



IVBP-Suite beta version

Quick Start Guide



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Department of Theoretical and Applied Sciences (DiSTA)
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Information

The software and models were developed by:

QSAR Research Unit in Environmental Chemistry and Ecotoxicology
Department of Theoretical and Applied Sciences (DiSTA)
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<https://dunant.dista.uninsubria.it/qsar/>

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<https://arnotresearch.com>

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Overview

IVBP-Suite beta version allows the user to input his molecular structures and get estimations and Applicability Domain for a desired QSAR model.

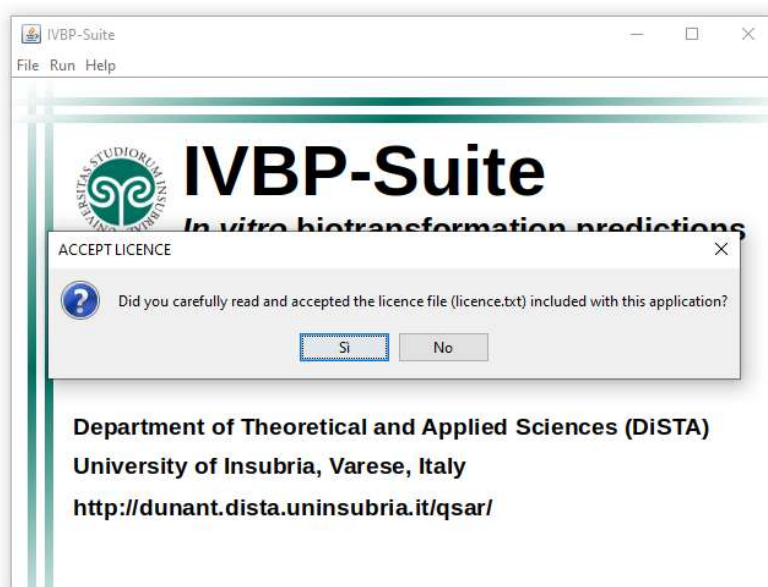
Minimal information required to obtain prediction are:

-Chemical structures files (e.g. .smi, .mol) (see below to see how to set a .smi file)

Tutorial

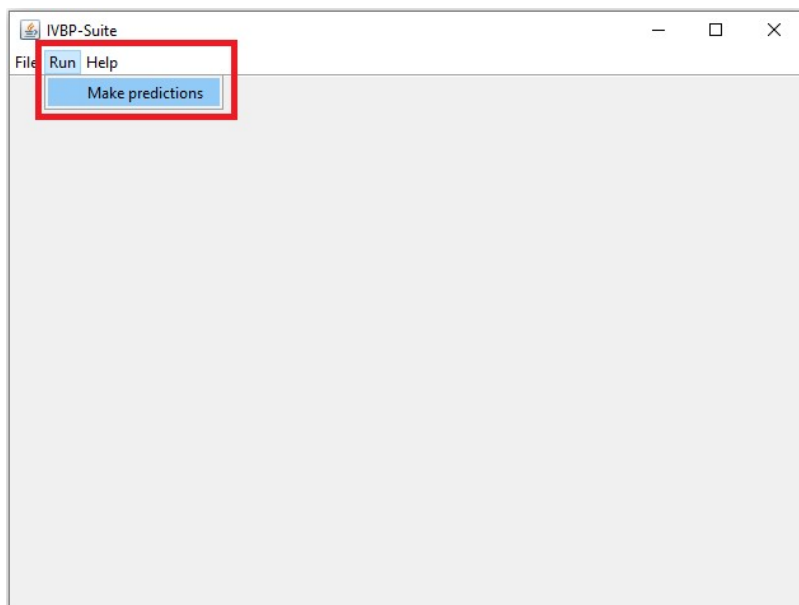
Launching program

Execute IVBP-Suite.jar (usually by double clicking on its icon. If it is not working, please ask your IT staff because it depends on whether, or how, the Java environment is configured on your machine). The first time you execute IVBP-Suite beta version, you need to read the Licence agreement and if you agree you can use IVBP-Suite beta version.



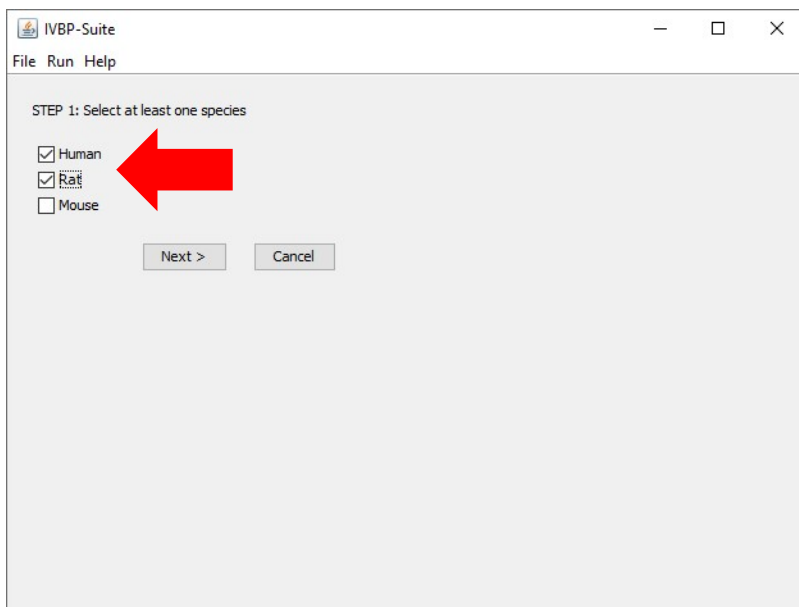
Begin setup for predictions

To start predicting the endpoint of the chemicals, select the “Run” menu and then “Make predictions”



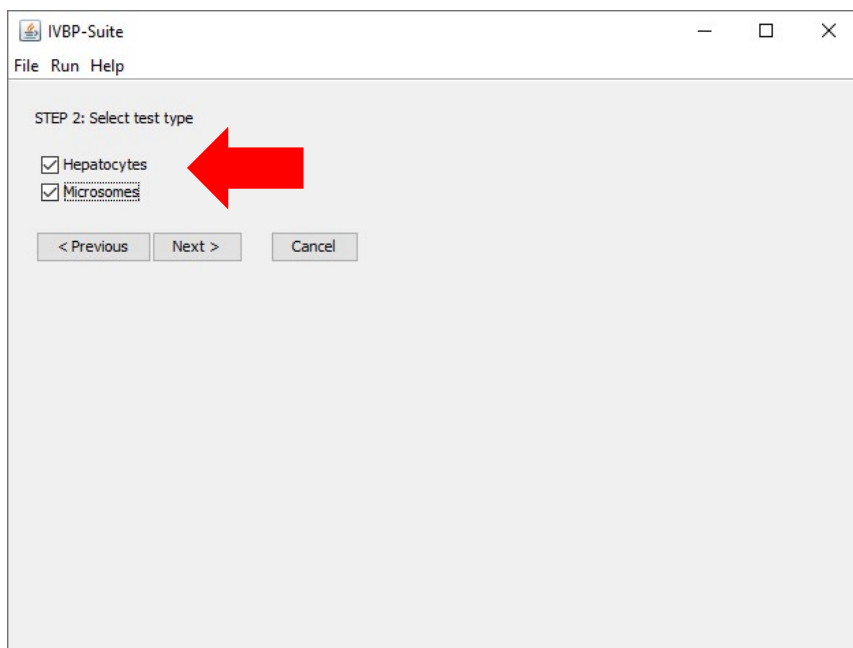
Step 1 – Choose species

Select the species of interest, then press “Next”



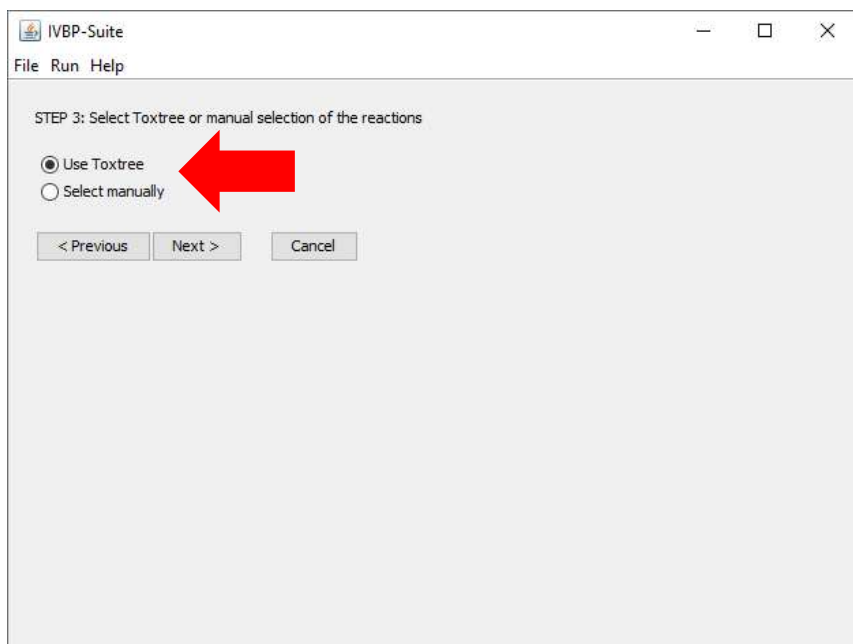
Step 2 – Choose test type

Select the test type of interest, then press “Next”



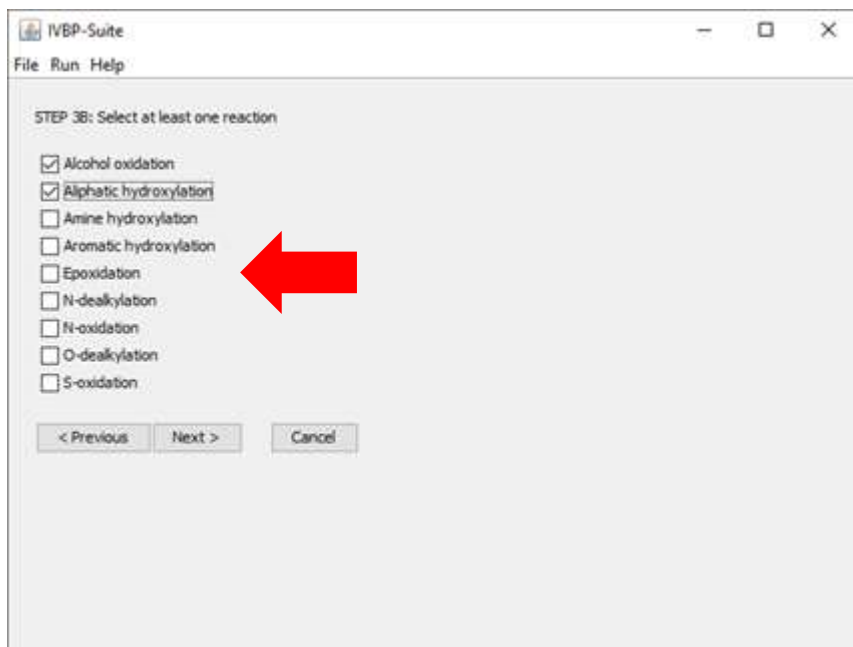
Step 3 – Choose for automated or manual reactions selection

Select “Use Toxtree” for an automated detection of most probable biotransformation reactions or “Select manually” if manual selection is preferred, then press “Next”



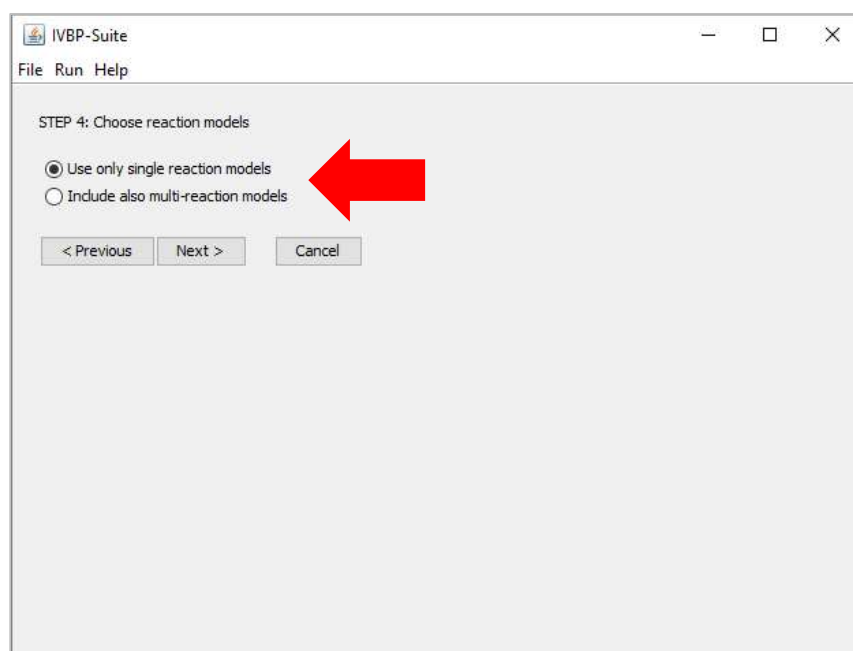
Step 3B – Choose reactions manually (if requested)

In case “Select manually” was selected at step 3, select the reactions of interest, then press “Next”



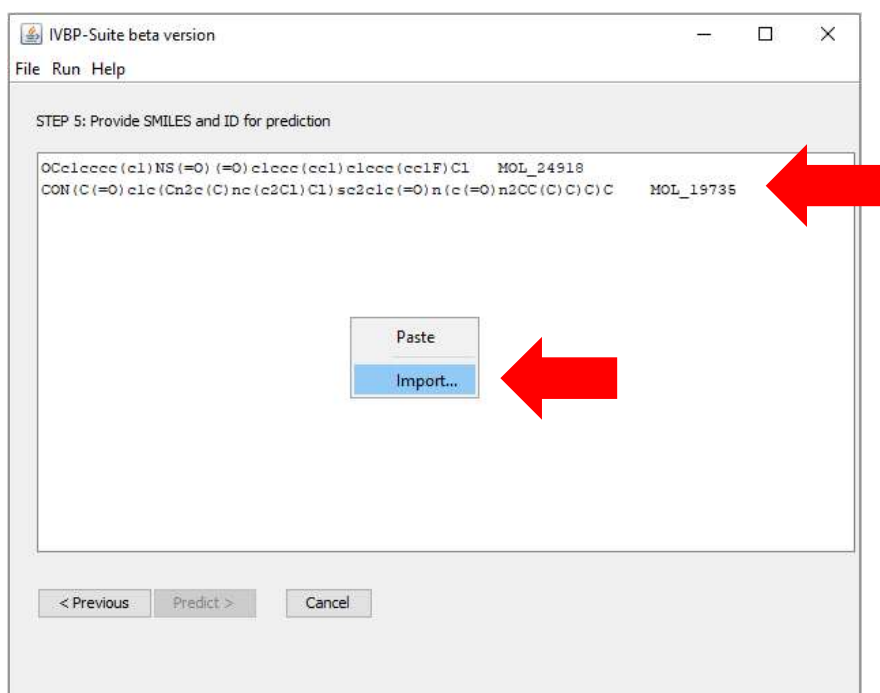
Step 4 – Choose for single or multiple reaction models

Choose whether only single-reaction based models have to be applied or also the more general models for multiple reactions (which could be less precise) should be included for prediction, then press “Next”



Step 5 – Provide SMILES and ID

Write the SMILES of the molecules whose biotransformation endpoint should be predicted. SMILES can be typed directly in the text box or alternatively pasted from another source or imported from a file. Accepted format is SMILES, followed by a white space (or, in alternative, tab) and then an arbitrary molecule ID, as shown in the figure below example. Once SMILES are entered press “Predict” to predict the endpoint of the chemicals, then wait till Toxtree (if previously selected) and PaDEL-Descriptor complete calculations (note: PaDEL-Descriptor can take significant time for calculations, depending on the number and/or complexity of the chemicals)



Output

The output of IVBP-Suite beta version is organized as a user-friendly table.

IVBP-Suite beta version										
File Run Help										
Rank 1	Rank 2	Rank 3	Rank 4							
Molecule	Organism	Test type	Reaction	Endpoint	Consensus weighted ALL	Consensus weighted AD	... Model ID 1	... Model ID 2	... Model ID 6	
MOL_01	Human	Hepatocytes	O-dealkylation	Log_CL in vitro, i...	0.67±0.61	0.67±0.61	-	-	-	
MOL_01	Human	Microsomes	O-dealkylation	Log_CL in vitro, i...	4.0e-02±0.19	-0.12±0.24	-	-	-	
MOL_01	Rat	Hepatocytes	O-dealkylation	LogClin vitro, int ...	0.29±0.57	0.29±0.57	-	-	-	
MOL_01	Rat	Microsomes	O-dealkylation	LogClin vitro, int ...	0.89±0.48	0.89±0.48	-	-	-	
MOL_01	No model available...	NA	NA	NA	NA	NA	-	-	-	
MOL_01	Mouse	Microsomes	O-dealkylation	LogClin vitro, int ...	0.67±0.73	NA	-	-	-	
MOL_02	Human	Hepatocytes	O-dealkylation	Log_CL in vitro, i...	0.41±0.61	0.41±0.61	-	-	-	
MOL_02	Human	Microsomes	O-dealkylation	Log_CL in vitro, i...	0.45±0.19	0.39±0.31	-	-	-	
MOL_02	Rat	Hepatocytes	O-dealkylation	LogClin vitro, int ...	0.72±0.59	0.72±0.59	-	-	-	
MOL_02	Rat	Microsomes	O-dealkylation	LogClin vitro, int ...	1.3±0.49	1.3±0.49	-	-	-	
MOL_02	No model available...	NA	NA	NA	NA	NA	-	-	-	
MOL_02	Mouse	Microsomes	O-dealkylation	LogClin vitro, int ...	0.51±0.68	0.51±0.68	-	-	-	
MOL_03	Human	Hepatocytes	Aliphatic hydr...	Log_CL in vitro, i...	1.6±0.52	NA	1.7±0.67 *#	1.5±0.81 *#	-	
MOL_03	Human	Microsomes	Aliphatic hydr...	Log_CL in vitro, i...	-0.38±0.29	-4.3e-02±0.58	-	-	-	
MOL_03	Rat	Hepatocytes	Aliphatic hydr...	LogClin vitro, int ...	0.16±0.53	0.21±0.62	-	-	-	
MOL_03	Rat	Microsomes	Aliphatic hydr...	LogClin vitro, int ...	0.90±0.39	0.67±0.45	-	-	-	
MOL_03	No model available...	NA	NA	NA	NA	NA	-	-	-	
MOL_03	Mouse	Microsomes	Aliphatic hydr...	LogClin vitro, int ...	0.93±0.47	0.93±0.47	-	-	-	
MOL_04	Human	Hepatocytes	Aromatic hydr...	Log_CL in vitro, i...	0.16±0.47	0.16±0.47	-	-	0.16±0.47	
MOL_04	Human	Microsomes	Aromatic hydr...	Log_CL in vitro, i...	0.30±0.25	0.64±0.31	-	-	-	
MOL_04	Rat	Hepatocytes	Aromatic hydr...	LogClin vitro, int ...	0.26±0.38	0.26±0.38	-	-	-	
MOL_04	Rat	Microsomes	Aromatic hydr...	LogClin vitro, int ...	0.52±0.23	0.55±0.24	-	-	-	
MOL_04	No model available...	NA	NA	NA	NA	NA	-	-	-	
MOL_04	Mouse	Microsomes	Aromatic hydr...	LogClin vitro, int ...	1.1±0.33	1.1±0.51	-	-	-	
MOL_05	Human	Hepatocytes	Epoxidation	Log_CL in vitro, i...	1.7±0.81	NA	-	-	-	
MOL_05	Human	Microsomes	Epoxidation	Log_CL in vitro, i...	1.7±0.79	NA	-	-	-	
MOL_05	No model available...	NA	NA	NA	NA	NA	-	-	-	
MOL_05	Rat	Microsomes	Epoxidation	LogClin vitro, int ...	0.54±0.61	NA	-	-	-	
MOL_05	No model available...	NA	NA	NA	NA	NA	-	-	-	
MOL_05	Mouse	Microsomes	Epoxidation	LogClin vitro, int ...	1.8±0.45	NA	-	-	-	
MOL_06	Human	Hepatocytes	Aromatic hydr...	Log_CL in vitro, i...	-1.2e-02±0.47	-1.2e-02±0.47	-	-	-1.2e-02±0.47	
MOL_06	Human	Microsomes	Aromatic hydr...	Log_CL in vitro, i...	0.35±0.24	0.40±0.31	-	-	-	
MOL_06	Rat	Hepatocytes	Aromatic hydr...	LogClin vitro, int ...	0.35±0.39	0.35±0.39	-	-	-	
MOL_06	Rat	Microsomes	Aromatic hydr...	LogClin vitro, int ...	1.1±0.25	0.61±0.35	-	-	-	
MOL_06	No model available...	NA	NA	NA	NA	NA	-	-	-	
MOL_06	Mouse	Microsomes	Aromatic hydr...	LogClin vitro, int ...	0.98±0.39	0.45±0.60	-	-	-	

If Toxtree was selected, four table ranked from 1 (most probable reactions) to 4 (least probable reactions) are provided, otherwise only one if manual selection of the reactions was performed (Step 3B).

Molecules can be filtered according to the available species and test type, by checking the pertinent menu voices as shown in the menu below.

☒ Human
 ☒ Rat
 ☒ Mouse

☒ Hepatocytes
 ☒ Microsomes

Copy

 Select all

 Save...

In addition data can be copied in the clipboard and/or saved as a text file.

Details of the output columns

Molecule: the name of the molecule.

Organism: the selected organism.

Test type: the select assay.

Reaction: the selected reaction (either manually or by Toxtree).

Endpoint: the endpoint of interest.

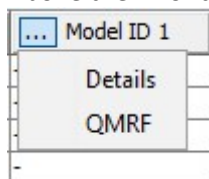
Consensus weighted ALL: weighted average¹ of the predictions of all models available.

Consensus weighted AD: weighted average¹ of the predictions of only the models for which the molecule is within the structural and response applicability domain.

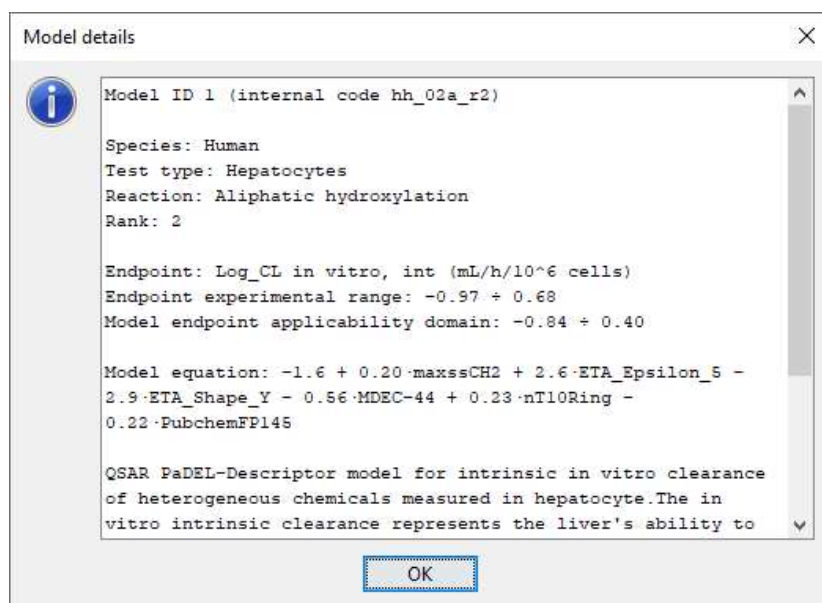
The predictions per model are shown in the subsequent columns (their number varies depending on the previous setup and the molecules). The format of the columns is **Model ID** - number of the model-. In case the prediction is out of the applicability domain the following codes are provided:

-> out of structural domain * -> out of endpoint domain.

Above the ID of the model, pressing the ... box as shown below allows for showing details of the model.




By selecting “Details”, details of the corresponding model are shown, as in the example below



¹ Italian edition of “An Introduction to Error Analysis, The Study of Uncertainties in Physical Measurements”, Taylor J.R., University Science Books, 1982.

By selecting “QMRF” a QMRF document is automatically opened as .pdf, as in the shown in the short extract below

	QMRF identifier (JRC Inventory): To be entered by JRC
	QMRF Title: InVitroHCL_HumanHep_AliphaticHydroxylation_a_rank2
	Printing Date: 28-mag-2021

1.QSAR identifier

1.1.QSAR identifier (title):

InVitroHCL_HumanHep_AliphaticHydroxylation_a_rank2

1.2.Other related models:

None

1.3.Software coding the model:

QSARINS

Software for QSAR MLR models development

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<http://dunant.dista.uninsubria.it/qsar/>

2.General information

2.1.Date of QMRF:

31/08/2020

2.2.QMRF author(s) and contact details:

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ester.papa@uninsubria.it <http://dunant.dista.uninsubria.it/qsar/>

2.3.Date of QMRF update(s):

Starting new predictions

To start new predictions, while deleting the current output, select the “Run” menu and then select “Make predictions” again.