

QSAR Toolboxの操作説明

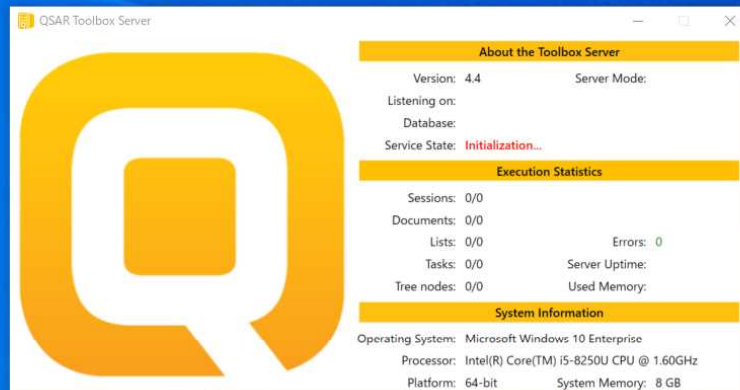
(独) 製品評価技術基盤機構 (NITE)
化学物質管理センター

立ち上げ(1)



←①ダブルクリック

②表示される→



立ち上げ(2)



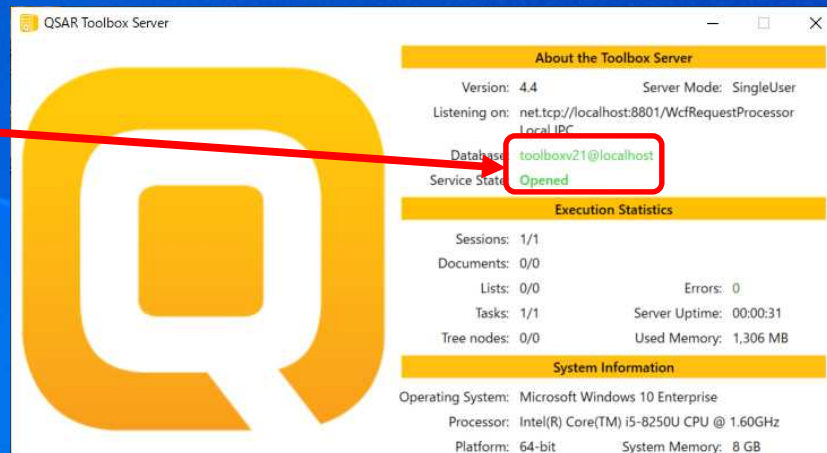
QSAR Toolbox 4.4
Desktop Client

←②ダブルクリック

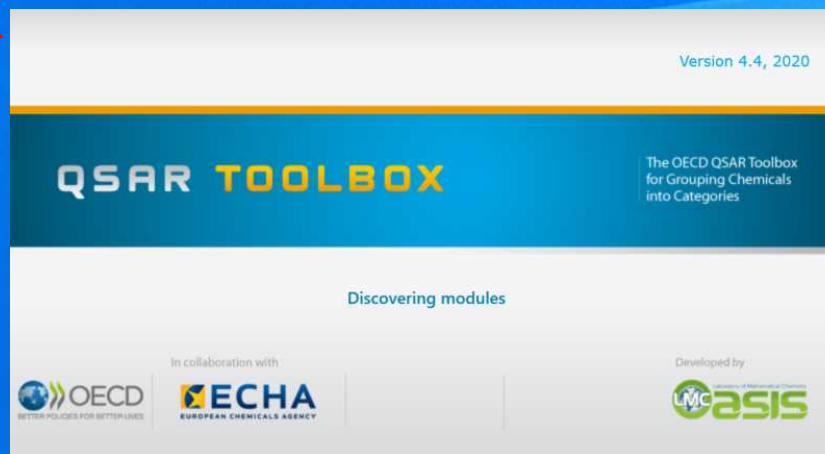


QSAR Toolbox 4.4
Server

①緑色になったことを確認



③表示される→
(数分待つ)

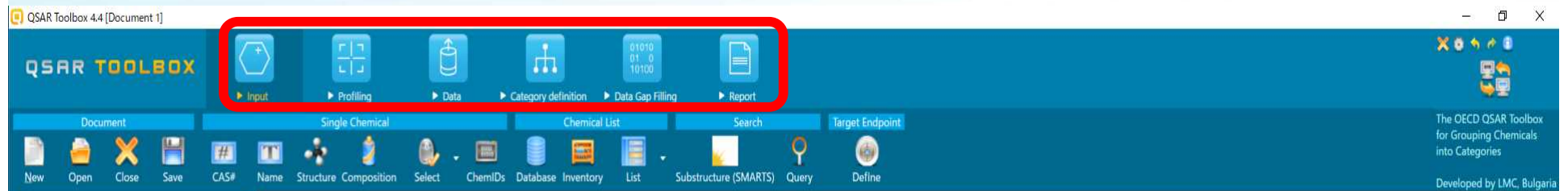


立ち上げ(3)



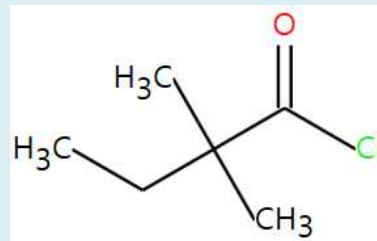
クリック

ワークフローに対応した6つのモジュール



リードアクロスの操作例

評価対象物質

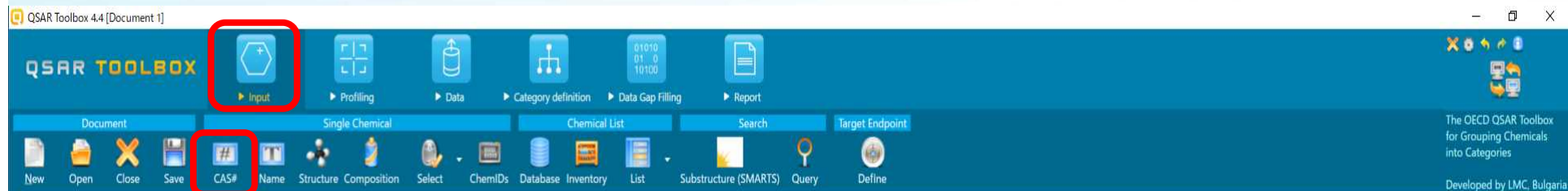


5856-77-9

対象エンドポイント

皮膚感作性

評価対象物質の入力



①クリック(CAS番号による入力を選択)

②入力
5856-77-9



Select All Unselect All Invert Selection Selected 1 of 1

1	CAS	5856-77-9	
	SMILES	CCC(C)(C)C(Cl)=O	
	CS Relation	High	
	Substance	Mono constituent	
<input checked="" type="checkbox"/>	Composition		
	Name	2,2-Dimethyl-buteryl chloride;2,2-	
	Sources	DSSTOX ECHA PR FINNCS	

評価対象物質の入力(結果)

The screenshot displays the QSAR Toolbox 4.4 interface. The top toolbar contains several icons, with the 'Insert' icon (a blue hexagon with a white plus sign) highlighted by a red circle. Below the toolbar, the 'Documents' panel on the left shows a list of documents, with the first document selected. A red arrow points from this document to the 'Structure info' panel in the main workspace. The 'Structure info' panel is also highlighted with a red circle. The main workspace displays the chemical structure of the selected substance, along with its properties and SMILES string.

①クリック(入力した物質の構造情報の確認)

EC Number:2274...
5856-77-9
High
2,2-dimethylbut...
C6H11ClO
Mono constituent
CCC(C)C(C)C(=O)O

プロファイリング

The screenshot shows the QSAR Toolbox 4.4 interface. The 'Profiling' tab is active in the top menu. A red box highlights the 'Profiling' icon in the top toolbar, with the annotation '① クリック'. Below it, the 'Apply' button in the 'Profiling' sub-menu is highlighted with a red box and the annotation '② クリック'. The 'Filter endpoint tree...' panel on the right shows a tree structure of endpoints. A red box highlights the 'Human Health Hazards' folder, with the annotation '③ クリック (評価対象エンドポイントに関連のあるプロファイラ/代謝シミュレータの確認→関連のあるものが強調表示される)'. The 'Profilers' panel on the left shows a list of profilers. A red box highlights the 'Protein binding by OASIS' entry, which is checked, with the annotation '④ "Protein binding by OASIS" にチェックを入れ、他のチェックを外す (使用するプロファイラの選択)'. The 'Metabolism' panel at the bottom shows a list of metabolism simulators. A red box highlights the 'Protein binding by OASIS' entry, which is unchecked, with the annotation '⑤ 全てチェックを外す (代謝シミュレータは使用しない)'. The 'Endpoints' panel on the right shows a list of endpoints. A red box highlights the 'Acylation' entry, with the annotation '⑦ 選択したプロファイラによるプロファイリングの結果'. A red arrow points from the 'Protein binding by OASIS' entry in the 'Profilers' panel to the 'Acylation' entry in the 'Endpoints' panel, with the annotation '⑥ クリック (選択したプロファイラによるプロファイリングの実行)'. A text box in the upper right contains the text 'プロファイリング: 評価対象物質がどのようなグループに属するのかを調べる'. The 'Structure' panel shows a chemical structure of a target molecule.

① クリック

② クリック

プロファイラ

③ クリック (評価対象エンドポイントに関連のあるプロファイラ/代謝シミュレータの確認→関連のあるものが強調表示される)

④ "Protein binding by OASIS" にチェックを入れ、他のチェックを外す (使用するプロファイラの選択)

⑤ 全てチェックを外す (代謝シミュレータは使用しない)

⑥ クリック (選択したプロファイラによるプロファイリングの実行)

⑦ 選択したプロファイラによるプロファイリングの結果

プロファイリング: 評価対象物質がどのようなグループに属するのかを調べる

エンドポイントツリー

代謝シミュレータ

プロファイリング結果の詳細の確認

③クリック

②ダブルクリック

①ダブルクリック

④ アシル化により蛋白結合を生じる物質のグループに属することを確認

Explanation for: Protein binding by OASIS -> Acylation -> Direct acylation involving a leaving group -> (Thi...)

Categories

Filter:

binding by OASIS
lation
(Thio)carbamoylation of protein
Isothiocyanates, Isocyanates
Acyl transfer via nucleophilic ad
Carbodiimides
Direct acylation involving a leav
(Thio)Acetates
(Thio)Acyl and (thio)carban
Anhydrides (sulphur analog
Azlactones and unsaturated
Carbamates
Diacyl peroxides, anhydride:
N-Acylsuccinimides

Definition

The reliability of the transformations 2, 3 and 4 is supported by Dr D. Roberts,
School of Pharmacy and Biomolecular Sciences, Liverpool John Moores
University,
Liverpool, England L3 3AF

Mechanistic Domain: Acylation

Mechanistic Alert: Direct acylation involving a leaving group

Structural Alert: (Thio)Acyl and (thio)carbamoyl halides, cyanides, azides, etc.

The chemical is a strong sensitizer as a result of **Protein acylation by (thio)acyl halides and (thio)carbamoyl derivatives:**

CC(C)C(=O)Cl

Map 1

$$\text{R}-\text{C}(=\text{O})-\text{Hal} \xrightarrow{\text{Pr}-\text{NH}_2} \text{R}-\text{C}(=\text{O})-\text{NH}-\text{Pr} + \text{H}-\text{Hal}$$

Hal = F, Cl, Br, I
R = any C

試験データの取得

① クリック

データベース

インベントリ (試験データはなし)

評価対象物質の試験データを取得する

② クリック (評価対象エンドポイントに関連のあるデータベースの確認→関連のあるものが強調表示される)

③ "Skin Sensitization"と"Skin Sensitization ECETOC"にチェックを入れ、他のチェックを全て外す(使用するデータベースの選択)

④ チェックを全て外す(類似物質検索(次のモジュール)にインベントリは使用しない)

⑤ クリック(選択したデータベースから評価対象物質の試験データを取得する)

試験データの取得

The screenshot shows the QSAR Toolbox 4.4 interface. The 'Data' menu item in the top toolbar is highlighted with a red box. Below it, the 'Databases' panel shows several databases selected, including 'Skin Sensitization' and 'Skin sensitization ECETOC'. The 'Filter endpoint tree...' panel on the right shows a list of endpoints, with 'AW SWAOP' selected. Two dialog boxes are overlaid on the interface. The first dialog, titled 'Read data?', has the 'All endpoints' radio button selected and the 'OK' button highlighted with a red box. The second dialog, titled 'There is no experimental data available for the chemicals of interest.', has the 'OK' button highlighted with a red box.

① クリック (全エンドポイントのデータを抽出)

② クリック (選択したデータベースにはデータがなかった)
→ よって、類似物質を用いたデータギャップ補完の検討に進む

カテゴリー定義

QSAR Toolbox 4.4 [Document 1]

QSAR TOOLBOX

Input Profiling Data **Category definition** Data Gap Filling Report

Categorize Category consistency

Define Define with metabolism Subcategorize Combine Clustering Category elements

① クリック

Document 1
[C: 1;Md: 0;P: 0] CAS: 58567...

Filter endpoint tree... 1 [target]

Structure

- Structure info
- Parameters
- Physical Chemical Properties
- Environmental Fate and Transport
- Ecotoxicological Information
- Human Health Hazards
 - Acute Toxicity
 - ADME
 - Bioaccumulation
 - Carcinogenicity
 - Developmental Toxicity / Teratogenicity
 - Genetic Toxicity
 - Immunotoxicity
 - Irritation / Corrosion
 - Neurotoxicity
 - Photoinduced toxicity
 - Repeated Dose Toxicity
 - Sensitisation
 - ToxCast
 - Toxicity to Reproduction
 - Toxicokinetics, Metabolism and Distribution
- Profiling
 - General Mechanistic
 - Protein binding by OASIS

Estrogen Receptor Binding
Hydrolysis half-life (Ka, pH 7)(Hydrowin)
Hydrolysis half-life (Ka, pH 8)(Hydrowin)
Hydrolysis half-life (Kb, pH 7)(Hydrowin)
Hydrolysis half-life (Kb, pH 8)(Hydrowin)
Hydrolysis half-life (pH 6.5-7.4)
Ionization at pH = 1
Ionization at pH = 4
Ionization at pH = 7.4
Ionization at pH = 9

Protein binding by OASIS

Protein binding by OASIS
Protein binding potency Cys (DPRA 13%)
Protein binding potency GSH
Protein binding potency Lys (DPRA 13%)
Toxic hazard classification by Cramer
Toxic hazard classification by Cramer (extended)
Ultimate biodeg
Uncouplers (MITOTOX)

② “Protein binding by OASIS”をクリック（グループ化に利用するプロファイラーを選択）

③ クリック（選択したプロファイラーにより、評価対象物質の類似物質の試験データを取得する（類似物質：選択したプロファイラーにより、同じグループに属する物質））

グループング方法（プロファイラ）

The OECD QSAR Toolbox for Grouping Chemicals into Categories
Developed by LMC, Bulgaria

カテゴリー定義

QSAR Toolbox 4.4 [Document 1]

QSAR TOOLBOX

Input Profiling Data **Category definition** Data Gap Filling Report

Define Define with metabolism Subcategorize Combine Clustering Category elements

Documents

Document 1
[C: 1;Md: 0;P: 0] CAS: 5856779

Grouping options (Protein binding by OASIS)

Target categories

Acylation

Acylation >> Direct acylation involving a leaving group

Acylation >> Direct acylation involving a leaving group >> (Thio)Acyl and (thio)carban

Options

Down Up Reset Options

All categories

(N/A)

Acylation >> (Tio)carbamylation of protein nucleophiles

Acylation >> (Tio)carbamylation of protein nucleophiles >> Isothiocyanates, Isocy

Acylation >> Acyl transfer via nucleophilic addition reaction

Acylation >> Acyl transfer via nucleophilic addition reaction >> Carbodiimides

Acylation >> Direct acylation involving a leaving group >> (Thio)Acetates

Acylation >> Direct acylation involving a leaving group >> Anhydrides (sulphur an

Acylation >> Direct acylation involving a leaving group >> Azlactones and unsatur

Acylation >> Direct acylation involving a leaving group >> Carbamates

Acylation >> Direct acylation involving a leaving group >> Diacyl peroxides, anhyd

Combine profiles

Invert result

AND OR Strict

Sort results

OK Cancel

① 評価対象物質が属するグループの確認(アシル化)

② クリック(類似物質の試験データの取得の実行)

カテゴリー定義

QSAR Toolbox 4.4 [Document 1]

Input Profiling Data **Category definition** Data Gap Filling Report

Define Define with metabolism Subcategorize Combine Clustering Category elements

Documents

- Document 1
 - # [C: 1;Md: 0;P: 0] CAS: 5856779
 - [C: 9;Md: 9;P: 0] Acylation<AND>Acylation
 - [C: 9;Md: 0;P: 0] Acylation<AND>Acylation

Filter endpoint tree... 1 [target] 2 3 4 5 6 7 8 9

Grouping results

9 chemical(s) found.

OK ① クリック(抽出物質数の確認)

Read data?

All endpoints Choose...

OK Cancel ② クリック(全てのエンドポイントの試験データを抽出)

Gather data

9 points added across 8 chemicals.

OK ③ クリック(試験データ数の確認)

Protein binding by OASIS

Options 1 Selected

- Select All Unselect All Invert About Option
- Estrogen Receptor Binding
- Hydrolysis half-life (Ka, pH 7)(Hydrowin)
- Hydrolysis half-life (Ka, pH 8)(Hydrowin)
- Hydrolysis half-life (Kb, pH 7)(Hydrowin)
- Hydrolysis half-life (Kb, pH 8)(Hydrowin)
- Hydrolysis half-life (pH 6.5-7.4)
- Ionization at pH = 1
- Ionization at pH = 4
- Ionization at pH = 7.4
- Ionization at pH = 9
- Protein binding by OASIS
- Protein binding by OECD
- Protein binding potency Cys (DPRA 13%)
- Protein binding potency GSH
- Protein binding potency Lys (DPRA 13%)
- Toxic hazard classification by Cramer
- Toxic hazard classification by Cramer (extended)
- Ultimate biodeg
- Uncouplers (MITOTOX)

類似物質の試験データの確認

QSAR Toolbox 4.4 [Document 1]

Input Profiling Data **Category definition** Data Gap Filling Report

Categorize Category consistency

Define Define with metabolism Subcategorize Combine Clustering Category elements

Documents

Document 1
[C: 1;Md: 0;P: 0] CAS: 5856779
[C: 9;Md: 9;P: 0] Acylation<AND>Acylation

Filter endpoint tree... 1 [target] 2 3 4 5 6 7 8 9

Structure

Structure info
Parameters
Physical Chemical Properties
Environmental Fate and Transport
Ecotoxicological Information
Human Health Hazards
Acute Toxicity
ADME
Bioaccumulation
Carcinogenicity
Developmental Toxicity / Teratogenicity
Genetic Toxicity
Immunotoxicity
Irritation / Corrosion
Neurotoxicity
Photoinduced toxicity
Repeated Dose Toxicity
Sensitisation
ToxCast
Toxicity to Reproduction
Toxicokinetics, Metabolism and Distribution
Profiling
General Mechanistic
Protein binding by OASIS

Protein binding by OASIS

Options 1 Selected

Select All Unselect All Invert About Options

Estrogen Receptor Binding
Hydrolysis half-life (Ka, pH 7)(Hydrowin)
Hydrolysis half-life (Ka, pH 8)(Hydrowin)
Hydrolysis half-life (Kb, pH 7)(Hydrowin)
Hydrolysis half-life (Kb, pH 8)(Hydrowin)
Hydrolysis half-life (pH 6.5-7.4)
Ionization at pH = 1
Ionization at pH = 4
Ionization at pH = 7.4
Ionization at pH = 9
Protein binding by OASIS
Protein binding by OECD
Protein binding potency Cys (DPRA 13%)
Protein binding potency GSH
Protein binding potency Lys (DPRA 13%)
Toxic hazard classification by Cramer
Toxic hazard classification by Cramer (extended)
Ultimate biodeg
Uncouplers (MITOTOX)

① クリック(ツリーを展開)

② ダブルクリック
(データの詳細の確認)

③ データの詳細が表示される

④ クリック

⑤ クリック

このエンドポイントは、8物質に対し9の試験データがある

試験データ (M:は実測の意味)

Datapoints	#	Value	Original value	Assay
Human Health Hazards;Sensitisation	1	M: 8.8 % (Skin sensitization EC3 (ratio))	8.8 % (Skin sensitization EC3(ratio))	LLNA

M: Strongly posit...:M: 0.23 % M: 1.8 % M: Strongly posit...:M: 2.7 % M: 8.8 % M: 2.7 % M: 2.3 %

データギャップ補完

QSAR Toolbox 4.4 [Document 1]

QSAR TOOLBOX

① クリック

データギャップ補完の方法

③ クリック(データギャップ補完の方法の指定: Read-across)

② クリック(データギャップ補完を行うエンドポイントの指定: LLNA EC3)

④ クリック(陽性/陰性の分類方法の選択)

Documents

Document 1

[C: 1; Md: 0; P: 0] CAS: 5856779

[C: 9; Md: 9; P: 0] Acylation<AND>Acylation

Filter endpoint tree...

Structure

Structure info

Parameters

Physical Chemical Properties

Environmental Fate and Transport

Ecotoxicological Information

Human Health Hazards

Acute Toxicity

ADME

Bioaccumulation

Carcinogenicity

Developmental Toxicity / Teratogenicity

Genetic Toxicity

Immunotoxicity

Irritation / Corrosion

Neurotoxicity

Photoinduced toxicity

Repeated Dose Toxicity

Sensitisation

Skin

in Vivo

LLNA

EC3

ToxCast

Toxicity to Reproduction

Toxicokinetics, Metabolism and Distribution

Profiling

General Mechanistic

Protein binding by OASIS

AW SWAOP

8/9

Strongly posit... M: 0.23 % M: 1.8 % M: Str

Acylation

Possible data inconsistency

Metadata

- Assay
 - LLNA (8 chemicals; 9 data)
- Endpoint
 - EC3 (8 chemicals; 9 data)
- Native scale/unit
 - Skin sensitisation I (Oasis) (2 chemicals; 2 data)
 - Skin sensitization EC3(ratio) (6 chemicals; 7 data)
- Organ
 - Skin (8 chemicals; 9 data)
- Type of method
 - in Vivo (8 chemicals; 9 data)

Select scale/unit to use

- Skin Sensitization (Danish EPA) [0 native data and 9 converted]
- Skin sensitisation I (Oasis) [2 native data and 7 converted]
- Skin sensitisation II (ECETOC) [0 native data and 9 converted]
- Skin sensitization EC3(ratio) [7 native data and 0 converted]
- Skin sensitization GHS (ordinal) [0 native data and 7 converted]

Converted data

2 from scale/unit Skin sensitisation I (Oasis)

7 from scale/unit Skin sensitization EC3(ratio)

Chemicals 8/8; Data 9/9

OK Cancel

データギャップ補完

QSAR Toolbox 4.4 [Document 1]

QSAR TOOLBOX

Input Profiling Data Category definition **Data Gap Filling** Report

Gap Filling Workflow

Trend analysis Read across (Q)SAR Standardized Automated

The OECD QSAR Toolbox for Grouping Chemicals

by LMC, Bulgaria

Confirm

Are you sure you want to accept this prediction?

Yes No

② クリック(承認の確認)

Repeated Dose Toxicity

- Sensitisation
 - Skin
 - in Vivo
 - LLNA
 - EC3 8/9 M: Strongly posit... M: 0.23 % M: 1.8 % M: Strongly posit... M: 2.7 % M: 8.8 % M: 2.7 % M: 2.3 %

- ToxCast
- Toxicity to Reproduction
- Toxicokinetics, Metabolism and Distribution
- Profiling
- General Mechanistic
 - Protein binding by OASIS Acylation

Data Gap Filling Settings

Only endpoint relevant

At this position:

QSARs 0
Automated workflows 0
Standardized workflows 0

In nodes below:

QSARs 0
Automated workflows 0
Standardized workflows 0

Descriptors

Prediction

Read-across prediction for EC3, based on 6 values
Predicted: Positive

Positive

Negative

log Kow

Active descriptor X log Kow

① クリック(予測結果の承認)

Accept prediction

● : 評価対象物質(予測)
● : 類似物質(実測; Read-acrossに使用)
● : 類似物質(実測; Read-acrossに未使用)
● : 選択されているプロット

データギャップ補完(結果)

QSAR Toolbox 4.4 [Document 1]

QSAR TOOLBOX

Input Profiling Data Category definition **Data Gap Filling** Report

Gap Filling Workflow

Trend analysis Read across (Q)SAR Standardized Automated

Documents

- Document 1
 - # [C: 1;Md: 0;P: 1] CAS: 5856779
 - [C: 9;Md: 9;P: 1] Acylation<AND>Acylat...
 - [C: 9;Md: 9;P: 1] Enter GF(RA)

Filter endpoint tree... 1 [target] 2 3 4 5 6 7 8 9

Structure

Structure info

Parameters

Physical Chemical Properties

Environmental Fate and Transport

Ecotoxicological Information

Human Health Hazards

- Acute Toxicity
- ADME
- Bioaccumulation
- Carcinogenicity
- Developmental Toxicity / Teratogenicity
- Genetic Toxicity
- Immunotoxicity
- Irritation / Corrosion
- Neurotoxicity
- Photoinduced toxicity
- Repeated Dose Toxicity
- Sensitisation
 - Skin
 - in Vivo
 - LLNA
 - EC3
- ToxCast
- Toxicity to Reproduction
- Toxicokinetics, Metabolism and Distribution

Profiling

- General Mechanistic
- Protein binding by OASIS

Acylation

9/10 R: Positive M: Strongly posit...M: 0.23 % M: 1.8 % M: Strongly posit...M: 2.7 % M: 8.8 % M: 2.7 % M: 2.3 %

Success

Prediction accepted successfully

OK

① クリック

予測データ
(R:はRead acrossの意味)

At this position:
Select a cell with a rigid (bold) path
Automated workflows 0
Standardized workflows 0

9

レポート作成

① クリック

② クリック(レポートを作成する予測結果を選択)

③ クリック(レポートの形式を選択: Data Matrix)

④ クリック(レポート作成の実行)

⑤ クリック

⑥ クリック(作成されたレポートを開く)

Generated report files

The following files were generated.
Select a file to open or save.

Data matrix

MS Excel file containing chemicals of the current Data Matrix along with their data for selected parameters, profiles and endpoint tree positions

Open Save as

Customize report content and appearance

Wizard pages

Data matrix

Options

Include 2D parameters
Select 2D parameters to report

Include profiles
Select profiles to report

Include experimental data
Select experimental data to report

Cancel Create report

9/10	Positive	Strongly posit...M: 0.23 %	M: 1.8 %	M: Strongly posit...M: 2.7 %	M: 8.8 %	M: 2.7 %	M: 2.3 %

レポート作成(結果)

Excel window: Data matrix_21_12_20_14_02_43_(1).xlsx - Excel

File Home Insert Drawing Page Layout Formulas Data References Send To Back Styles Layout Cell Editing Tools

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V			
1			Chemical #1		Chemical #2		Chemical #3		Chemical #4		Chemical #5		Chemical #6												
2	Substance identity																								
3	Structure																								
4	CAS number		5856-77-9		3282-30-2		98-88-4		764-85-2		625-36-5		36727-29-4												
5	Chemical name		2,2-Dimethylbutyryl chloride		pivaloyl chloride		Benzoyl chloride		Nonanoyl chloride		3-chloropropanoyl chloride		O=C(CCC(C)(C)C)Cl												
6	Other identifier																								
7	SMILES		CCC(C)C(C)Cl=O		CC(C)C(C)C(C)Cl=O		ClC(=O)c1ccccc1		CCCCCCCCC(C)Cl=O		ClCCC(C)Cl=O		CC(C)C(C)Cl=O		CCC(C)C(C)Cl=O										
8																									
9	Profilers																								
10	General Mechanistic																								
11	Protein binding by OASIS		Acylation >> Direct acylation involving a leaving group Acylation >> Direct acylation involving a leaving group >> (Thio)Acyl and																						
12																									
13	Measured and predicted data																								
14	Human Health Hazards#Sensitisation																								
	sublevel	endpoint	value	unit	species, duration, test type, type of method, assay, strain, test guideline, year, reference, database	value	unit	species, duration, test type, type of method, assay, strain, test guideline, year, reference, database	value	unit	species, duration, test type, type of method, assay, strain, test guideline, year, reference, database	value	unit	species, duration, test type, type of method, assay, strain, test guideline, year, reference, database	value	unit	species, duration, test type, type of method, assay, strain, test guideline, year, reference, database	value	unit	species, duration, test type, type of method, assay, strain, test guideline, year, reference, database	value	unit			
15	Sensitisation	EC3			Test organisms (species): mouse Endpoint: EC3 Type of method: in Vivo Assay: LLNA Year: 2007 Reference source: Regulatory Toxicology and Pharmacology, 48: 225-239 Author: Patlewicz G, Dimitrov SD, Low LK, Kern PS, Dimitrova GD, Comber ML, Ashby AD, Phillips	0.23	%	Test organisms (species): mouse Endpoint: EC3 Type of method: in Vivo Assay: LLNA Author: P&G			Test organisms (species): mouse Endpoint: EC3 Type of method: in Vivo Assay: LLNA Year: 2005 Reference source: Dermatitis, 16 (4): 1-46 Author: Gerberick, G.F., Ryan, C.A., Kern, P.S., Schlatter, H., Dearman, R.J., Kimber, I., Patlewicz, C.V., Basketter, D.A.	1.8	%	Test organisms (species): mouse Endpoint: EC3 Type of method: in Vivo Assay: LLNA Year: 2007 Reference source: Regulatory Toxicology and Pharmacology, 48: 225-239 Author: Patlewicz G, Dimitrov SD, Low LK, Kern PS, Dimitrova GD, Comber ML, Ashby AD, Phillips			Test organisms (species): mouse Endpoint: EC3 Type of method: in Vivo Assay: LLNA Year: 2005 Reference source: Dermatitis, 16 (4): 1-46 Author: Gerberick, G.F., Ryan, C.A., Kern, P.S., Schlatter, H., Dearman, R.J., Kimber, I., Patlewicz, C.V., Basketter, D.A.	2.7	%	Test organisms (species): mouse Endpoint: EC3 Type of method: in Vivo Assay: LLNA Year: 2007 Reference source: Regulatory Toxicology and Pharmacology, 48: 225-239 Author: Patlewicz G, Dimitrov SD, Low LK, Kern PS, Dimitrova GD, Comber ML, Ashby AD, Phillips			Test organisms (species): mouse Endpoint: EC3 Type of method: in Vivo Assay: LLNA Year: 2005 Reference source: Dermatitis, 16 (4): 1-46 Author: Gerberick, G.F., Ryan, C.A., Kern, P.S., Schlatter, H., Dearman, R.J., Kimber, I., Patlewicz, C.V., Basketter, D.A.	8.8	%

Sheet1 | 表示設定 | 100%

ユーザーマニュアル(和訳)

<https://www.nite.go.jp/chem/qsar/toolbox.html#section2>

QSAR Toolboxマニュアル類

<NITEの仮訳>

OECDのQSAR Toolbox ページに公開されている一部のマニュアルをNITEで仮訳いたしました。ぜひご活用ください。

• [OECD QSAR Toolbox v.4の操作マニュアル](#)

(QSAR Toolbox v4.1に基づいたマニュアル)

原文 [Application manual of OECD QSAR Toolbox v.4](#) 【PDF:外部サイト】

• [OECD QSAR Toolboxユーザーマニュアルスタートガイド](#)

(QSAR Toolbox v3.0に基づいた使い方マニュアル)

原文 [QSAR Toolbox Manual for getting started](#) 【PDF:外部サイト】

• OECD QSAR Toolbox4.4のインストールマニュアル (現在準備中)

原文 [Toolbox 4.4 Installation Manual](#) 【PDF:外部サイト】

<NITEのマニュアル>

QSAR Toolboxの使用方法について、NITE独自でマニュアルを作成しております。こちらをご覧ください。

• [OECD QSAR Toolbox version 3.2を用いた公開データの活用方法に関するマニュアル](#)

OECD QSAR Toolbox v.4.1

のアプリケーション マニュアル

(F1 help)



本翻訳物は、OECD より公開された QSAR_Toolbox_TB41_August2017, (<http://www.oecd.org/chemicalsafety/risk-assessment/oecd-qsar-toolbox.htm>, バージョン 4.1) を NITE が仮訳したものです。正確には原文をあたってください。原文と本翻訳に相違がある場合は、原文を優先してください。