

NAMASTOX WORKFLOW DEFINITION FORMAT

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Introduction

In NAMASTOX custom workflows can be defined using tables, where each line represents a node and each column a piece of information for this node.

The table must be entered using TSV format, with fields separated by tabs (\t). It is important that the text does not contain Unicode text, only plain text.

The table must contain all of the following columns, with the following column names: id, label, result_type, name, category, description, method_type, method_link, next_node, next_yes, next_no

Example:

| | A | B | C | D | E | F | G | H | I | J | K |
|---|-------|-------|-------------|-------------|----------|----------------------|-------------|---|-----------|----------|---------|
| 1 | id | label | result_type | name | category | description | method_type | method_link | next_node | next_yes | next_no |
| 2 | A0001 | AAA0 | text | First node | TASK | Description First | expert | | A0002 | | |
| 3 | A0002 | AAA0 | text | Second node | TASK | Description Second | expert | https://phi.upf.edu | A0003 | | |
| 4 | A0003 | DDD0 | bool | Question | LOGICAL | Description question | | | | A0004 | A0005 |
| 5 | A0004 | BBB0 | value | Third node | TASK | Description Second | expert | | Z0001 | | |
| 6 | A0005 | BBB1 | value | Fourth node | TASK | Description Second | expert | | Z0001 | | |
| 7 | Z0001 | EXIT1 | text | Exit | END | Final report | | | | | |
| 8 | | | | | | | | | | | |

We recommend using LibreOffice for editing the TSV files, but any other text editor can also be suitable. The filename can have any extension (even if .csv or .tsv are recommended), but it is important that the filename does not contain spaces. Please use only letters, numbers and the underscore and hyphen signs.

Column definition

id

Any text indicating the node ID. Must be unique. The first letter could be used to group the nodes in colored blocks: 'H' for HAZARD, 'B' for ADME and 'E' for EXPOSURE.

label

Any text, Will be shown as a label for this node.

result_type

Indicates the type of input expected. It can be “text”, “bool” or “value”. Depending on the type, the node will have a different aspect, for entering free text (text) or values (value).

category

Indicates the type of node. It can be “TASK”, “LOGICAL” or “END”

method type

Indicate how the values will be entered. It is only orientative.

method link

When nonempty, the link will be shown in the interface. If it contains “local_models”, the node will call an endpoint for retrieving any Flame models present in the current host.

next_node

Only for TASK nodes. Shows the ID of the following node. This information is compulsory and should make reference to an existing node. It is possible to add the IDs or several nodes, separated by comma.

next_yes

Only for LOGICAL nodes. Shows the ID of the node linked to the YES option. This information is compulsory and should make reference to an existing node. It is possible to add the IDs or several nodes, separated by comma.

next_no

Only for LOGICAL nodes. Shows the ID of the node linked to the NO option. This information is compulsory and should make reference to an existing node. It is possible to add the IDs or several nodes, separated by comma.