GUI for the QDB archive creation

Structure of the QDB archive
Description of the archive

Add name for your archive.

Add description for your archive. It is usually abstract of the article.

Adding compounds to the archive 1/3

Import compounds from external file

Add new compound

- Compound's ID
- Compound's name
- Compound's label
- Compound's CAS no.
- Compound's InChI code
Adding compounds to the archive 2/3

ID, Name, CAS and InChI fields are automatically recognised.

Other fields must be assigned manually.

Import data into your archive.

Adding compounds to the archive 3/3

All the fields (except Id) can be edited later on in the Compounds panel.
Adding properties to the archive 1/4

Import property values from external file
Add new property

Property’s ID
Name of the property
QMRF endpoints list
Species used in the experiment

Adding properties to the archive 2/4

Assign created property to the corresponding field in external file
Adding properties to the archive 3/4

Use DOI to add reference to experimental data

Download bibtex file from the Internet

Adding properties to the archive 4/4

Check if the bibtex file is correct and add it to the archive
Adding descriptors to the archive 1/3

Assign IDs to the descriptors from the external file.

Adding descriptors to the archive 2/3

- Descriptor’s ID
- Descriptor’s name
- Software used for descriptor calculation
- Create new descriptor field
Adding descriptors to the archive 3/3

Descriptors are assigned one by one

Adding model to the archive 1/2

Select descriptors to the model

Model’s ID
Model name
Property used for modelling
Create new MLR model
Adding model to the archive 2/2

Add coefficients to your MLR model

Adding predictions to the archive 2/2

Import predictions from external file

Predictions ID
Predictions name
Software used for modelling
Model used for predictions
Datasets type:
Training
Validation
Testing
Validation of the archive

Validate your QDB archive

Visualization of the models