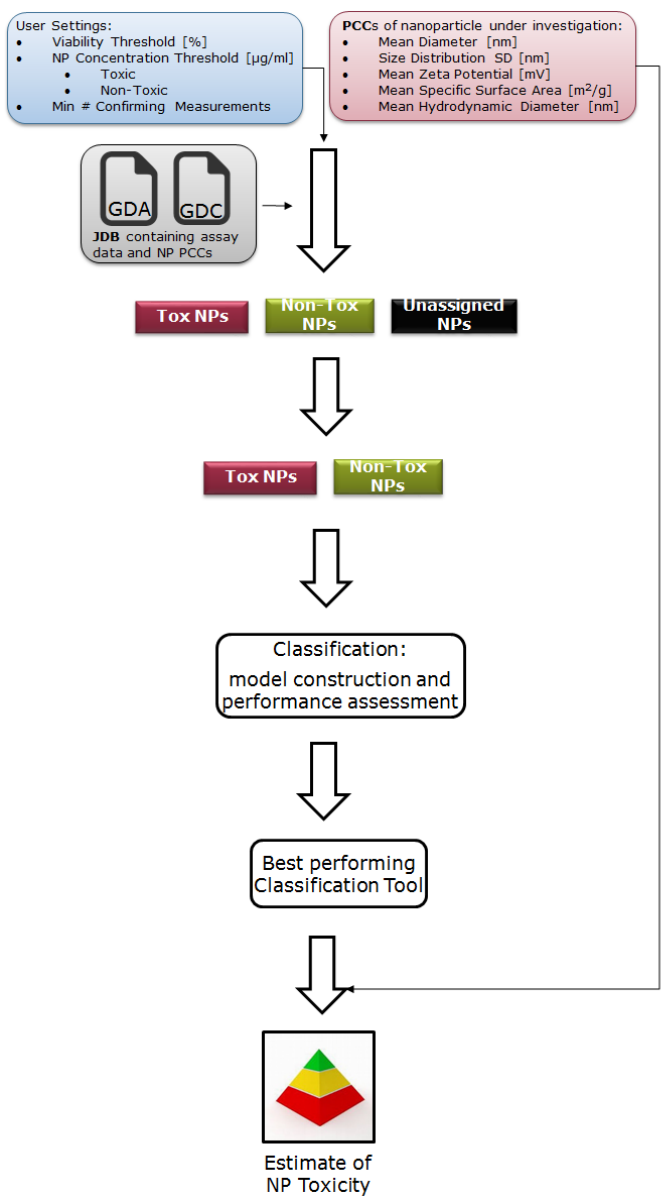


Figure 1: Proportion of different types of assays populating the newly designed database.

Assays consists of physico-chemical, viability, oxidative stress, pro-inflammation, genotoxicity and apoptosis/necrosis. Left: for silica NP, Right: for ZnO NP

**MOD-ENP-TOX:**

Modeling Assays Platform "MAP" for hazard ranking of engineered nanoparticles



1. Input Parameters from user
2. Extraction of Assay Data and PCCs of nanoparticles from JDB
3. Toxicity Assignment of nanoparticles in JDB based on user's input settings (blue)
4. Toxicity groups (toxic and non-toxic) populated with nanoparticles and their PCCs are input for classification model construction and performance assessment
5. Model Construction of classification tools is created and misclassification rates are computed to identify best performing classifier
6. Best performing classification tool applied to user's PCC input from NP under investigation
7. Classification tool returns toxicity estimate from 0 (non-toxic) to 1 (toxic)

**Figure 2: The individual steps of the classification tool.**

The input parameters from user (user settings corresponding to toxicity assignment of NP in database in blue; PCCs of NP under investigation in red) are taken from the graphical user interface in step 1. The toxicity assignment settings (blue) are used to assign the NP in database to the toxic or non-toxic group depending on the available assay data (Step 2 and 3). Those NP which could not be assigned to a group (toxic/non-toxic) are discarded (Step 4). The toxicity assigned NP and their PCCs are used to construct classification models for the implemented classification methods and the best performing method is selected from area under the curves of the ROCs (Step 5). The best classification method is then applied to the PCCs of the NP under investigation inserted by the user (Step 6) and a toxicity estimate is returned (Step 7).

**MOD-ENP-TOX:**  
Modeling Assays Platform "MAP" for hazard ranking of engineered nanoparticles

**Galaxy / MOD-ENP-TOX** Analyze Data Workflow Shared Data Visualization Admin Help User Using 3.0 MB

**Tools**

search tools

**MOD-ENP-TOX**

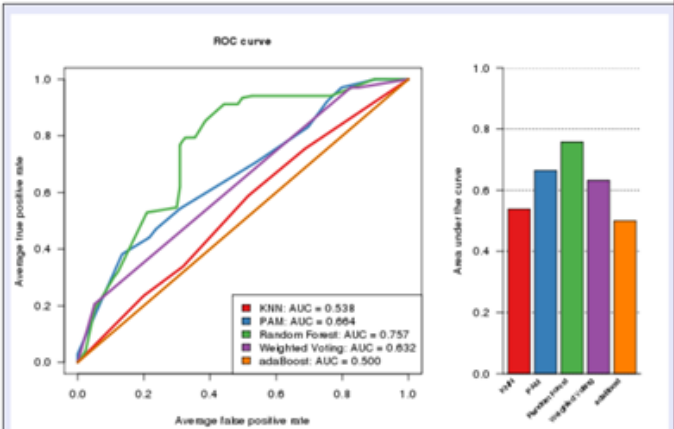
Predict Nanoparticle Toxicity based on physicochemical characteristics

**Workflows**

**Global Toxicity Class Prediction:**

	Probability
Toxic	0.10
Non-Toxic	0.90

This prediction was performed by applying the supervised classification algorithm Random Forest, which performed best in a nested cross-validation experiment in which the prediction accuracy of diverse classifiers was compared. The averaged ROC curves obtained from cross-validation are shown below:



**History**

search datasets

**Results\_dmertens**  
3 shown, 4 deleted

1.3 MB

**7: Predict Nanoparticle Toxicity**

**6: Predict Nanoparticle Toxicity**

1.8 KB  
format: html, database: 2

HTML file

**5: Predict Nanoparticle Toxicity**

**Tool: Predict Nanoparticle Toxicity**

Name: Predict Nanoparticle Toxicity  
Created: Thu Jan 7 08:38:11 2016 (UTC)  
Filesize: 1.8 KB  
Dbkey: ?  
Format: html  
Galaxy Tool ID: predToxCClass  
Galaxy Tool Version: 1.0.0  
Job End Time: 2016-01-07 09:38:18  
Job Start Time: 2016-01-07 09:38:13  
Cores Allocated: 1  
Job Runtime (Wall Clock): 5 seconds

Input Parameter	Value	Note for rerun
Mean Diameter [nm]	101.4	
SD/Range Size-Distribution SD [nm]	292.8	
Mean Zeta-Potential [mV]	191.2	
Mean Specific Surface Area [m2/g]	456.8	
Mean Hydrodynamic Diameter [nm]	178.2	
Use Default Settings	yes	

**Download Results**

1 job has been successfully added to the queue - resulting in the following datasets:

**7: Predict Nanoparticle Toxicity**

You can check the status of queued jobs and view the resulting data by refreshing the History pane. When the job has been run the status will change from 'running' to 'finished' if completed successfully or 'error' if problems were encountered.

**Figure 3: Results Management of the modelling platform.** Classification results are stored and outputs can be reviewed at any stage (shown in red). The information about input parameters is now available and stored for every single analysis (shown in blue). Images and underlying data can be downloaded using the Download button (shown in yellow).

**MOD-ENP-TOX:**

Modeling Assays Platform "MAP" for hazard ranking of engineered nanoparticles



# MOD-ENP-TOX

