QSAR Toolbox prediction for single chemical

The template of the current report is based on "GUIDANCE DOCUMENT ON THE VALIDATION OF (QUANTITATIVE) STRUCTURE-ACTIVITY RELATIONSHIPS MODELS" published by OECD (September, 2007) and "GUIDANCE ON INFORMATION REQUIREMENTS AND CHEMICAL SAFETY ASSESSMENT / CHAPTER R.6: QSARS AND GROUPING OF CHEMICALS" published by ECHA (May, 2008).

The report provides information about the target substance, chemical characteristics used for the grouping, the resulting boundaries of the group of chemicals (applicability domain), the type of data gap filling approach that was applied (read-across, trend analysis or QSAR models), the predicted result(s) and in the Annex information about the category members or training set and test set chemicals.

The chemicals are ordered by the distance to the target substance within the descriptors space. Only chemicals with experimental data are listed as category members.

Depending on the settings selected by the user, detailed information (incl. 2D image and profiling results) is provided for some chemicals while more limited information (CAS, name, SMILES) is provided for others.

If not otherwise specified, the experimental values are reported in bold, recalculated experimental values are reported in bold & italic and calculated values are reported in regular font.

Table of content

Summary 3

1. Target substance

1.1. CAS number 4
1.2. Other regulatory numbers 4
1.3. Chemical name(s) 4
1.4. Structural formula 4
1.5. Structure codes 4
1.6. Quality of structure identity (CAS/2D quality) 5

2. General information

2.1. Date of report generation 5
2.2. Report author(s) and contact details 5

3. Category definition

3.1. Category definition 5
3.2. Category justification 6
3.3. Data matrix 6

4. Prediction

4.1. Defined endpoint (OECD Principle 1) 7
4.2. Unambiguous algorithm (OECD Principle 2) 7
4.3. Applicability domain (OECD Principle 3) 8
4.4. Uncertainty of the prediction (OECD Principle 4) 8
4.5. Chemical and biological mechanisms (OECD Principle 5) 8

5. Adequacy

5.1. Regulatory purpose 10
5.2. Approach for regulatory interpretation of the model result 10
5.3. Outcome 10
5.4. Conclusion 10

Appendix 1 - Category members 11

Appendix 2 - Data matrix 20

Appendix 3 - QMRF 21

Appendix 4 - QMRF, training set 21

Appendix 5 - QMRF, test set 21

Appendix 6 - Additional information from QSAR 21

Appendix 7 - Chemical components 22

QSAR Toolbox prediction based on read-across

Prediction of Summary carcinogenicity for 2-bromopropane

Summary

Toxicity of the target chemical (Negative) is predicted from category members using read-across based on 18 values (Positive x6, Equivocal x3, Negative x9) from 4 nearest neighbours compared by prediction descriptors. Category members are single chemicals or mixtures and are selected based on the profile of the target chemical. Only chemicals having experimental data are listed in the category.

The target chemical FALLS within applicability domain of the prediction (see Section 4.3 for details).

The data used for calculating the current prediction is taken from 18 experimental values selected from the following database(s):

1. Carcinogenic Potency Database (CPDB)
2. Carcinogenicity&mutagenicity ISSCAN

Below is a summary table for endpoint & descriptor values for the target chemical and the category members.
Experimental values from data matrix are presented in bold font. Recalculated endpoint values (if required by selected data usage option in Gap Filling) are presented in italic font. Recalculated endpoint values based on experimental data only are presented in bold and italic font.

	Endpoint(s)	***Descriptor(s)***
	Human Health Hazards; Carcinogenicity	**log Kow**
	Carcinogenicity I (ISSCAN)	-
Target chemical	-	2.08
Cat. member No. 1	***Positive (4)*** ***Equivocal (2)***	1.67
Cat. member No. 2	***Negative (4)***	2.56
Cat. member No. 3	***Negative*** ***Positive (2)*** ***Equivocal***	1.58
Cat. member No. 4	***Negative (4)***	1.18

Section 1 - *Target chemical*

1.1. CAS number:

75-26-3

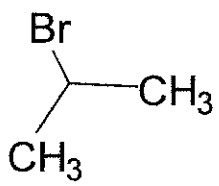
1.2. Other regulatory numbers:

Not reported

1.3. Chemical name(s):

2-bromopropane
iso-propyl bromide
propane, 2-bromo-
2bromopropane
isopropyl bromide

1.4. Structural formula:



1.5. Structure codes:

a. SMILES:

CC(C)Br

b. Input structure code (if different from SMILES):

Not available

c. Stereochemical features: *manually editable field*

Not provided by the user

1.6. Quality of structure identity (CAS/2D quality):

High Quality

Databases to which the target chemical belongs are:

Aquatic Japan MoE
Bacterial mutagenicity ISSSTY
Biodegradation NITE
Developmental & Reproductive Toxicity (DART)
ECHA CHEM
Eye Irritation ECETOC
Genotoxicity OASIS
Phys-chem EPISUITE
Rodent Inhalation Toxicity Database
Skin Iirritation

Section 2 - *General information*

2.1. Date of report generation:

23.07.2015

2.2. Report author(s) and contact details:

manually editable field

Not provided by the user

Section 3 - *Category definition and category members*

3.1. Category definition:

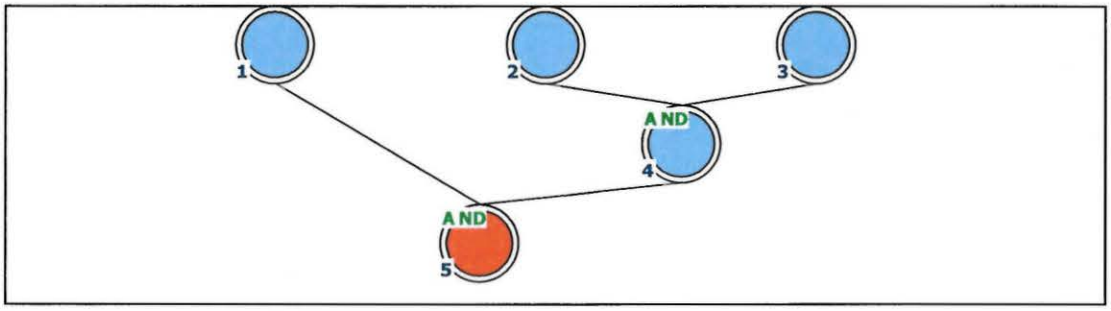
a. Category hypothesis:

manually editable field

Not provided by the user

b. Applicability domain of the category:

The applicability domain is defined by following scheme



1) Referential boundary:

The target chemical should be classified as SN2 AND SN2 >> Alkylation by epoxide metabolically formed after E2 reaction AND SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes AND SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom AND SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes AND SN2 >> Nucleophilic substitution after carbenium ion formation AND SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes by DNA alerts for AMES, MN and CA by OASIS v.1.3

2) Parametric boundary:

The target chemical should have a value of log Kow which is >= 1.18

3) Parametric boundary:

The target chemical should have a value of log Kow which is <= 2.56

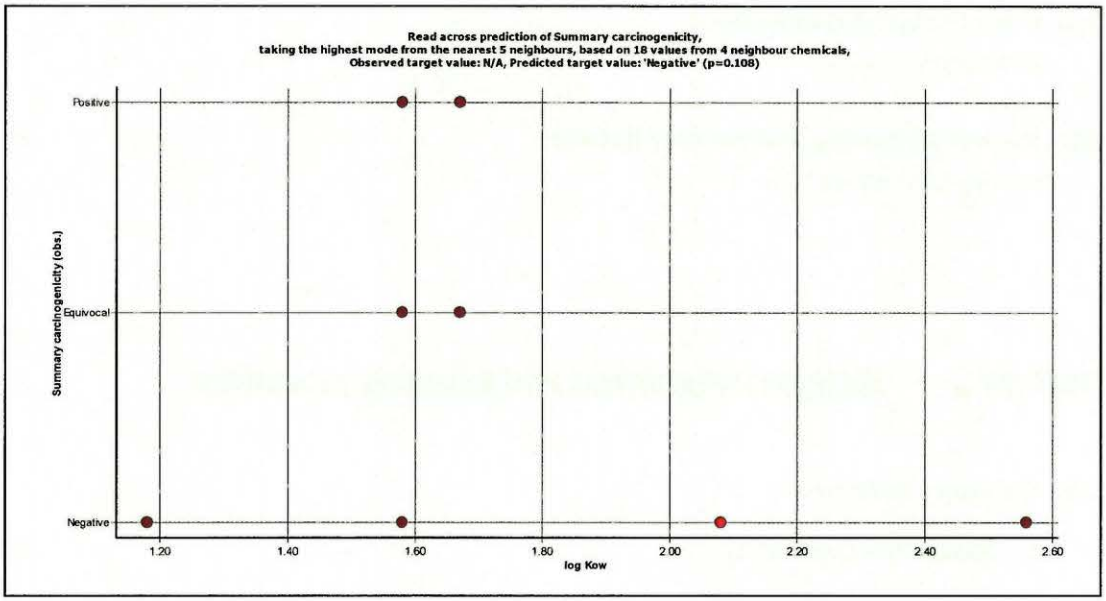
c. Endpoints covered: *manually editable field*

Not provided by the user

d. Category members:

The list of the category members is available in **Appendix 1**

The category members shown with respect to the descriptor **log Kow**



3.2. Category justification: *manually editable field*

Not provided by the user

3.3. Data matrix:

The data matrix is available in **Appendix 2**

Section 4 - *Prediction*

4.1. Defined Endpoint (OECD Principle 1):

a. Endpoint (e.g. Acute toxicity to fish): *manually editable field*

Summary carcinogenicity

Materials & methods / type of method:

In Vivo

b. Dependent variable (e.g. LC50): *manually editable field*

(Summary carcinogenicity)

c. Units: *manually editable field*

Not provided by the user

d. Duration: *manually editable field*

Not provided by the user

e. Species: *manually editable field*

Rat
Mouse

4.2. Unambiguous algorithm (OECD Principle 2):

a. Prediction approach: *manually editable field*

Read-across from category members
Experimental values for the target chemical (if any) were not used in prediction calculations

b. Calculation approach:

Takes highest mode value from the 5 nearest neighbours

c. Model name:

Not applicable

d. Model version:

Not applicable

e. Reference to QMRF:

Not applicable

f. Input for prediction (target chemical):

SMILES

g. Descriptor and endpoint values for target chemical (if applicable):

Descriptor(s)	
log Kow	2.08
Endpoint (dep. variable)	
Human Health Hazards; Carcinogenicity	-

h. Additional chemicals eliminations (not determined by domain):

Not available

i. Additional data eliminations (not determined by domain):

Not available

j. Predicted value (model result):

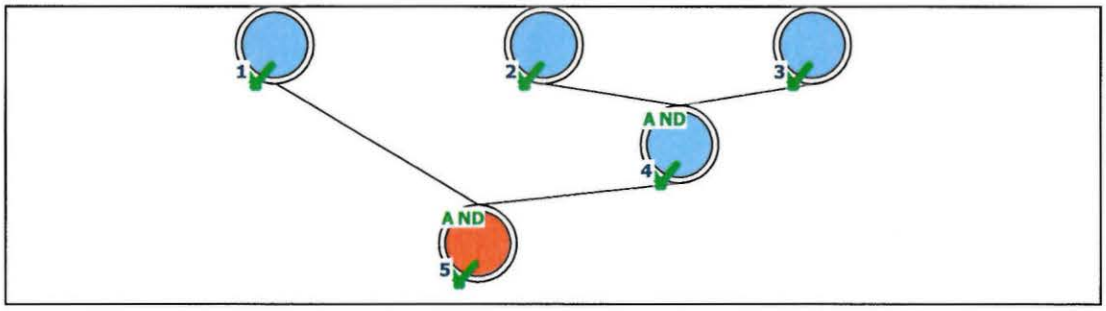
Negative

k. Predicted value (comments): *manually editable field*

Not provided by the user

4.3. Applicability domain (OECD Principle 3):

The target chemical FALLS within applicability domain
(see Section 3.1.b for detailed description of the domain)



4.4. Uncertainty of the prediction (OECD Principle 4): *manually editable field*

The prediction is based on 18 neighbours' values, 9 of them equal to prediction.
Prediction confidence is measured by the p-value = 0.108 (no confidence)

4.5. Chemical and biological mechanisms (OECD Principle 5):

Profiling results for the target substance:

DNA binding by OASIS v.1.3

SN2

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes

SN2 >> Nucleophilic substitution after carbenium ion formation

SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes

DNA binding by OECD

SN2

SN2 >> SN2 at an sp3 Carbon atom

SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Neutral Organics

Comments:

Not provided by the user *manually editable field*

Section 5 - *Adequacy*

5.1. Regulatory purpose: *manually editable field*

Not provided by the user

5.2. Approach for regulatory interpretation of the model result: *manually editable field*

Not provided by the user

5.3. Outcome: *manually editable field*

Not provided by the user

5.4. Conclusion: *manually editable field*

Not provided by the user

QSAR Toolbox prediction based on read-across

Prediction of Summary carcinogenicity for 2-bromopropane

APPENDIX 1 - Category members

The 4 category members are reported in more detail

1. Cat. member No.1: ***used for read-across***

1.1. CAS number:

74-96-4

1.2. Other regulatory numbers:

Not reported

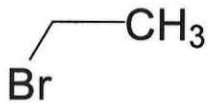
1.3. Chemical name(s):

bromoethane
ethane, bromo-
bromoethane(ethyl bromide)
ethyl bromide

1.4. Structural formula:

SMILES

CCBr



1.5. Profiling results:

DNA binding by OASIS v.1.3

SN2

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes

SN2 >> Nucleophilic substitution after carbenium ion formation

SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes

DNA binding by OECD

SN2

SN2 >> SN2 at an sp3 Carbon atom

SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Neutral Organics

2. Cat. member No.2: *used for read-across*

2.1. CAS number:

109-69-3

2.2. Other regulatory numbers:

Not reported

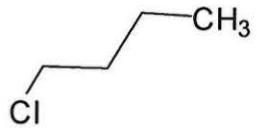
2.3. Chemical name(s):

1-chlorobutane,
1-chlorobutane
butane, 1-chloro-
n-butyl chloride
butyl chloride, n-

2.4. Structural formula:

SMILES

CCCCCl



2.5. Profiling results:

DNA binding by OASIS v.1.3

SN2

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes

SN2 >> Nucleophilic substitution after carbenium ion formation

SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes

DNA binding by OECD

SN2

SN2 >> SN2 at an sp3 Carbon atom

SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Neutral Organics

3. Cat. member No.3: *used for read-across*

3.1. CAS number:

75-00-3

3.2. Other regulatory numbers:

Not reported

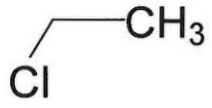
3.3. Chemical name(s):

chloroethane
ethyl chloride
ethane, chloro-

3.4. Structural formula:

SMILES

CCCl



3.5. Profiling results:

DNA binding by OASIS v.1.3

SN2

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes

SN2 >> Nucleophilic substitution after carbenium ion formation

SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes

DNA binding by OECD

SN2

SN2 >> SN2 at an sp3 Carbon atom

SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Neutral Organics

4. Cat. member No.4: *used for read-across*

4.1. CAS number:

74-83-9

4.2. Other regulatory numbers:

Not reported

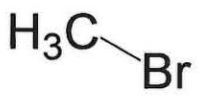
4.3. Chemical name(s):

methyl bromide
methane, bromo-
bromomethane
bromomethane(methyl bromide iso)
methyl bromide [bsi:iso]
methane, bromo-""""

4.4. Structural formula:

SMILES

CBr



4.5. Profiling results:

DNA binding by OASIS v.1.3

SN2

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes

SN2 >> Nucleophilic substitution after carbenium ion formation

SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes

DNA binding by OECD

SN2

SN2 >> SN2 at an sp3 Carbon atom

SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Neutral Organics

QSAR Toolbox prediction based on read-across

Prediction of Summary carcinogenicity for 2-bromopropane

APPENDIX 2 - Data matrix

OMITTED BY THE USER

QSAR Toolbox prediction based on read-across

Prediction of Summary carcinogenicity for 2-bromopropane

APPENDIX 3 - QMRF

APPENDIX 4 - QMRF, training set chemicals

APPENDIX 5 - QMRF, test set chemicals

APPENDIX 6 - Additional information from (Q)SAR

NOT APPLICABLE

QSAR Toolbox prediction based on read-across

Prediction of Summary carcinogenicity for 2-bromopropane

APPENDIX 7 - Chemical components

NOT APPLICABLE

QSAR Toolbox prediction for single chemical

The template of the current report is based on "GUIDANCE DOCUMENT ON THE VALIDATION OF (QUANTITATIVE) STRUCTURE-ACTIVITY RELATIONSHIPS MODELS" published by OECD (September, 2007) and "GUIDANCE ON INFORMATION REQUIREMENTS AND CHEMICAL SAFETY ASSESSMENT / CHAPTER R.6: QSARS AND GROUPING OF CHEMICALS" published by ECHA (May, 2008).

The report provides information about the target substance, chemical characteristics used for the grouping, the resulting boundaries of the group of chemicals (applicability domain), the type of data gap filling approach that was applied (read-across, trend analysis or QSAR models), the predicted result(s) and in the Annex information about the category members or training set and test set chemicals.

The chemicals are ordered by the distance to the target substance within the descriptors space. Only chemicals with experimental data are listed as category members.

Depending on the settings selected by the user, detailed information (incl. 2D image and profiling results) is provided for some chemicals while more limited information (CAS, name, SMILES) is provided for others.

If not otherwise specified, the experimental values are reported in bold, recalculated experimental values are reported in bold & italic and calculated values are reported in regular font.

Table of content

Summary 3

1. Target substance

1.1. CAS number 5
1.2. Other regulatory numbers 5
1.3. Chemical name(s) 5
1.4. Structural formula 5
1.5. Structure codes 5
1.6. Quality of structure identity (CAS/2D quality) 6

2. General information

2.1. Date of report generation 6
2.2. Report author(s) and contact details 6

3. Category definition

3.1. Category definition 6
3.2. Category justification 8
3.3. Data matrix 8

4. Prediction

4.1. Defined endpoint (OECD Principle 1) 8
4.2. Unambiguous algorithm (OECD Principle 2) 9
4.3. Applicability domain (OECD Principle 3) 9
4.4. Uncertainty of the prediction (OECD Principle 4) 10
4.5. Chemical and biological mechanisms (OECD Principle 5) 10

5. Adequacy

5.1. Regulatory purpose 12
5.2. Approach for regulatory interpretation of the model result 12
5.3. Outcome 12
5.4. Conclusion 12

Appendix 1 - Category members 13
Appendix 2 - Data matrix 35
Appendix 3 - QMRF 36
Appendix 4 - QMRF, training set 36
Appendix 5 - QMRF, test set 36
Appendix 6 - Additional information from QSAR 36
Appendix 7 - Chemical components 37

QSAR Toolbox prediction based on read-across

Prediction of Gene mutation for 1-bromopropane

Summary

Toxicity of the target chemical (Negative) is predicted from category members using read-across based on 60 values (Positive x17, Equivocal x2, Negative x41) from 5 nearest neighbours compared by prediction descriptors. Category members are single chemicals or mixtures and are selected based on the profile of the target chemical. Only chemicals having experimental data are listed in the category.

The target chemical FALLS within applicability domain of the prediction (see Section 4.3 for details).

The data used for calculating the current prediction is taken from 60 experimental values selected from the following database(s):

1. Bacterial mutagenicity ISSSTY
2. Genotoxicity OASIS

Below is a summary table for endpoint & descriptor values for the target chemical and the first 10 category members.
Experimental values from data matrix are presented in bold font. Recalculated endpoint values (if required by selected data usage option in Gap Filling) are presented in italic font. Recalculated endpoint values based on experimental data only are presented in bold and italic font.

	Endpoint(s)	***Descriptor(s)***
	Human Health Hazards; Genetic Toxicity	**log Kow**
	Gene mutation I	-
Target chemical	***Negative (13)***	2.16
Cat. member No. 1	***Positive (11)*** ***Negative (6)***	2.01
Cat. member No. 2	***Negative (3)***	1.94
Cat. member No. 3	***Equivocal (2)*** ***Negative (8)*** ***Positive***	2.43
Cat. member No. 4	***Negative (13)*** ***Positive (3)***	2.50
Cat. member No. 5	***Negative (11)*** ***Positive (2)***	1.79
Cat. member No. 6	***Positive (4)***	2.58
Cat. member No. 7	***Positive (6)*** ***Negative (3)*** ***Equivocal***	1.67
Cat. member No. 8	***Positive (5)*** ***Negative (4)***	2.65

	Endpoint(s)	***Descriptor(s)***
	Human Health Hazards; Genetic Toxicity	**log Kow**
	Gene mutation I	-
Cat. member No. 9	***Positive (2)*** ***Negative (3)***	2.77
Cat. member No. 10	***Equivocal*** ***Positive (3)*** ***Negative (2)***	2.77

Section 1 - *Target chemical*

1.1. CAS number:

106-94-5

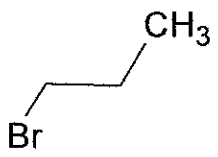
1.2. Other regulatory numbers:

Not reported

1.3. Chemical name(s):

1-bromopropane
propane, 1-bromo-
n-propyl bromide
1bromopropane
npropyl bromide

1.4. Structural formula:



1.5. Structure codes:

a. SMILES:

CCCBr

b. Input structure code (if different from SMILES):

Not available

c. Stereochemical features: *manually editable field*

Not provided by the user

1.6. Quality of structure identity (CAS/2D quality):

High Quality

Databases to which the target chemical belongs are:

Aquatic OASIS
Bacterial mutagenicity ISSSTY
Biodegradation NITE
Developmental & Reproductive Toxicity (DART)
ECHA CHEM
ECOTOX
Genotoxicity OASIS
Micronucleus ISSMIC
Phys-chem EPISUITE
Rodent Inhalation Toxicity Database

Section 2 - *General information*

2.1. Date of report generation:

22.07.2015

2.2. Report author(s) and contact details: *manually editable field*

Not provided by the user

Section 3 - *Category definition and category members*

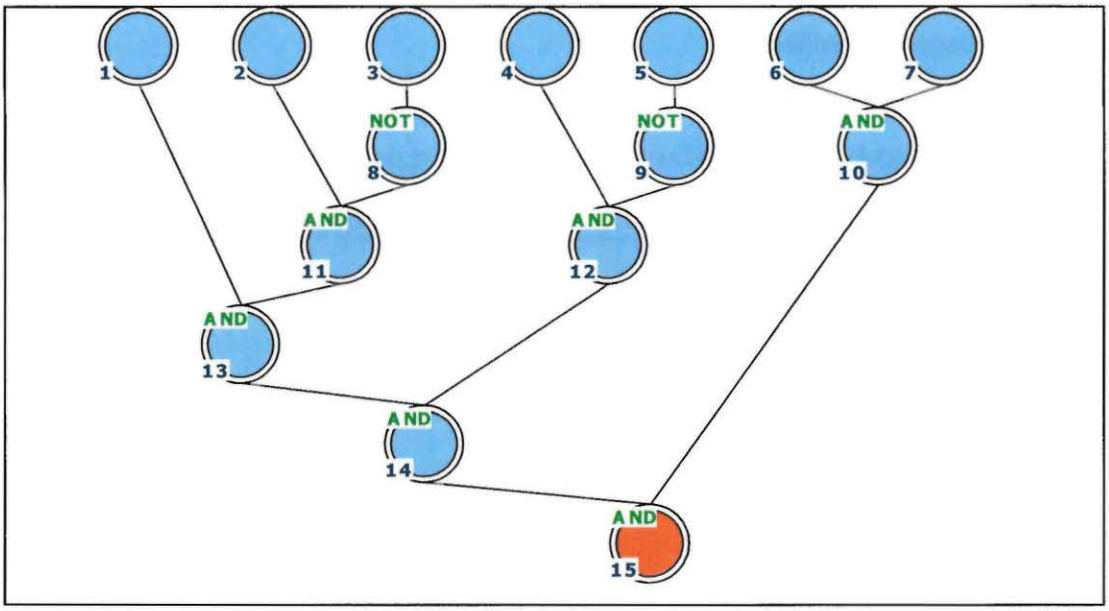
3.1. Category definition:

a. Category hypothesis: *manually editable field*

Not provided by the user

b. Applicability domain of the category:

The applicability domain is defined by following scheme



1) Referential boundary:

The target chemical should be classified as Aliphatic halogens (Genotox) AND Structural alert for genotoxic carcinogenicity by Carcinogenicity (genotox and nongenotox) alerts by ISS

2) Referential boundary:

The target chemical should be classified as Group 14 - Carbon C AND Group 17 - Halogens Br AND Group 17 - Halogens F,Cl,Br,I,At by Chemical elements

3) Referential boundary:

The target chemical should be classified as Group 1 - Alkali Earth Li,Na,K,Rb,Cs,Fr OR Group 10 - Trans.Metals Ni,Pd,Pt OR Group 14 - Metalloids Si,Ge OR Group 15 - Nitrogen N OR Group 15 - Phosphorus P OR Group 16 - Oxygen O OR Group 16 - Sulfur S OR Group 17 - Halogens Cl OR Group 17 - Halogens F OR Group 17 - Halogens I OR Group 2 - Alkaline Earth Be,Mg,Ca,Sr,Ba,Ra OR Unknown chemical element by Chemical elements

4) Referential boundary:

The target chemical should be classified as Alkyl halide by Organic Functional groups

5) Referential boundary:

The target chemical should be classified as Alkane branched with quaternary carbon OR Alkene OR Alkenyl halide OR Alkyl arenes OR Alkyne OR Allyl OR Anthracene OR Aryl OR Benzyl OR Fused carbocyclic aromatic OR Isopropyl OR Naphtalene OR Perhalogenated carbons derivatives OR Phenanthrene OR tert-Butyl by Organic Functional groups

6) Parametric boundary:

The target chemical should have a value of log Kow which is >= 1.79

7) Parametric boundary:

The target chemical should have a value of log Kow which is <= 2.5

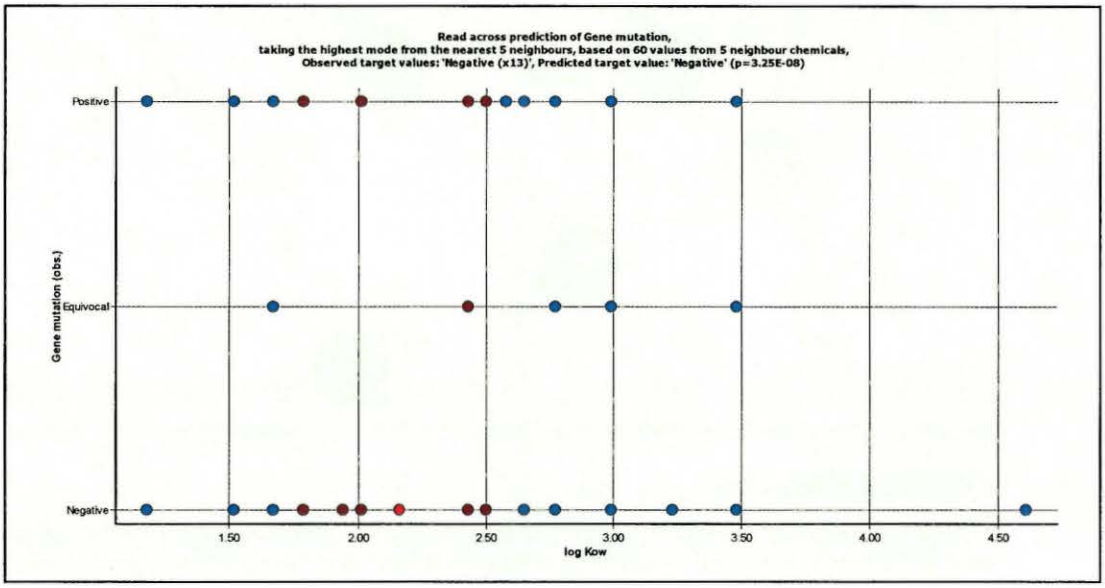
c. Endpoints covered: *manually editable field*

Not provided by the user

d. Category members:

The list of the category members is available in **Appendix 1**

The category members shown with respect to the descriptor **log Kow**



3.2. Category justification: *manually editable field*

Not provided by the user

3.3. Data matrix:

The data matrix is available in **Appendix 2**

Section 4 - *Prediction*

4.1. Defined Endpoint (OECD Principle 1):

a. Endpoint (e.g. Acute toxicity to fish): *manually editable field*

Gene mutation

Materials & methods / type of method:

In Vitro

Test chemical / test type:

Bacterial reverse mutation assay (e.g. Ames test)

b. Dependent variable (e.g. LC50): *manually editable field*

(Gene mutation)

c. Units: *manually editable field*

Not provided by the user

d. Duration: *manually editable field*

Not provided by the user

e. Species: *manually editable field*

Salmonella typhimurium

4.2. Unambiguous algorithm (OECD Principle 2):

a. Prediction approach: *manually editable field*

Read-across from category members
Experimental values for the target chemical (if any) were not used in prediction calculations

b. Calculation approach:

Takes highest mode value from the 5 nearest neighbours

c. Model name:

Not applicable

d. Model version:

Not applicable

e. Reference to QMRF:

Not applicable

f. Input for prediction (target chemical):

SMILES

g. Descriptor and endpoint values for target chemical (if applicable):

Descriptor(s)	
log Kow	2.16
Endpoint (dep. variable)	
Human Health Hazards; Genetic Toxicity	***Negative*** (x 13)

h. Additional chemicals eliminations (not determined by domain):

Not available

i. Additional data eliminations (not determined by domain):

Not available

j. Predicted value (model result):

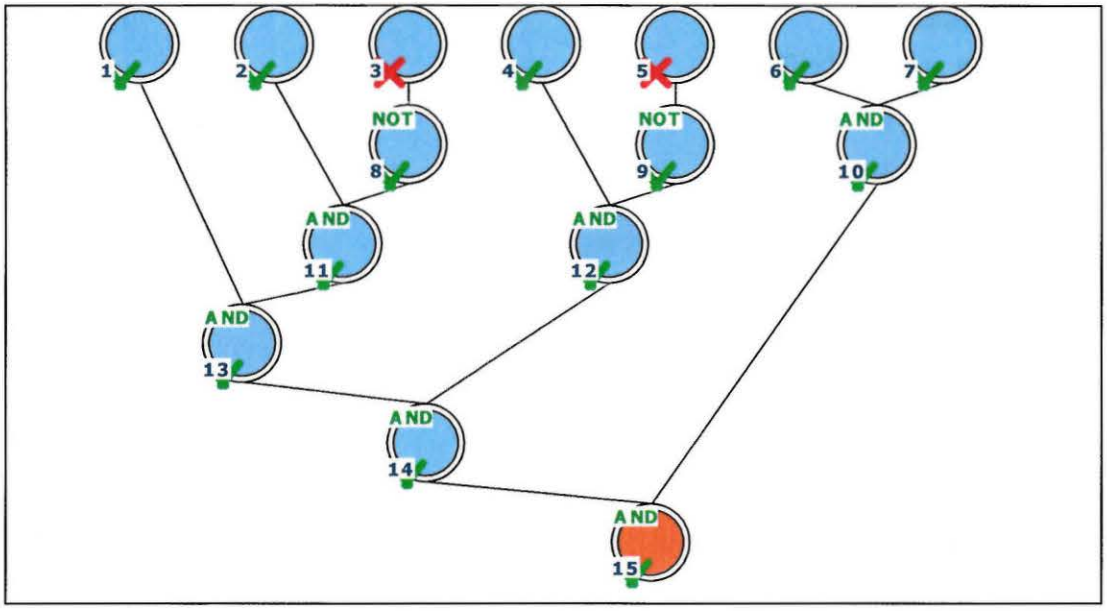
Negative

k. Predicted value (comments): *manually editable field*

Not provided by the user

4.3. Applicability domain (OECD Principle 3):

The target chemical FALLS within applicability domain
(see Section 3.1.b for detailed description of the domain)



4.4. Uncertainty of the prediction (OECD Principle 4):

manually editable field

The prediction is based on 60 neighbours' values, 41 of them equal to prediction.
Prediction confidence is measured by the p-value = 3.25E-08 (very strong confidence)

4.5. Chemical and biological mechanisms (OECD Principle 5):

Profiling results for the target substance:

DNA binding by OASIS v.1.3

SN2

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes

SN2 >> Nucleophilic substitution after carbenium ion formation

SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes

DNA binding by OECD

SN2

SN2 >> SN2 at an sp3 Carbon atom

SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Neutral Organics

Comments:

Not provided by the user *manually editable field*

Section 5 - *Adequacy*

5.1. Regulatory purpose: *manually editable field*

Not provided by the user

5.2. Approach for regulatory interpretation of the model result: *manually editable field*

Not provided by the user

5.3. Outcome: *manually editable field*

Not provided by the user

5.4. Conclusion: *manually editable field*

Not provided by the user

QSAR Toolbox prediction based on read-across

Prediction of Gene mutation for 1-bromopropane

APPENDIX 1 - Category members

From 16 category members, 10 chemicals are reported in more detail,
the remaining category members are listed in a table with basic information

1. Cat. member No.1: *used for read-across*

1.1. CAS number:

106-93-4

1.2. Other regulatory numbers:

Not reported

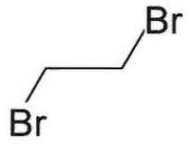
1.3. Chemical name(s):

1,2-dibromoethane
dibromoethane, 1,2-
ethylene dibromide
ethane, 1,2-dibromo-
1,2,dibromoethane
1,2dibromoethane
ethylene dibromide (edb)

1.4. Structural formula:

SMILES

BrCCBr



1.5. Profiling results:

DNA binding by OASIS v.1.3

SN2

SN2 >> DNA alkylation

SN2 >> DNA alkylation >> Vicinal Dihaloalkanes

SN2 >> Internal SN2 reaction with aziridinium and/or cyclic sulfonium ion formation (enzymatic)

SN2 >> Internal SN2 reaction with aziridinium and/or cyclic sulfonium ion formation (enzymatic) >> Vicinal Dihaloalkanes

DNA binding by OECD

SN2

SN2 >> Episulfonium Ion Formation

SN2 >> Episulfonium Ion Formation >> 1,2-Dihaloalkanes

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> Episulfonium Ion Formation

SN2 >> Episulfonium Ion Formation >> 1,2-Dihaloalkane

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Not categorized

2. Cat. member No.2: **used for read-across**

2.1. CAS number:

557-91-5

2.2. Other regulatory numbers:

Not reported

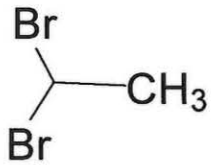
2.3. Chemical name(s):

1,1-dibromoethane
ethane, 1,1-dibromo-

2.4. Structural formula:

SMILES

CC(Br)Br



2.5. Profiling results:

DNA binding by OASIS v.1.3

AN2

AN2 >> Schiff base formation by aldehyde formed after metabolic activation

AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives

AN2 >> Shiff base formation for aldehydes

AN2 >> Shiff base formation for aldehydes >> Geminal Polyhaloalkane Derivatives

Radical

Radical >> Radical mechanism via ROS formation (indirect)

Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane Derivatives

SN2

SN2 >> Acylation involving a leaving group

SN2 >> Acylation involving a leaving group >> Geminal Polyhaloalkane Derivatives

SN2 >> Acylation involving a leaving group after metabolic activation

SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives

SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation

SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives

DNA binding by OECD

Acylation

Acylation >> P450 Mediated Activation to Acyl Halides

Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

No alert found

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Not categorized

3. Cat. member No.3: ***used for read-across***

3.1. CAS number:

78-75-1

3.2. Other regulatory numbers:

Not reported

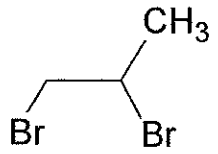
3.3. Chemical name(s):

1,2-dibromopropane
propane, 1,2-dibromo-

3.4. Structural formula:

SMILES

CC(Br)CBr



3.5. Profiling results:

DNA binding by OASIS v.1.3

SN2

SN2 >> DNA alkylation

SN2 >> DNA alkylation >> Vicinal Dihaloalkanes

SN2 >> Internal SN2 reaction with aziridinium and/or cyclic sulfonium ion formation (enzymatic)

SN2 >> Internal SN2 reaction with aziridinium and/or cyclic sulfonium ion formation (enzymatic) >> Vicinal Dihaloalkanes

DNA binding by OECD

SN2

SN2 >> Episulfonium Ion Formation

SN2 >> Episulfonium Ion Formation >> 1,2-Dihaloalkanes

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> Episulfonium Ion Formation

SN2 >> Episulfonium Ion Formation >> 1,2-Dihaloalkane

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Not categorized

4. Cat. member No.4: *used for read-across*

4.1. CAS number:

109-64-8

4.2. Other regulatory numbers:

Not reported

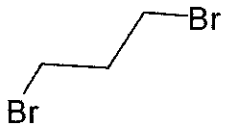
4.3. Chemical name(s):

1,3-dibromopropane
propane, 1,3-dibromo-

4.4. Structural formula:

SMILES

BrCCCBr



4.5. Profiling results:

DNA binding by OASIS v.1.3

No alert found

DNA binding by OECD

SN2

SN2 >> SN2 at an sp3 Carbon atom

SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Not categorized

5. Cat. member No.5: *used for read-across*

5.1. CAS number:

75-25-2

5.2. Other regulatory numbers:

Not reported

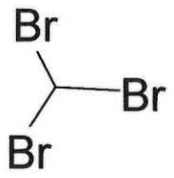
5.3. Chemical name(s):

tribromomethane
bromoform
methane, tribromo-

5.4. Structural formula:

SMILES

BrC(Br)Br



5.5. Profiling results:

DNA binding by OASIS v.1.3

AN2

AN2 >> Schiff base formation by aldehyde formed after metabolic activation

AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives

AN2 >> Shiff base formation for aldehydes

AN2 >> Shiff base formation for aldehydes >> Geminal Polyhaloalkane Derivatives

Radical

Radical >> Radical mechanism via ROS formation (indirect)

Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane Derivatives

SN2

SN2 >> Acylation involving a leaving group

SN2 >> Acylation involving a leaving group >> Geminal Polyhaloalkane Derivatives

SN2 >> Acylation involving a leaving group after metabolic activation

SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives

SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation

SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives

DNA binding by OECD

No alert found

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

No alert found

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

BrC(Br)Br

Has superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Not categorized

6. Cat. member No.6:

6.1. CAS number:

78-76-2

6.2. Other regulatory numbers:

Not reported

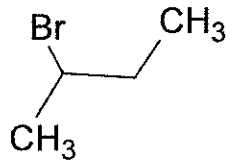
6.3. Chemical name(s):

sec-butyl bromide
bromo-2-butane
2-bromobutane
butane, 2-bromo-

6.4. Structural formula:

SMILES

CCC(C)Br



6.5. Profiling results:

DNA binding by OASIS v.1.3

SN2

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes

SN2 >> Nucleophilic substitution after carbenium ion formation

SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes

DNA binding by OECD

SN2

SN2 >> SN2 at an sp3 Carbon atom

SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Neutral Organics

7. Cat. member No.7:

7.1. CAS number:

74-96-4

7.2. Other regulatory numbers:

Not reported

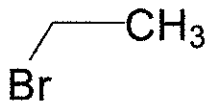
7.3. Chemical name(s):

bromoethane
ethane, bromo-
bromoethane(ethyl bromide)
ethyl bromide

7.4. Structural formula:

SMILES

CCBr



7.5. Profiling results:

DNA binding by OASIS v.1.3

SN2

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes

SN2 >> Nucleophilic substitution after carbenium ion formation

SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes

DNA binding by OECD

SN2

SN2 >> SN2 at an sp3 Carbon atom

SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Neutral Organics

8. Cat. member No.8:

8.1. CAS number:

109-65-9

8.2. Other regulatory numbers:

Not reported

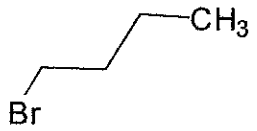
8.3. Chemical name(s):

1-bromobutane
butyl bromide
butane, 1-bromo-
butylbrom

8.4. Structural formula:

SMILES

CCCCBr



8.5. Profiling results:

DNA binding by OASIS v.1.3

SN2

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes

SN2 >> Nucleophilic substitution after carbenium ion formation

SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes

DNA binding by OECD

SN2

SN2 >> SN2 at an sp3 Carbon atom

SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Neutral Organics

9. Cat. member No.9:

9.1. CAS number:

23511-78-6

9.2. Other regulatory numbers:

Not reported

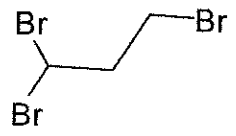
9.3. Chemical name(s):

1,1,3-tribromopropane

9.4. Structural formula:

SMILES

BrCCC(Br)Br



9.5. Profiling results:

DNA binding by OASIS v.1.3

AN2

AN2 >> Schiff base formation by aldehyde formed after metabolic activation

AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives

AN2 >> Shiff base formation for aldehydes

AN2 >> Shiff base formation for aldehydes >> Geminal Polyhaloalkane Derivatives

Radical

Radical >> Radical mechanism via ROS formation (indirect)

Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane Derivatives

SN2

SN2 >> Acylation involving a leaving group

SN2 >> Acylation involving a leaving group >> Geminal Polyhaloalkane Derivatives

SN2 >> Acylation involving a leaving group after metabolic activation

SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives

SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation

SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives

DNA binding by OECD

Acylation

Acylation >> P450 Mediated Activation to Acyl Halides

Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes

SN2

SN2 >> SN2 at an sp3 Carbon atom

SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Not categorized

10. Cat. member No.10:

10.1. CAS number:

96-11-7

10.2. Other regulatory numbers:

Not reported

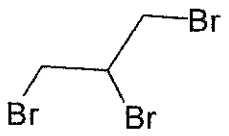
10.3. Chemical name(s):

1,2,3-tribromopropane
propane, 1,2,3-tribromo-

10.4. Structural formula:

SMILES

BrCC(Br)CBr



10.5. Profiling results:

DNA binding by OASIS v.1.3

SN2

SN2 >> DNA alkylation

SN2 >> DNA alkylation >> Vicinal Dihaloalkanes

SN2 >> Internal SN2 reaction with aziridinium and/or cyclic sulfonium ion formation (enzymatic)

SN2 >> Internal SN2 reaction with aziridinium and/or cyclic sulfonium ion formation (enzymatic) >> Vicinal Dihaloalkanes

DNA binding by OECD

SN2

SN2 >> Episulfonium Ion Formation

SN2 >> Episulfonium Ion Formation >> 1,2-Dihaloalkanes

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> Episulfonium Ion Formation

SN2 >> Episulfonium Ion Formation >> 1,2-Dihaloalkane

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Not categorized

Chemical(s) No. 11 - 16 are reported below:

No.	CAS	Chem. name	SMILES	RA
11	74-95-3	dibromomethane	BrCBr	
12	110-52-1	1.4-dibromobutane	BrCCCCBr	
13	74-83-9	methyl bromide	CBr	
14	631-28-7	1,2,3-tribromo-2-methylpropane	CC(Br)(CBr)CBr	
15	111-24-0	1,5-dibromopentane	BrCCCCCBr	
16	111-83-1	1-bromooctane	CCCCCCCCBr	

QSAR Toolbox prediction based on read-across

Prediction of Gene mutation for 1-bromopropane

APPENDIX 2 - Data matrix

OMITTED BY THE USER

QSAR Toolbox prediction based on read-across

Prediction of Gene mutation for 1-bromopropane

APPENDIX 3 - QMRF

APPENDIX 4 - QMRF, training set chemicals

APPENDIX 5 - QMRF, test set chemicals

APPENDIX 6 - Additional information from (Q)SAR

NOT APPLICABLE

QSAR Toolbox prediction based on read-across

Prediction of Gene mutation for 1-bromopropane

APPENDIX 7 - Chemical components

NOT APPLICABLE

QSAR Toolbox prediction for single chemical

The template of the current report is based on "GUIDANCE DOCUMENT ON THE VALIDATION OF (QUANTITATIVE) STRUCTURE-ACTIVITY RELATIONSHIPS MODELS" published by OECD (September, 2007) and "GUIDANCE ON INFORMATION REQUIREMENTS AND CHEMICAL SAFETY ASSESSMENT / CHAPTER R.6: QSARS AND GROUPING OF CHEMICALS" published by ECHA (May, 2008).

The report provides information about the target substance, chemical characteristics used for the grouping, the resulting boundaries of the group of chemicals (applicability domain), the type of data gap filling approach that was applied (read-across, trend analysis or QSAR models), the predicted result(s) and in the Annex information about the category members or training set and test set chemicals.

The chemicals are ordered by the distance to the target substance within the descriptors space. Only chemicals with experimental data are listed as category members.

Depending on the settings selected by the user, detailed information (incl. 2D image and profiling results) is provided for some chemicals while more limited information (CAS, name, SMILES) is provided for others.

If not otherwise specified, the experimental values are reported in bold, recalculated experimental values are reported in bold & italic and calculated values are reported in regular font.

Table of content

Summary 3

1. Target substance

1.1. CAS number 4
1.2. Other regulatory numbers 4
1.3. Chemical name(s) 4
1.4. Structural formula 4
1.5. Structure codes 4
1.6. Quality of structure identity (CAS/2D quality) 5

2. General information

2.1. Date of report generation 5
2.2. Report author(s) and contact details 5

3. Category definition

3.1. Category definition 5
3.2. Category justification 6
3.3. Data matrix 6

4. Prediction

4.1. Defined endpoint (OECD Principle 1) 7
4.2. Unambiguous algorithm (OECD Principle 2) 7
4.3. Applicability domain (OECD Principle 3) 8
4.4. Uncertainty of the prediction (OECD Principle 4) 8
4.5. Chemical and biological mechanisms (OECD Principle 5) 8

5. Adequacy

5.1. Regulatory purpose 10
5.2. Approach for regulatory interpretation of the model result 10
5.3. Outcome 10
5.4. Conclusion 10

Appendix 1 - Category members 11
Appendix 2 - Data matrix 16
Appendix 3 - QMRF 17
Appendix 4 - QMRF, training set 17
Appendix 5 - QMRF, test set 17
Appendix 6 - Additional information from QSAR 17
Appendix 7 - Chemical components 18

QSAR Toolbox prediction based on read-across

Prediction of Chromosome aberration for 1-bromopropane

Summary

Toxicity of the target chemical (Negative) is predicted from category members using read-across based on 2 values (Negative x2) from 2 nearest neighbours compared by prediction descriptors. Category members are single chemicals or mixtures and are selected based on the profile of the target chemical. Only chemicals having experimental data are listed in the category.

The target chemical FALLS within applicability domain of the prediction (see Section 4.3 for details).

The data used for calculating the current prediction is taken from 2 experimental values selected from the following database(s):

1. Genotoxicity OASIS

Below is a summary table for endpoint & descriptor values for the target chemical and the category members.
Experimental values from data matrix are presented in bold font. Recalculated endpoint values (if required by selected data usage option in Gap Filling) are presented in italic font. Recalculated endpoint values based on experimental data only are presented in bold and italic font.

	Endpoint(s)	***Descriptor(s)***
	Human Health Hazards; Genetic Toxicity	**log Kow**
	Chromosome aberration I (Oasis)	-
Target chemical	-	2.16
Cat. member No. 1	**Negative**	2.56
Cat. member No. 2	**Negative**	1.67

Section 1 - *Target chemical*

1.1. CAS number:

106-94-5

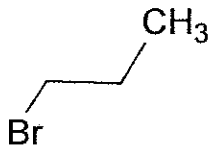
1.2. Other regulatory numbers:

Not reported

1.3. Chemical name(s):

1-bromopropane
propane, 1-bromo-
n-propyl bromide
1bromopropane
npropyl bromide

1.4. Structural formula:



1.5. Structure codes:

a. SMILES:

CCCBr

b. Input structure code (if different from SMILES):

Not available

c. Stereochemical features: *manually editable field*

Not provided by the user

1.6. Quality of structure identity (CAS/2D quality):

High Quality

Databases to which the target chemical belongs are:

Aquatic OASIS
Bacterial mutagenicity ISSSTY
Biodegradation NITE
Developmental & Reproductive Toxicity (DART)
ECHA CHEM
ECOTOX
Genotoxicity OASIS
Micronucleus ISSMIC
Phys-chem EPISUITE
Rodent Inhalation Toxicity Database

Section 2 - *General information*

2.1. Date of report generation:

22.07.2015

2.2. Report author(s) and contact details:

manually editable field

Not provided by the user

Section 3 - *Category definition and category members*

3.1. Category definition:

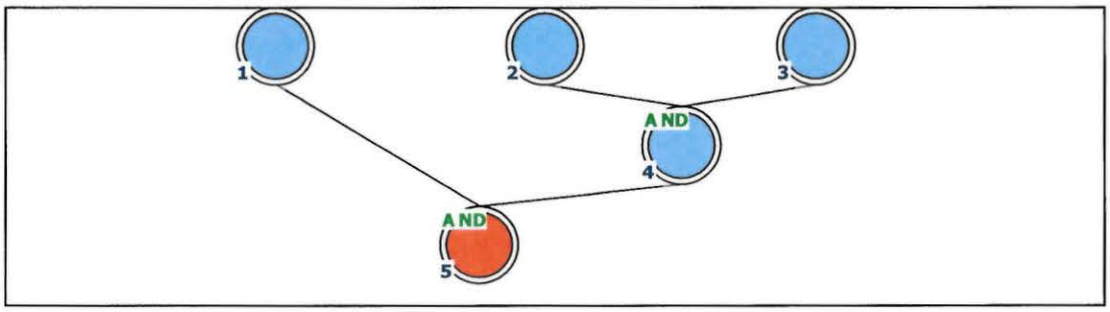
a. Category hypothesis:

manually editable field

Not provided by the user

b. Applicability domain of the category:

The applicability domain is defined by following scheme



1) Referential boundary:

The target chemical should be classified as SN2 AND SN2 >> Alkylation by epoxide metabolically formed after E2 reaction AND SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes AND SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom AND SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes AND SN2 >> Nucleophilic substitution after carbenium ion formation AND SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes by DNA alerts for AMES, MN and CA by OASIS v.1.3

2) Parametric boundary:

The target chemical should have a value of log Kow which is >= 1.67

3) Parametric boundary:

The target chemical should have a value of log Kow which is <= 2.56

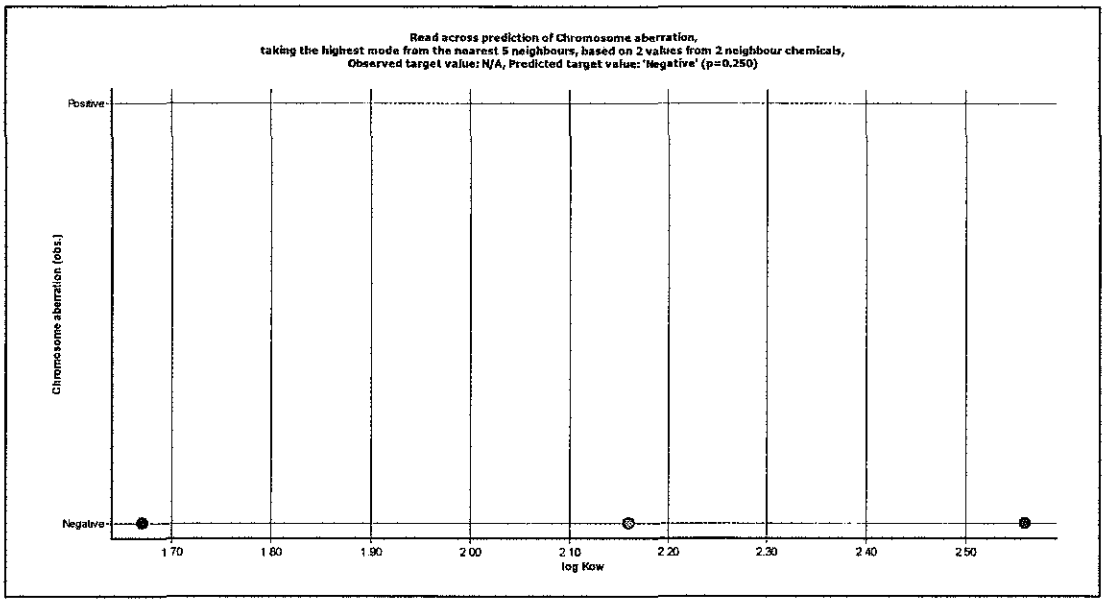
c. Endpoints covered: *manually editable field*

Not provided by the user

d. Category members:

The list of the category members is available in **Appendix 1**

The category members shown with respect to the descriptor **log Kow**



3.2. Category justification: *manually editable field*

Not provided by the user

3.3. Data matrix:

The data matrix is available in **Appendix 2**

Section 4 - *Prediction*

4.1. Defined Endpoint (OECD Principle 1):

a. Endpoint (e.g. Acute toxicity to fish): *manually editable field*

Chromosome aberration

Materials & methods / type of method:

In Vitro

Test chemical / test type:

In Vitro mammalian chromosome aberration test

b. Dependent variable (e.g. LC50): *manually editable field*

(Chromosome aberration)

c. Units: *manually editable field*

Not provided by the user

d. Duration: *manually editable field*

Not provided by the user

e. Species: *manually editable field*

Not provided by the user

4.2. Unambiguous algorithm (OECD Principle 2):

a. Prediction approach: *manually editable field*

Read-across from category members
Experimental values for the target chemical (if any) were not used in prediction calculations

b. Calculation approach:

Takes highest mode value from the 5 nearest neighbours

c. Model name:

Not applicable

d. Model version:

Not applicable

e. Reference to QMRF:

Not applicable

f. Input for prediction (target chemical):

SMILES

g. Descriptor and endpoint values for target chemical (if applicable):

Descriptor(s)	
log Kow	2.16
Endpoint (dep. variable)	
Human Health Hazards; Genetic Toxicity	-

h. Additional chemicals eliminations (not determined by domain):

Not available

i. Additional data eliminations (not determined by domain):

Not available

j. Predicted value (model result):

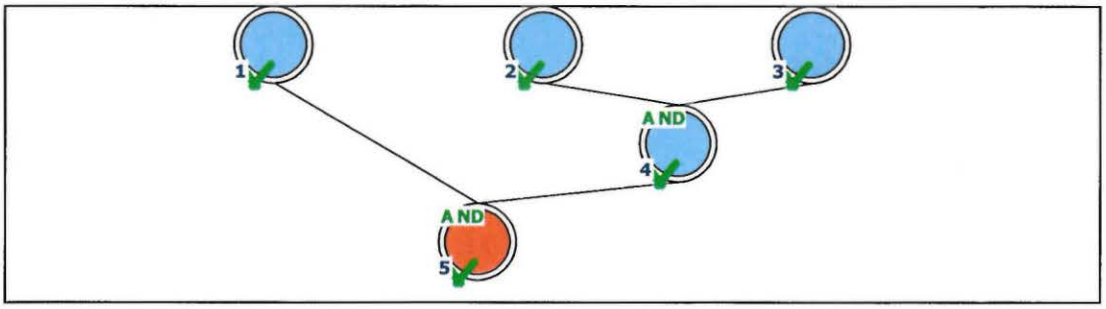
Negative

k. Predicted value (comments): *manually editable field*

Not provided by the user

4.3. Applicability domain (OECD Principle 3):

The target chemical FALLS within applicability domain
(see Section 3.1.b for detailed description of the domain)



4.4. Uncertainty of the prediction (OECD Principle 4): *manually editable field*

The prediction is based on 2 neighbours' values, 2 of them equal to prediction.
Prediction confidence is measured by the p-value = 0.250 (no confidence)

4.5. Chemical and biological mechanisms (OECD Principle 5):

Profiling results for the target substance:

DNA binding by OASIS v.1.3

SN2

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes

SN2 >> Nucleophilic substitution after carbenium ion formation

SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes

DNA binding by OECD

SN2

SN2 >> SN2 at an sp3 Carbon atom

SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Neutral Organics

Comments:

Not provided by the user *manually editable field*

Section 5 - *Adequacy*

5.1. Regulatory purpose: *manually editable field*

Not provided by the user

5.2. Approach for regulatory interpretation of the model result: *manually editable field*

Not provided by the user

5.3. Outcome: *manually editable field*

Not provided by the user

5.4. Conclusion: *manually editable field*

Not provided by the user

QSAR Toolbox prediction based on read-across

Prediction of Chromosome aberration for 1-bromopropane

APPENDIX 1 - Category members

The 2 category members are reported in more detail

1. Cat. member No.1: *used for read-across*

1.1. CAS number:

109-69-3

1.2. Other regulatory numbers:

Not reported

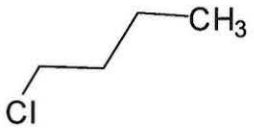
1.3. Chemical name(s):

1-chlorobutane,
1-chlorobutane
butane, 1-chloro-
n-butyl chloride
butyl chloride, n-

1.4. Structural formula:

SMILES

CCCCCl



1.5. Profiling results:

DNA binding by OASIS v.1.3

SN2

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes

SN2 >> Nucleophilic substitution after carbenium ion formation

SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes

DNA binding by OECD

SN2

SN2 >> SN2 at an sp3 Carbon atom

SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Neutral Organics

2. Cat. member No.2: *used for read-across*

2.1. CAS number:

74-96-4

2.2. Other regulatory numbers:

Not reported

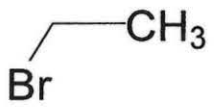
2.3. Chemical name(s):

bromoethane
ethane, bromo-
bromoethane(ethyl bromide)
ethyl bromide

2.4. Structural formula:

SMILES

CCBr



2.5. Profiling results:

DNA binding by OASIS v.1.3

SN2

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes

SN2 >> Nucleophilic substitution after carbenium ion formation

SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes

DNA binding by OECD

SN2

SN2 >> SN2 at an sp3 Carbon atom

SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Neutral Organics

QSAR Toolbox prediction based on read-across

Prediction of Chromosome aberration for 1-bromopropane

APPENDIX 2 - Data matrix

OMITTED BY THE USER

QSAR Toolbox prediction based on read-across

Prediction of Chromosome aberration for 1-bromopropane

APPENDIX 3 - QMRF

APPENDIX 4 - QMRF, training set chemicals

APPENDIX 5 - QMRF, test set chemicals

APPENDIX 6 - Additional information from (Q)SAR

NOT APPLICABLE

QSAR Toolbox prediction based on read-across

Prediction of Chromosome aberration for 1-bromopropane

APPENDIX 7 - Chemical components

NOT APPLICABLE

QSAR Toolbox prediction for single chemical

The template of the current report is based on "GUIDANCE DOCUMENT ON THE VALIDATION OF (QUANTITATIVE) STRUCTURE-ACTIVITY RELATIONSHIPS MODELS" published by OECD (September, 2007) and "GUIDANCE ON INFORMATION REQUIREMENTS AND CHEMICAL SAFETY ASSESSMENT / CHAPTER R.6: QSARS AND GROUPING OF CHEMICALS" published by ECHA (May, 2008).

The report provides information about the target substance, chemical characteristics used for the grouping, the resulting boundaries of the group of chemicals (applicability domain), the type of data gap filling approach that was applied (read-across, trend analysis or QSAR models), the predicted result(s) and in the Annex information about the category members or training set and test set chemicals.

The chemicals are ordered by the distance to the target substance within the descriptors space. Only chemicals with experimental data are listed as category members.

Depending on the settings selected by the user, detailed information (incl. 2D image and profiling results) is provided for some chemicals while more limited information (CAS, name, SMILES) is provided for others.

If not otherwise specified, the experimental values are reported in bold, recalculated experimental values are reported in bold & italic and calculated values are reported in regular font.

Table of content

Summary 3

1. Target substance

1.1. CAS number 4
1.2. Other regulatory numbers 4
1.3. Chemical name(s) 4
1.4. Structural formula 4
1.5. Structure codes 4
1.6. Quality of structure identity (CAS/2D quality) 5

2. General information

2.1. Date of report generation 5
2.2. Report author(s) and contact details 5

3. Category definition

3.1. Category definition 5
3.2. Category justification 6
3.3. Data matrix 6

4. Prediction

4.1. Defined endpoint (OECD Principle 1) 7
4.2. Unambiguous algorithm (OECD Principle 2) 7
4.3. Applicability domain (OECD Principle 3) 8
4.4. Uncertainty of the prediction (OECD Principle 4) 8
4.5. Chemical and biological mechanisms (OECD Principle 5) 8

5. Adequacy

5.1. Regulatory purpose 10
5.2. Approach for regulatory interpretation of the model result 10
5.3. Outcome 10
5.4. Conclusion 10

Appendix 1 - Category members 11

Appendix 2 - Data matrix 20

Appendix 3 - QMRF 21

Appendix 4 - QMRF, training set 21

Appendix 5 - QMRF, test set 21

Appendix 6 - Additional information from QSAR 21

Appendix 7 - Chemical components 22

QSAR Toolbox prediction based on read-across

Prediction of Summary carcinogenicity for 1-bromopropane

Summary

Toxicity of the target chemical (Negative) is predicted from category members using read-across based on 18 values (Positive x6, Equivocal x3, Negative x9) from 4 nearest neighbours compared by prediction descriptors. Category members are single chemicals or mixtures and are selected based on the profile of the target chemical. Only chemicals having experimental data are listed in the category.

The target chemical FALLS within applicability domain of the prediction (see Section 4.3 for details).

The data used for calculating the current prediction is taken from 18 experimental values selected from the following database(s):

1. Carcinogenic Potency Database (CPDB)
2. Carcinogenicity&mutagenicity ISSCAN

Below is a summary table for endpoint & descriptor values for the target chemical and the category members.
Experimental values from data matrix are presented in bold font. Recalculated endpoint values (if required by selected data usage option in Gap Filling) are presented in italic font. Recalculated endpoint values based on experimental data only are presented in bold and italic font.

	Endpoint(s)	***Descriptor(s)***
	Human Health Hazards; Carcinogenicity	**log Kow**
	Carcinogenicity I (ISSCAN)	-
Target chemical	-	2.16
Cat. member No. 1	***Negative (4)***	2.56
Cat. member No. 2	***Positive (4)*** ***Equivocal (2)***	1.67
Cat. member No. 3	***Negative*** ***Positive (2)*** ***Equivocal***	1.58
Cat. member No. 4	***Negative (4)***	1.18

Section 1 - *Target chemical*

1.1. CAS number:

106-94-5

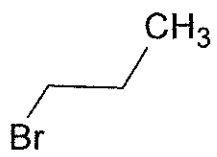
1.2. Other regulatory numbers:

Not reported

1.3. Chemical name(s):

1-bromopropane
propane, 1-bromo-
n-propyl bromide
1bromopropane
npropyl bromide

1.4. Structural formula:



1.5. Structure codes:

a. SMILES:

CCCBr

b. Input structure code (if different from SMILES):

Not available

c. Stereochemical features: *manually editable field*

Not provided by the user

1.6. Quality of structure identity (CAS/2D quality):

High Quality

Databases to which the target chemical belongs are:

Aquatic OASIS
Bacterial mutagenicity ISSSTY
Biodegradation NITE
Developmental & Reproductive Toxicity (DART)
ECHA CHEM
ECOTOX
Genotoxicity OASIS
Micronucleus ISSMIC
Phys-chem EPISUITE
Rodent Inhalation Toxicity Database

Section 2 - *General information*

2.1. Date of report generation:

22.07.2015

2.2. Report author(s) and contact details: *manually editable field*

Not provided by the user

Section 3 - *Category definition and category members*

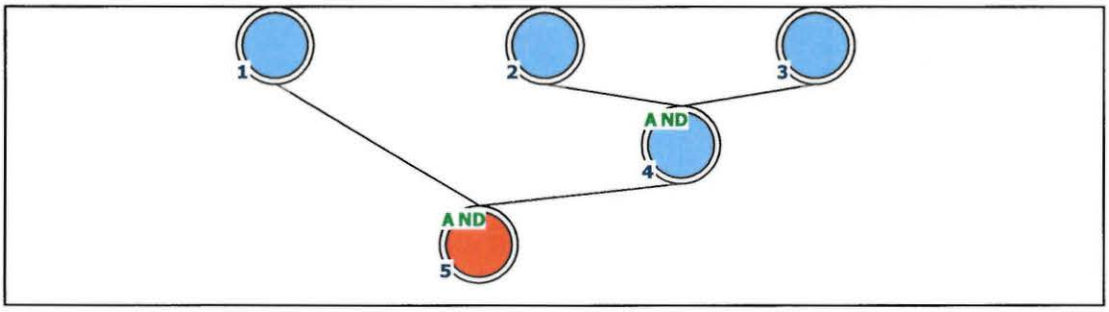
3.1. Category definition:

a. Category hypothesis: *manually editable field*

Not provided by the user

b. Applicability domain of the category:

The applicability domain is defined by following scheme



1) Referential boundary:

The target chemical should be classified as SN2 AND SN2 >> Alkylation by epoxide metabolically formed after E2 reaction AND SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes AND SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom AND SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes AND SN2 >> Nucleophilic substitution after carbenium ion formation AND SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes by DNA alerts for AMES, MN and CA by OASIS v.1.3

2) Parametric boundary:

The target chemical should have a value of log Kow which is >= 1.18

3) Parametric boundary:

The target chemical should have a value of log Kow which is <= 2.56

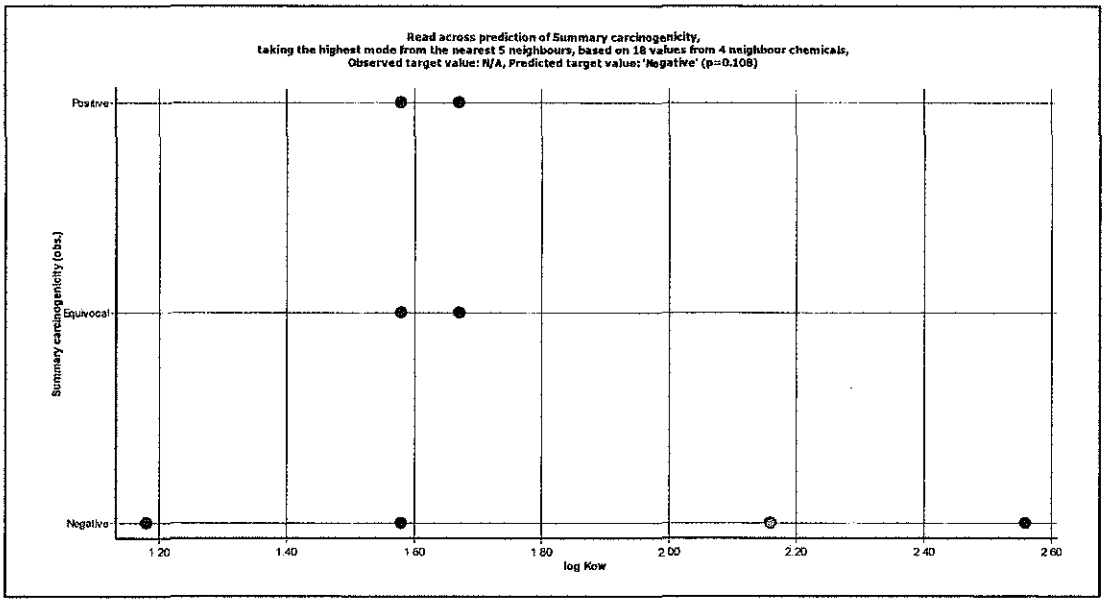
c. Endpoints covered: *manually editable field*

Not provided by the user

d. Category members:

The list of the category members is available in **Appendix 1**

The category members shown with respect to the descriptor **log Kow**



3.2. Category justification: *manually editable field*

Not provided by the user

3.3. Data matrix:

The data matrix is available in **Appendix 2**

Section 4 - *Prediction*

4.1. Defined Endpoint (OECD Principle 1):

a. Endpoint (e.g. Acute toxicity to fish): *manually editable field*

Summary carcinogenicity

Materials & methods / type of method:

In Vivo

b. Dependent variable (e.g. LC50): *manually editable field*

(Summary carcinogenicity)

c. Units: *manually editable field*

Not provided by the user

d. Duration: *manually editable field*

Not provided by the user

e. Species: *manually editable field*

Rat
Mouse

4.2. Unambiguous algorithm (OECD Principle 2):

a. Prediction approach: *manually editable field*

Read-across from category members
Experimental values for the target chemical (if any) were not used in prediction calculations

b. Calculation approach:

Takes highest mode value from the 5 nearest neighbours

c. Model name:

Not applicable

d. Model version:

Not applicable

e. Reference to QMRF:

Not applicable

f. Input for prediction (target chemical):

SMILES

g. Descriptor and endpoint values for target chemical (if applicable):

Descriptor(s)	
log Kow	2.16
Endpoint (dep. variable)	
Human Health Hazards; Carcinogenicity	-

h. Additional chemicals eliminations (not determined by domain):

Not available

i. Additional data eliminations (not determined by domain):

Not available

j. Predicted value (model result):

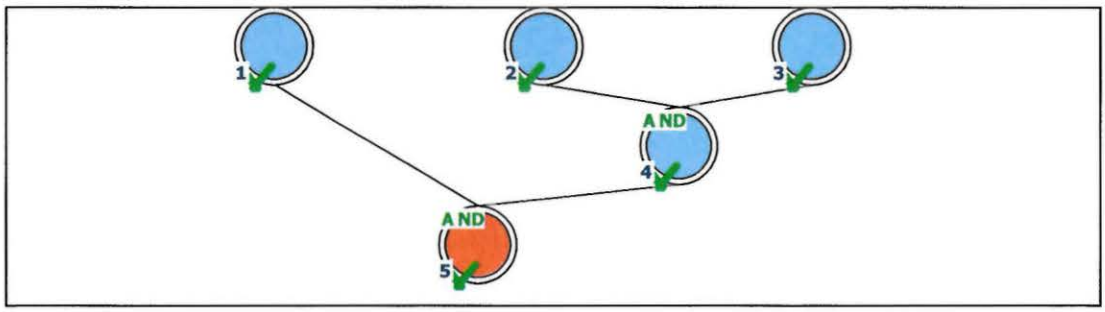
Negative

k. Predicted value (comments): *manually editable field*

Not provided by the user

4.3. Applicability domain (OECD Principle 3):

The target chemical FALLS within applicability domain
(see Section 3.1.b for detailed description of the domain)



4.4. Uncertainty of the prediction (OECD Principle 4): *manually editable field*

The prediction is based on 18 neighbours' values, 9 of them equal to prediction.
Prediction confidence is measured by the p-value = 0.108 (no confidence)

4.5. Chemical and biological mechanisms (OECD Principle 5):

Profiling results for the target substance:

DNA binding by OASIS v.1.3

SN2

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes

SN2 >> Nucleophilic substitution after carbenium ion formation

SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes

DNA binding by OECD

SN2

SN2 >> SN2 at an sp3 Carbon atom

SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Neutral Organics

Comments:

Not provided by the user *manually editable field*

Section 5 - *Adequacy*

5.1. Regulatory purpose: *manually editable field*

Not provided by the user

5.2. Approach for regulatory interpretation of the model result: *manually editable field*

Not provided by the user

5.3. Outcome: *manually editable field*

Not provided by the user

5.4. Conclusion: *manually editable field*

Not provided by the user

QSAR Toolbox prediction based on read-across

Prediction of Summary carcinogenicity for 1-bromopropane

APPENDIX 1 - Category members

The 4 category members are reported in more detail

1. Cat. member No.1: *used for read-across*

1.1. CAS number:

109-69-3

1.2. Other regulatory numbers:

Not reported

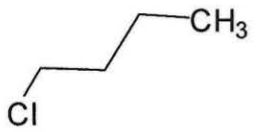
1.3. Chemical name(s):

1-chlorobutane,
1-chlorobutane
butane, 1-chloro-
n-butyl chloride
butyl chloride, n-

1.4. Structural formula:

SMILES

CCCCCl



1.5. Profiling results:

DNA binding by OASIS v.1.3

SN2

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes

SN2 >> Nucleophilic substitution after carbenium ion formation

SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes

DNA binding by OECD

SN2

SN2 >> SN2 at an sp3 Carbon atom

SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Neutral Organics

2. Cat. member No.2: **used for read-across**

2.1. CAS number:

74-96-4

2.2. Other regulatory numbers:

Not reported

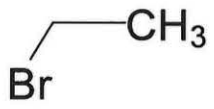
2.3. Chemical name(s):

bromoethane
ethane, bromo-
bromoethane(ethyl bromide)
ethyl bromide

2.4. Structural formula:

SMILES

CCBr



2.5. Profiling results:

DNA binding by OASIS v.1.3

SN2

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes

SN2 >> Nucleophilic substitution after carbenium ion formation

SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes

DNA binding by OECD

SN2

SN2 >> SN2 at an sp3 Carbon atom

SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Neutral Organics

3. Cat. member No.3: **used for read-across**

3.1. CAS number:

75-00-3

3.2. Other regulatory numbers:

Not reported

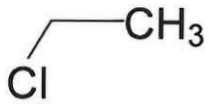
3.3. Chemical name(s):

chloroethane
ethyl chloride
ethane, chloro-

3.4. Structural formula:

SMILES

CCCl



3.5. Profiling results:

DNA binding by OASIS v.1.3

SN2

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes

SN2 >> Nucleophilic substitution after carbenium ion formation

SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes

DNA binding by OECD

SN2

SN2 >> SN2 at an sp3 Carbon atom

SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Neutral Organics

4. Cat. member No.4: *used for read-across*

4.1. CAS number:

74-83-9

4.2. Other regulatory numbers:

Not reported

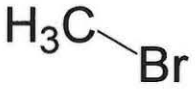
4.3. Chemical name(s):

methyl bromide
methane, bromo-
bromomethane
bromomethane(methyl bromide iso)
methyl bromide [bsi:iso]
methane, bromo-"""

4.4. Structural formula:

SMILES

CBr



4.5. Profiling results:

DNA binding by OASIS v.1.3

SN2

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes

SN2 >> Nucleophilic substitution after carbenium ion formation

SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes

DNA binding by OECD

SN2

SN2 >> SN2 at an sp3 Carbon atom

SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Neutral Organics

QSAR Toolbox prediction based on read-across

Prediction of Summary carcinogenicity for 1-bromopropane

APPENDIX 2 - Data matrix

OMITTED BY THE USER

QSAR Toolbox prediction based on read-across

Prediction of Summary carcinogenicity for 1-bromopropane

APPENDIX 3 - QMRF

APPENDIX 4 - QMRF, training set chemicals

APPENDIX 5 - QMRF, test set chemicals

APPENDIX 6 - Additional information from (Q)SAR

NOT APPLICABLE

QSAR Toolbox prediction based on read-across

Prediction of Summary carcinogenicity for 1-bromopropane

APPENDIX 7 - Chemical components

NOT APPLICABLE

QSAR Toolbox prediction for single chemical

The template of the current report is based on "GUIDANCE DOCUMENT ON THE VALIDATION OF (QUANTITATIVE) STRUCTURE-ACTIVITY RELATIONSHIPS MODELS" published by OECD (September, 2007) and "GUIDANCE ON INFORMATION REQUIREMENTS AND CHEMICAL SAFETY ASSESSMENT / CHAPTER R.6: QSARS AND GROUPING OF CHEMICALS" published by ECHA (May, 2008).

The report provides information about the target substance, chemical characteristics used for the grouping, the resulting boundaries of the group of chemicals (applicability domain), the type of data gap filling approach that was applied (read-across, trend analysis or QSAR models), the predicted result(s) and in the Annex information about the category members or training set and test set chemicals.

The chemicals are ordered by the distance to the target substance within the descriptors space. Only chemicals with experimental data are listed as category members.

Depending on the settings selected by the user, detailed information (incl. 2D image and profiling results) is provided for some chemicals while more limited information (CAS, name, SMILES) is provided for others.

If not otherwise specified, the experimental values are reported in bold, recalculated experimental values are reported in bold & italic and calculated values are reported in regular font.

Table of content

Summary 3

1. Target substance

1.1. CAS number 4
1.2. Other regulatory numbers 4
1.3. Chemical name(s) 4
1.4. Structural formula 4
1.5. Structure codes 4
1.6. Quality of structure identity (CAS/2D quality) 5

2. General information

2.1. Date of report generation 5
2.2. Report author(s) and contact details 5

3. Category definition

3.1. Category definition 5
3.2. Category justification 6
3.3. Data matrix 6

4. Prediction

4.1. Defined endpoint (OECD Principle 1) 7
4.2. Unambiguous algorithm (OECD Principle 2) 7
4.3. Applicability domain (OECD Principle 3) 8
4.4. Uncertainty of the prediction (OECD Principle 4) 8
4.5. Chemical and biological mechanisms (OECD Principle 5) 8

5. Adequacy

5.1. Regulatory purpose 10
5.2. Approach for regulatory interpretation of the model result 10
5.3. Outcome 10
5.4. Conclusion 10

Appendix 1 - Category members 11

Appendix 2 - Data matrix 16

Appendix 3 - QMRF 17

Appendix 4 - QMRF, training set 17

Appendix 5 - QMRF, test set 17

Appendix 6 - Additional information from QSAR 17

Appendix 7 - Chemical components 18

QSAR Toolbox prediction based on read-across

Prediction of Chromosome aberration for 2-bromopropane

Summary

Toxicity of the target chemical (Positive) is predicted from category members using read-across based on 2 values (Positive x1, Inconclusive x1) from 2 nearest neighbours compared by prediction descriptors. Category members are single chemicals or mixtures and are selected based on the profile of the target chemical. Only chemicals having experimental data are listed in the category.

The target chemical FALLS within applicability domain of the prediction (see Section 4.3 for details).

The data used for calculating the current prediction is taken from 2 experimental values selected from the following database(s):

1. Micronucleus ISSMIC

Below is a summary table for endpoint & descriptor values for the target chemical and the category members.
Experimental values from data matrix are presented in bold font. Recalculated endpoint values (if required by selected data usage option in Gap Filling) are presented in italic font. Recalculated endpoint values based on experimental data only are presented in bold and italic font.

	Endpoint(s)	***Descriptor(s)***
	Human Health Hazards; Genetic Toxicity	**log Kow**
	Micronucleus II	-
Target chemical	-	2.08
Cat. member No. 1	**Inconclusive**	2.16
Cat. member No. 2	**Positive**	1.18

Section 1 - *Target chemical*

1.1. CAS number:

75-26-3

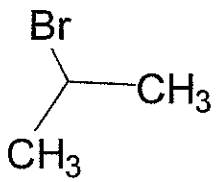
1.2. Other regulatory numbers:

Not reported

1.3. Chemical name(s):

2-bromopropane
iso-propyl bromide
propane, 2-bromo-
2bromopropane
isopropyl bromide

1.4. Structural formula:



1.5. Structure codes:

a. SMILES:

CC(C)Br

b. Input structure code (if different from SMILES):

Not available

c. Stereochemical features:

manually editable field

Not provided by the user

1.6. Quality of structure identity (CAS/2D quality):

High Quality

Databases to which the target chemical belongs are:

Aquatic Japan MoE
Bacterial mutagenicity ISSSTY
Biodegradation NITE
Developmental & Reproductive Toxicity (DART)
ECHA CHEM
Eye Irritation ECETOC
Genotoxicity OASIS
Phys-chem EPISUITE
Rodent Inhalation Toxicity Database
Skin Iirritation

Section 2 - *General information*

2.1. Date of report generation:

03.08.2015

2.2. Report author(s) and contact details: *manually editable field*

Not provided by the user

Section 3 - *Category definition and category members*

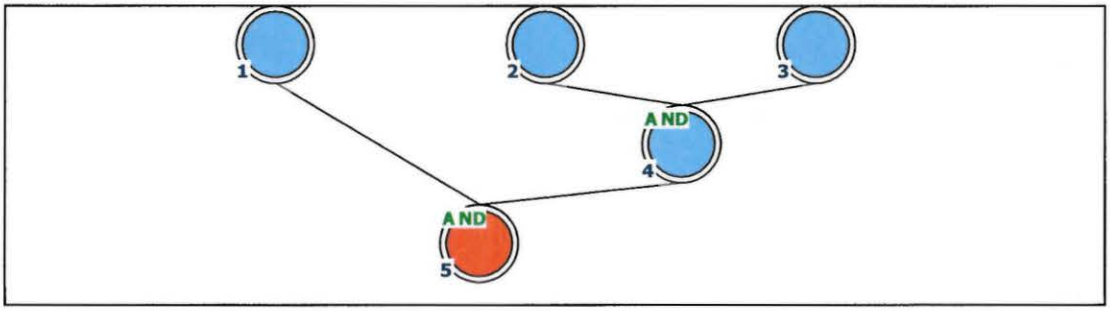
3.1. Category definition:

a. Category hypothesis: *manually editable field*

Not provided by the user

b. Applicability domain of the category:

The applicability domain is defined by following scheme



1) Referential boundary:

The target chemical should be classified as SN2 AND SN2 >> Alkylation by epoxide metabolically formed after E2 reaction AND SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes AND SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom AND SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes AND SN2 >> Nucleophilic substitution after carbenium ion formation AND SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes by DNA alerts for AMES, MN and CA by OASIS v.1.3

2) Parametric boundary:

The target chemical should have a value of log Kow which is >= 1.18

3) Parametric boundary:

The target chemical should have a value of log Kow which is <= 2.16

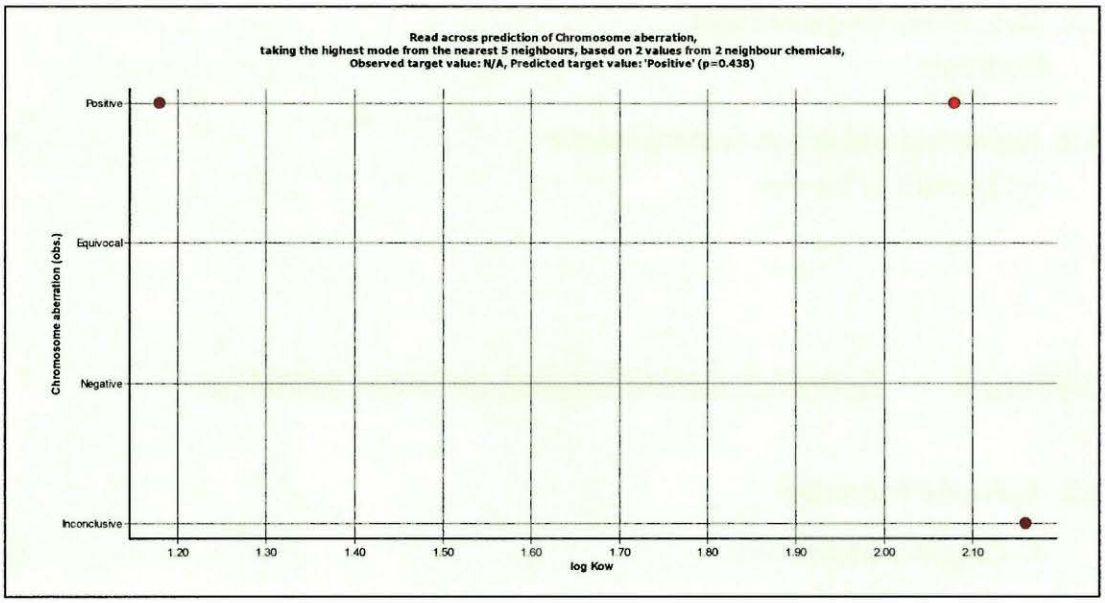
c. Endpoints covered: *manually editable field*

Not provided by the user

d. Category members:

The list of the category members is available in **Appendix 1**

The category members shown with respect to the descriptor **log Kow**



3.2. Category justification: *manually editable field*

Not provided by the user

3.3. Data matrix:

The data matrix is available in **Appendix 2**

Section 4 - *Prediction*

4.1. Defined Endpoint (OECD Principle 1):

a. Endpoint (e.g. Acute toxicity to fish): *manually editable field*

Chromosome aberration

Materials & methods / type of method:

In Vivo

Test chemical / test type:

micronucleus assay

b. Dependent variable (e.g. LC50): *manually editable field*

(Chromosome aberration)

c. Units: *manually editable field*

Not provided by the user

d. Duration: *manually editable field*

Not provided by the user

e. Species: *manually editable field*

Mouse

4.2. Unambiguous algorithm (OECD Principle 2):

a. Prediction approach: *manually editable field*

Read-across from category members
Experimental values for the target chemical (if any) were not used in prediction calculations

b. Calculation approach:

Takes highest mode value from the 5 nearest neighbours

c. Model name:

Not applicable

d. Model version:

Not applicable

e. Reference to QMRF:

Not applicable

f. Input for prediction (target chemical):

SMILES

g. Descriptor and endpoint values for target chemical (if applicable):

Descriptor(s)	
log Kow	2.08
Endpoint (dep. variable)	
Human Health Hazards; Genetic Toxicity	-

h. Additional chemicals eliminations (not determined by domain):

Not available

i. Additional data eliminations (not determined by domain):

Not available

j. Predicted value (model result):

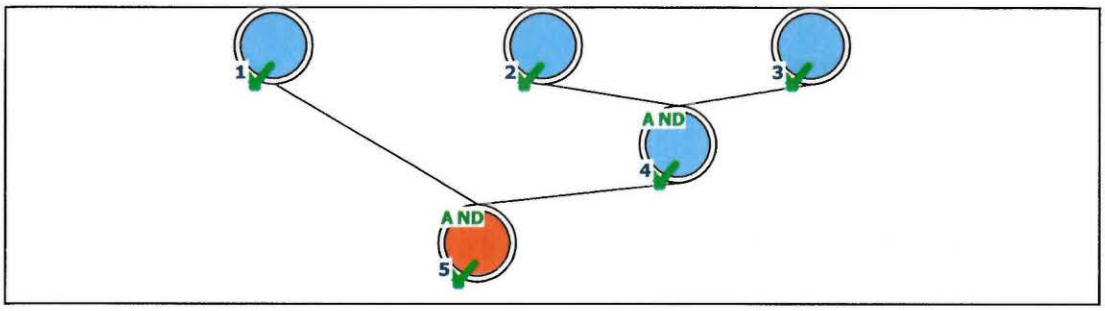
Positive

k. Predicted value (comments): *manually editable field*

Not provided by the user

4.3. Applicability domain (OECD Principle 3):

The target chemical FALLS within applicability domain
(see Section 3.1.b for detailed description of the domain)



4.4. Uncertainty of the prediction (OECD Principle 4): *manually editable field*

The prediction is based on 2 neighbours' values, 1 of them equal to prediction.
Prediction confidence is measured by the p-value = 0.438 (no confidence)

4.5. Chemical and biological mechanisms (OECD Principle 5):

Profiling results for the target substance:

DNA binding by OASIS v.1.3

SN2

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes

SN2 >> Nucleophilic substitution after carbenium ion formation

SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes

DNA binding by OECD

SN2

SN2 >> SN2 at an sp3 Carbon atom

SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Neutral Organics

Comments:

Not provided by the user *manually editable field*

Section 5 - *Adequacy*

5.1. Regulatory purpose: *manually editable field*

Not provided by the user

5.2. Approach for regulatory interpretation of the model result: *manually editable field*

Not provided by the user

5.3. Outcome: *manually editable field*

Not provided by the user

5.4. Conclusion: *manually editable field*

Not provided by the user

QSAR Toolbox prediction based on read-across

Prediction of Chromosome aberration for 2-bromopropane

APPENDIX 1 - Category members

The 2 category members are reported in more detail

1. Cat. member No.1: *used for read-across*

1.1. CAS number:

106-94-5

1.2. Other regulatory numbers:

Not reported

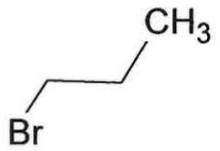
1.3. Chemical name(s):

1-bromopropane
propane, 1-bromo-
n-propyl bromide
1bromopropane
npropyl bromide

1.4. Structural formula:

SMILES

CCCBr



1.5. Profiling results:

DNA binding by OASIS v.1.3

SN2

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes

SN2 >> Nucleophilic substitution after carbenium ion formation

SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes

DNA binding by OECD

SN2

SN2 >> SN2 at an sp3 Carbon atom

SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Neutral Organics

2. Cat. member No.2: ***used for read-across***

2.1. CAS number:

74-83-9

2.2. Other regulatory numbers:

Not reported

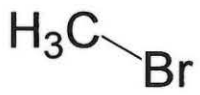
2.3. Chemical name(s):

methyl bromide
methane, bromo-
bromomethane
bromomethane(methyl bromide iso)
methyl bromide [bsi:iso]
methane, bromo-"""

2.4. Structural formula:

SMILES

CBr



2.5. Profiling results:

DNA binding by OASIS v.1.3

SN2

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction

SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Monohaloalkanes

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom

SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Monohaloalkanes

SN2 >> Nucleophilic substitution after carbenium ion formation

SN2 >> Nucleophilic substitution after carbenium ion formation >> Monohaloalkanes

DNA binding by OECD

SN2

SN2 >> SN2 at an sp3 Carbon atom

SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides

Estrogen Receptor Binding

Non binder, non cyclic structure

OECD HPV Chemical Categories

Not categorized

Protein binding by OASIS v1.3

SN2

SN2 >> Nucleophilic substitution at sp3 carbon atom

SN2 >> Nucleophilic substitution at sp3 carbon atom >> Alkyl halides

Protein binding by OECD

SN2

SN2 >> SN2 reaction at sp3 carbon atom

SN2 >> SN2 reaction at sp3 carbon atom >> Alkyl halides

Protein binding potency

Not possible to classify according to these rules (GSH)

Superfragments

No superfragment

Toxic hazard classification by Cramer (extension)

High (Class III)

Toxic hazard classification by Cramer (original)

High (Class III)

US-EPA New Chemical Categories

Neutral Organics

QSAR Toolbox prediction based on read-across

Prediction of Chromosome aberration for 2-bromopropane

APPENDIX 2 - Data matrix

OMITTED BY THE USER

QSAR Toolbox prediction based on read-across

Prediction of Chromosome aberration for 2-bromopropane

APPENDIX 3 - QMRF

APPENDIX 4 - QMRF, training set chemicals

APPENDIX 5 - QMRF, test set chemicals

APPENDIX 6 - Additional information from (Q)SAR

NOT APPLICABLE

QSAR Toolbox prediction based on read-across

Prediction of Chromosome aberration for 2-bromopropane

APPENDIX 7 - Chemical components

NOT APPLICABLE

U.S. National Library of Medicine TOXNET TOXICOLOGY DATA NETWORK

Mobile | Help | FAQs | TOXNET Fact Sheet | Training Manual & Schedule

CCRIS: 2-BROMOPROPANE

CASRN: 75-26-3 This record appears in multiple databases.

View record in another database: CCRIS

Download this Record Print Select Record My List Permalink

TABLE OF CONTENTS

Show Selected Items Clear Expand all Collapse all

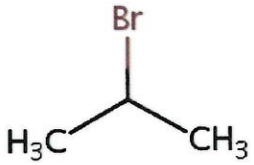
Full Record

+ Substance Identification
+ Studies Data
+ Administrative Information

Show Selected Items Clear

2-BROMOPROPANE

CASRN: 75-26-3



FULL RECORD DISPLAY

Displays all fields in the record.

For other data, click on the Table of Contents

Substance Identification:

Substance Name:

2-BROMOPROPANE

CAS Registry Number:

75-26-3

Major Use:

INTERMEDIATES (Alkylating Agent)

Data Type:

Mutagenicity

Studies Data:

Mutagenicity Studies:

Test System:	AMES SALMONELLA TYPHIMURIUM
Strain Indicator:	TA100

Metabolic Activation: NONE

Method: PREINCUBATION

Dose: 50-5000 UG/PLATE (TEST MATERIAL SOLVENT: DMSO)

Results: NEGATIVE

Reference:

[MAENG,SH AND YU,IJ; MUTAGENICITY OF 2-BROMOPROPANE; IND. HEALTH 35(1):87-95, 1997]

Test System: AMES SALMONELLA TYPHIMURIUM

Strain Indicator: TA100

Metabolic Activation: RAT, LIVER, S-9, PHENOBARBITAL AND 5,6-BENZOFLAVONE

Method: PREINCUBATION

Dose: 50-5000 UG/PLATE (TEST MATERIAL SOLVENT: DMSO)

Results: POSITIVE

Reference:

[MAENG,SH AND YU,IJ; MUTAGENICITY OF 2-BROMOPROPANE; IND. HEALTH 35(1):87-95, 1997]

Test System: AMES SALMONELLA TYPHIMURIUM

Strain Indicator: TA1535

Metabolic Activation: NONE

Method: PREINCUBATION

Dose: 50-5000 UG/PLATE (TEST MATERIAL SOLVENT: DMSO)

Results: POSITIVE

Reference:

[MAENG,SH AND YU,IJ; MUTAGENICITY OF 2-BROMOPROPANE; IND. HEALTH 35(1):87-95, 1997]

Test System: AMES SALMONELLA TYPHIMURIUM

Strain Indicator: TA1535

Metabolic Activation: RAT, LIVER, S-9, PHENOBARBITAL AND 5,6-BENZOFLAVONE

Method: PREINCUBATION

Dose: 50-5000 UG/PLATE (TEST MATERIAL SOLVENT: DMSO)

Results: POSITIVE

Reference:

[MAENG,SH AND YU,IJ; MUTAGENICITY OF 2-BROMOPROPANE; IND. HEALTH 35(1):87-95, 1997]

Test System: AMES SALMONELLA TYPHIMURIUM

Strain Indicator: TA98

Metabolic Activation: NONE

Method: PREINCUBATION

Dose: 50-5000 UG/PLATE (TEST MATERIAL SOLVENT: DMSO)

Results: NEGATIVE

Reference:

[MAENG,SH AND YU,IJ; MUTAGENICITY OF 2-BROMOPROPANE; IND. HEALTH 35(1):87-95, 1997]

Test System: AMES SALMONELLA TYPHIMURIUM

Strain Indicator: TA98

Metabolic Activation: RAT, LIVER, S-9, PHENOBARBITAL AND 5,6-BENZOFLAVONE

Method: PREINCUBATION

Dose: 50-5000 UG/PLATE (TEST MATERIAL SOLVENT: DMSO)

Results: NEGATIVE

Reference:

[MAENG,SH AND YU,IJ; MUTAGENICITY OF 2-BROMOPROPANE; IND. HEALTH 35(1):87-95, 1997]

Test System: AMES SALMONELLA TYPHIMURIUM

Strain Indicator: TA1537

Metabolic Activation: NONE

Method: PREINCUBATION

Dose: 50-5000 UG/PLATE (TEST MATERIAL SOLVENT: DMSO)

Results: NEGATIVE

Reference:

[MAENG,SH AND YU,IJ; MUTAGENICITY OF 2-BROMOPROPANE; IND. HEALTH 35(1):87-95, 1997]

Test System: AMES SALMONELLA TYPHIMURIUM

Strain Indicator: TA1537

Metabolic Activation: RAT, LIVER, S-9, PHENOBARBITAL AND 5,6-BENZOFLAVONE

Method: PREINCUBATION

Dose: 50-5000 UG/PLATE (TEST MATERIAL SOLVENT: DMSO)

Results: NEGATIVE

Reference:

[MAENG,SH AND YU,IJ; MUTAGENICITY OF 2-BROMOPROPANE; IND. HEALTH 35(1):87-95, 1997]

Test System: E. COLI

Strain Indicator: WP2 UVRA

Metabolic Activation: NONE

Method: PREINCUBATION

Dose: 50-5000 UG/PLATE (TEST MATERIAL SOLVENT: DMSO)

Results: NEGATIVE

Reference:

[MAENG,SH AND YU,IJ; MUTAGENICITY OF 2-BROMOPROPANE; IND. HEALTH 35(1):87-95, 1997]

Test System:	E. COLI
Strain Indicator:	WP2 UVRA
Metabolic Activation:	RAT, LIVER, S-9, PHENOBARBITAL AND 5,6-BENZOFLAVONE
Method:	PREINCUBATION
Dose:	50-5000 UG/PLATE (TEST MATERIAL SOLVENT: DMSO)
Results:	NEGATIVE
Reference:	

[MAENG,SH AND YU,IJ; MUTAGENICITY OF 2-BROMOPROPANE; IND. HEALTH 35(1):87-95, 1997]

Test System:	AMES SALMONELLA TYPHIMURIUM
Strain Indicator:	TA100
Metabolic Activation:	NONE
Method:	PREINCUBATION
Dose:	9.77-5000 UG/PLATE (TEST MATERIAL SOLVENT: DMSO)
Results:	POSITIVE
Reference:	

[JAPAN CHEMICAL INDUSTRY ECOLOGY- TOXICOLOGY AND INFORMATION CENTER, JAPAN; MUTAGENICITY TEST DATA OF EXISTING CHEMICAL SUBSTANCES BASED ON THE TOXICITY INVESTIGATION OF THE INDUSTRIAL SAFETY AND HEALTH LAW; 1996]

Test System:	AMES SALMONELLA TYPHIMURIUM
Strain Indicator:	TA100
Metabolic Activation:	RAT LIVER S-9, PHENOBARBITAL AND BETA-NAPHTHOFLAVONE
Method:	PREINCUBATION
Dose:	9.77-5000 UG/PLATE (TEST MATERIAL SOLVENT: DMSO)
Results:	POSITIVE
Reference:	

[JAPAN CHEMICAL INDUSTRY ECOLOGY- TOXICOLOGY AND INFORMATION CENTER, JAPAN; MUTAGENICITY TEST DATA OF EXISTING CHEMICAL SUBSTANCES BASED ON THE TOXICITY INVESTIGATION OF THE INDUSTRIAL SAFETY AND HEALTH LAW; 1996]

Test System:	AMES SALMONELLA TYPHIMURIUM
Strain Indicator:	TA1535
Metabolic Activation:	NONE
Method:	PREINCUBATION
Dose:	9.77-5000 UG/PLATE (TEST MATERIAL SOLVENT: DMSO)
Results:	POSITIVE

Reference:

[JAPAN CHEMICAL INDUSTRY ECOLOGY- TOXICOLOGY AND INFORMATION CENTER, JAPAN; MUTAGENICITY TEST DATA OF EXISTING CHEMICAL SUBSTANCES BASED ON THE TOXICITY INVESTIGATION OF THE INDUSTRIAL SAFETY AND HEALTH LAW; 1996]

Test System:	AMES SALMONELLA TYPHIMURIUM
Strain Indicator:	TA1535
Metabolic Activation:	RAT LIVER S-9, PHENOBARBITAL AND BETA-NAPHTHOFLAVONE
Method:	PREINCUBATION
Dose:	9.77-5000 UG/PLATE (TEST MATERIAL SOLVENT: DMSO)
Results:	POSITIVE
Reference:	

[JAPAN CHEMICAL INDUSTRY ECOLOGY- TOXICOLOGY AND INFORMATION CENTER, JAPAN; MUTAGENICITY TEST DATA OF EXISTING CHEMICAL SUBSTANCES BASED ON THE TOXICITY INVESTIGATION OF THE INDUSTRIAL SAFETY AND HEALTH LAW; 1996]

Test System:	AMES SALMONELLA TYPHIMURIUM
Strain Indicator:	TA100
Metabolic Activation:	RAT LIVER S-9, PHENOBARBITAL AND BETA-NAPHTHOFLAVONE
Method:	PREINCUBATION
Dose:	78.1-5000 UG/PLATE (TEST MATERIAL SOLVENT: DMSO)
Results:	NEGATIVE
Reference:	

[JAPAN CHEMICAL INDUSTRY ECOLOGY- TOXICOLOGY AND INFORMATION CENTER, JAPAN; MUTAGENICITY TEST DATA OF EXISTING CHEMICAL SUBSTANCES BASED ON THE TOXICITY INVESTIGATION OF THE INDUSTRIAL SAFETY AND HEALTH LAW; 1996]

Test System:	AMES SALMONELLA TYPHIMURIUM
Strain Indicator:	TA98
Metabolic Activation:	NONE
Method:	PREINCUBATION
Dose:	9.77-5000 UG/PLATE (TEST MATERIAL SOLVENT: DMSO)
Results:	NEGATIVE
Reference:	

[JAPAN CHEMICAL INDUSTRY ECOLOGY- TOXICOLOGY AND INFORMATION CENTER, JAPAN; MUTAGENICITY TEST DATA OF EXISTING CHEMICAL SUBSTANCES BASED ON THE TOXICITY INVESTIGATION OF THE INDUSTRIAL SAFETY AND HEALTH LAW; 1996]

Test System:	AMES SALMONELLA TYPHIMURIUM
Strain Indicator:	TA98
Metabolic Activation:	RAT LIVER S-9, PHENOBARBITAL AND BETA-NAPHTHOFLAVONE

Method: PREINCUBATION

Dose: 9.77-5000 UG/PLATE (TEST MATERIAL SOLVENT: DMSO)

Results: NEGATIVE

Reference:

[JAPAN CHEMICAL INDUSTRY ECOLOGY- TOXICOLOGY AND INFORMATION CENTER, JAPAN; MUTAGENICITY TEST DATA OF EXISTING CHEMICAL SUBSTANCES BASED ON THE TOXICITY INVESTIGATION OF THE INDUSTRIAL SAFETY AND HEALTH LAW; 1996]

Test System: AMES SALMONELLA TYPHIMURIUM

Strain Indicator: TA1537

Metabolic Activation: NONE

Method: PREINCUBATION

Dose: 9.77-5000 UG/PLATE (TEST MATERIAL SOLVENT: DMSO)

Results: NEGATIVE

Reference:

[JAPAN CHEMICAL INDUSTRY ECOLOGY- TOXICOLOGY AND INFORMATION CENTER, JAPAN; MUTAGENICITY TEST DATA OF EXISTING CHEMICAL SUBSTANCES BASED ON THE TOXICITY INVESTIGATION OF THE INDUSTRIAL SAFETY AND HEALTH LAW; 1996]

Test System: AMES SALMONELLA TYPHIMURIUM

Strain Indicator: TA1537

Metabolic Activation: RAT LIVER S-9, PHENOBARBITAL AND BETA-NAPHTHOFLAVONE

Method: PREINCUBATION

Dose: 9.77-5000 UG/PLATE (TEST MATERIAL SOLVENT: DMSO)

Results: NEGATIVE

Reference:

[JAPAN CHEMICAL INDUSTRY ECOLOGY- TOXICOLOGY AND INFORMATION CENTER, JAPAN; MUTAGENICITY TEST DATA OF EXISTING CHEMICAL SUBSTANCES BASED ON THE TOXICITY INVESTIGATION OF THE INDUSTRIAL SAFETY AND HEALTH LAW; 1996]

Test System: E.COLI

Strain Indicator: WP2UVRA

Metabolic Activation: RAT LIVER S-9, PHENOBARBITAL AND BETA-NAPHTHOFLAVONE

Method: PREINCUBATION

Dose: 9.77-5000 UG/PLATE (TEST MATERIAL SOLVENT: DMSO)

Results: NEGATIVE

Reference:

[JAPAN CHEMICAL INDUSTRY ECOLOGY- TOXICOLOGY AND INFORMATION CENTER, JAPAN; MUTAGENICITY TEST DATA OF EXISTING CHEMICAL SUBSTANCES BASED ON THE TOXICITY INVESTIGATION OF THE INDUSTRIAL SAFETY AND HEALTH LAW; 1996]

Test System:	E.COLI
Strain Indicator:	WP2UVRA
Metabolic Activation:	RAT LIVER S-9, PHENOBARBITAL AND BETA-NAPHTHOFLAVONE
Method:	PREINCUBATION
Dose:	78.1-5000 UG/PLATE (TEST MATERIAL SOLVENT: DMSO)
Results:	POSITIVE
Reference:	

[JAPAN CHEMICAL INDUSTRY ECOLOGY- TOXICOLOGY AND INFORMATION CENTER, JAPAN; MUTAGENICITY TEST DATA OF EXISTING CHEMICAL SUBSTANCES BASED ON THE TOXICITY INVESTIGATION OF THE INDUSTRIAL SAFETY AND HEALTH LAW; 1996]

Test System:	E.COLI
Strain Indicator:	WP2UVRA
Metabolic Activation:	NONE
Method:	PREINCUBATION
Dose:	9.77-5000 UG/PLATE (TEST MATERIAL SOLVENT: DMSO)
Results:	POSITIVE
Reference:	

[JAPAN CHEMICAL INDUSTRY ECOLOGY- TOXICOLOGY AND INFORMATION CENTER, JAPAN; MUTAGENICITY TEST DATA OF EXISTING CHEMICAL SUBSTANCES BASED ON THE TOXICITY INVESTIGATION OF THE INDUSTRIAL SAFETY AND HEALTH LAW; 1996]

Test System:	E.COLI
Strain Indicator:	WP2UVRA
Metabolic Activation:	NONE
Method:	PREINCUBATION
Dose:	78.1-5000 UG/PLATE (TEST MATERIAL SOLVENT: DMSO)
Results:	NEGATIVE
Reference:	

[JAPAN CHEMICAL INDUSTRY ECOLOGY- TOXICOLOGY AND INFORMATION CENTER, JAPAN; MUTAGENICITY TEST DATA OF EXISTING CHEMICAL SUBSTANCES BASED ON THE TOXICITY INVESTIGATION OF THE INDUSTRIAL SAFETY AND HEALTH LAW; 1996]

Test System:	Chinese Hamster Ovary (CHO-WBL) cells
End Point:	In vitro micronucleus
Metabolic Activation:	None
Dose:	0; 3,472; 4,167; 5,000 ug/ml (Test Material Solvent: DMSO)
Dose Regimen:	24 hr continuous treatment
Results:	Negative
Reference:	

[SOBOL,Z, ENGEL,ME, RUBITSKI,E, KU,WW, AUBRECHT,J AND SCHIESTL,RH; GENOTOXICTY PROFILES OF COMMON ALKYL HALIDES AND ESTERS WITH ALKYLATING ACTIVITY; MUTAT. RES., GEN. TOXICOL. ENVIRON. MUTAGEN. 633(2):80-94, 2007]

Administrative Information:

CCRIS Record Number:

7919

Last Revision Date:

20080115

Update History:

Complete Update on 2008-01-15
Complete Update on 12/01/2003, 2 fields added/edited/deleted.
Complete Update on 02/24/1999, 4 fields added/edited/deleted.

About | Contact Us | SIS Home | Copyright | Privacy | Accessibility | Viewers and Players

U.S. National Library of Medicine 8600 Rockville Pike, Bethesda, MD 20894
National Institutes of Health, Health & Human Services