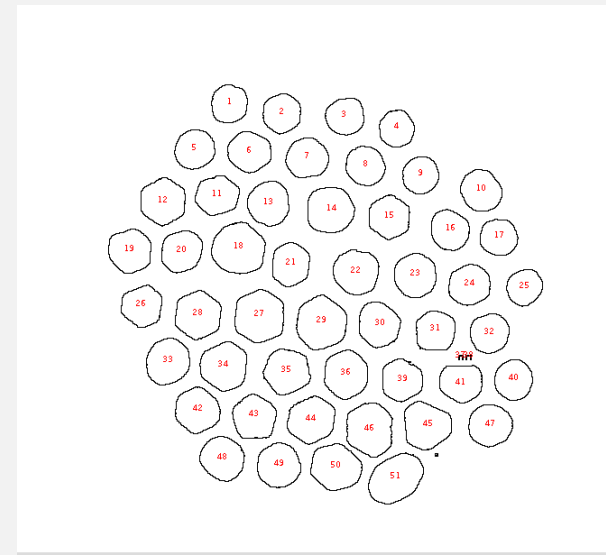
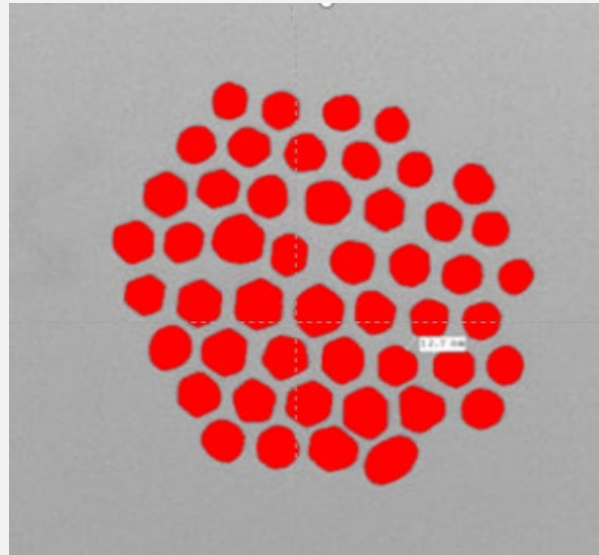
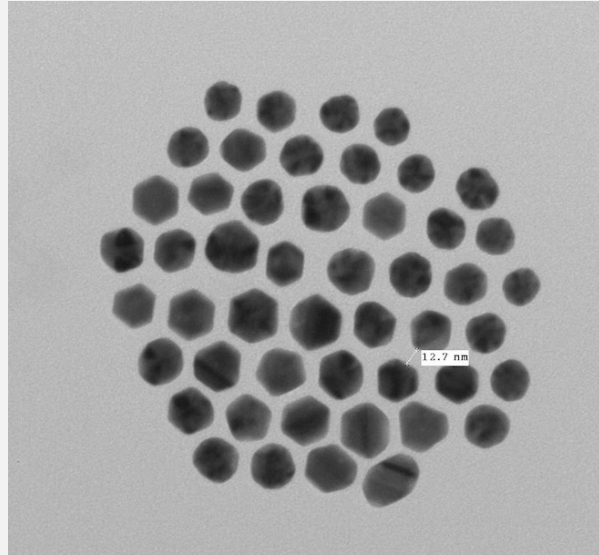
Select Descriptors:

| | | | | | |
|---|-------------------------------------|---|---|--|--|
| <input type="checkbox"/> Angle | <input type="checkbox"/> Area | <input type="checkbox"/> Aspect Ratio | <input type="checkbox"/> Circularity | <input type="checkbox"/> Feret Angle | <input type="checkbox"/> Grey Deviation |
| <input type="checkbox"/> Integrated Density | <input type="checkbox"/> Kurtosis | <input type="checkbox"/> Major Axis | <input type="checkbox"/> Max Grey Value | <input type="checkbox"/> Mean Grey Value | <input type="checkbox"/> Min Grey Value |
| <input type="checkbox"/> Min Feret | <input type="checkbox"/> Minor Axis | <input type="checkbox"/> Modal Grey Value | <input type="checkbox"/> Perimeter | <input type="checkbox"/> Porosity | <input type="checkbox"/> Roundness |
| <input type="checkbox"/> Skewness | <input type="checkbox"/> Solidity | <input type="checkbox"/> Sphericity | <input type="checkbox"/> Surface Diameter | <input type="checkbox"/> Volume | <input type="checkbox"/> Volume to Surface |

Results of this tool are derived from ImageJ, with additional descriptors provided, as described in:
Philip Doganis, Georgia Tsiliki, Haralambos Sarimveis, Haralambos Chomenidis, Georgios Drakakis, Egon Willighagen, Barry Hardy. (2015, April 29). Deliverable Report D4.2 Descriptor Calculation Algorithms and Methods. Zenodo. <http://doi.org/10.5281/zenodo.376609>



Calculating image descriptors for spherical nanomaterials




Calculating image descriptors for spherical nanomaterials


| List of Properties | | | | | | | | | | |
|--------------------|----------|----------|--------------|-------------|-------------|----------------|--------------------|-------------|------------|----|
| (1 of 3) 1 2 3 25 | | | | | | | | | | |
| id | Angle | Area | Aspect Ratio | Circularity | Feret Angle | Grey deviation | Integrated Density | Kurtosis | Major Axis | |
| Average Particle | 96.13313 | 780.2823 | 1.0759023 | 0.8592815 | 97.67603 | 21.327768 | 53979.883 | -0.44196674 | 32.50095 | 1: |
| 1 | 31.853 | 514.877 | 1.049 | 0.889 | 22.620 | 20.576 | 38233.001 | -0.810 | 26.222 | 1: |
| 2 | 23.957 | 562.506 | 1.061 | 0.846 | 158.587 | 16.775 | 46490.280 | -0.733 | 27.320 | 1: |
| 3 | 4.397 | 476.167 | 1.058 | 0.862 | 170.910 | 24.161 | 33538.219 | -0.988 | 25.329 | 1: |
| 4 | 110.551 | 433.125 | 1.013 | 0.886 | 111.801 | 20.821 | 35176.785 | -0.698 | 23.633 | 1: |
| 5 | 106.344 | 813.192 | 1.125 | 0.852 | 103.627 | 24.343 | 50797.166 | -0.422 | 34.125 | 1: |
| 6 | 131.483 | 631.550 | 1.099 | 0.904 | 109.654 | 23.437 | 43264.853 | -0.708 | 29.726 | 1: |
| 7 | 84.296 | 569.543 | 1.074 | 0.841 | 82.875 | 24.121 | 40191.019 | -1.008 | 27.661 | 1: |
| 8 | 25.308 | 655.643 | 1.089 | 0.887 | 32.106 | 22.161 | 44481.122 | -0.506 | 30.148 | 1: |
| 9 | 106.995 | 769.609 | 1.190 | 0.857 | 94.205 | 19.459 | 58704.946 | -0.626 | 34.141 | 1: |
| 10 | 138.673 | 523.269 | 1.112 | 0.880 | 162.582 | 19.736 | 39727.846 | -0.525 | 27.217 | 1: |
| 11 | 170.300 | 851.091 | 1.067 | 0.868 | 147.724 | 25.882 | 44428.605 | -0.206 | 34.011 | 1: |
| 12 | 162.309 | 707.347 | 1.032 | 0.845 | 142.943 | 20.357 | 50640.700 | -0.664 | 30.490 | 1: |
| 13 | 124.555 | 693.000 | 1.049 | 0.862 | 146.310 | 20.356 | 49973.146 | -0.491 | 30.430 | 1: |
| 14 | 70.426 | 836.202 | 1.154 | 0.872 | 52.633 | 22.376 | 51461.472 | -0.118 | 35.048 | 1: |
| 15 | 143.629 | 845.406 | 1.073 | 0.884 | 110.556 | 22.381 | 54884.242 | -0.403 | 33.977 | 1: |
| 16 | 63.841 | 531.119 | 1.031 | 0.889 | 23.629 | 20.101 | 37434.179 | -0.321 | 26.400 | 1: |
| 17 | 46.369 | 602.044 | 1.141 | 0.857 | 23.070 | 20.942 | 47170.286 | -0.910 | 29.568 | 1: |
| 18 | 51.225 | 743.621 | 1.028 | 0.861 | 79.046 | 22.626 | 52225.667 | -0.724 | 31.202 | 1: |
| 19 | 33.415 | 624.241 | 1.042 | 0.881 | 40.061 | 22.603 | 40840.706 | -0.457 | 28.774 | 1: |
| 20 | 58.898 | 705.994 | 1.056 | 0.885 | 51.633 | 24.296 | 46138.366 | -0.647 | 30.816 | 1: |
| 21 | 57.115 | 770.421 | 1.071 | 0.894 | 52.595 | 21.787 | 50777.405 | -0.292 | 32.416 | 1: |
| 22 | 79.090 | 870.852 | 1.100 | 0.824 | 81.870 | 14.121 | 76792.515 | -0.466 | 34.924 | 1: |
| 23 | 140.855 | 832.412 | 1.018 | 0.836 | 80.538 | 21.035 | 62232.207 | -0.601 | 32.850 | 1: |
| 24 | 104.264 | 1026.235 | 1.136 | 0.863 | 84.668 | 23.455 | 59227.132 | 0.062 | 38.526 | 1: |

Download Spherical Descriptors:    



Calculating descriptors for carbon nanotubes



MENU 

Nanotubes

Image Preview

Insert

Parameters

Sigma:

Lower Threshold:

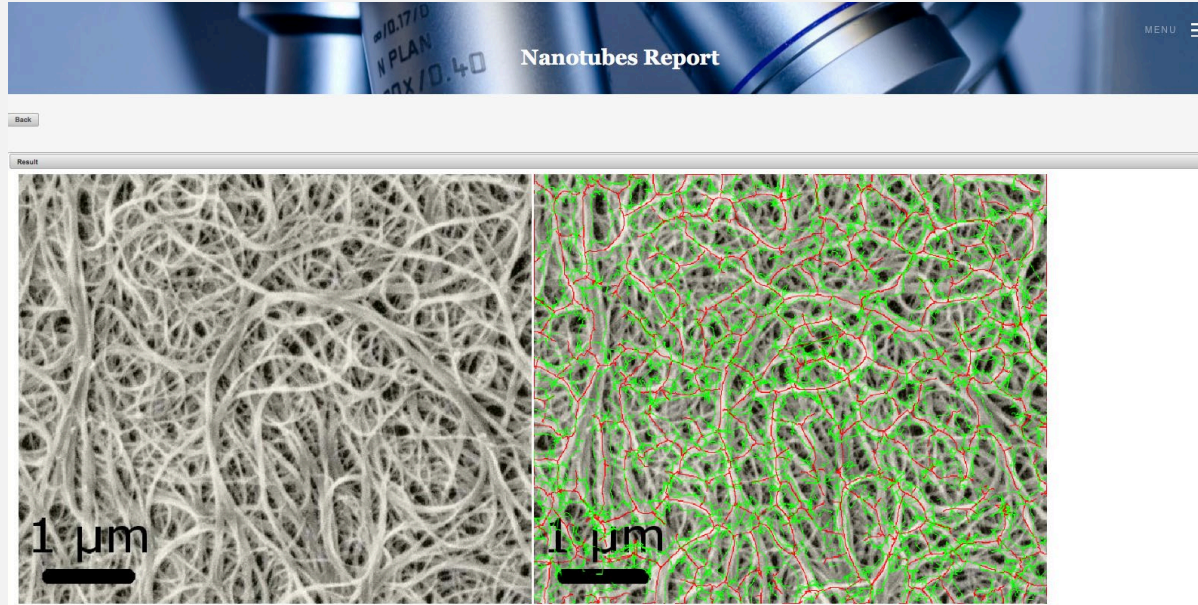
Upper Threshold:

Pixel to nm ratio: 1:

Results of this tool are derived from the Ridge Detection plugin of ImageJ.
For more information, please refer to: https://imagej.net/Ridge_Detection Steger, C., 1998. An unbiased detector of curvilinear structures. IEEE Transactions on Pattern Analysis and Machine Intelligence, 20(2), pp.113-125.
For comments on calculated descriptors please refer to: <https://github.com/thorstenwagner/i-ridgedetection/issues>



Calculating descriptors for carbon nanotubes



Calculating descriptors for carbon nanotubes

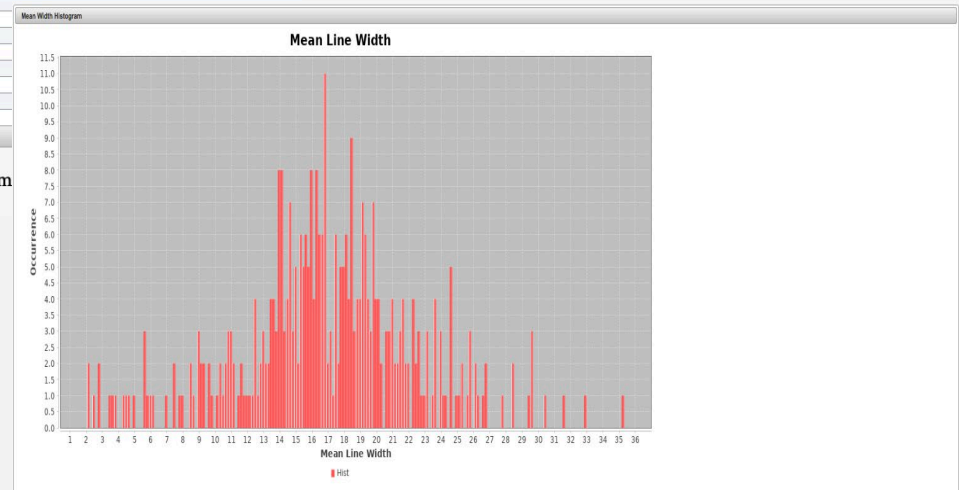
Summary per Nanotube

(1 of 18) | 1 2 3 4 5 6 7 8 9 10 | 25

| Contour Id. | Length | Mean Line Width |
|-------------|--------|-----------------|
| Average | 48.454 | 19.366 |
| 1898 | 19.418 | 28.483 |
| 1879 | 17.790 | 24.792 |
| 2763 | 7.478 | 25.183 |
| 2149 | 46.242 | 25.178 |
| 2294 | 14.275 | 16.801 |
| 3027 | 32.286 | 12.935 |
| 1903 | 14.343 | 26.992 |
| 2919 | 13.759 | 1.604 |
| 2971 | 83.469 | 20.631 |
| 2962 | 90.604 | 16.003 |
| 2227 | 7.791 | 10.702 |
| 2958 | 21.103 | 21.867 |
| 2774 | 9.903 | 9.732 |
| 2986 | 81.181 | 24.179 |
| 2207 | 16.636 | 26.074 |
| 2977 | 10.734 | 10.881 |
| 2781 | 17.560 | 30.725 |
| 2235 | 4.865 | 26.727 |
| 2160 | 13.263 | 28.741 |
| 2243 | 30.053 | 16.465 |
| 1654 | 30.000 | 26.611 |
| 2916 | 89.276 | 11.774 |
| 1867 | 40.501 | 23.434 |
| 1897 | 30.406 | 27.627 |

(1 of 18) | 1 2 3 4 5 6 7 8 9 10 | 25

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Jaqpot: Other services

ToxFlow¹: a read-across methodology, considers the multi-perspective characterization of nanoparticles and selects neighbour based on both physicochemical and biological similarity criteria, <http://147.102.86.129:3838/toxflow>¹

Dose-response modelling : a web implementation of the Benchmark Dose (BMD) approach for estimating derived no-effect levels (DNELs). Integrates the PROAST open-source software developed by RIVM

Biodescriptor calculations² : descriptors which are derived by enriching high-throughput omics data with biological-pathway information

Biokinetics: Integration of high-throughput toxicokinetics (httk) and PK-Sim software platforms

¹Varsou DD, Tsiliki G, Nymark P, Kohonen P, Grafström R, Sarimveis H. (2018) toxFlow: A Web-Based Application for Read-Across Toxicity Prediction Using Omics and Physicochemical Data, J Chem Inf Model. 2018 Mar 26;58(3):543-549. doi: 10.1021/acs.jcim.7b00160

²Tsiliki G, Nymark P, Kohonen P, Grafström R, Sarimveis H. (2017) Enriching Nanomaterials Omics Data: An Integration Technique to Generate Biological Descriptors, Small Methods; 1700139.



Jaqpot in EOSC Catalogue

The screenshot shows the Jaqpot service page in the EOSC Catalogue. At the top, the EOSC logo is on the left, and navigation links (About, Governance, Services & Resources, Policy, EOSC in practice, Media, For Providers) are on the right. A dark blue header contains the text 'Home Jaqpot' and a search bar. The main content area features the service title 'Jaqpot' with a subtitle 'Generate, store and share predictive statistical and machine learning models'. Below this are user ratings (5 stars), a heart icon (1), and an eye icon (29). A 'Categorization' section shows 'SOFTWARE' and 'PLATFORM'. The description states that Jaqpot is a user-friendly web-based e-infrastructure for data analysis and modelling. A 'Tags' section lists various scientific domains. On the right, there are buttons for 'SERVICE HOMEPAGE' and 'SERVICE ORDER', and a 'CONTRACTUAL INFO' section with links for 'Service level agreement' and 'Terms of use'. At the bottom, there are sections for 'Usage' (Technology Readiness Level) and 'Service coverage' (Countries serviced by Jaqpot).

EUROPEAN OPEN SCIENCE CLOUD CATALOGUE

About Governance Services & Resources Policy EOSC in practice Media For 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

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SERVICE HOMEPAGE

SERVICE ORDER

CONTRACTUAL INFO

Service level agreement →
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Usage
TECHNOLOGY READINESS LEVEL

Service coverage
Countries serviced by Jaqpot =

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





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Transnational access

The NanoCommons Transnational Access (TA) is the ability of nanosafety Researchers from industry, academia and regulatory bodies to access the state-of-the-art NanoCommons expertise free of charge and take advantage of the NanoCommons services, facilities and knowledge to advance their work, solve problems and take their research to the next level.

NanoCommons is designed to provide innovative solutions for data mining, harmonisation, utilisation and re-utilisation, including incorporation of a range of modelling and decision support tools that require organised high-quality datasets on which to run, provided via an Open Access, federated Knowledge Commons platform. Access to the platform and the supporting tools will be provided to the nanosafety community and its broadest set of stakeholders (enterprise, regulators, insurance and society broadly) via funded calls for Transnational access, as well as development of demonstration User case studies targeting the key stakeholders (academia, industry, regulators).

NanoCommons is envisaged as a bridge between academic research organisation and industry, and subsequently regulatory bodies, focused as it is on implementing the recommendations of the NanoSafety Cluster “Closer to the Market” Research Roadmap, and with its emphasis on co-development of solutions to industry challenges around safety-by-design and Life cycle assessment whilst also needing to maintain desired functionality and competitive market positioning.

Access the NanoCommons e-infrastructure

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Conclusions

Jaqqot constitutes a **universal platform** that **produces and exchanges** semantically annotated datasets and machine learning **predictive models** .

- Jaqqot is an **open source web infrastructure** with a flexible structure:
 - **generalization across disciplines**
 - **integration to third-party tools** in order to fulfil modelling needs on the Cloud
 - **easy integration** to diverse **architectures/ontologies/knowledge domains**.
- Jaqqot 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**.





Thank you!

