	QMRF identifier (JRC Inventory): **Q17-23a-0036**
	QMRF Title: **Artificial Intelligence Expert Predictive System (AIEPS) model for biodegradation**
	Printing Date: **Dec 11, 2019**

1.QSAR identifier

1.1.QSAR identifier (title):

Artificial Intelligence Expert Predictive System (AIEPS) model for biodegradation

1.2.Other related models:

1.3.Software coding the model:

Accelrys Accord Chemistry SDK v 6.1

Accord Software Development Kit

BIOVIA 5005 Wateridge Vista Drive, San Diego, CA 92121 USA Tel: +1 858 799 5000

http://accelrys.com/; http://accelrys.com/products/datasheets/accord-chemistry-cartridge.pdf

Accelrys Accord Chemistry Control 6 Runtime

Active X Chemistry control - database files used by windows installer

BIOVIA 5005 Wateridge Vista Drive, San Diego, CA 92121 USA Tel: +1 858 799 5000

http://accelrys.com/; http://accelrys.com/products/datasheets/accord-chemistry-control.pdf

2.General information

2.1.Date of QMRF:

24 December, 2015

2.2.QMRF author(s) and contact details:

Mark Lewis Health Canada 99 Metcalfe St., Ottawa, Ontario, Canada, K1A 0K9

mark.lewis@canada.ca http://www.hc-sc.gc.ca/ewh-semt/index-eng.php

2.3.Date of QMRF update(s):

2.4.QMRF update(s):

2.5.Model developer(s) and contact details:

Stefan P. Niculescu Scientific Consultant spniculescu@gmail.com

2.6.Date of model development and/or publication:

9 November 2012

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

[1]Kaiser KLE and Niculescu SP (2001). Modeling acute toxicity of chemicals to Daphnia magna: A probabilistic neural network approach. Environmental toxicology and chemistry 20 (2) 420-431. http://onlinelibrary.wiley.com/doi/10.1002/etc.5620200225/full

[2]Niculescu SP, Kaiser KLE and Schultz TW (2000). Modeling the toxicity of chemicals to Tetrahymena pyriformis using molecular fragment descriptors and probabilistic neural networks. Archives of environmental contamination and toxicology 39 (3) 289-329 http://link.springer.com/article/10.1007/s002440010107

[3]Niculescu SP, Atkinson A, Hammond G & Lewis M (2004). Using fragment chemistry data mining and probabilistic neural networks in screening chemicals for acute toxicity to the fathead minnow. SAR and QSAR in Environmental Research 15 (4) 293-309. http://www.tandfonline.com/doi/abs/10.1080/10629360410001724941

[4]Niculescu SP, Lewis MA and Tigner J (2008). Probabilistic neural networks modeling of the 48-h LC50 acute toxicity endpoint to Daphnia magna. SAR and QSAR in Environmental Research 19 (7-8) 735-750. http://www.tandfonline.com/doi/abs/10.1080/10629360802550556

[5]Masters T (1993) Practical Neural Network Recipes in C++. Academic Press, San Diego" https://books.google.ca/books?id=7Ez_Pq0sp2EC&lpg=PR17&ots=e05FixTiqW&dq=Masters%20T%20(1993)%20Practical%20Neural%20Network%20Recipes%20in%20C%2B%2B.%20Academic%20Press%2C%20San%20Diego%E2%80%9D&lr&pg=PR17#v=onepage&q&f=false

2.8.Availability of information about the model:

The model is not proprietary. The Accelrys Chemistry Control Runtime might be required to run the interface. Consult with Accelrys/Biovia.

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

3.Defining the endpoint - OECD Principle 1

3.1.Species:

N/A

3.2.Endpoint:

2.Environmental fate parameters 2.3.a.Persistence: Biodegradation. Ready/not ready biodegradability

3.3.Comment on endpoint:

Computation of the Percentage Biodegradation 28-d (BOD) (Biological oxygen demand/ Theoretical oxygen demand)

3.4.Endpoint units:

Percent

3.5.Dependent variable:

The dependent variable is the oxygen demand (consumption) over the 28 day bacterial biodegradation test.

3.6.Experimental protocol:

Ready Biodegradation tests:

MITI I (OECD 301C)

Closed Bottle Test (OECD 301D)

Inherent Biodegradation tests:

MITI II (OECD 302C)

A small fraction of test data from comparable protocols were also used.

3.7.Endpoint data quality and variability:

The percentage biodegradation 28-d (BOD) information used for modeling and testing purposes is public domain and originates from [sect.9.2/ ref.6] and [sect.9.2/ ref.7]. The training set consisted of 851 chemicals.

4.Defining the algorithm - OECD Principle 2

4.1.Type of model:

Probabilistic Neural Network with Gaussian kernel (statistical corrections) included

4.2.Explicit algorithm:

PNN Algorithm

Probabilistic Neural Network with Gaussian kernel (statistical corrections) included

see Attachment

Details on PNN methodology may be found here:
Masters T (1993) Practical Neural Network Recipes in C++. Academic
Press, San Diego

4.3.Descriptors in the model:

[1]number of bromine atoms count number of bromine atoms
[2]number of carbon atoms count number of carbon atoms
[3]number of chlorine atoms count number of chlorine atoms
[4]number of fluorine atoms count number of fluorine atoms
[5]number of iodine atoms count number of iodine atoms
[6]number of nitrogen atoms count number of nitrogen atoms
[7]cumulative number of sodium, potassium and lithium atoms count cumulative number of sodium, potassium and lithium atoms
[8]number of oxygen atoms count number of oxygen atoms
[9]number of phosphorus atoms count number of phosphorus atoms
[10]Number of lead atoms count Number of lead atoms
[11]number of sulfur atoms count number of sulfur atoms
[12]Number of silicon atoms count Number of silicon atoms
[13]Number of tin atoms count Number of tin atoms
[14]ratio between the cumulative number of nitrogen and oxygen atoms in the molecule over the cumulative number of nitrogen, oxygen and carbon atoms (1 for inorganics) count ratio between the cumulative number of nitrogen and oxygen atoms in the molecule over the cumulative number of nitrogen, oxygen and carbon atoms (1 for inorganics)
[15]number of identified combinations of pairs of =O connected to cyclohexane count number of identified combinations of pairs of =O connected to cyclohexane
[16]number of methyl groups count number of methyl groups
[17]number of triple bonds between carbon atoms count number of triple bonds between carbon atoms
[18]number of C-C#N groups count number of C-C#N groups
[19]number of C#N, carbonitrile excluded count number of C#N, carbonitrile excluded
[20]number of N=C=S groups count number of N=C=S groups
[21]number of C=S groups, isothiocyanat excluded count number of C=S groups, isothiocyanat excluded
[22]number of S-C#N groups count number of S-C#N groups
[23]number of S-C groups, thiocyanat excluded count number of S-C groups, thiocyanat excluded
[24]Cumulative number of N-N, N=N and N#N groups count Cumulative number of N-N, N=N and N#N groups
[25]number of amide groups attached to carbons from rings count number of amide groups attached to carbons from rings
[26]number of amide groups attached to carbons not part of rings count number of amide groups attached to carbons not part of rings
[27]number of amide groups not connected to carbons count number of amide groups not connected to carbons
[28]number of amine groups attached to carbons from rings count number of amine groups attached to carbons from rings

[29]number of amine groups attached to carbons not part of rings, amides excluded count number of amine groups attached to carbons not part of rings, amides excluded
[30]number of amine groups not attached to carbons count number of amine groups not attached to carbons
[31]number of carbon-halogen bonds where the carbons are in rings count number of carbon-halogen bonds where the carbons are in rings
[32]number of CF3 groups number of CF3 groups
[33]number of CCl3 groups number of CCl3 groups
[34]number of carbon-halogen bonds where the carbons are not part of rings, number of carbon-halogen bonds where the carbons are not part of rings,
[35]CF3 and CCl3 excluded CF3 and CCl3 excluded
[36]number of OH groups attached to carbons from rings number of OH groups attached to carbons from rings
[37]number of C-O groups where C is part of a ring, RingC-OH excluded number of C-O groups where C is part of a ring, RingC-OH excluded
[38]number of ester bridges number of ester bridges
[39]number of ether bridges, ester bridges excluded number of ether bridges, ester bridges excluded

[40]number of carboxyl groups attached to carbons from rings number of carboxyl groups attached to carbons from rings
[41]number of carboxyl groups, RingC-carboxyl excluded number of carboxyl groups, RingC-carboxyl excluded
[42]number of C-OH groups where C is not is ring, carboxyls excluded number of C-OH groups where C is not is ring, carboxyls excluded
[43]number of O-C(=O)([]) bridges, carboxyls and esters excluded number of O-C(=O)([]) bridges, carboxyls and esters excluded
[44]number of C=O groups where the carbon is not part of a ring, and excluding those included in amides, carboxyls, ester bridges, isocyanat and aldehydes, but including those part of OC(=O)O groups number of C=O groups where the carbon is not part of a ring, and excluding those included in amides, carboxyls, ester bridges, isocyanat and aldehydes, but including those part of OC(=O)O groups
[45]number of OH groups attached to nitrogen number of OH groups attached to nitrogen
[46]number of nitrogen-halogens bonds number of nitrogen-halogens bonds
[47]number of NO2 groups number of NO2 groups
[48]Number of N=O groups, NO2 excluded Number of N=O groups, NO2 excluded
[49]ratio between the cumulative number of nitrogen and oxygen atoms in the molecule which are not part of N(=O)=O groups over the number of carbons (0 for inorganics) ratio between the cumulative number of nitrogen and oxygen atoms in the molecule which are not part of N(=O)=O groups over the number of carbons (0 for inorganics)
[50]number of aldehyde groups number of aldehyde groups
[51]number of bridges consisting of a sulphur atom connected with only three oxygens and made of two S=O and one S-O subgroups number of bridges consisting of a sulphur atom connected with only three oxygens and made of two S=O and one S-O subgroups
[52]number of bridges consisting of a sulphur atom connected with four oxygens and made of two S=O and two S-O subgroups number of bridges consisting of a sulphur atom connected with four oxygens and made of two S=O and two S-O subgroups

[53]number of bridges consisting of a sulphur atom connected with two oxygens through double bonds, excluding sulfonic and sulfate bridges number of bridges consisting of a sulphur atom connected with two oxygens through double bonds, excluding sulfonic and sulfate bridges
[54]number of S=O groups not part of S(=O)=O bridges number of S=O groups not part of S(=O)=O bridges
[55]number of quinone groups number of quinone groups
[56]number of C=O groups where C is in ring, CC(=O)C groups where all carbons are in ring excluded number of C=O groups where C is in ring, CC(=O)C groups where all carbons are in ring excluded
[57]number of sulphur-hydrogen bonds number of sulphur-hydrogen bonds
[58]number of bridges consisting of a nitrogen atom connected through single bonds to four carbons number of bridges consisting of a nitrogen atom connected through single bonds to four carbons
[59]number of S=P(S)(O)O bridges g/mole number of S=P(S)(O)O bridges
[60]number of S=P(O)(O)O bridges number of S=P(O)(O)O bridges
[61]number of C1CC1 rings number of C1CC1 rings
[62]number of single phosphorus-nitrogen bonds number of single phosphorus-nitrogen bonds
[63]number of P-OH groups number of P-OH groups
[64]number of P-O- groups, P-OH excluded number of P-O- groups, P-OH excluded
[65]number of single carbon-metal bonds number of single carbon-metal bonds
[66]number of single oxygen-metal bonds number of single oxygen-metal bonds
[67]Number of single sulphur-metal bonds Number of single sulphur-metal bonds
[68]number of carbon atoms in rings number of carbon atoms in rings
[69]number of nitrogen atoms in rings number of nitrogen atoms in rings
[70]number of sulphur atoms in rings number of sulphur atoms in rings
[71]ratio of the number of atoms in aromatic rings over the total number of atoms in the molecule ratio of the number of atoms in aromatic rings over the total number of atoms in the molecule
[72]ratio of the number of atoms in non-aromatic rings over the total number of atoms in the molecule ratio of the number of atoms in non-aromatic rings over the total number of atoms in the molecule
[73]number of carbons in the longest carbon atoms chain whose bonds are not part of any ring and at least one extremity is not part of a ring number of carbons in the longest carbon atoms chain whose bonds are not part of any ring and at least one extremity is not part of a ring
[74]number of bonds in non-isolated rings minus the corresponding number of atoms number of bonds in non-isolated rings minus the corresponding number of atoms
[75]number of vinyl groups number of vinyl groups
[76]Length of the longest CH2 chain in the molecule where none of the carbons is part of any ring Length of the longest CH2 chain in the molecule where none of the carbons is part of any ring
[77]Cumulative number of lactone groups Cumulative number of lactone groups
[78]number of terminal N([H])([H])([H])([H]) groups number of terminal N([H])([H])([H])([H]) groups
[79]number of O=C-C=O bridges where the bond between carbons is not part of any ring number of O=C-C=O bridges where the bond between carbons is not part of any ring
[80]number of O-C-C-O bridges where the bond between carbons is not part of any ring number of O-C-C-O bridges where the bond between carbons is not part of any ring
[81]number of Cc1c([H])c([H])c(C)c([H])c([H])1 bridges number of Cc1c([H])c([H])c(C)c([H])c([H])1 bridges
[82]number of Cc1c([H])c(O)c([H])c([H])c([H])1 bridges number of Cc1c([H])c(O)c([H])c([H])c([H])1

bridges
[83]number of CN([H])C bridges number of CN([H])C bridges
[84]number of CN(C)C bridges number of CN(C)C bridges
[85]number of C1CO1 rings number of C1CO1 rings
[86]number of peroxyde bridges COO number of peroxyde bridges COO
[87]number of branch C(=C)(C)C nodes number of branch C(=C)(C)C nodes
[88]number of branch C([H])(C)(C)C nodes number of branch C([H])(C)(C)C nodes
[89]number of branch C(C)(C)(C)C nodes number of branch C(C)(C)(C)C nodes
[90]number of terminal CC([H])=CH2 fragments number of terminal CC([H])=CH2 fragments
[91]total number of non-ring carbons with two hydrogens attached to them total number of non-ring carbons with two hydrogens attached to them
[92]total number of C#C bonds not included in rings total number of C#C bonds not included in rings
[93]total number of C-[CH]=[CH]C fragments not part of rings total number of C-[CH]=[CH]C fragments not part of rings
[94]number of carbons in rings with two hydrogen attached to them number of carbons in rings with two hydrogen attached to them
[95]number of carbons in aromatic rings with one hydrogen attached to them number of carbons in aromatic rings with one hydrogen attached to them
[96]number of phtalate groups number of phtalate groups
[97]number of terminal OC(=O)c1c([H])c([H])c([H])c([H])c([H])1 fragments number of terminal OC(=O)c1c([H])c([H])c([H])c([H])c([H])1 fragments
[98]number of terminal OC([H])([H])c1c([H])c([H])c([H])c([H])c([H])1 fragments number of terminal OC([H])([H])c1c([H])c([H])c([H])c([H])c([H])1 fragments
[99]number of terminal Oc1c([H])c([H])c([H])c([H])c([H])1 fragments number of terminal Oc1c([H])c([H])c([H])c([H])c([H])1 fragments
[100]number of terminal Oc1c([H])c([H])c(C(C([H])([H])[H])C([H])([H])[H])c([H])c([H])1 fragments number of terminal Oc1c([H])c([H])c(C(C([H])([H])[H])C([H])([H])[H])c([H])c([H])1 fragments
[101]number of terminal Oc1c([H])c(C([H])([H])[H])c([H])c(C([H])([H])[H])c([H])1 fragments number of terminal Oc1c([H])c(C([H])([H])[H])c([H])c(C([H])([H])[H])c([H])1 fragments
[102]molecular weight molecular weight

4.4.Descriptor selection:

102 descriptors were chosen in the final model. The list started with those descriptors (78) used to develop a PNN model for estimating fathead minnow LC50. These were based on structural information in the training set. Refinements of the descriptors were based on partial model experiments where combinations of descriptors on approximately 80% of the training substances (random selection) was examined on the remaining 20% for potential impact on the predictive quality. Through this process descriptors were eliminated or added.

4.5.Algorithm and descriptor generation:

See attachment (AIEPS 3.0 - Biodegradation 28-d (BOD) PNN Model Validation Study.doc), section 4, for the discussion of the derivation and refinement of the PNN algorithm. As a starting point the multivariate Bayesian density estimator is used in combination with a mapping tool similar to the Maximum Likelihood Estimation method. The best probability density associated with the accumulative distribution

of the cases in the training set is determined using Meisels' algorithm.
Details can be found in Masters T (1993) Practical Neural Network
Recipes in C++. Academic Press, San Diego.

4.6.Software name and version for descriptor generation:

Accelerys - Accord Chemistry Control 6.0.1 and Accord SDK 6.01
Runtime versions of these are included with the distributed program. The descriptors are automatically generated from the SMILES string during the data minning stage prior to prediction generation.
Accelrys.com

4.7.Chemicals/Descriptors ratio:

The number of chemicals in training set to descriptors ratio is 2400/59
= 40.67

5.Defining the applicability domain - OECD Principle 3

5.1.Description of the applicability domain of the model:

Based on the continuity of the mathematical functions involved in the model's computation algorithm, predictions are expected to be reliable when the values of the model input values are in the range between the minimum and maximum values of the corresponding descriptors encountered in the model's training data set, or outside close to them.

5.2.Method used to assess the applicability domain:

The substance of interest should have chemical descriptors which fall within the minimum or maximum values of those used in the training set. In addition, the model provides means to compare the substance of interest to those in the training set through Tanimoto indices. In other words, a prediction may be deemed acceptable when the Tanimoto maximum similarity indicator with the compounds in the model's training set is higher than a professionally determined value. For each prediction, the AIEPS provides the functionality of generating a similarity with the model's training dataset report, where the 10 most similar compounds are identified and the corresponding measured information reported in table format. Another table allows comparison between the values used as model input with the ranges of the corresponding training set descriptors. So, all necessary elements to judge the reliability of the predictions are made available to the user. Based on this information, is up to the user to decide if the predicted value is reliable or not.

5.3.Software name and version for applicability domain assessment:

5.4.Limits of applicability:

The model targets only small molecules consisting of less than 200 atoms. It is not recommended to use it for larger structures.
Basically, the model is targeting organic compounds. The algorithm can handle inorganic structures, but the predictions may not be reliable at all for the reason that only very limited information on biodegradation of inorganics was available (one compound). Consequently, we advise do not use it for inorganics.
With few exceptions the model cannot account for the differences between

structural isomers. The exceptions occur when the combination of the model fragment descriptors is able to recognize them.
Predictions may not be accurate when the target structure involves atoms and/or fragments not accounted for by the existing model descriptors.

6.Internal validation - OECD Principle 4

6.1.Availability of the training set:

Yes

6.2.Available information for the training set:

CAS RN: Yes
Chemical Name: Yes
Smiles: Yes
Formula: No
INChI: No
MOL file: No

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

All

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

All

6.5.Other information about the training set:

Most of the data is the result of performing ready and inherent biodegradation tests (MITI I, MITI II and the Closed Bottle Test). The external test set of 74 compounds was randomly selected (via random number generator) from a complete training set of 925 compounds.

6.6.Pre-processing of data before modelling:

6.7.Statistics for goodness-of-fit:

Minimum Residuals -57.9566
Maximum Residuals 86.7654
Average Residuals 5.88E-09
Standard Deviation of Residuals 16.5402
Sum of Square Residuals 232542.12
Average Square Residuals 273.25749
Coefficient of determination between measured and model predicted values 0.7848
Coefficient of correlation between measured and model predicted values 0.8859

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

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

6.10.Robustness - Statistics obtained by Y-scrambling:

6.11.Robustness - Statistics obtained by bootstrap:

6.12.Robustness - Statistics obtained by other methods:

External test (74 compounds) set and comparison with CATABOL
Statistical Indicator/Model PNN Catabol
Minimum Residuals -61.3355 -91
Maximum Residuals 78.3002 49
Average Residuals 2.5522 -8.3203

Standard Deviation of Residuals 23.4580 23.9120

Sum of Square Residuals 40652.33 46863.07

Average Square Residuals 549.3558 633.2847

Coefficient of determination between measured and model predicted values

0.6049 0.6262

Coefficient of correlation between measured and model predicted values

0.7778 0.7913

7.External validation - OECD Principle 4

7.1.Availability of the external validation set:

Yes

7.2.Available information for the external validation set:

CAS RN: Yes

Chemical Name: Yes

Smiles: Yes

Formula: No

INChI: No

MOL file: No

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

All

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

All

7.5.Other information about the external validation set:

74 substances were used as the external validation set for the Biodegradation PNN model.

These were selected randomly from the whole dataset of 925 substances.

These 74 substances were also used to compare with predictions from Catabol (v 4.5.4.2) and were deemed to be honest candidates based on input from the following sources

74 substances were used as the external validation set for the Biodegradation PNN model.

These were selected randomly from the whole dataset of 925 substances.

These 74 substances were also used to compare with predictions from Catabol (v 4.5.4.2) and were deemed to be honest candidates based on input from the following sources:[sect.9.2/ ref.8 & 9]

7.6.Experimental design of test set:

Experimental data was randomly set aside before modeling

7.7.Predictivity - Statistics obtained by external validation:

Minimum Residuals -61.3355

Maximum Residuals 54.2679

Average Residuals 1.5145

Standard Deviation of Residuals 21.8435

Sum of Square Residuals 34521.41

Average Square Residuals 472.8960

Coefficient of determination between measured and model predicted values

0.6460

Coefficient of correlation between measured and model predicted values
0.8037
Sample size 73 (1 outlier removed)

7.8.Predictivity - Assessment of the external validation set:

Predictability was conducted through a comparison with Catabol (v 4.5.4.2) from the Laboratory of Mathematical Chemistry, University of Bulgaria, Bourgas, Bulgaria.

7.9.Comments on the external validation of the model:

It is concluded that the PNN model at least matches the Catabol predictive performance if not slightly superior.

8.Providing a mechanistic interpretation - OECD Principle 5

8.1.Mechanistic basis of the model:

The mechanistic approach of the present model is supported by the use of the specific atoms, bonds, and molecular fragments involved in the model descriptors.

8.2.A priori or a posteriori mechanistic interpretation:

The mechanistic interpretation was determined a posteriori by interpreting and modifying the final set of descriptors which contributed to the best fit.

8.3.Other information about the mechanistic interpretation:

9.Miscellaneous information

9.1.Comments:

9.2.Bibliography:

[1]Kaiser KLE and Niculescu SP (2001). Modeling acute toxicity of chemicals to Daphnia magna: A probabilistic neural network approach. Environmental toxicology and chemistry 20 (2) 420-431. http://onlinelibrary.wiley.com/doi/10.1002/etc.5620200225/full

[2]Niculescu SP, Kaiser KLE and Schultz TW (2000). Modeling the toxicity of chemicals to Tetrahymena pyriformis using molecular fragment descriptors and probabilistic neural networks. Archives of environmental contamination and toxicology 39 (3) 289-329 http://link.springer.com/article/10.1007/s002440010107

[3]Niculescu SP, Atkinson A, Hammond G & Lewis M (2004). Using fragment chemistry data mining and probabilistic neural networks in screening chemicals for acute toxicity to the fathead minnow. SAR and QSAR in Environmental Research 15 (4) 293-309. http://www.tandfonline.com/doi/abs/10.1080/10629360410001724941

[4]Niculescu SP, Lewis MA and Tigner J (2008). Probabilistic neural networks modeling of the 48-h LC50 acute toxicity endpoint to Daphnia magna. SAR and QSAR in Environmental Research 19 (7-8) 735-750. http://www.tandfonline.com/doi/abs/10.1080/10629360802550556

[5]Masters T (1993) Practical Neural Network Recipes in C++. Academic Press, San Diego" https://books.google.ca/books?id=7Ez_Pq0sp2EC&lpg=PR17&ots=e05FixTiqW&dq=Masters%20T%20(1993)%20Practical%20Neural%20Network%20Recipes%20in%20C%2B%2B.%20Academic%20Press%2C%20San%20Diego%E2%80%9D&lr&pg=PR17#v=onepage&q&f=false

[6]CITI (1992). Biodegradation and Bioaccumulation Data of Existing Chemicals Based on CSCL Japan. Japan Chemical Industry Ecology-Toxicology and Information Center, Chemicals Inspection and Testing Institute, Tokyo. ISBN 4-89074-101-1

[7]NITE (2011). Biodegradation and Bioconcentration of the Existing Chemical Substances under the Chemical Substances Control Law Database. National Institute of Technology and Evaluation, Tokyo, Japan. http://www.safe.nite.go.jp/english/kizon/KIZON_start_hazkizon.html
[8]Pavan M, Worth AP (2006). Review of QSAR Models for Ready Biodegradation. Report EUR 22355 EN, European Commission, Directorate-General Joint Research Centre, Institute for Health and Consumer Protection, Ispra (VA), Italy.
[9]Sakuratani Y, Yamada J, Kasai K, Noguchi Y, Nishihara T (2005). External validation of the biodegradability prediction model CATABOL using data sets of existing and new chemicals under the Japanese Chemical Substances Control Law. SAR and QSAR in Environmental Research 16, 403-431

9.3.Supporting information:

qmrf519_AIEPS 3.0 - Biodeg Training Set_851.sdf	http://qsardb.jrc.ec.europa.eu/qmrf/protocol/Q17-23a-0036/attachment/A1110
qmrf519_AIEPS 3.0 -Biodeg Validation_74.sdf	http://qsardb.jrc.ec.europa.eu/qmrf/protocol/Q17-23a-0036/attachment/A1111

Test set(s)

10.Summary (JRC QSAR Model Database)

Supporting information

10.1.QMRF number:

Q17-23a-0036

10.2.Publication date:

2017-09-27

10.3.Keywords:

Artificial Intelligence Expert Predictive System;AIEPS;biodegradation;MITI test;

10.4.Comments:

old# Q52-55-56-519