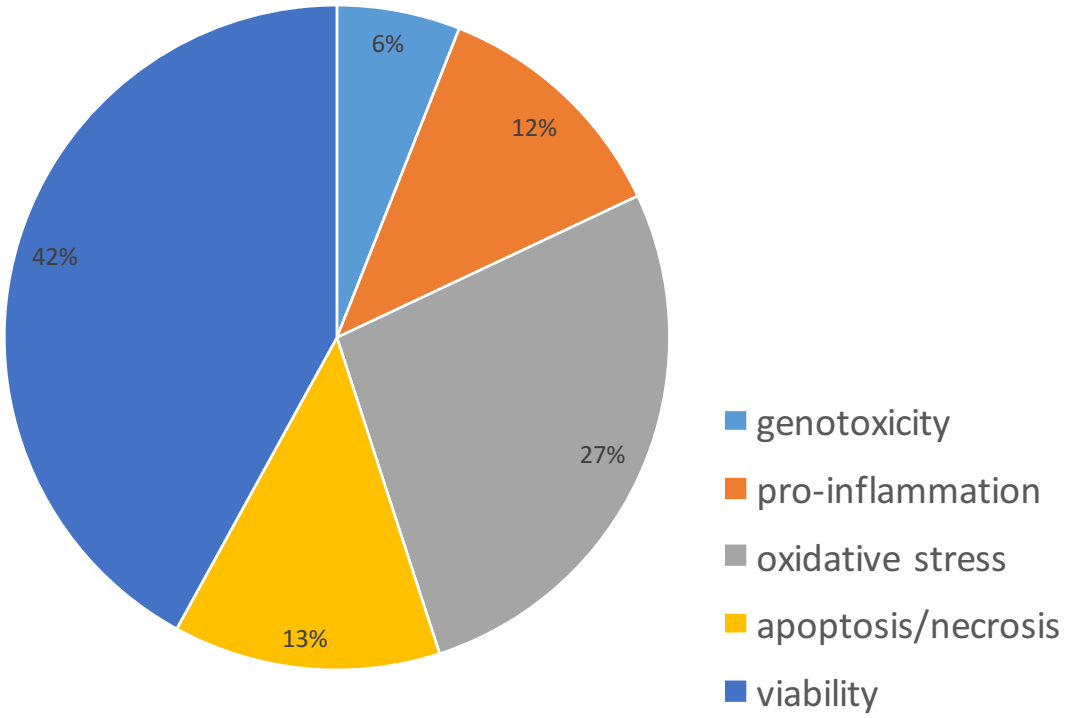

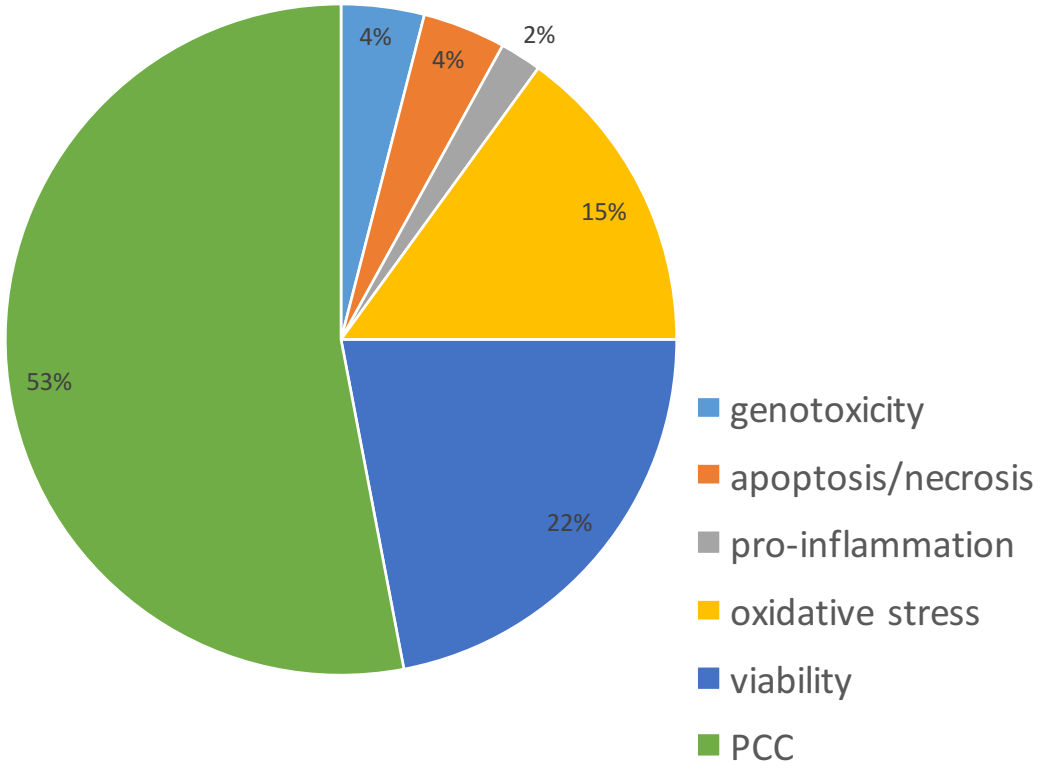

Figure 1: Proportion of different types of assays populating the newly designed database.
Assays consists of physico-chemical, viability, oxidative stress, pro-inflammation, genotoxicity and apoptosis/necrosis. Left: for silica NP, Right: for ZnO NP

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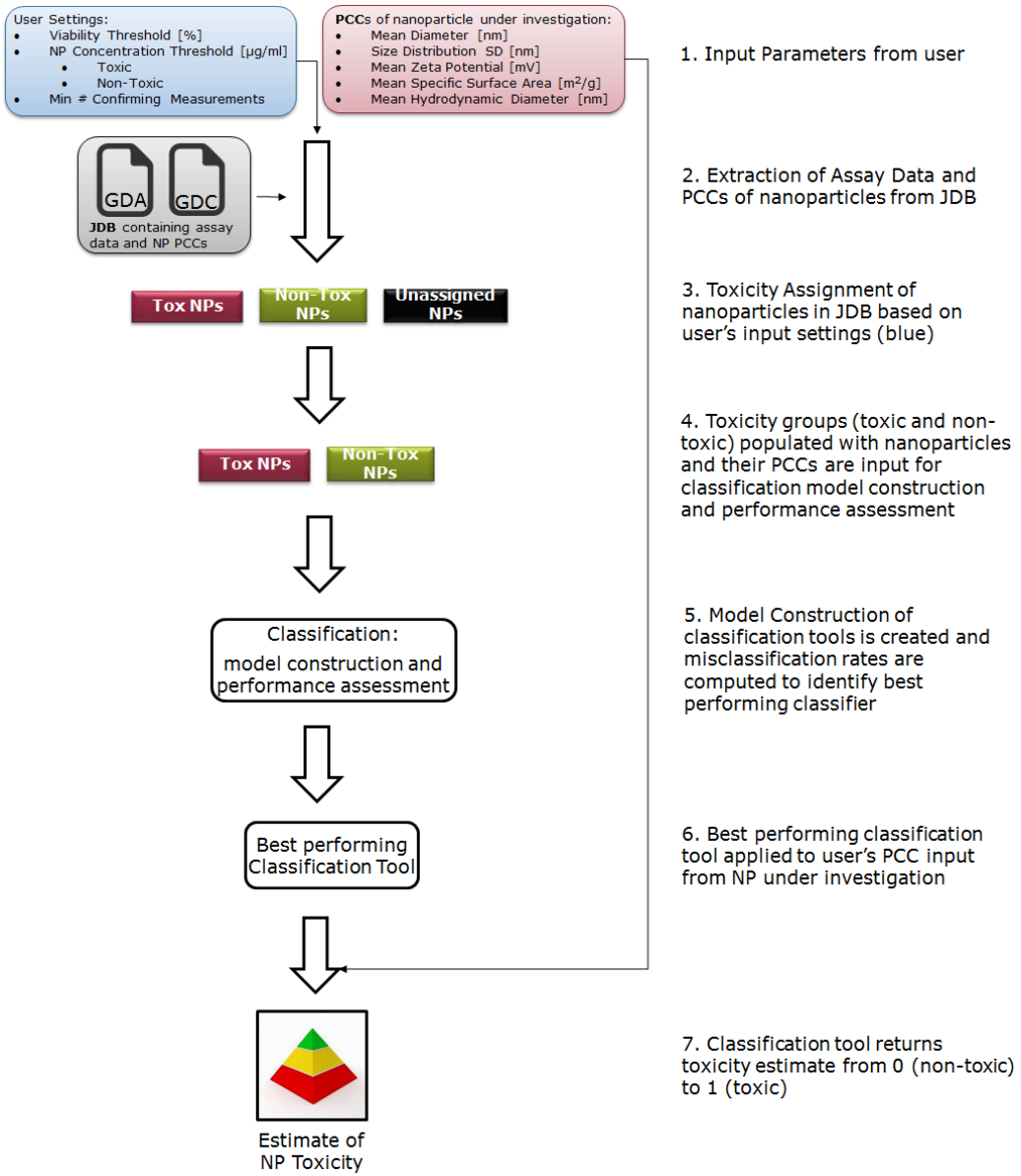

Figure 2: The individual steps of the classification tool.

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 (Step7).

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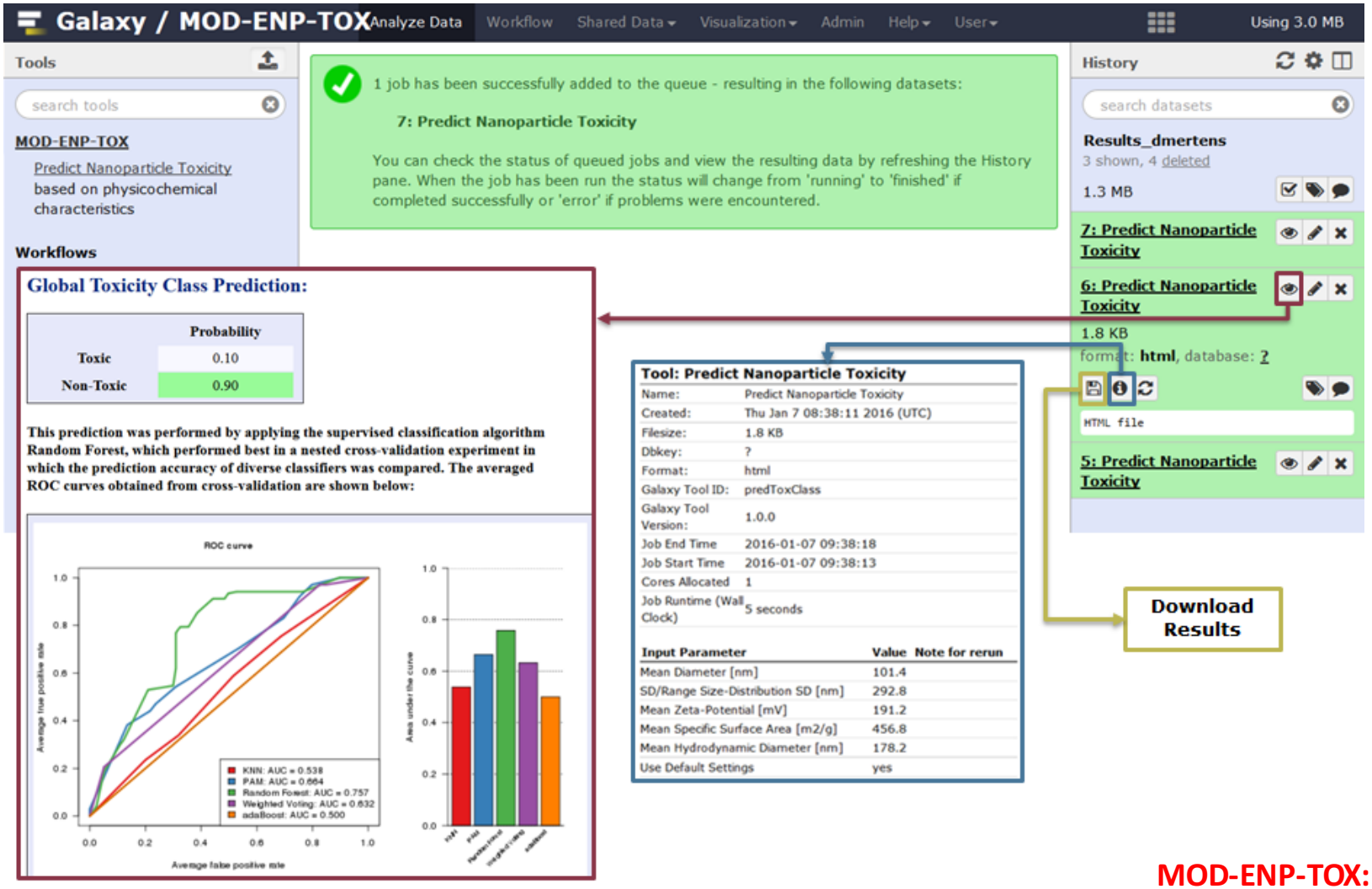

Figure 3: Results Management of the modelling platform.
Classification results are stored and outputs can be reviewed at any stage (shown in red). The information about input parameters is now available and stored for every single analysis (shown in blue). Images and underlying data can be downloaded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

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