	QMRF identifier (JRC Inventory): **To be entered by JRC**
	QMRF Title: **VEGA implementation of Verhaar scheme - v. 1.0.1**
	Printing Date: **September 2022**

1.QSAR identifier

1.1.QSAR identifier (title):

VEGA implementation of Verhaar scheme (version 1.0.1)

1.2.Other related models:

This is the description of the VEGA model that mimic the Verhaar scheme as implemented in the software ToxTree version 3.2

1.3.Software coding the model:

VEGA (https://www.vegahub.eu/)

The VEGA software provides QSAR models to predict tox, ecotox, environ, phys-chem and toxicokinetic properties of chemical substances.

emilio.benfenati@marionegri.it

2.General information

2.1.Date of QMRF:

September 2022

2.2.QMRF author(s) and contact details:

[1] Emilio Benfenati Istituto di Ricerche Farmacologiche Mario Negri - IRCSS Via Mario Negri 2, 20156 Milano, Italy emilio.benfenati@marionegri.it https://www.marionegri.it/

[2] Erika Colombo Istituto di Ricerche Farmacologiche Mario Negri - IRCSS Via Mario Negri 2, 20156 Milano, Italy erika.colombo@marionegri.it https://www.marionegri.it/

2.3.Date of QMRF update(s):

No update

2.4.QMRF update(s):

No update

2.5.Model developer(s) and contact details:

The original model implements the conceptual scheme developed by Verhaar et al. For the implementation in ToxTree: Nina jeliazkova; IDEA Consult, Joseph II straat 40 B1, 1000 Brussels, Belgium; jeliazkova.nina@gmail.com

For the implementation in VEGA of the Toxtree model: Alberto Manganaro; IRCCS-Istituto di Ricerche Farmacologiche Mario Negri, Via La Masa 19, 20156 Milano, Italy; alberto.manganaro@marionegri.it

2.6.Date of model development and/or publication:

2020 in VEGA

2.7.Reference(s) to main scientific papers and/or software package:

Verhaar, H.J.M., van Leeuwen, C.J., Hermens, J.L.M., 1992. Classifying environmental-pollutants. 1. 481 Structure-activity-relationships for prediction of aquatic toxicity. Chemosphere 25, 471-491.

2.8.Availability of information about the model:

The model is non-proprietary.

2.9.Availability of another QMRF for exactly the same model:

Another QMRF is not available.

3.Defining the endpoint - OECD Principle 1

3.1.Species:

Fish

3.2.Endpoint:

This model identifies the mechanism of action of substances for fish acute toxicity

3.3.Comment on endpoint:

The model gives a classification based on the mechanism of action of the substance to help in the assessment of the acute toxicity towards fish.

3.4.Endpoint units:

Adimensional.

3.5.Dependent variable:

The dependent variable is the mechanism of action organized in four classes:

Class 1 (narcosis or baseline toxicity)

Class 2 (less inert compounds)

Class 3 (unspecific reactivity)

Class 4 (compounds and groups of compounds acting by a specific mechanism)

Class 5 (Not possible to classify according to these rules)

3.6.Experimental protocol:

NA

3.7.Endpoint data quality and variability:

NA

4.Defining the algorithm - OECD Principle 2

4.1.Type of model:

Structure-based model

4.2.Explicit algorithm:

The Verhaar classification is based on the same scheme as implemented in ToxTree, which is an open source application. The scheme is expert-based

4.3.Descriptors in the model:

The model is a structure-based model and does not make use of descriptors

4.4.Descriptor selection:

No descriptor is used.

4.5.Algorithm and descriptor generation:

A decision tree has been implemented within Toxtree, and the same tree is implemented in VEGA.

4.6.Software name and version for descriptor generation:

Ad hoc decision tree has been implemented within Toxtree

4.7.Chemicals/Descriptors ratio:

Not applicable; the software is an expert system, not a statistical one.

5.Defining the applicability domain - OECD Principle 3

5.1.Description of the applicability domain of the model:

Not available. The scheme is expert-based.

5.2.Method used to assess the applicability domain:

Not applicable.

5.3.Software name and version for applicability domain assessment:

Not applicable.

5.4.Limits of applicability:

NA

6.Internal validation - OECD Principle 4

6.1.Availability of the training set:

NA

6.2.Available information for the training set:

NA

6.3.Data for each descriptor variable for the training set:

NA

6.4.Data for the dependent variable for the training set:

NA

6.5.Other information about the training set:

NA

6.6.Pre-processing of data before modelling:

NA

6.7.Statistics for goodness-of-fit:

NA

6.8.Robustness - Statistics obtained by leave-one-out cross-validation:

NA

6.9.Robustness - Statistics obtained by leave-many-out cross-validation:

NA

6.10.Robustness - Statistics obtained by Y-scrambling:

NA

6.11.Robustness - Statistics obtained by bootstrap:

NA

6.12.Robustness - Statistics obtained by other methods:

NA

7.External validation - OECD Principle 4

7.1.Availability of the external validation set:

NA

7.2.Available information for the external validation set:

NA

7.3.Data for each descriptor variable for the external validation set:

NA

7.4.Data for the dependent variable for the external validation set:

All

7.5.Other information about the external validation set:

NA

7.6.Experimental design of test set:

NA

7.7.Predictivity - Statistics obtained by external validation:

NA

7.8.Predictivity - Assessment of the external validation set:

NA

7.9.Comments on the external validation of the model:

NA

8.Providing a mechanistic interpretation - OECD Principle 5

8.1.Mechanistic basis of the model:

The fragments and features use by the scheme of the Verhaar et al. model have been described and discussed within the original paper:

Verhaar, H.J.M., van Leeuwen, C.J., Hermens, J.L.M., 1992. Classifying environmental-pollutants. 1. 481 Structure-activity-relationships for prediction of aquatic toxicity. Chemosphere 25, 471-491.

Four classes are identified, related to the mechanism of action.

8.2.A priori or a posteriori mechanistic interpretation:

A priori.

8.3.Other information about the mechanistic interpretation:

NA

9.Miscellaneous information

9.1.Comments:

NA

9.2.Bibliography:

Verhaar, H.J.M., van Leeuwen, C.J., Hermens, J.L.M., 1992. Classifying environmental-pollutants. 1. 481 Structure-activity-relationships for prediction of aquatic toxicity. Chemosphere 25, 471-491.

9.3.Supporting information:

Training set(s)Test set(s)Supporting information:

10.Summary (JRC QSAR Model Database)

10.1.QMRF number:

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10.2.Publication date:

To be entered by JRC

10.3.Keywords:

To be entered by JRC

10.4.Comments:

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