

NAMASTOX Quick starting guide

Introduction

This document will guide you step-by-step in creating a new risk-assessment project (so-called RA), applying the ASPA risk-assessment workflow, presenting the tasks that should be carried out, and collecting the results. At some points, you will be asked to make decisions based on the results obtained so far, combined with your expertise, which will determine your path in the workflow. These decisions will also be collected and documented.

The process illustrated in this document often requires a lot of time to complete because some tasks involve experimental work or data compilation from heterogeneous sources. Also, the process can involve a team of contributors. For these reasons, NAMASTOX is a tool accessible online, which will track all the actions and facilitate their revision. Reports summarizing the results obtained in editable formats can be easily generated. The current status of the work can also be exported, imported and backed up.

RA creation

Open the NAMASTOX interface and click the three-line icon (\equiv) on the top left corner to open the toolbar. Press the first button (New RA). This will open a dialog box like the following

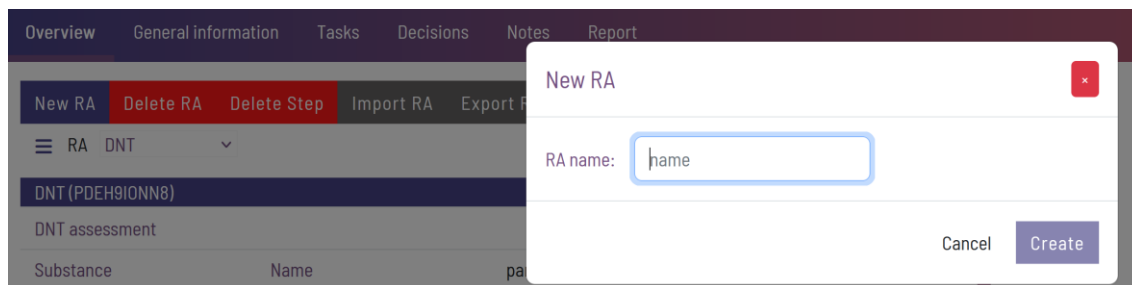


Figure 1. Dialogue for creating a New RA

Enter a suitable name for your project. In this guide, we will use MyFirstRA. Press the Create button. A screen like the following will be displayed:

Overview General information Tasks Decisions Notes Report

ASPIS RISK HUNT3R

RA MyFirstRA

Title: Descriptive name for this study

General description: Descriptive text about this study

Background: Any relevant information

Endpoint: Toxicological endpoint(s) of interest

Administration route: Administration routes of the toxicant to be considered

Regulatory framework: Regulatory bodies for which this study can be of interest

Species: Biological species to be considered

Uncertainty: Comments about the acceptable uncertainty levels

workflow undefined

...

Reset

Figure 2. General information form

Please note that the new RA has been added to the list of available RA projects besides the lines icon (≡).

The next step is to enter general information about this project.

Entering General Information

You must start entering relevant information about your project, like a title and general description, assessment background, endpoint, etc. None of the fields are compulsory, and the information entered can be edited later.

A critical section is the identification of the substance being studied.

Substance: Name(s) Substance name or names separated by a colon

ID(s) Substance ID or IDs separated by a colon

CAS-RN(s) undefined

Structure

Examinar... No se ha seleccionado ningún archivo.

Autocomplete

Figure 3. Section of the General Information identifying the substance of interest

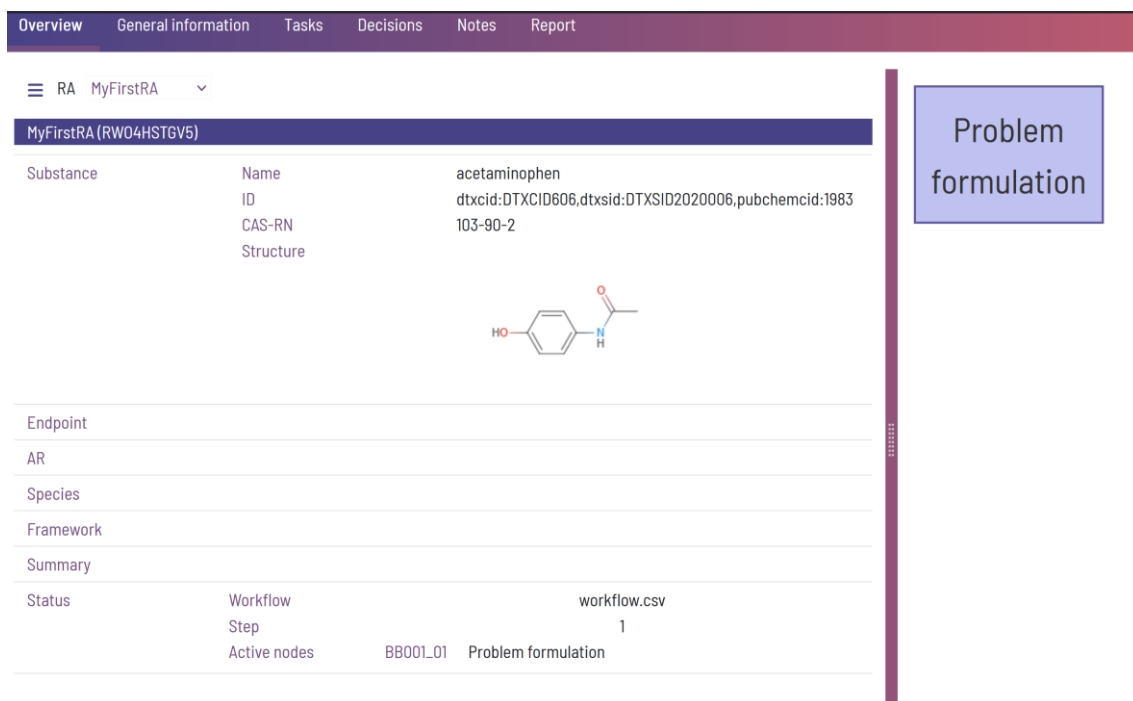
In this form, enter the Name or the CAS-RN and press Autocomplete. For many known compounds, the rest of the fields (IDs and chemical structure) can be completed automatically by pressing the Autocomplete button.

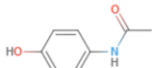
By default, NAMASTOX will use the most updated version of the ASPA workflow (1.9 when writing this guide). Still, we can use a customized workflow by uploading a workflow definition file at the bottom of the dialogue.

Press the Submit button at the bottom of the page to complete this step.

What to do next?

The NAMASTOX interface depicts the workflow on the right-hand side, representing only the task already carried out (in grey) and the following tasks (in light violet colour).



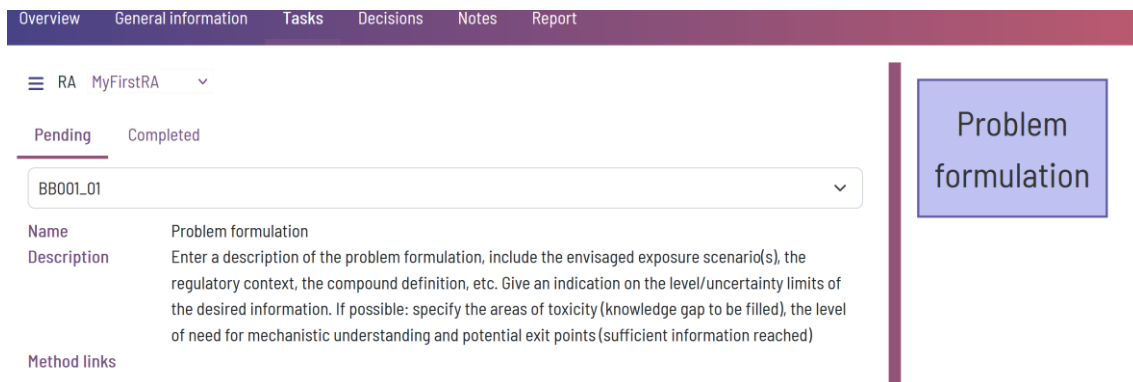
Substance	Name	acetaminophen
	ID	dtxcid:DTXCID606,dtxsid:DTXSID2020006, pubchemcid:1983
	CAS-RN	103-90-2
	Structure	

Endpoint
AR

Summary		
Status	Workflow	workflow.csv
	Step	1
	Active nodes	BB001_01 Problem formulation

Figure 4. Initial status of the RA.

The user should click on an active node to progress in the assessment. This will show a description of this task, with detailed instructions about what the user should do, sometimes including links to guidance documents or useful resources.



Pending	Completed
BB001_01	

Name	Description
Problem formulation	Enter a description of the problem formulation, include the envisaged exposure scenario(s), the regulatory context, the compound definition, etc. Give an indication on the level/uncertainty limits of the desired information. If possible: specify the areas of toxicity (knowledge gap to be filled), the level of need for mechanistic understanding and potential exit points (sufficient information reached)

Figure 5. Description of the task

In most cases, the user can close the interface and exit if carrying out these tasks will require time and effort.

At a later stage, once the tasks are completed, the user can reopen the interface, select the RA on the list of RAs on top and click again on the task to enter the results together with any relevant documentation.

It should be stressed that the NAMASTOX interface does not require entering all the information in a single session or by a single user. The RA can be visited an unlimited

number of times for consulting on the following tasks: entering new results, editing existing results, retrieving the data entered, or generating reports. RAs will be stored in a repository and remain there until explicitly removed.

Entering and documenting task results

Once the task has been completed, the results can be entered by clicking the corresponding box on the right-hand side. Only active boxes, depicted in light violet, can be selected to enter new results.

If the expected results are text, like in the task “Problem formulation”) the aspect of the interface is this

The interface for entering text results consists of several components. At the top, there is a 'Results*' label followed by a large text input field with a placeholder text: 'Results obtained for the tasks specified in the description (compulsory field)'. Below this, there is a 'Documentation:' label followed by a row of controls: a button labeled 'Examinar...', a button labeled 'No se ha seleccionado archivo.', a checked checkbox labeled 'Include', a text input field labeled 'label', and a red arrow icon. Below the documentation controls, there is a 'Summary:' label followed by a text input field with a placeholder text: 'Concise description of the results obtained or the decisions made'. At the bottom right, there is a blue 'Submit' button.

Figure 6. Interface for entering the results of a task producing text results.

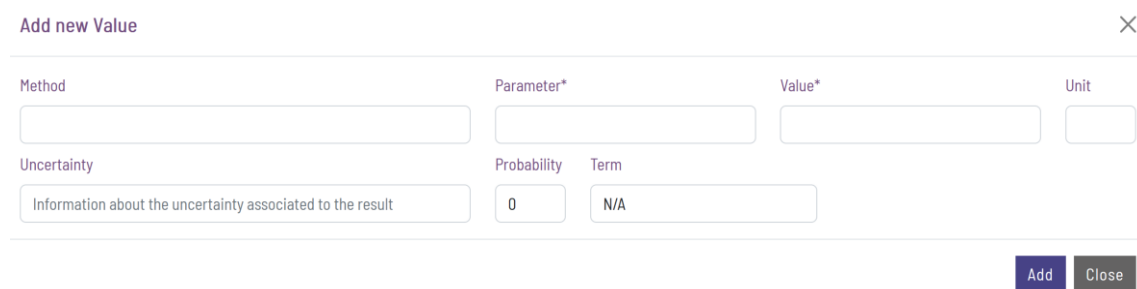
You must enter a descriptive text in the field Results (compulsory). Additionally, it is strongly recommended that you enter a shorter version in the summary field and any number of relevant documents to provide further information. It is possible to upload documents in text (.txt, .csv, .tsv), PDF and Microsoft Office formats (.doc, .docx, .xls, .xlsx). Bitmaps in .png and .jpeg formats can also be imported.

In the case of tasks that are expected to produce values, the interface aspect is slightly different, even if the Documentation and Summary fields are identical.

The interface for entering value results is similar to the one for text results but includes additional controls at the top right. Above the 'Documentation:' label, there are three buttons: 'Add value', 'Import Table', and 'Predict'. The 'Documentation:' label is followed by the same row of controls as in Figure 6: 'Examinar...', 'No se ha seleccionado archivo.', 'Include' (checked), 'label', and a red arrow icon. Below this, there is a 'Summary:' label followed by a text input field with a placeholder text: 'Concise description of the results obtained or the decisions made'. At the bottom right, there is a blue 'Submit' button.

Figure 7. Interface for entering the results of a task producing value results.

Values can be entered one by one using the Add Value button. This will create the following dialogue.



Add new Value

Method Parameter* Value* Unit

Uncertainty Probability Term

Information about the uncertainty associated to the result 0 N/A

Add Close

Figure 8. Dialogue for entering values.

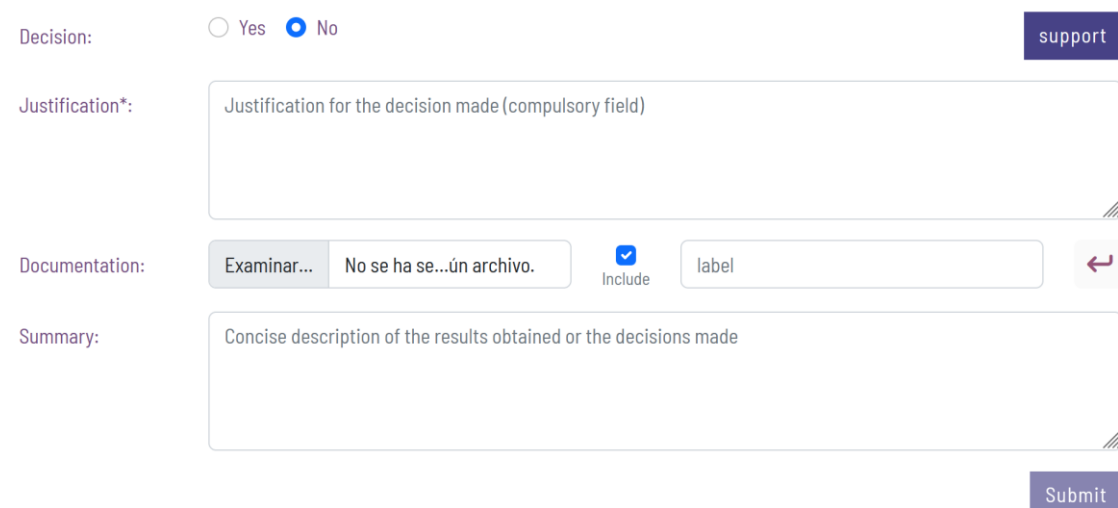
Complete at least the Parameter and Value fields and press Add to enter a new value. The uncertainty associated with the values can be entered in the form of free text, a probability value or a predefined term when available.

You can also enter multiple values simultaneously by importing a pre-formatted table in .tsv format by pressing the Import Table button.

In some tasks, it is also possible to run predictions for the substance defined in the General Information by pressing the Predict button.

Making and documenting decisions

Some tasks require that the user make a decision. Decisions are always binary (yes or no) and must be justified. The interface has the following aspect



Decision: ☐ Yes ☒ No

Justification*: Justification for the decision made (compulsory field)

Documentation: Examinar... No se ha se...ún archivo. Include label

Summary: Concise description of the results obtained or the decisions made

support Submit

Figure 9. Interface for entering decisions.

As in the case of the task, it is possible to add a summary and attach documents to justify the decision further.

The button support opens a dialogue where the results of upstream nodes are presented, together with their associated uncertainties, to facilitate the decision-making process.

Generating reports

Press the tab reports at the top to show the following page.

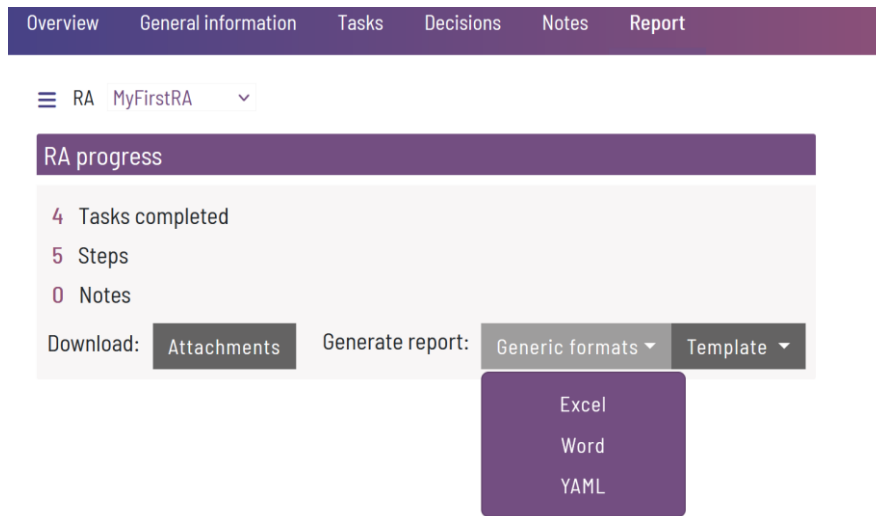


Figure 10. Interface for producing reports in different formats.

This page summarises the work carried out so far and offers the possibility of generating a report in Excel or Word (YAML format is computer-readable). It is also possible to download all the documents attached in compressed format by pressing the Attachment button. If it is decompressed in the same folder of the file, the report will link the attached documents.

Exporting and importing projects

RAs can be exported by pressing the three lines icon (≡) on the top left corner to open the toolbar and pressing the Export RA button (for exporting the current RA)

The button Import RA allows the user to select a file with a previously exported RA and import it into the current repository.

The import and export features can be used to back up RAs.

Managing projects

RAs can be deleted by pressing the three lines icon (≡) on the top left corner to open the toolbar and pressing the Delete RA button.

The Delete Step command will only remove the last step of the current RA. Please use it with care because this option cannot be reverted.