



QSAR Toolboxの概要・操作説明

(独)製品評価技術基盤機構 化学物質管理センター

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QSAR Toolboxの概要

QSAR Toolboxとは？

- OECDがECHA（欧州化学品庁）と共同で開発を行っているカテゴリーアプローチを支援するためのソフトウェア。
- 物理化学的性状、分解性、蓄積性、生態毒性、反復投与毒性などの様々なエンドポイント*に関するデータベースと化学物質をグループ分けするために必要な機能などが備わっている。
- 2008年3月にver.1.0が公開され、現行の最新版であるver.4.6 が2023年5月に公開。
- フリーソフトウェア
（OECDのWebsite上にて公開。ユーザー登録が必要。）
- 公開サイト：<https://qsartoolbox.org/>

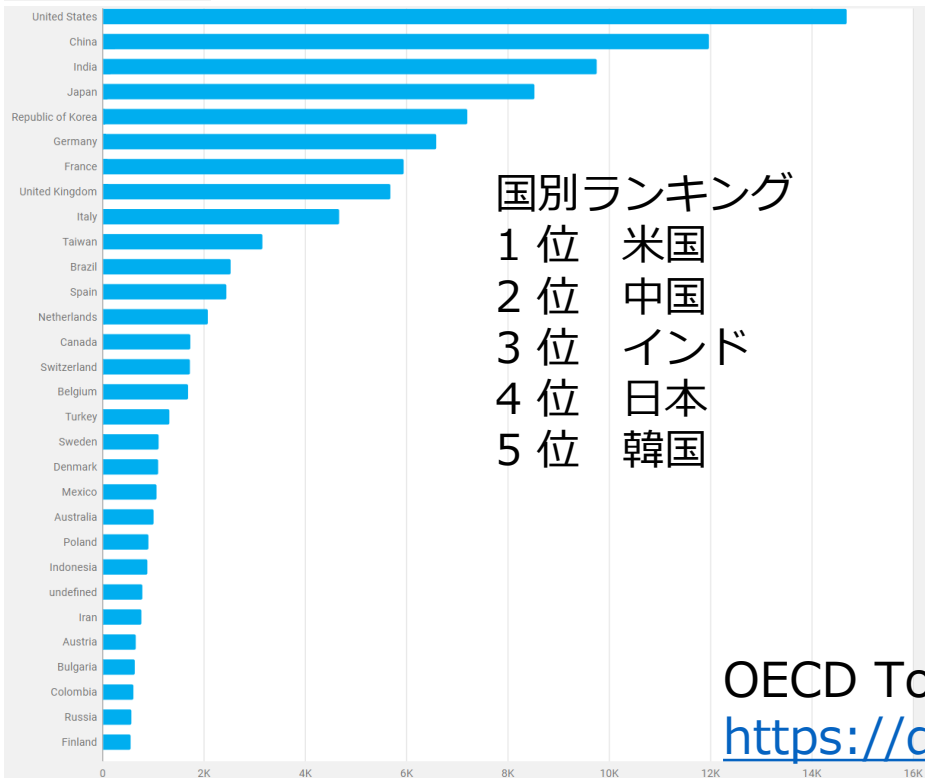
QSAR Toolboxのユーザは？

ダウンロード数: 57,300

Top 30 Countries

Top Country Statistics

■ Downloads



国別ランキング

1 位 米国

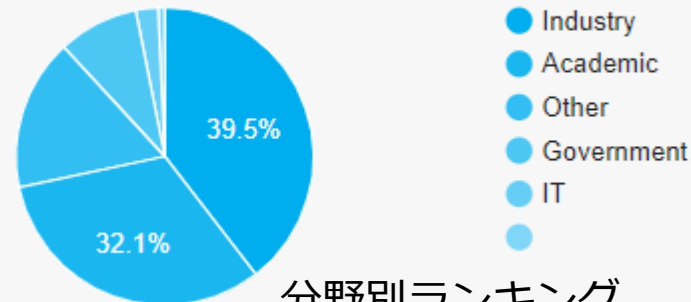
2 位 中国

3 位 インド

4 位 日本

5 位 韓国

Overall Downloads by Type



分野別ランキング

1 位 産業

2 位 学術

3 位 そのほか

4 位 行政

5 位 IT

OECD Toolbox HPより (2024/7/16 確認)

<https://qsartoolbox.org/download/statistics/>

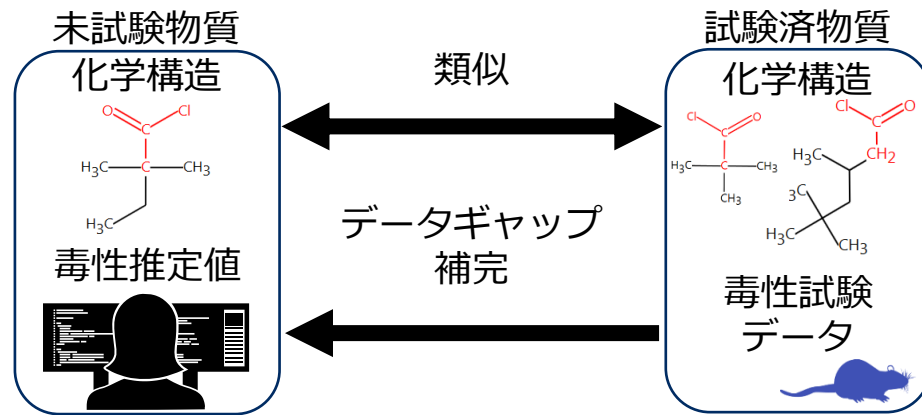
QSAR Toolboxの開発の経緯

- 2005年頃の開発当初は、各種Q S A Rモデルを集めたライブラリの構築を計画。
- 開発メンバー間における議論において、QSARモデルの予測結果のみでは行政利用における判断根拠としては不十分であるとの認識が高まる。
- 最終的には、カテゴリー作成を支援する機能及びカテゴリーアプローチによるデータギャップ補完を支援する機能と共に、カテゴリー化の根拠を第三者に明確に示す機能が主体のシステムとして公開。

“for Grouping chemicals into categories”

QSAR Toolboxの機能概要

- グルーピングを行うための、毒性発現の原因となる部分構造を認識する機能（プロファイラー）と、各国から提供された各種エンドポイントの実測試験データベースが実装されている。
- プロファイラーにより、毒性発現の原因となる共通の部分構造を有する、カテゴリーの候補物質群を効率よく探すことができる。また、実測試験データベースから、これら物質群の実測試験データを収集できる。
- 収集した実測試験データを基に毒性発現の傾向を解析することにより、カテゴリーを構築し、未試験物質のデータを予測（データギャップ補完）することができる。



QSAR Toolboxでできること

実測試験データベース

- ・物理化学的性状、環境中運命と移送、生態毒性情報、人健康有害性分野における62データベースに、10万物質、300万件の実測データを収載
- ・日本からは化審法データ（分解性、蓄積性、生態毒性、人健康有害性）、光感作性データを提供

プロファイラー

- ・70 プロファイラー
- ・日本からはHESSカテゴリーを提供

QSAR

- ・254 QSARモデル
- ・日本からはKATEを提供

その他

- ・11インベントリー(約318,000物質)
- ・代謝DBとシミュレーター



実測試験データの検索



代謝産物の探索やシミュレート



QSAR予測の実行



類似物質の検索とカテゴリ構築



類似物質データからデータギャップ補完



データマトリックス・レポートの作成

QSAR Toolbox 4.6の操作説明

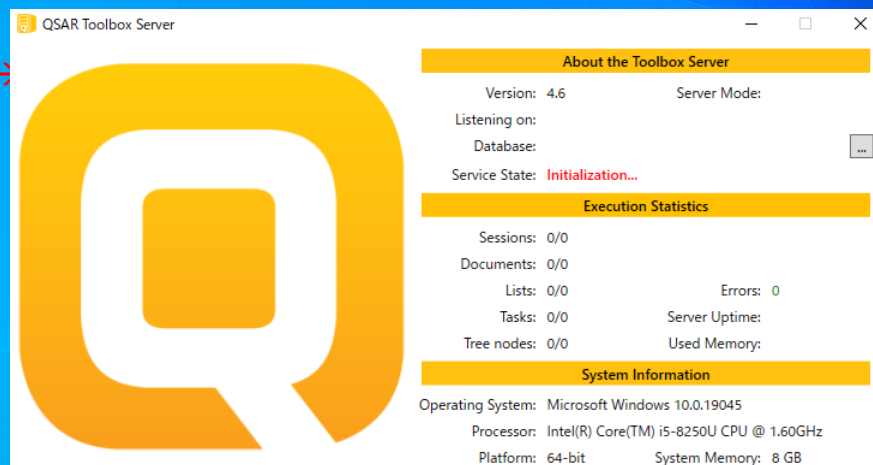
立ち上げ（１）

←①ダブルクリック

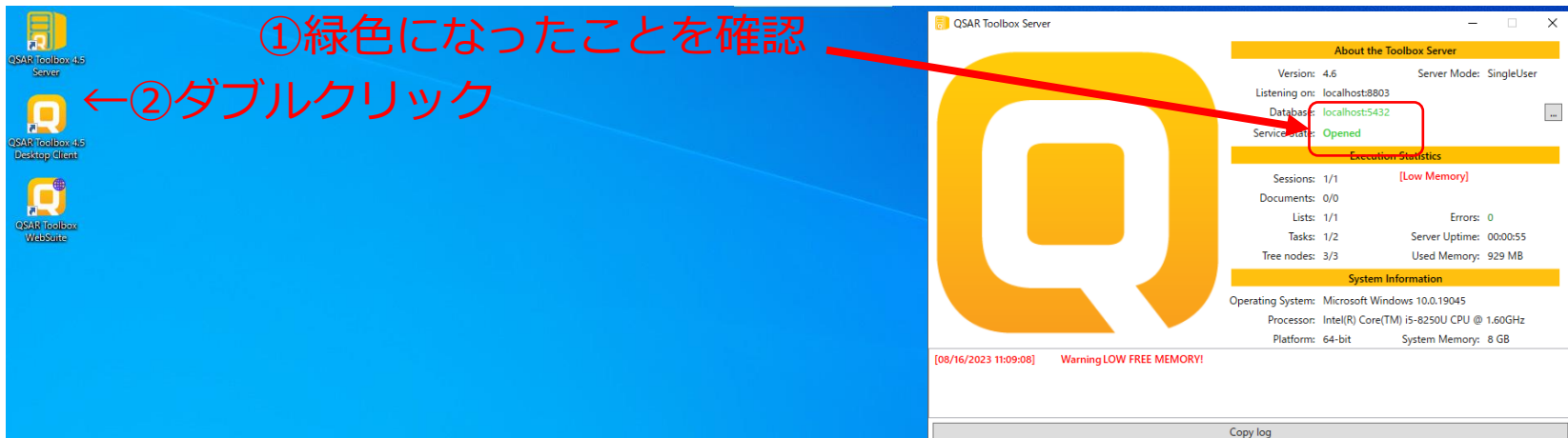
Q SAR Toolbox 4.5
Desktop client

Q SAR Toolbox
WebSuite

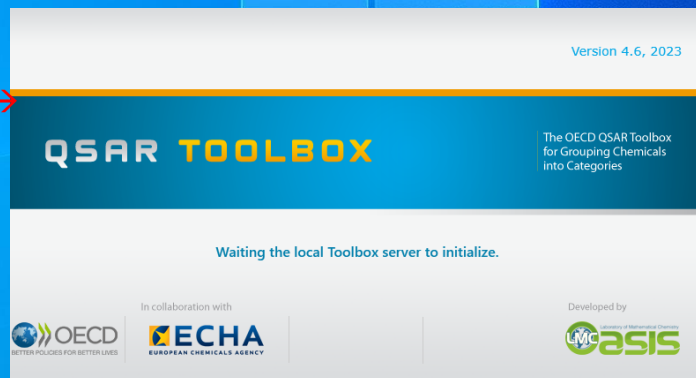
②表示される→



立ち上げ（２）



③ 表示される→
(数分待つ)



立ち上げ (3)

QSAR Toolbox Version 4.6, 2023

Start with:

-  **Simplified User Interface**
New QSAR Toolbox interface developed to perform basic tasks in a simplified environment
-  **Classical User Interface**
The classical QSAR Toolbox interface with full functionalities

☐ Remember the choice

After you select one of the interfaces from above, you can still switch between the two options later within the Toolbox

QSAR Toolbox Server

About the Toolbox Server

Version: 4.6 Server Mode: SingleUser
Listening on: localhost:8803
Database: localhost:5432
Service State: **Opened**

Execution Statistics

Sessions: 1/1 **[Low Memory]**
Documents: 0/0
Lists: 1/1 Errors: 0
Tasks: 1/2 Server Uptime: 00:00:55
Tree nodes: 3/3 Used Memory: 929 MB

System Information

Operating System: Microsoft Windows 10.0.19045
Processor: Intel(R) Core(TM) i5-8250U CPU @ 1.60GHz
Platform: 64-bit System Memory: 8 GB

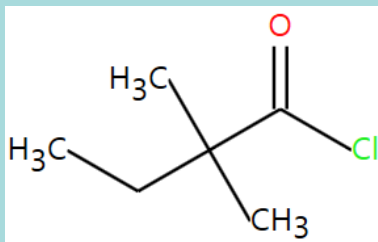
Warning LOW FREE MEMORY!

Copy log

クリック

リードアクロスの操作例

評価対象物質



対象エンドポイント
皮膚感作性

CAS RN: 5856-77-9

QSAR Toolboxのワークフロー

Input

①評価対象物質の入力

Profiling

②カテゴリー属性等の抽出

Data

③DBから実測試験データの抽出

Category
Definition

④類似物質データの抽出

Data Gap
Filling

⑤データギャップ補完

Report

⑥レポートの作成

QSAR Toolboxの基本画面構成

ワークフローに対応した6つのモジュール

Input

Profiling

Data

Category Definition

Data Gap Filling

Report

QSAR Toolbox 4.6 [Document 1]

The screenshot displays the QSAR Toolbox 4.6 interface. The top navigation bar includes six modules: Input, Profiling, Data, Category Definition, Data Gap Filling, and Report. The main workspace is divided into several panels:

- Documents:** Shows the current document and its contents.
- Structure:** Displays the chemical structure of the selected compound.
- Structure info:** Provides details about the structure, including EC Number, CAS Number, and SMILES.
- Parameters:** Lists various parameters used in the QSAR models, such as Acute Toxicity, Carcinogenicity, and Developmental Toxicity.
- Table of Contents:** A sidebar on the right showing the structure of the report, including sections like Introduction, Welcome, User interface, Workflow, and Input.

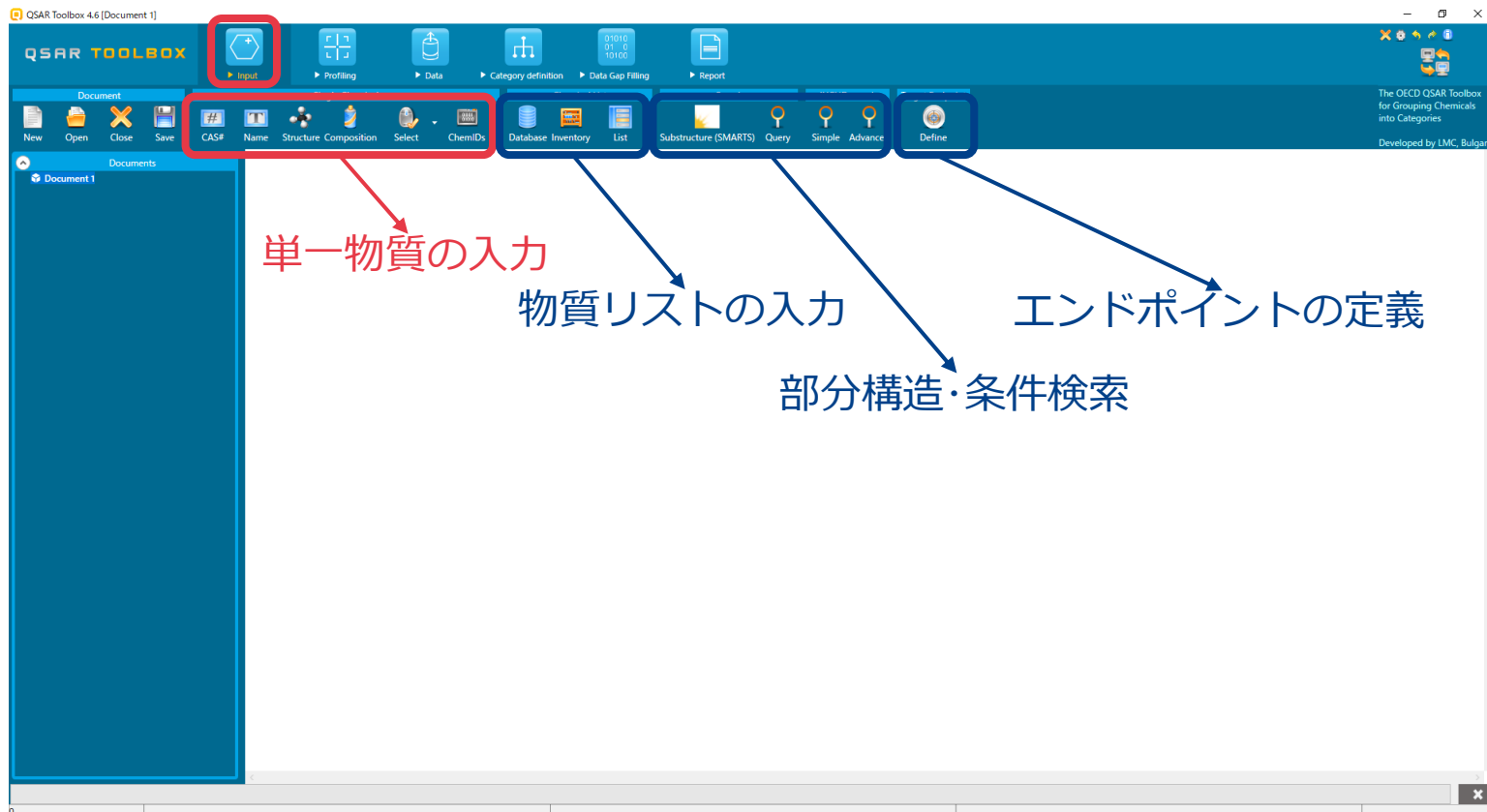
Red annotations highlight key features:

- 評価対象構造 (Evaluation Target Structure):** Points to the chemical structure input field.
- 類似物質 (Similar Substances):** Points to the list of similar chemical structures.
- データマトリクス (Data Matrix):** Points to the table displaying the results of the QSAR models.
- F1 ボタンでヘルプ画面を見ることができます。 (You can see the help screen with the F1 button.):** A text box indicating the function of the F1 key.
- エンドポイントツリー (Endpoint Tree):** Points to the tree view of the endpoints used in the models.

EC Number	2274785	2219216	2603308	2027108	2121312	2108904	2531684	
EC Number	2274785	2219216	2603308	2027108	2121312	2108904	2531684	
CAS Number	5856-77-9	816431-72-8	3282-30-2	56677-60-2	98-88-4	65055-17-6	764-85-2	36727-29-4
CAS SMILES relation	High	High	High	High	Low	High	High	High
Chemical name(s)	2,2-Dimethyl-butyl c...	4-((2-methoxyphenyl...	2,2-Dimethylpropano...	Carbonochloric acid...	Benzoil chloride	3-Chloro-4-fluoroben...	Nonanoyl chloride	3-chloropropanoyl chl...
Identify	Sources:7	Sources:12	Sources:12	Sources:22	Sources:12	Sources:10	Sources:13	Sources:13
Molecular formula	C9H17ClO	C15H12ClNO5S	C5H9ClO	C7H9ClO2	C7H9ClO2	C9H17ClO	C3H4ClO2	C9H17ClO
Defined substance type	Mono constituent	Mono constituent	Mono constituent	Mono constituent	Mono constituent	Mono constituent	Mono constituent	Mono constituent
SMILES	CCCC(C)(C)C(=O)O	COc1ccc(C(=O)O)ns1	CC(C)(C)C(=O)O	CCCCCCCCCCCCCCCC(C(=O)O)c1ccc1	FC1ccc(C(=O)C(C)O)cc1	CCCCCCCC(C)C(=O)O	CCCCCCCC(C)C(=O)O	CC(C)(C)O=C(C)C(C)C

Inputモジュール 画面構成

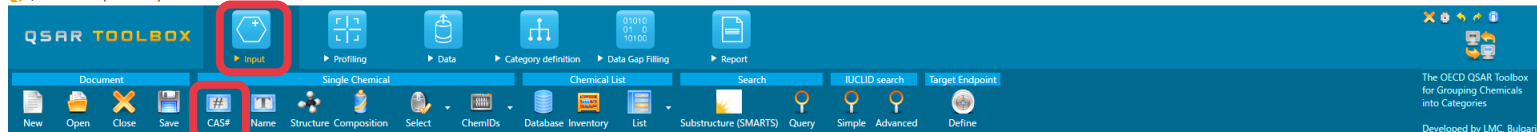
Input: 評価対象物質の入力



評価対象物質の入力

① Inputモジュールクリック

QSAR Toolbox 4.6 [Document 1]



② クリック (CAS番号による入力を選択)

③ 入力
5856-77-9

Search by CAS #

④ クリック

5856-77-9 Search

OK

Cancel

⑤ クリック

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	
	Identity	Sources:7	
	Name	2,2-Dimethyl-butyl chloride;2,2-dimethylbutyryl chloride	
	Sources	DSSTOX ECHA PR FINFCS	

評価対象物質の入力(結果)

QSAR Toolbox 4.6 [Document 1]

QSAR TOOLBOX

Input Profiling Data Category definitions Data Gap Filling Report

Document Single Chemical Chemical List Search IUCLID search Target Endpoint

New Open Close Save CAS# Name Structure Composition Select ChemIDs Database Inventory List Substructure (SMARTS) Query Simple Advanced Define

Documents

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

Filter endpoint tree... 1 [target]

Structure

Structure Info
Parameters
Physical Chemical Properties
Environmental Fate and Transport
Ecotoxicological Information
Human Health Hazards

① クリック
(入力した物質の構造情報の確認)

Profilingモジュール 画面構成

Profiling: カテゴリー属性等の抽出

QSAR Toolbox 4.6 [Document 1]

プロファイラー

評価対象構造

プロファイリング結果の詳細説明画面

各カテゴリーの説明タブ

カテゴリーリスト

構造条件

毒性発現のメカニズムに関する情報

評価対象物質

代謝シミュレーター

プロファイラーに対する属性（該当するカテゴリー）

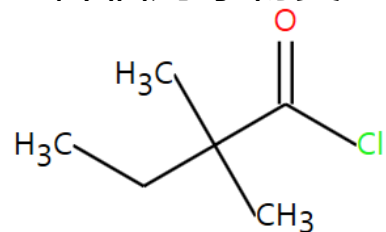
プロファイラーによる該当するカテゴリーの特定

皮膚感作性のための蛋白結合アラートプロファイラー

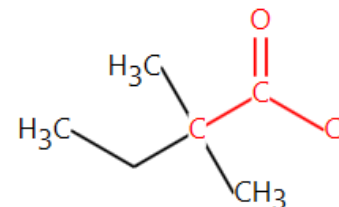
評価対象物質

プロファイラ

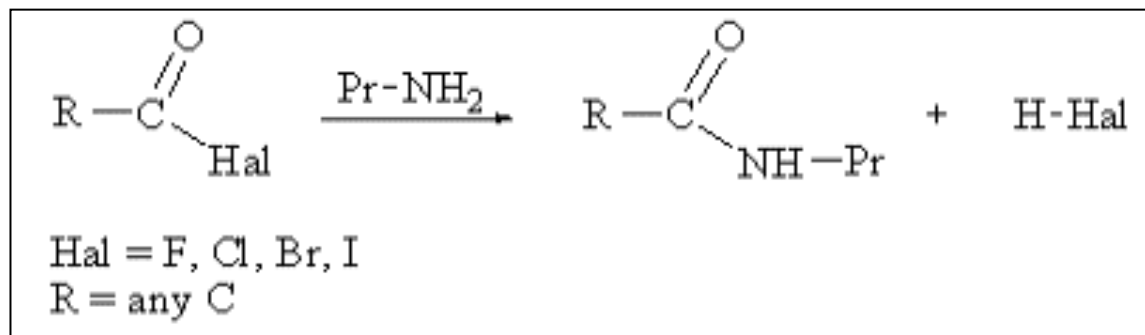
プロファイリング結果



皮膚感作性のための
蛋白質結合ア
ラート



>> (Thio)Acyl and
(thio)carbamoyl halides and
cyanides



毒性発現の原因となる部分構造を特定

プロファイリング

① Profiling モジュールクリック

QSAR Toolbox 4.6 [Document 1]

④ “Endpoint Specific”の“Protein binding alerts for skin sensitization 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）

② クリック（人健康関連エンドポイントのツリーを開く）

③ セル選択（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）

緑 ■ : 評価対象エンドポイントのためのデータや知見により開発されたプロファイラ
 オレンジ ■ : 評価対象エンドポイントに何らかの形で関係性があるデータや知見により開発されたプロファイラ
 強調なし □ : 評価対象エンドポイントと開発に用いられたデータや知見の間に関連性があるというエビデンスがないプロファイラ

代謝情報・シミュレータ

プロファイリング

① 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）

QSAR Toolbox 4.6 [Document 1]

Input Profiling Data Category definition Data Gap Filling Report

Documents

Document 1
[C: 1Mid: 0P: 0] CAS: 5856779

Filter endpoint tree... 1 [target]

Structure

Structure Info
Parameters
Physical Chemical Properties
Environmental Fate and Transport
Ecotoxicological Information
Human Health Hazards
Acute Toxicity
ADME
Carcinogenicity
Developmental Toxicity / Teratogenicity
Genetic Toxicity
Immunotoxicity
Irritation / Corrosion
Neurotoxicity
Photoinduced toxicity
Repeated Dose Toxicity
Sensitisation
Toxicokinetics, Metabolism and Distribution

Profiling

Endpoint Specific
Protein binding alerts for skin sensitization... Acylation

Metabolism/Transformations

Options
Select All Unselect All Invert

Autoxidation simulator
Autoxidation simulator (alkaline medium)
Desiccation simulator
Hydrolysis simulator (acidic)
Hydrolysis simulator (basic)
Hydrolysis simulator (neutral)
in vivo Rat metabolism simulator
Microbial metabolism simulator
Rat liver S9 metabolism simulator
Skin metabolism simulator
Tautomerism

② 選択したプロファイラによるプロファイリングの結果

プロファイリング結果の詳細の確認

QSAR Toolbox 4.6 [Document 1]

QSAR TOOLBOX

Input Profiling Data Category definition Data Gap Filling Report

Profiling Custom profile Apply View New Delete

Document 1 Documents
[C: 1M: 0P: 0] CAS: 5856779

Filter endpoint tree... [target]

Structure

Structure info
Parameters
Physical Chemical Properties
Environmental Fate and Transport
Ecotoxicological Information
Human Health Hazards
Acute Toxicity
ADME
Carcinogenicity
Developmental Toxicity / Teratogenicity
Genetic Toxicity
Immunotoxicity
Irritation / Corrosion
Neurotoxicity
Photoinduced Toxicity
Repeated Dose Toxicity
Sensitisation
Toxicant
Toxicity to Reproduction
Toxicokinetics, Metabolism and Distribution

Profiling
Endpoint Specific
Protein binding alerts for skin sensitiz...

Protein binding alerts for skin sensitization by OASIS

Options
Select All Unselect All Invert About Option
in vitro mutagenicity (Ames test) alerts by ISS
in vivo mutagenicity (Micronucleus) alerts by ISS
Keratinocyte gene expression
OncoLogic Primary Classification
Protein binding alerts for Chromosomal aberrations
Protein binding alerts for skin sensitization by OASIS
Protein binding alerts for skin sensitization by OASIS
Protein Binding Potency h-CLAT
Respiratory sensitisation
Retinoic Acid Receptor Binding
ITER Expert System - USEPA

Metabolism/Transformations
Options
Select All Unselect All Invert
Autoxidation simulator
Autoxidation simulator (alkaline medium)
Dissociation simulator
Hydrolysis simulator (acidic)
Hydrolysis simulator (basic)
Hydrolysis simulator (neutral)
in vivo Rat metabolism simulator
Microbial metabolism simulator
Rat liver S9 metabolism simulator
Skin metabolism simulator
Tautomerism

Explainer

Acylation
Direct acylation involving a leaving group
(Thio)Acyl and (thio)carbamoyl halides and cyanides

② クリック

Details

③ クリック

① ダブルクリック

④ Literatureタブ選択

Explanation for Protein binding alerts for skin sensitization by OASIS -> Acylation -> Direct acylation involving a leaving group -> ...

Categories

Filter:

binding alerts for skin sensitization by OASIS
(Thio)carbamoylation of protein in isocyanates, isothiocyanates
Acyl transfer via nucleophilic addition
Carbodiimides
Direct acylation involving a leaving group
(Thio)Acetates
(Thio)Acyl and (thio)carbamoyl halides and cyanides
Anhydrides (sulphur analogues)
Azlactones and unsaturated lactones
Carbamates
Diacyl peroxides, anhydrides (N-Acyl)oxysuccinimides
N-Carbonyl heterocyclic amines
N-Halocarbonyl amides

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:

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

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

⑤ アシルハライド基が蛋白結合を誘発するグループに属することを確認

Dataモジュール 画面構成

Data: DBから実測試験データの抽出

データベース

選択したデータベースから
実測試験データを抽出

データ詳細確認画面

Datapoints	#	Value	Original value	Assigned SMILES	Database	Endpoint	Experimental condition	Qualifier	Reference source	Substance/Test material
Physical Chemical Properties, Boiling point	1	Mt. 132 °C (Temperature)	132 °C (Temperature)	False	Phys-chem EPISUITE	Boiling point	760+ mm Hg	No qualifier	SRC	Equal

試験データの取得

① Dataモジュールクリック

QSAR Toolbox 4.6 [Document 1]

QSAR TOOLBOX

Input Profiling Data Category definition Data Gap Filling Report

Data Import Export Delete

Gather Import IUCLID6 IUCLID6 Database Inventory

Documents

Document 1
[C: tMdl: QP: O] CAS: 5856779

Databases

Options Select All Unselect All Invert About Options

3 Selected

REACH Skin sensitisation database (norm) ☒
 Receptor Mediated Effects ☐
 Rep Dose Tox Fraunhofer ITEM ☐
 Repeated Dose Toxicity HESS ☐
 Rodent Inhalation Toxicity Database ☐
 Skin Irritation ☐
 Skin Sensitization ☒
 Skin Sensitization ECETOC ☒
 Skin Sensitization OASIS (normalized) ☒
 ToxCastDB ☐
 Toxicity data on pharmaceuticals (US F) ☐

Inventories

Options Select All Unselect All Invert

0 Selected

IIC ☐
 anada DSL ☐
 OSING ☐
 SSTOX ☐
 OIA PR ☐
 nIrc ☐
 PVC OECD ☐
 IETI Japan ☐
 EACB ECB ☐
 SCA ☐
 HPV Challenge Program ☐

Filter endpoint tree...

Structure

Structure Info ☐
 Parameters ☐
 Physical Chemical Properties ☐
 Environmental Fate and Transport ☐
 Ecotoxicological Information ☐
 Human Health Hazards ☐
 Acute Toxicity ☐
 ADME ☐
 Carcinogenicity ☐
 Developmental Toxicity / Teratogenicity ☐
 Genetic Toxicity ☐
 Immunotoxicity ☐
 Irritation / Corrosion ☐
 Neurotoxicity ☐
 Photodynamic toxicity ☐
 Repeated Dose Toxicity ☐
 Sensitisation ☐
 ToxCast ☐
 Toxicity to Reproduction ☐
 Toxicokinetics, Metabolism and Distribution ☐
 Profiling ☐
 Endpoint Specific ☐
 Protein binding alerts for skin sensitiz... ☐

AW SW ACP ☒

Acylation

Chemical structure: CC(=O)OCC

緑■：評価対象エンドポイントのデータが掲載されているDB
 強調なし□：評価対象エンドポイントのデータが掲載されていないDB

② セル選択（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 “Human Health Hazards”の“Skin Sensitization”、“Skin Sensitization ECETOC”、“Skin Sensitization OASIS (normalized)”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）

インベントリ
 （試験データはなし）

試験データの取得

① 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）

The screenshot shows the QSAR Toolbox 4.6 interface. The 'Data' menu is highlighted in the top toolbar. The 'Databases' panel on the left shows a list of databases, with 'REACH Skin sensitisation database (normal)' selected. The 'Inventories' panel shows a list of inventories, with 'ABC' selected. The 'Filter endpoint tree...' panel on the right shows a list of endpoints, with 'Acylation' selected. The 'Read data?' dialog box is open, showing the 'All endpoints' radio button selected. The 'No experimental data are available on the chemicals of interest.' message box is also shown, with the 'OK' button highlighted.

② クリック（全エンドポイントのデータを抽出）

③ 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

Category Definitionモジュール 画面構成

Category Definition: 類似物質データの抽出

(類似物質: 選択したプロファイラーにより、同じカテゴリーに属する物質)

QSAR Toolbox 4.6 [Document 1]

類似物質

プロファイラー

選択したプロファイラーに対し、
評価対象物質と同じカテゴリーに
属する類似物質データが抽出される。

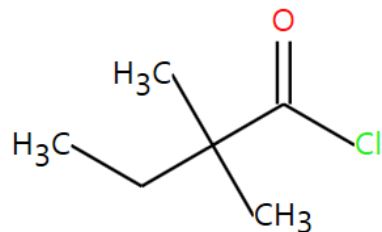
M : 実測
R : Read-across
T : Trend analysis
Q : QSAR

Structure	EC Number:2274785	EC Number:22719216	EC Number:2603308	EC Number:2027108	EC Number:2121312	EC Number:2108904	EC Number:2531684	EC
<chem>CC(C)C(C)C=O</chem>	816431-72-8	3282-30-2	56677-60-2	98-88-4	65055-17-6	764-85-2	625-36-5	11;
High	High	High	Low	Low	High	High	High	Hi
2,2-Dimethyl-butyl c...	4-[[[2-methoxyphenyl]...	2,2-Dimethylpropano...	Carbonochloridic acid...	Benzoyl chloride	3-Chloro-4-fluoroben...	Nonanoyl chloride	3-chloropropanoyl ch...	3,3,5-trimethylhexano...
Sources:7	Sources:12	Sources:8	Sources:22	Sources:10	Sources:12	Sources:10	Sources:12	So
C6H11ClO	C15H12ClNO5S	C5H9ClO	C15H29ClO2	C7H5ClO	C7H3Cl2FO	C9H17ClO	C3H4Cl2O	C9H17ClO
Mono constituent	Mono constituent	Mono constituent	Mono constituent	Mono constituent	Mono constituent	Mono constituent	Mono constituent	Mono constituent
CCCC(C)C(C)C=O	CCOC1CCCC1C(=O)N...	CC(C)C(C)C=O	CCCCCCCCCCCCCCCC...	CC(C=O)C1CCCC1	Fe1CCCC1C(C)C(C)...	CCCCCCCC(C)C=O	CCCC(C)C=O	CC(C)C(C)C=O
Parameters	Parameters	Parameters	Parameters	Parameters	Parameters	Parameters	Parameters	Parameters
Physical Chemical Properties	Physical Chemical Properties	Physical Chemical Properties	Physical Chemical Properties	Physical Chemical Properties	Physical Chemical Properties	Physical Chemical Properties	Physical Chemical Properties	Physical Chemical Properties
Environmental Fate and Transport	Environmental Fate and Transport	Environmental Fate and Transport	Environmental Fate and Transport	Environmental Fate and Transport	Environmental Fate and Transport	Environmental Fate and Transport	Environmental Fate and Transport	Environmental Fate and Transport
Ecotoxicological Information	Ecotoxicological Information	Ecotoxicological Information	Ecotoxicological Information	Ecotoxicological Information	Ecotoxicological Information	Ecotoxicological Information	Ecotoxicological Information	Ecotoxicological Information
Human Health Hazards	Human Health Hazards	Human Health Hazards	Human Health Hazards	Human Health Hazards	Human Health Hazards	Human Health Hazards	Human Health Hazards	Human Health Hazards
Acute Toxicity	Acute Toxicity	Acute Toxicity	Acute Toxicity	Acute Toxicity	Acute Toxicity	Acute Toxicity	Acute Toxicity	Acute Toxicity
ADME	ADME	ADME	ADME	ADME	ADME	ADME	ADME	ADME
Carcinogenicity	Carcinogenicity	Carcinogenicity	Carcinogenicity	Carcinogenicity	Carcinogenicity	Carcinogenicity	Carcinogenicity	Carcinogenicity
Developmental Toxicity / Teratogenicity	Developmental Toxicity / Teratogenicity	Developmental Toxicity / Teratogenicity	Developmental Toxicity / Teratogenicity	Developmental Toxicity / Teratogenicity	Developmental Toxicity / Teratogenicity	Developmental Toxicity / Teratogenicity	Developmental Toxicity / Teratogenicity	Developmental Toxicity / Teratogenicity
Genetic Toxicity	Genetic Toxicity	Genetic Toxicity	Genetic Toxicity	Genetic Toxicity	Genetic Toxicity	Genetic Toxicity	Genetic Toxicity	Genetic Toxicity
Immunotoxicity	Immunotoxicity	Immunotoxicity	Immunotoxicity	Immunotoxicity	Immunotoxicity	Immunotoxicity	Immunotoxicity	Immunotoxicity
Irritation / Corrosion	Irritation / Corrosion	Irritation / Corrosion	Irritation / Corrosion	Irritation / Corrosion	Irritation / Corrosion	Irritation / Corrosion	Irritation / Corrosion	Irritation / Corrosion
Neurotoxicity	Neurotoxicity	Neurotoxicity	Neurotoxicity	Neurotoxicity	Neurotoxicity	Neurotoxicity	Neurotoxicity	Neurotoxicity
Photoinduced toxicity	Photoinduced toxicity	Photoinduced toxicity	Photoinduced toxicity	Photoinduced toxicity	Photoinduced toxicity	Photoinduced toxicity	Photoinduced toxicity	Photoinduced toxicity
Repeated Dose Toxicity	Repeated Dose Toxicity	Repeated Dose Toxicity	Repeated Dose Toxicity	Repeated Dose Toxicity	Repeated Dose Toxicity	Repeated Dose Toxicity	Repeated Dose Toxicity	Repeated Dose Toxicity
Sensitisation	Sensitisation	Sensitisation	Sensitisation	Sensitisation	Sensitisation	Sensitisation	Sensitisation	Sensitisation
Skin	Skin	Skin	Skin	Skin	Skin	Skin	Skin	Skin
In Vivo	In Vivo	In Vivo	In Vivo	In Vivo	In Vivo	In Vivo	In Vivo	In Vivo
LLNA	LLNA	LLNA	LLNA	LLNA	LLNA	LLNA	LLNA	LLNA
EC3	EC3	EC3	EC3	EC3	EC3	EC3	EC3	EC3
11/16	M: Negative	M: Strongly positive	M: 2.9 %	M: 0.23 %	M: 7.8 %	M: 1.8 %	M: Strongly positive	M: 2.7 %
ToxCast	ToxCast	ToxCast	ToxCast	ToxCast	ToxCast	ToxCast	ToxCast	ToxCast
Toxicity to Reproduction	Toxicity to Reproduction	Toxicity to Reproduction	Toxicity to Reproduction	Toxicity to Reproduction	Toxicity to Reproduction	Toxicity to Reproduction	Toxicity to Reproduction	Toxicity to Reproduction
Toxicokinetics, Metabolism and Distribution	Toxicokinetics, Metabolism and Distribution	Toxicokinetics, Metabolism and Distribution	Toxicokinetics, Metabolism and Distribution	Toxicokinetics, Metabolism and Distribution	Toxicokinetics, Metabolism and Distribution	Toxicokinetics, Metabolism and Distribution	Toxicokinetics, Metabolism and Distribution	Toxicokinetics, Metabolism and Distribution
Profiling	Profiling	Profiling	Profiling	Profiling	Profiling	Profiling	Profiling	Profiling
General Mechanistic	General Mechanistic	General Mechanistic	General Mechanistic	General Mechanistic	General Mechanistic	General Mechanistic	General Mechanistic	General Mechanistic

抽出される類似物質

皮膚感作性のための蛋白結合アラートプロファイラー

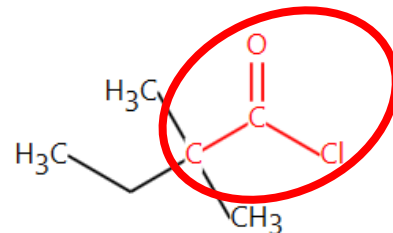
評価対象物質



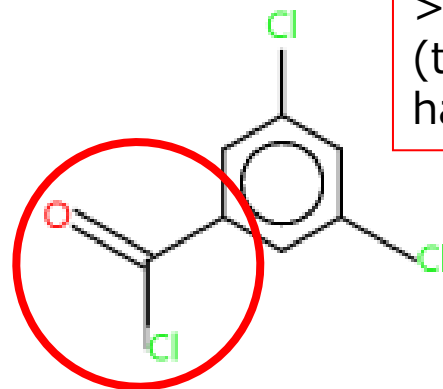
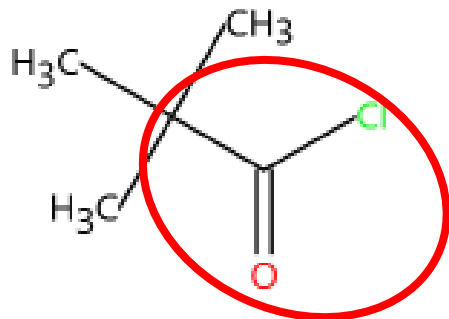
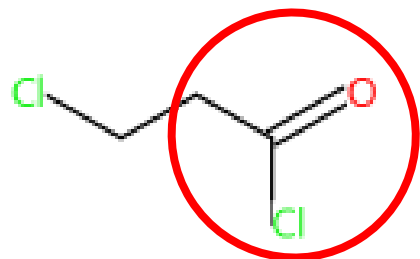
プロファイラ

皮膚感作性のための
蛋白質結合アラート

プロファイリング結果



>> (Thio)Acyl and
(thio)carbamoyl
halides and cyanides



同じカテゴリの類似物質が抽出される

カテゴリー定義

① Category Definitionクリック

③ クリック（選択したプロファイラーにより、評価対象物質と同じカテゴリーに属する物質の試験データを前のモジュールで選択したデータベースから取得する）

② “Endpoint Specific”の“Protein binding alerts for skin sensitization by OASIS”をクリック（カテゴリーによるグループ化に利用するプロファイラーを選択）

グルーピング方法
(プロファイラ)

カテゴリー定義

QSAR Toolbox 4.6 [Document 1]

QSAR TOOLBOX

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

Category consistency

Define Define with metabolism Subcategorize Combine Clustering Category elements

Documents

Protein binding alerts for skin sensitization by OASIS

Options 1 Selected

Toxic hazard classification by Gramer

Ultimate biodeg

Uncouples (MITOTOX)

ipoint Specific

Acute aquatic toxicity classification by Verhaar (Mc)

Acute aquatic toxicity MOA by OASIS

Acute Oral Toxicity

Aquatic toxicity classification by ECOSAR

Bioaccumulation - metabolism alerts

Bioaccumulation - metabolism half-lives

Biodegradation fragments (BioWIN MITI)

Carcinogenicity (genotox and nongenotox) alerts

DART scheme

DNA alerts for Ames, CA and MNT by OASIS

Eye irritation/corrosion Exclusion rules by BfR

Eye irritation/corrosion Inclusion rules by BfR

In vitro mutagenicity (Ames test) alerts by ISS

In vivo mutagenicity (Micronucleus) alerts by ISS

Keratinocyte gene expression

Oncologic Primary Classification

Protein binding alerts for Chromosomal aberration

Protein binding alerts for skin sensitization according

Protein binding alerts for skin sensitization by OASIS

Protein Binding Potency h-CLAT

Respiratory sensitisation

Retroic Acid Receptor Binding

rER Export System - USEPA

Skin irritation/corrosion Exclusion rules by BfR

Skin irritation/corrosion Inclusion rules by BfR

piric

Chemical elements

Groups of elements

Lipinski Rule base

Organic functional groups

Organic functional groups (nested)

Organic functional groups (US EPA)

Organic functional groups, Norbert Haider (check)

Structure similarity

Tautomers unstable

ecological

Repeated dose (HESS)

atom

Example Prioritization Scheme (PBT)

Filter endpoint tree...

Structure

Structure info

Parameters

Physical Chemical Properties

Environmental Fate and Transport

Ecotoxicological Information

Human Health Hazards

Acute Toxicity

ADME

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

Endpoint Specific

Protein binding alerts for skin sensitization by OASIS

Acylation

Grouping options (Protein binding alerts for skin sensitization by OASIS)

Target categories

Acylation

Acylation >> Direct acylation involving a leaving group

Acylation >> Direct acylation involving a leaving group >> (Thio)Acyl and (thio)carbamoyl halides and cyanides

Options

Down Up Reset Options

All categories (N/A)

Acylation >> (Thio)carbamoylation of protein nucleophiles

Acylation >> (Thio)carbamoylation of protein nucleophiles >> Isocyanates, Isothiocyanates

Combine profiles

☒ AND ☐ OR

☐ Invert result

☐ Strict

☐ Sort results

OK Cancel

Grouping with "Protein binding alerts for skin sensitization by OASIS"

You have selected <AND> from different hierarchy levels!
Selecting most informative level(s) will have the same result!
Do you want to continue?

Do not show this dialog

Yes No

① 評価対象物質が属するグループの確認
(アシル化に関するカテゴリーの階層が表示されている 大：ドメイン、中：メカニズム、小：物質群)

② クリック (類似物質の試験データの取得の実行)

③ クリック (グループの複数階層をANDで結んで選択しているので、最も詳細な階層のみを選択した結果と同じになるがよい?)

カテゴリー定義

QSAR Toolbox 4.6 [Document 1]

QSAR TOOLBOX

Category definition

Documents

Protein binding alerts for skin sensitization by OASIS

Options

1 Selected

Select All Unselect All Invert About Options

Toxic hazard classification by Cramer

Ultimate biodeg

Uncouplers (MITOTOX)

Point Specific

Acute aquatic toxicity classification by Verhaar (Mn)

Acute aquatic toxicity MOA by OASIS

Acute Oral Toxicity

Aquatic toxicity classification by ECOSAR

Bioaccumulation - metabolism alerts

Bioaccumulation - metabolism half-lives

Biodegradation fragments (BioWIN MITI)

Carcinogenicity (genotox and nongenotox) alerts

DART scheme

DNA alerts for Ames, CA and MNT by OASIS

Eye irritation/corrosion Exclusion rules by BfR

Eye irritation/corrosion Inclusion rules by BfR

In vitro mutagenicity (Ames test) alerts by ISS

In vivo mutagenicity (Macronucleus) alerts by ISS

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Protein binding alerts for skin sensitization by OASIS

Protein Binding Potency h-CLAT

Respiratory sensitisation

Retinoic Acid Receptor Binding

rER Expert System - USEPA

Skin irritation/corrosion Exclusion rules by BfR

Skin irritation/corrosion Inclusion rules by BfR

pinic

Chemical elements

Groups of elements

Leibniz Rule Oass

Organic functional groups

Organic functional groups (nested)

Organic functional groups (US EPA)

Organic functional groups, Norbert Haider (check)

Structure similarity

Tautomers unstable

ecological

Repeated dose (HESS)

itom

Example Prioritization Scheme (PBT)

Filter endpoint tree...

1 [target]

2

3

4

5

6

7

8

9

10

Structure

Structure info

Parameters

Physical Chemical Properties

Environmental Fate and Transport

Ecotoxicological Information

Human Health Hazards

Acute Toxicity

ADME

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

Endpoint Specific

Protein binding alerts for skin sensitization

Acylation

Grouping results

12 chemical(s) found.

Copy

OK

Read data?

All endpoints Choose...

OK

Cancel

Gather data

16 points added across 11 chemicals.

Copy

OK

① クリック（抽出物質数の確認）

② クリック（全てのエンドポイントの試験データを抽出）

③ クリック（試験データ数の確認）

類似物質の試験データの確認

QSAR Toolbox 4.6 [Document 1]

Category definition

データマトリックス

① クリック (ツリーを展開)

このエンドポイントは、11物質に対し16の試験データがある

試験データ (M : は実測の意味)

1 [target]	2	3	4	5	6	7	8	9	10
Structure									
Structure info									
Additional Ids	EC Number:2274785	EC Number:2219216	EC Number:2603308	EC Number:2027108	EC Number:2121312	EC Number:2108904	EC Number:2531684	EC Number:2039967	
CAS Number	5856-77-9	816431-72-8	3282-30-2	56677-60-2	98-88-4	65055-17-6	764-85-2	625-36-5	36727-29-4
CAS-SMILES relation	High	High	High	High	High	Low	High	High	High
Chemical name(s)	2,2-Dimethyl-butyl c...	4-[[2-(methoxypheny)...	2,2-Dimethylpropanoy...	Carbonochloridic acid...	Benzoyl chloride	3-Chloro-4-fluoroben...	Nonanoyl chloride	3-chloropropanoyl chl...	3,3,5-trimethylhexano...
Identity	Sources:7	Sources:5	Sources:12	Sources:8	Sources:22	Sources:2	Sources:10	Sources:13	Sources:10
Molecular formula	C6H11ClO	C15H12ClNO5S	C5H9ClO	C15H29ClO2	C7H5ClO	C7H3Cl2FO	C9H17ClO	C3H4Cl2O	C9H17ClO
Predefined substance type	Mono constituent	Mono constituent	Mono constituent	Mono constituent	Mono constituent	Mono constituent	Mono constituent	Mono constituent	Mono constituent
SMILES	CCC(C)(C)C(Cl)=O	CCc1cccc1C(=O)NS...	CC(C)(C)C(Cl)=O	CCCCCCCCCCCCCCCCC...	C1C(=O)c1cccc1	Fc1ccc(cc1C)C(Cl)=O	CCCCCCCC(C)C(Cl)=O	C1CCCC(C)C(Cl)=O	CC(C)(C)C(Cl)=O
Parameters									
Physical Chemical Properties									
Environmental Fate and Transport									
Ecotoxicological Information									
Human Health Hazards									
Acute Toxicity									
ADME									
Carcinogenicity									
Developmental Toxicity / Teratogenicity									
Genetic Toxicity									
Immunotoxicity									
Irritation / Corrosion									
Neurotoxicity									
Phototoxicity									
Reproductive Toxicity									
Sensitization									
ToxCast									
Toxicity to Reproduction									
Toxicokinetics, Metabolism and Distribution									
Profiling									
Endpoint Specific									
11/16	M: Negative	M: Strongly positive	M: 2.9 %	M: 0.23 %	M: 7.8 %	M: 1.8 %	M: Strongly positive	M: 2.7 %	M: 8.8 %

類似物質の試験データの確認

QSAR Toolbox 4.6 [Document 1]

QSAR TOOLBOX

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

Category: Category consistency

Define Define with metabolism Subcategorize Combine Clustering Category elements

Documents

ation >> Direct acylation involving a leaving group

Structure

Structure info

- Additional ids
- CAS Number
- CAS-SMILES relation
- Chemical name(s)
- Identity
- Molecular formula
- Predefined substance type
- SMILES
- Parameters
- Physical Chemical Properties
- Environmental Fate and Transport
- Ecotoxicological Information
- Human Health Hazards
- Acute Toxicity
- ADME
- Carcinogenicity
- Developmental Toxicity / Teratogenicity
- Genetic Toxicity
- Immunotoxicity
- Irritation / Corrosion
- Neurotoxicity
- Photoinduced toxicity
- Repeated Dose Toxicity
- Sensitization
 - Skin
 - In Vivo
 - LLNA
 - EC3
- ToxCast
- Toxicity to Reproduction
- Toxicokinetics, Metabolism and Distribution
- Profiling
- Endpoint Specific

Filter endpoint tree...

Target

11/16

M: Negative M: Strongly positive M: 2.9 % M: 0.23 % M: 7.8 % M: 1.8 % M: Strongly positive M: 2.7 % M: 8.8 %

② ダブルクリック (データの詳細の確認)

Data points

Datapoints	#	Value	Original value	Assay	Assigned SMILES	Comments	Database
Human Health Hazards;Sensitization;Skin;in Vivo;LLNA;EC3	1	M: 2.9 % (Skin sensitization EC3 (ratio))	2.9 % (Skin sensitization EC3(ratio))	LLNA	False	According to Skin sensitisation II (ECETOC) scale: Positive: EC3 < 50%; Negative: EC3 >= 50%	Skin Sensitization OAS (normalized)

③ データの詳細が表示される

Data Gap Filling: データギャップ補完



類似物質の試験データ
(毒性影響が類似して
いない)

毒性影響が類似するよ
うにサブカテゴリ化

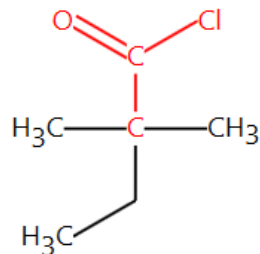
類似物質の試験データ確認
(毒性影響が類似していない場合には、サブカテゴリー化による類似物質の検討が必要)

データギャップ補完

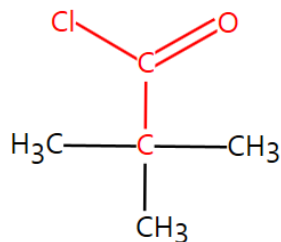
皮膚感作性のための蛋白結合アラートプロファイラー

類似構造
(Common functional group)

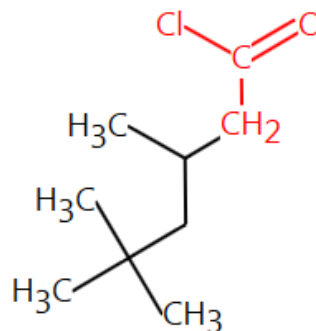
評価対象物質



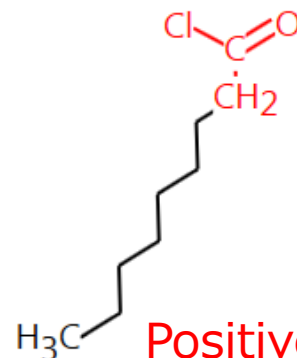
Positive
(Read-across)



Positive
(in vivo)



Positive
(in vivo)



Positive
(in vivo)

類似する毒性影響

データギャップ補完

① Data Gap Fillingクリック

QSAR Toolbox 4.6 [Document 1]

③ クリック (データギャップ補完の方法の指定: Read-across)

② セル選択 (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)

データギャップ補完

QSAR Toolbox 4.6 [Document 1]

QSAR TOOLBOX

Input Profiling Data Data Case Filter Report

Gap Filling Workflow Editor

Fixed analysis Read across (QSAR) Automated Standardized New Import Export Delete

Documents

Document 1

IC 13M: 0-P: 0 CAS: 585679

IC 12M: 16-P: 0 Acylation->AND>Acylation >> Direct acyl

IC 12M: 16-P: 0 Enter GF(RA)

Filter endpoint tree...

Structure

CAS-SMILES relation

Chemical names

Identify

Molecular formula

Predicted substance type

SMILES

Parameters

Physical Chemical Properties

Environmental Fate and Transport

Ecotoxicological Information

Human Health Hazards

Acute Toxicity

ADME

Carcinogenicity

Developmental Toxicity / Teratogenicity

Genetic Toxicity

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

Select / filter data

Gap filling approach

Descriptors / data

Model/QSAR

Calculation options

Visual options

Information

Miscellaneous

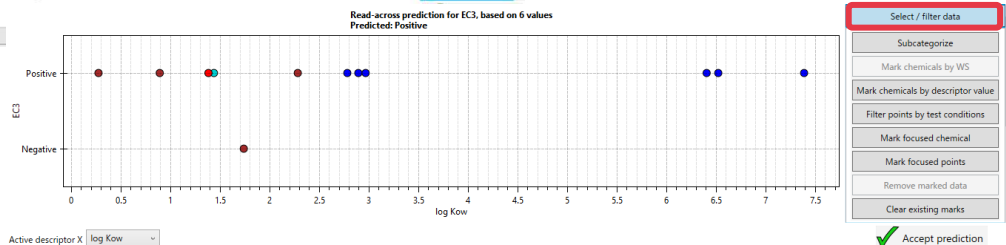
グラフで特性の類似性/規則性を確認する

予測がNegativeのデータが一つ含まれるのでサブカテゴリ化を行う。

① Select/filter dataをクリック

② Subcategorizeをクリック

- : 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

QSAR Toolbox 4.6 [Document 1]

QSAR TOOLBOX

Input Data Category definition Data Gap Filling Report

Gap Filling Workflow Editor

Documents

Document 1

- # [C: 1; Md: 0; P: 0] CAS: 5856779
- [C: 12; Md: 16; P: 0] Acylation<AND>Acylation >> Direct acyl
- [C: 12; Md: 16; P: 0] Enter GF(RA)

Filter endpoint tree...

Structure

CAS-SMILES relation
Chemical name(s)
Identity
Molecular formula
Predefined substance type
SMILES

Parameters

- Physical Chemical Properties
- Environmental Fate and Transport
- Ecotoxicological Information
- Human Health Hazards
- Acute Toxicity
- ADME
- Carcinogenicity
- Developmental Toxicity / Teratogenicity
- Genetic Toxicity
- Immunotoxicity

Descriptors

Prediction

Read-across prediction for EC
Predicted: Positive

EC

log Kow

Active descriptor X log Kow

Group by: Category

Sort by: Name

Color by: Target endpoint Legend

② Color byでTarget endpointを選択し、Legendをクリック

① Optionをクリック

Subcategorization

Options

Select All Unselect All Invert

0 Selected

Predefined

- Database Affiliation
- Inventory Affiliation
- OECD HPV Chemical Categories
- Substance type
- US-EPA New Chemical Categories

General Mechanistic

- Biodeg BioHC half-life (Biowin)
- Biodegradation primary (Biowin 4)
- Biodegradation probability (Biowin 1)
- Biodegradation probability (Biowin 2)
- Biodegradation probability (Biowin 5)
- Biodegradation probability (Biowin 6)
- Biodegradation probability (Biowin 7)
- Biodegradation ultimate (Biowin 3)
- DNA binding by OASIS

Options

Select All Unselect All Invert

0 Selected

Do not account metabolism

Documented

- Observed Mammalian metabolism
- Observed Microbial metabolism
- Observed Rat In vivo metabolism
- Observed rat liver metabolism with quantitative data
- Observed Rat Liver S9 metabolism

Simulated

- Autoxidation simulator
- Autoxidation simulator (alkaline medium)
- Dissociation simulator
- Hydrolysis simulator (acidic)
- Hydrolysis simulator (basic)
- Hydrolysis simulator (neutral)
- In vivo Rat metabolism simulator
- Microbial metabolism simulator

Adjust options

Target

Differ from target by

- At least one category
- All categories

[STOP]

Analogues

Selected

Select different

Remove selected

データギャップ補完

QSAR Toolbox 4.6 [Document 1]

① Group byでTarget endpointを選択し、Legendをクリック

② クリック

Subcategorization

Options Select All Unselect All Invert

Predefined

- Database Affiliation
- Inventory Affiliation
- OECD HPV Chemical Categories
- Substance type
- US-EPA New Chemical Categories

General Mechanistic

- Biodegradation BioHC half-life (Biowin 1)
- Biodegradation primary (Biowin 4)
- Biodegradation probability (Biowin 1)
- Biodegradation probability (Biowin 2)
- Biodegradation probability (Biowin 5)
- Biodegradation probability (Biowin 6)
- Biodegradation probability (Biowin 7)
- Biodegradation ultimate (Biowin 3)
- DNA binding by OASIS

Legend

Target endpoint

- Suitable
- Plausible
- Unclassified

OK

Metabolisms

Options Select All Unselect All Invert

Do not account metabolism

Documented

- Observed Mammalian metabolism
- Observed Microbial metabolism
- Observed Rat In vivo metabolism
- Observed rat liver metabolism with quantitative data
- Observed Rat Liver S9 metabolism

Simulated

- Autoxidation simulator
- Autoxidation simulator (alkaline medium)
- Dissociation simulator
- Hydrolysis simulator (acidic)
- Hydrolysis simulator (basic)
- Hydrolysis simulator (neutral)
- In vivo Rat metabolism simulator
- Microbial metabolism simulator

Selected

Select different

Remove selected

データギャップ補完

QSAR Toolbox 4.6 [Document 1]

グルーピングの対象から外れる候補

グルーピングに適したプロファイルの候補が表示される

① Protein binding by OASISをクリック

Subcategorization

Options: Select All, Unselect All, Invert

1 Selected

Target: Adjust options

Protein binding alerts for skin sensitization according to GHS

Protein binding alerts for skin sensitization by OASIS

Protein binding by OASIS

Plausible

Aquatic toxicity classification by ECOSAR

Chemical elements

Groups of elements

Keratinocyte gene expression

Lipinski Rule Oas

OECD HPV Chemical Categories

Organic functional groups

Organic functional groups (nested)

Organic functional groups (US EPA)

Do not account metabolism

Documented

Observed Mammalian metabolism

Observed Microbial metabolism

Observed Rat In vivo metabolism

Observed rat liver metabolism with quantitative data

Observed Rat Liver S9 metabolism

Simulated

Autoxidation simulator

Autoxidation simulator (alkaline medium)

Dissociation simulator

Hydrolysis simulator (acidic)

Hydrolysis simulator (basic)

Hydrolysis simulator (neutral)

Selected 2 (9/11)

Selected different

Remove selected

Legend:

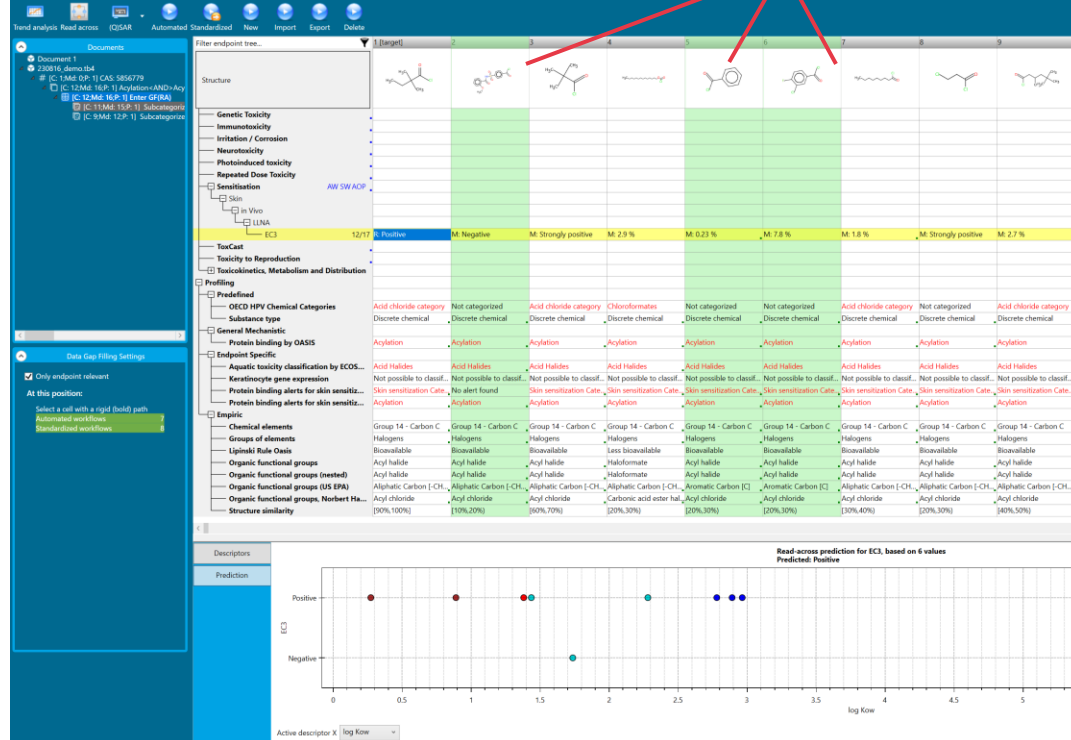
- : 評価対象物質 (予測)
- : 類似物質 (実測 ; Read-acrossに使用)
- : 異なる作用機序を示すと予想された類似物質
- : 削除対象とされた物質

データギャップ補完

QSAR Toolbox 4.6 (200816_demo.th4)



グルーピングの対象から外れる候補



Subcategorization

Options f Select All Unselect All Invert About Options

1 Selected

Options f Select All Unselect All Invert

0 Selected

Options f Select All Unselect All Invert

Adjust options

Target

Acyl halide

① Organic functional groupsをクリック

Organic functional group (nested)

Organic functional groups (US EPA)

Organic functional groups, Norbert Haider (checkmol)

Protein binding by OECD

Protein binding potency Gys (OPRA 13%)

Protein binding potency GSH

Protein Binding Potency h-CLAT

Protein binding potency Lys (DPRA 13%)

Respiratory sensitisation

Structure similarity

Options f Select All Unselect All Invert

Metabolisms

0 Selected

Options f Select All Unselect All Invert

Do not account metabolism

Documented

Observed Mammalian metabolism

Observed Microbial metabolism

Observed Rat In vivo metabolism

Observed Rat liver metabolism with quantitative data

Observed Rat Liver S9 metabolism

Simulated

Autoxidation simulator

Autoxidation simulator (alkaline medium)

Disassociation simulator

Hydrolysis simulator (acidic)

Hydrolysis simulator (basic)

Hydrolysis simulator (neutral)

In vivo Rat metabolism simulator

Microbial metabolism simulator

Rat liver S9 metabolism simulator

Skin metabolism simulator

Tautomerism

Analogs

(10) Acyl halide

(1) Alkane, branched with quaternary carbon

(1) Alkane, branched with tertiary carbon

(1) Alkoxy moiety

(1) Alkyl halide

(3) Aryl

(1) Aryl halide

(1) Benzamide

(1) Ether moiety

(1) Halofomate

(1) Isopropyl

(1) Sulfonamide

(2) tert-Butyl

Selected 3 (8/11)

Select different

Remove selected

② AnaloguesのうちArylをクリック

③ Remove selectedをクリック

[illegible]

- : 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

② クリック（承認の確認）

① Accept prediction **クリック**
(予測結果の承認)

データギャップ補完

QSAR TOOLBOX 4.6 [230816_demo.tst]

Gap Filling Workflow Editor

Documents

- Document 1
- 230816_demo.tst
- # [C: 9MA8_6P-2] CAS: 9554779
- [C: 12MA8_16P-2] Acylation<AND>Ac
- [C: 12MA8_16P-2] Enter GF(0A)
- [C: 12MA8_16P-2] Subcategory
- [C: 9MA8_12P-2] Subcategory
- [C: 9MA8_12P-2] Subcategory

Filter endpoint tree

- Structure
- Parameters
- Physical Chemical Properties
- Environmental Fate and Transport
- Ecotoxicological Information
- Human Health Hazards
 - Acute Toxicity
 - ADME
 - Carcinogenicity
 - Developmental Toxicity / Teratogenicity
 - Genetic Toxicity
 - Immunotoxicity
 - Irritation / Corrosion
 - Neurotoxicity
 - Photoinduced toxicity
 - Repeated Dose Toxicity
 - Sensitisation
 - In Vivo
 - LLNA
 - EC3
- ToxCast
- Toxicity to Reproduction
- Toxicokinetics, Metabolism and Distribution
- Profiling
- Endpoint Specific
 - Protein binding alerts for skin sensitiz...

12 [R: Positive] M: Negative M: Strongly positive M: 2.9 % M: 0.23 % M: 7.8 % M: 1.8 % M: Strongly positive M: 2.7 % M: 8.8 % M: 2.7 % M: 2.3 %

予測データ
(R : はRead acrossの意味)

Success

Prediction accepted successfully

Copy OK

① クリック

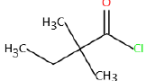
データギャップ補完

Prediction of EC3 for 2,2-Dimethylbutyryl chloride

1 / 9

QSAR Toolbox prediction for single chemical

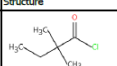
Date: 2 8 2011
Author(s):
Contact details:

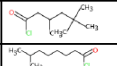
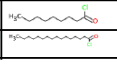
Target information		
Structural information	Numerical identifiers	Chemical names
SMILES: <chem>CCCC(C)(C)Cl=O</chem>	CAS#: 5856-77-9 Other: EC Number: 2274785	2,2-dimethylbutanoyl chloride 2,2-Dimethylbutyryl chloride 2,2-Dimethyl-butyl chloride
Structure		
		

Prediction summary
Predicted endpoint: EC3; No effect specified; No species specified; No duration specified; No guideline specified
Predicted value: Positive
Unit/scale: Skin sensitisation II (ECETOC)
Data gap filling method: Read-across analysis
Summary: manually editable field
Not provided by the user

Category

manually editable field
manually editable field

Structure


ited parameters

manually editable field

評価結果をPDFのレポートやデータマトリックス形式で出力可

Data matrix_2_8_21_19_09_36.xlsx												
A	B	C	D	E	F	G	H	I	J	K	L	M
1	2	3	4	5	6	7	8	9	10	11	12	13
Substance identity	Target chemical	Neighbour #1	Neighbour #2	Neighbour #3								
Structure												
CAS number	5856-77-9	3282-30-2	36727-29-4	57077-56-8								
Chemical name	2,2-Dimethylbutyryl chloride	pivaloyl chloride	O=C(C)(CC(C)(C)C)C(C)C	Isononanoyl chloride								
Other identifier												
SMILES	<chem>CCCC(C)(C)Cl=O</chem>	<chem>CC(C)(C)C(C)Cl=O</chem>	<chem>CC(C)(C)C(C)Cl=O</chem>	<chem>CCCCCCCC(C)Cl=O</chem>								
Profiles												
Acylation >> Direct acylation involving a leaving	Acylation >> Direct acylation involving a leaving	Acylation >> Direct acylation involving a leaving	Acylation >> Direct acylation involving a leaving	Acylation >> Direct acylation involving a leaving								
Acid chloride category	Acid chloride category	Acid chloride category	Acid chloride category	Acid chloride category								
Acyl halide	Acyl halide	Acyl halide	Acyl halide	Acyl halide								
Discrete chemical	Discrete chemical	Discrete chemical	Discrete chemical	Discrete chemical								
Acid Chlorides	Acid Chlorides	Acid Chlorides	Acid Chlorides	Acid Chlorides								
Grey zone 9-21% (DPRA 13%)	Grey zone 9-21% (DPRA 13%)	Grey zone 9-21% (DPRA 13%)	Grey zone 9-21% (DPRA 13%)	Grey zone 9-21% (DPRA 13%)								
Acylation	Acylation	Acylation	Acylation	Acylation								
DPRA above 21% (DPRA 13%)	DPRA above 21% (DPRA 13%)	DPRA above 21% (DPRA 13%)	DPRA above 21% (DPRA 13%)	DPRA above 21% (DPRA 13%)								
Not possible to classify according to these	Not possible to classify according to these	Not possible to classify according to these	Not possible to classify according to these	Not possible to classify according to these								
Acylation	Acylation	Acylation	Acylation	Acylation								

QSAR Toolbox 4.4.1
Database version: 4.4.1

QSAR TOOLBOX

TPRF v4.4.1

QSAR Toolbox 4.4.1
Database version: 4.4.1

QSAR TOOLBOX

TPRF v4.4.1

レポート作成

The screenshot displays the QSAR TOOLBOX 4.6 (200816, demo.8d) interface. The top menu bar includes 'Input', 'Data', 'Category definition', 'Data Gap filling', and 'Report'. The 'Report' menu is highlighted with a red box and labeled '① Reportクリック'. The left sidebar shows a 'Documents' tree with a red box around the 'Data Matrix' icon, labeled '③クリック (レポートの形式を選択 : Data Matrix)'. The main workspace shows a 'Structure' panel on the left and a table of results on the right. The table has columns for chemical structures and various endpoints. The 'Toxicity' endpoint is highlighted with a red box and labeled '② クリック (レポートを作成する予測結果を選択)'. The table contains data for various chemical structures, including 12/19, 12/20, 12/21, 12/22, 12/23, 12/24, 12/25, 12/26, 12/27, 12/28, 12/29, 12/30, 12/31, 12/32, 12/33, 12/34, 12/35, 12/36, 12/37, 12/38, 12/39, 12/40, 12/41, 12/42, 12/43, 12/44, 12/45, 12/46, 12/47, 12/48, 12/49, 12/50, 12/51, 12/52, 12/53, 12/54, 12/55, 12/56, 12/57, 12/58, 12/59, 12/60, 12/61, 12/62, 12/63, 12/64, 12/65, 12/66, 12/67, 12/68, 12/69, 12/70, 12/71, 12/72, 12/73, 12/74, 12/75, 12/76, 12/77, 12/78, 12/79, 12/80, 12/81, 12/82, 12/83, 12/84, 12/85, 12/86, 12/87, 12/88, 12/89, 12/90, 12/91, 12/92, 12/93, 12/94, 12/95, 12/96, 12/97, 12/98, 12/99, 12/100.

① Report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)

レポート作成

The screenshot displays the QSAR Toolbox 4.6 (230816_demo.tb4) interface. The top toolbar features several icons, with the 'Report' icon (a document with a checkmark) highlighted by a red box. Below the toolbar, the 'Wizard pages' dialog box is open, showing the 'Data matrix' section with the following options:

- ☒ Include profiles
- ☒ Select profiles to report
- ☒ Include measured and predicted data
- ☒ Select experimental data to report
- ☒ Include predictions

The 'Create report' button at the bottom right of the wizard is also highlighted with a red box. To the right, the 'Generated report files' dialog box is open, displaying the text: 'The following files were generated. Select a file to open or save.' Below this, a list box contains the entry 'Data matrix', which is highlighted with a red box. The 'Open' button at the bottom of this dialog is also highlighted with a red box.

① クリック (レポート作成の実行)

② 保存したいファイルを選択

③ クリック (作成されたレポートを開く)

作成されるレポートファイルのリスト

レポート作成(結果)

Substance Identity		Chemical #1	Chemical #2	Chemical #3	Chemical #4	Chemical #5	Chemical #6	Chemical #7	Chemical #8	Chemical #9
Structure										
CAS number		5856-77-9	3782-30-2	56877-60-2	764-85-2	6275-36-5	36777-29-4	112-67-4	57077-36-8	112-76-5
Chemical name		2,2-Dimethylbutyl chloride	pivaloyl chloride	Tetradecyl chloroformate	Nonanoyl chloride	3-chloropentanol chloride	3,3,5-trimethylhexanoyl chloride	palmitoyl chloride	homonanoyl chloride	stearoyl chloride
Other identifier		CCCC(C)(C)Cl-O	CC(C)(C)C(=O)Cl-O	CCCCCCCCCCCCCCCC(=O)Cl-O	CCCCCCCCCCCC(=O)Cl-O	CCCC(C)Cl-O	CC(C)(C)C(C)(C)C(=O)Cl-O	CCCCCCCCCCCCCCCC(=O)Cl-O	CCCC(C)CCCC(C)Cl-O	CCCCCCCCCCCCCCCC(=O)Cl-O
SMILES		CCCC(C)(C)Cl-O	CC(C)(C)C(=O)Cl-O	CCCCCCCCCCCCCCCC(=O)Cl-O	CCCCCCCCCCCC(=O)Cl-O	CCCC(C)Cl-O	CC(C)(C)C(C)(C)C(=O)Cl-O	CCCCCCCCCCCCCCCC(=O)Cl-O	CCCC(C)CCCC(C)Cl-O	CCCCCCCCCCCCCCCC(=O)Cl-O
Profilers										
13 OECD HPV Chemical Categories		Acid chloride category	Acid chloride category	Chloroformates	Acid chloride category	Not categorized	Acid chloride category	Acid chloride category	Acid chloride category	Acid chloride category
14 US EPA New Chemical Categories		Acid Chlorides	Acid Chlorides	Not categorized	Acid Chlorides	Not categorized	Acid Chlorides	Acid Chlorides	Acid Chlorides	Acid Chlorides
15 Substance type		Discrete chemical	Discrete chemical	Discrete chemical	Discrete chemical	Discrete chemical	Discrete chemical	Discrete chemical	Discrete chemical	Discrete chemical
16 General Mechanistic										
17 Protein binding by OASIS		Acylation	Acylation	Acylation	Acylation	Acylation	Acylation	Acylation	Acylation	Acylation
18 Uncoverables (MITOGEN)		Non concern for uncoupling of OePhos	Non concern for uncoupling of OePhos	Out of mechanistic domain	Out of mechanistic domain	Out of mechanistic domain	Out of mechanistic domain	Out of mechanistic domain	Out of mechanistic domain	Out of mechanistic domain
19 Protein binding potency (DPRA 13%)		Grey zone 9-21% (DPRA 13%)	Grey zone 9-21% (DPRA 13%)	Out of mechanistic domain	Out of mechanistic domain	Out of mechanistic domain	Grey zone 9-21% (DPRA 13%)	Out of mechanistic domain	Grey zone 9-21% (DPRA 13%)	Out of mechanistic domain
20 Protein binding by OASIS, with Hydrolysis		2 x No alert found	2 x No alert found	1 x No alert found	2 x No alert found	1 x No alert found	2 x No alert found	2 x No alert found	2 x No alert found	2 x No alert found
21 Endpoints Specific										
22 Aquatic toxicity classification by ECDAR		Acid Halides	Acid Halides	Acid Halides	Acid Halides	Acid Halides	Acid Halides	Acid Halides	Acid Halides	Acid Halides
23 Acute aquatic toxicity classification by Verhaar		Class 3 (unspecific reactivity)	Class 3 (unspecific reactivity)	Class 5 (Not possible to classify according to these)	Class 3 (unspecific reactivity)	Class 3 (unspecific reactivity)	Class 3 (unspecific reactivity)	Class 5 (Not possible to classify according to these)	Class 3 (unspecific reactivity)	Class 5 (Not possible to classify according to these)
24 Protein binding alerts for skin sensitization by 1		Acylation	Acylation	Acylation	Acylation	Acylation	Acylation	Acylation	Acylation	Acylation
25 Keratinocyte gene expression		Not possible to classify according to these	Not possible to classify according to these	Not possible to classify according to these	Not possible to classify according to these	Not possible to classify according to these	Not possible to classify according to these	Not possible to classify according to these	Not possible to classify according to these	Not possible to classify according to these
26 Protein binding alerts for skin sensitization by 2		Skin sensitization Category 1B	Skin sensitization Category 1B	Skin sensitization Category 1B	Skin sensitization Category 1B	Skin sensitization Category 1B	Skin sensitization Category 1B	Skin sensitization Category 1B	Skin sensitization Category 1B	Skin sensitization Category 1B
27 Acute Oral Toxicity		Not categorized	Not categorized	Not categorized	Not categorized	Not categorized	Not categorized	Not categorized	Not categorized	Not categorized
28 Protein binding alerts for skin sensitization by 3		No metabolites	No metabolites	No metabolites	No metabolites	No metabolites	No metabolites	No metabolites	No metabolites	No metabolites
29 Protein binding alerts for skin sensitization by 4		1 x No alert found	5 x No alert found	2 x No alert found	No metabolites	No metabolites	2 x No alert found	No metabolites	1 x No alert found	3 x No alert found
30 Protein binding alerts for skin sensitization by 5		No metabolites	No metabolites	No metabolites	No metabolites	No metabolites	No metabolites	No metabolites	No metabolites	No metabolites
31 Protein binding alerts for skin sensitization by 6		2 x No alert found	2 x No alert found	4 x No alert found	2 x No alert found	1 x No alert found	2 x No alert found	2 x No alert found	2 x No alert found	2 x No alert found
32 Empiric										
33 Structure similarity		[20%,100%]	[20%,100%]	[20%,100%]	[20%,100%]	[20%,100%]	[20%,100%]	[20%,100%]	[20%,100%]	[20%,100%]
34 Organic functional groups		Alkyl halide	Alkyl halide	Haloformate	Alkyl halide	Alkyl halide	Alkyl halide	Alkyl halide	Alkyl halide	Alkyl halide
35 Groups of elements		Halogens	Halogens	Halogens	Halogens	Halogens	Halogens	Halogens	Halogens	Halogens
36 Chemical elements		Group 14 - Carbon C	Group 14 - Carbon C	Group 14 - Carbon C	Group 14 - Carbon C	Group 14 - Carbon C	Group 14 - Carbon C	Group 14 - Carbon C	Group 14 - Carbon C	Group 14 - Carbon C
37 Upstream Rule Davis		Bioavailable	Bioavailable	Less bioavailable	Bioavailable	Bioavailable	Bioavailable	Less bioavailable	Bioavailable	Less bioavailable
38 Organic functional groups (revised)		Alkyl halide	Alkyl halide	Haloformate	Alkyl halide	Alkyl halide	Alkyl halide	Alkyl halide	Alkyl halide	Alkyl halide
39 Organic functional groups (US EPA)		Aliphatic Carbon [-CH2-]	Aliphatic Carbon [-CH2-]	Aliphatic Carbon [-CH2-]	Aliphatic Carbon [-CH2-]	Aliphatic Carbon [-CH2-]	Aliphatic Carbon [-CH2-]	Aliphatic Carbon [-CH2-]	Aliphatic Carbon [-CH2-]	Aliphatic Carbon [-CH2-]
40 Organic functional groups, Norbert Halder		Aryl chloride	Aryl chloride	Carboxylic acid ester halide	Aryl chloride	Aryl chloride	Aryl chloride	Aryl chloride	Aryl chloride	Aryl chloride
41 Organic functional groups, with Autoxidation		No metabolites	No metabolites	No metabolites	No metabolites	No metabolites	No metabolites	No metabolites	No metabolites	No metabolites
42 Organic functional groups, with Dissociation		No metabolites	No metabolites	No metabolites	No metabolites	No metabolites	No metabolites	No metabolites	No metabolites	No metabolites
43 Organic functional groups, with Hydrolysis		1 x Carboxylic acid	1 x Carboxylic acid	1 x Alcohol	1 x Carboxylic acid	1 x Alkane, branched with quaternary	1 x Carboxylic acid	1 x Carboxylic acid	1 x Alkane, branched with tertiary carbon	1 x Carboxylic acid
44 Organic functional groups, with Autoxidation		No metabolites	No metabolites	No metabolites	No metabolites	No metabolites	No metabolites	No metabolites	No metabolites	No metabolites
45 Measured and predicted data										
46 Human Health Hazard/Sensitization										
sublabel	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
46				Test organisms (species): mouse Endpoint: EC3 Type of method: In Vivo Assay: LLNA Year: 2007 Reference source: Regulatory Toxicology			Test organisms (species): mouse Endpoint: EC3 Type of method: In Vivo Assay: LLNA Year: 2007 Reference source: Regulatory Toxicology			Test organisms (species): mouse Endpoint: EC3 Type of method: In Vivo Assay: LLNA Year: 2007 Reference source: Regulatory Toxicology

参考情報

QSAR Toolbox Website

<https://qsartoolbox.org/>

- QSAR Toolboxのダウンロード
- Guidance Documents and Training Materials
- Webinar
- Help Desk
- Public Discussion Forum
etc.

The OECD QSAR Toolbox

To increase the regulatory acceptance of (Q)SAR methods, the OECD is developing a QSAR Toolbox to make (Q)SAR technology readily accessible, transparent, and less demanding in terms of infrastructure costs.

[Download the Toolbox](#) [Guidance Documents and Training Materials](#) [Webinar](#) [Help Desk](#) [Public Discussion Forum](#)

WHAT'S NEW?

16 May 2023 – A new version of the OECD QSAR Toolbox is now available: New Toolbox offers extended connectivity with IUCLID, better docking capacity for external models and explicit references to the test material identity for REACH database.

The **OECD QSAR Toolbox 4.6** is now available for [download](#).

This update includes, among others, an extended IUCLID connectivity and searches, optimised execution of external QSARs, and an update to the Web Client and report functionalities. Furthermore, it offers a new perspective on the REACH database, where experimental results can now be consulted according to the material that was tested.

15 years of work on the OECD QSAR Toolbox have led to the development of a freely available software that supports and transparent chemical hazard assessment without new tests on animals. Co-developed by ECHA and OECD also with great support from member countries and QSAR community, the QSAR Toolbox has now over 30 000 users from private and public sector across the world and it is widely used under REACH and beyond.

The release of the Toolbox 4.6 is yet another step forward for the reduction of animal testing in chemical hazard assessment.

For the complete list of changes, please see the [release notes](#), Download the QSAR Toolbox and find more information on the [QSAR Toolbox website](#), and [access the new repository](#).

ユーザーマニュアル（和訳）

当機構HPにおいてユーザマニュアル・インストールマニュアル等の和訳を公開
<https://www.nite.go.jp/chem/qsar/toolbox.html>

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](#) 【ZIP : 33MB】 

（QSAR Toolbox v4.1に基づいたマニュアル）

 （原文）OECD QSAR Toolbox v.4の操作マニュアル 

 [OECD QSAR Toolboxユーザーマニュアルスタートガイド](#) 【PDF : 4MB】 

（QSAR Toolbox v3.0に基づいた使い方マニュアル）

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

 [OECD QSAR Toolbox4.4のインストールマニュアル](#) 【PDF : 2MB】 

（QSAR Toolbox v4.4に基づいたインストールマニュアル）

 OECD QSAR Toolbox4.6のインストールマニュアル 

<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](#) 【PDF : 3MB】 

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。

QSAR Toolbox のHelp Desk

次のようなトラブルについては、下記URLのヘルプデスクに照会して下さい。

- ユーザー登録
- ソフトウェアのダウンロード及びインストール
- ソフトウェアの基本的な使い方
- バグなどの情報

OECDのHP:

<https://qsartoolbox.org/support/#help>

動画講習/学習教材サイト

リードアクロス講習の動画等の
学習教材を公開しています。

1. リードアクロス講習
2. リードアクロス関連ガイダンスとサイトのご案内

NITEのHP:

<https://www.nite.go.jp/chem/qsar/ReadAcrossTraining.html>

ご清聴ありがとうございました

安全とあなたの未来を支えます

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