

ユーザーデータの追加方法

2014年7月1日(火)
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内容

- 準備するファイル
- 登録方法
- 登録したデータの確認
- その他(他のサブデータベースの利用)

準備するファイル

毒性徴候表ファイル(.docx)

ファイル名: S10001.docx, S10002.docx, S10003.docx,

| | | |
|----------------------|--|--------|
| S10001 | R10001 | C10001 |
| Cas No. | 95-78-3 | |
| Study type | Repeated Dose Toxicity Study (28 days) | |
| Species | Rat (SD) | |
| Route | Oral (Gavage) | |
| Solvent | Corn oil | |
| Dose level | 3 doses (12, 60, 300 mg/kg/day) | |
| Death | - | |
| NOEL | ♂♀: 12 mg/kg/day | |
| NOAEL | - | |
| Clinical observation | Staggering gait: 300♂♀ Lacrimation: 300♂♀ Salivation: 300♂♀ | |
| FOB | | |
| Body weight | Body weight gain↓: 300♂ | |
| Food consumption | ↓: 300♂ | |
| Water consumption | ↑: 300♂♀ | |
| Urinalysis | Volumet: 300♂♀ Specific gravity↓: 300♂♀ pH↓: 300♂ | |
| Hematology | RBC↓: 300♂♀ HCT↓: 300♂♀ HGB↓: 300♂♀ MCHC↓: 300♂ Met-HGB↑: 300♂♀ RET↑: 300♂♀ NEUT↑: 300♂ LYMPH↓: 300♂ PT↑: 300♀ | |

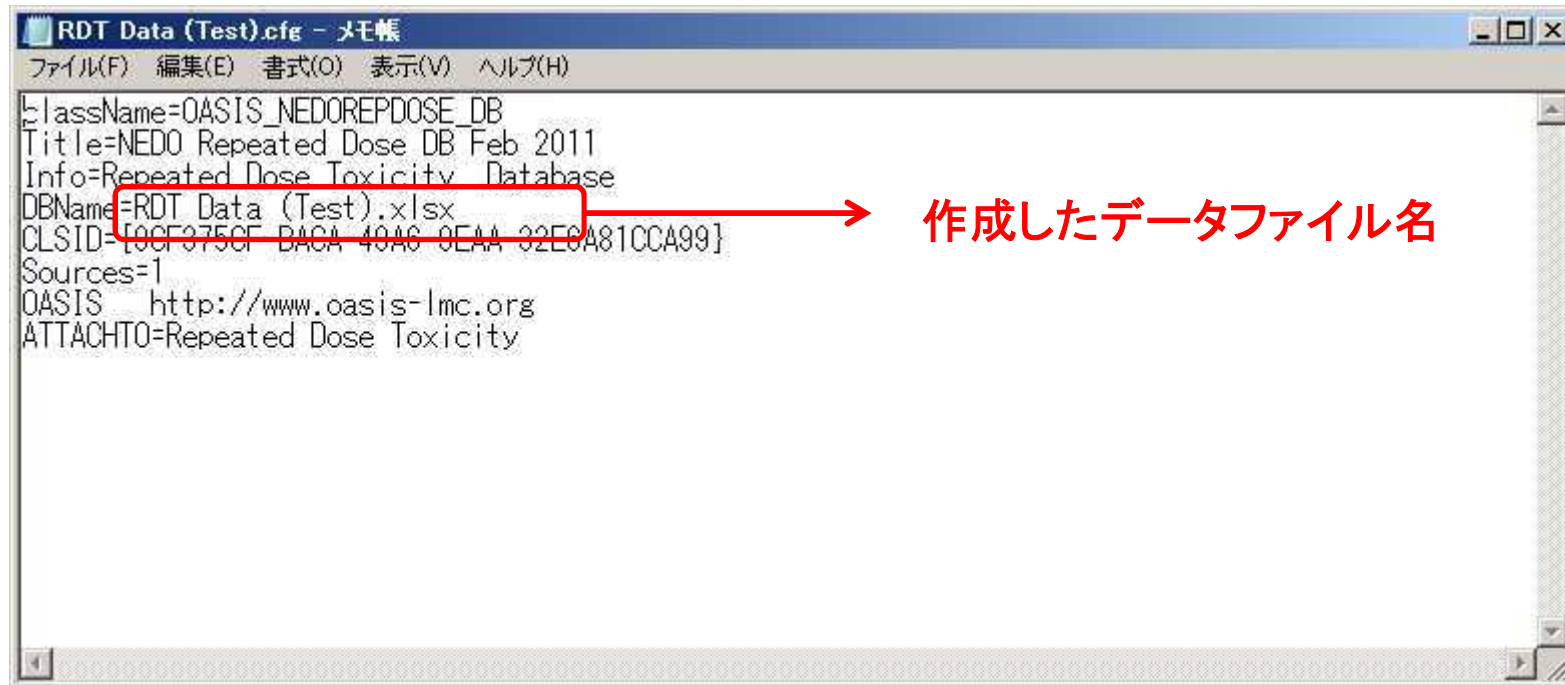
毒性試験データファイル(.xlsx)

ファイル名: RDT Data (Test).xlsx

| | A | B | C | D | E | F | G | H | I | J | K | L | M | N | O | P | Q |
|---|----|---|---|---|---|---------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|---|-------------|--------------|--------------|-----------------|---------|---|
| 1 | ID | | | | | CAS No. | 95783 | 95783 | 95783 | 95783 | 959557 | 959557 | 88415 | 88415 | | | |
| 2 | ID | | | | | Name | 2,5-xylylene | 2,5-xylylene | 2,5-xylylene | 2,5-xylylene | Benzylidene | Benzylidene | 2-tert-Butyl | 2-tert-Butyl | cyclohexan-1-yl | acetate | |
| 3 | ID | | | | | Smiles | c1(Cc2c3ccccc3cc2)c1(C)c4ccccc4 | c1(Cc2c3ccccc3cc2)c1(C)c4ccccc4 | c1(Cc2c3ccccc3cc2)c1(C)c4ccccc4 | c1(Cc2c3ccccc3cc2)c1(C)c4ccccc4 | c1(Cc2c3ccccc3cc2)c1(Cc2c | | | | | | |

コンフィグファイル(.cfg))

ファイル名: RDT Data (Test).cfg



登録方法

登録方法

1. 毒性徴候表ファイル(S10001-S10003)は、[HESSをインストールしたドライブ名(CまたはDなど)]:¥Program Files¥Hazard Evaluation Support System¥HESS 2.8¥Summary sheets に保存
2. データファイル(RDT Data (Test).xlsx)とコンフィグファイル(RDT Data (Test).cfg)はC:¥ユーザー¥[ユーザー名]¥マイドキュメント¥Hazard Evaluation Support System¥UserDir に保存。
3. [HESSをインストールしたドライブ名(CまたはDなど)]:¥Program Files¥Hazard Evaluation Support System¥HESS 2.8に保存されている。RDTProfilers.xlsx に登録するデータファイルのデータを追記する。

Reset Options Help

Help

Input

NO SELECTED TARGET

SMILES

metabolism mode...

Filter endpoint tree...

- ☐ Biomarker DB
- ☐ COSMOS DB
- ☐ HESS Repeated Dose Toxicity
- ☐ HESS Repeated Dose Toxicity (CSCL New Chemicals)
- ☐ ToxRef DB

⊕ Substance Identity

Repeated Dose Toxicity

Biomarker

abc

Hazard Evaluation Support System

Reset Options Help

Input
Profiling
RDT Data
Categories
Gap Filling
Report
Metabolism

Chemical name:
CAS No
SMILES

NO SELECTED TARGET

to data matrix -> metabolism mode...

Gather

Databases

- ☐ Biomarker DB
- ☐ COSMOS DB
- ☐ HESS Repeated Dose Toxicity
- ☐ HESS Repeated Dose Toxicity (CSCL New Chemicals)
- ☐ ToxRef DB

Structure

Filter endpoint tree...

- ☒ Substance Identity
- ☐ Repeated Dose Toxicity
- ☒ Biomarker

Delete Database
Select all
Unselect all
Invert selection
Add...

Import... Generic Excel Import...
HESS DB Import...

C:\¥ユーザー¥usr30 ¥ マイドキュメント¥Hazard Evaluation Support System¥UserDir → RDT Data (Test).cfg

①点線で囲まれたあたりで右クリックし、HESS DB importを選択

②コンフィグファイルのディレクトリ

③"New file"を選択

④任意のデータベース名を入力

⑤クリック

HESS DB format import...

Import file... C:\¥Users¥YTNH0910¥Documents¥Hazard Evaluation Support System¥UserDir¥RDT Data

Import to New file Database title My DB

Close Start import

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Hazard Evaluation Support System

ResetOptionsHelp

Input

Profiling

RDT Data

Categories

Gap Filling

Report

Metabolism

NO SELECTED TARGET

Chemical name:
CAS No
SMILES

to data matrix ->metabolism mode...

Gather

Databases

☐ Biomarker DB

☐ COSMOS DB

☐ HESS Repeated Dose Toxicity

☐ HESS Repeated Dose Toxicity (CSCL New Chemicals)

☐ ToxRef DB

Filter endpoint tree...

Structure

☒ Substance Identity

☐ Repeated Dose Toxicity

☐ Biomarker

NITE HESS

Import completed!

OK

HESS DB format import...

Import file...

C:\Users\YTNH0910\Documents\Hazard Evaluation Support System\UserDir\RDT Dai

Close

Start import

Import to

New file

Database title

My DB

0 Document

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Hazard Evaluation Support System Reset Options Help

Reset

Options

Help


Input

Profiling

Profiling

RDT Data

Categories

Gap Filling

Report

Metabolism

| | |
|--------------------|--|
| NO SELECTED TARGET | Chemical name: |
| | CAS No |
| | SMILES |
| | <div>to data matrix+></div> <div>metabolism mode...</div> |

Chemical name:

CAS No.

SMILES

to data matrix ->

metabolism mode...

Gather.

Databases

☐ Biomarker DB☐ COSMOS DB
☐ HESS Repeated Dose Toxicity☐ HESS Repeated Dose Toxicity (CSCI New Chemicals)☐ HESS Repeated Dose Toxicity (CSCL New Chemicals)☒ My DB☒ My DB

Filter endpoint tree...

Structure

⊕ Substance Identity

Repeated Dose Toxicity

| Biomarker |
|-----------|
|-----------|

登録したデータの確認

Hazard Evaluation Support System

Reset Options Help

Input ①

Profiling

RDT Data

Categories

Gap Filling

Report

Metabolism

Chemical name:
CAS No
SMILES

NO SELECTED TARGET

to data matrix -> metabolism mode...

登録したデータベースを確認する。

Set target Add to post-targets list CAS# Chemical name Drawing RDT tests Database User List Load DB Load Inventory ②

CAS # Search

Chemical name:

一度、HESSを閉じ、再び立ち上げる。

↓

①、②をクリック

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Hazard Evaluation Support System

Reset Options Help

Input
Profiling
RDT Data
Categories
Gap Filling
Report
Metabolism

Chemical name:
CAS No
SMILES

NO SELECTED TARGET

to data matrix -> metabolism mode...

Set target Add to post-targets list CAS# Chemical name Drawing RDT tests Database User List Load DB Load Inventory

CAS # Search

Chemical name:

Select database

- Biomarker DB
- COSMOS DB
- HESS Repeated Dose Toxicity
- HESS Repeated Dose Toxicity (CSCL New Chemicals)
- My DB**
- Parents in Rat Liver Metabolism DB
- ToxRef DB

OK Cancel

①登録したデータベースを選択する。

②クリック

Document Load database 12/7/8 Developed by LMC, Bulgaria 15

Hazard Evaluation Support System
Reset Options Help

Input
Profiling
RDT Data
Categories
Gap Filling
Report
Metabolism

Chemical name:
CAS No
SMILES
to data matrix -> metabolism mode...

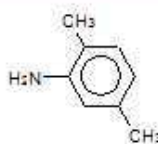
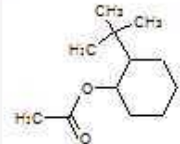
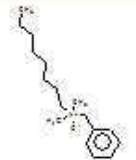
NO SELECTED TARGET
①選択

Show Boundaries **Apply** New Scheme

Profiling methods
Empiric
☐ Chemical elements
☐ Groups of elements
☐ Lipinski Rule Oasis
☐ Organic functional groups
☐ Organic functional groups (nested)
☐ Organic functional groups (US EPA)
☐ Organic functional groups, Norbert
☒ Study No. (Link to SSRDT)
☒ Chemical No. (Link to HESS DB)
☒ RDT Report No.
☐ CSCL Class
☒ Rat Liver Metabolism Database
Toxicological
☒ Repeated dose (HESS)

Metabolism
Documented
☐ Observed Rat Liver metabolism
Simulated
☐ Dissociation simulation
☐ Liver Metabolism Simulator
☐ NEDO In Vitro Rat Cellular Metabo
☐ NEDO In Vitro Rat Microsomal Met

Filter endpoint tree...

| | 1 | 2 | 3 |
|------------------------|---|---|---|
| Structure |  |  |  |
| Substance Identity | | | |
| Repeated Dose Toxicity | | | |
| Biomarker | | | |

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①選択

②クリック

Hazard Evaluation Support System

Hazard Evaluation Support System
ResetOptionsHelp

Input

Profiling

RDT Data

Categories

Gap Filling

Report

Metabolism

Chemical name:

CAS No

SMILES

NO SELECTED TARGET

to data matrix-->

metabolism mode...

Show Boundaries

Apply

New Scheme

Filter endpoint tree...

Structure

Substance Identity

Repeated Dose Toxicity

Biomarker

Profile

Study No. (Link to SSRDT)

Chemical No. (Link to HES...)

RDT Report No.

Rat Liver Metabolism Data...

Repeated dose (HESS)

1

CH₃

H₂N

CH₃

CH₃

CH₃

H₃C

CH₃

H₃C

O

CH₃

CH₃

CH₃

H₃C

CH₃

H₃C

O

CH₃

CH₃

CH₃

H₃C

CH₃

H₃C

O

CH₃

2

CH₃

CH₃

H₃C

CH₃

H₃C

O

CH₃

CH₃

CH₃

H₃C

CH₃

H₃C

O

CH₃

CH₃

CH₃

H₃C

CH₃

H₃C

O

CH₃

3

CH₃

CH₃

H₃C

CH₃

H₃C

O

CH₃

CH₃

CH₃

H₃C

CH₃

H₃C

O

CH₃

CH₃

CH₃

H₃C

CH₃

H₃C

O

CH₃

Profiling methods

Empiric

Chemical elements

Groups of elements

Lipinski Rule Oasis

Organic functional groups

Organic functional groups (nested)

Organic functional groups (US EPA)

Organic functional groups, Norbert

Study No. (Link to SSRDT)

Chemical No. (Link to HESS DB)

RDT Report No.

CSCL Class

Rat Liver Metabolism Database

Toxicological

Repeated dose (HESS)

Metabolism

Documented

Observed Rat Liver metabolism

Simulated

Dissociation simulation

Liver Metabolism Simulator

NEDO In Vitro Rat Cellular Metabo

NEDO In Vitro Rat Microsomal Mat

10001

10003

10002

10001

10003

10002

10001

10003

10002

Root of map No. 61

N/A

N/A

Anilines (Hemolytic...

Not categorized

Not categorized

Anilines (Hepatotox...

Not categorized

Not categorized

3

My DB

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毒性徴候表を表示させる。

①クリック

毒性徴候表ファイルの表示

| | |
|----------------------|--|
| §10001 R10001 C10001 | |
| Cas No. | 95-78-3 |
| Study type | Repeated Dose Toxicity Study (28 days) |
| Species | Rat (SD) |
| Route | Oral (Gavage) |
| Solvent | Corn oil |
| Dose level | 3 doses (12, 60, 300 mg/kg/day) |
| Death | - |
| NOEL | ♂♀: 12 mg/kg/day |
| NOAEL | - |
| | |
| Clinical observation | Staggering gait: 300♂♀, Lacrimation: 300♂♀, Salivation: 300♂♀ |
| FOB | - |
| Body weight | Body weight gain†: 300♂ |
| Food consumption | †: 300♂ |
| Water consumption | †: 300♂♀ |
| Urinalysis | Volume†: 300♂♀, Specific gravity†: 300♂♀, pH†: 300♂ |
| Hematology | RBC†: 300♂♀, HCT†: 300♂♀, HGB†: 300♂♀, MCHC†: 300♂, Met-HGB†: 300♂♀, RET†: 300♂♀, NEUT†: 300♂, LYMPH†: 300♂ |

Help

Metabolism

metabolism mode...

| | | | |
|-------------------------------|-------|-------|-------|
| Study No. (Link to SSRDT) | 10001 | 10003 | 10002 |
| Chemical No. (Link to HES...) | 10001 | 10003 | 10002 |
| RDT Report No. | 10001 | 10003 | 10002 |



その他 (他のサブデータベースの利用)

Hazard Evaluation Support System

Reset Options Help

Input ①選択

Chemical name:
CAS No
SMILES

NO SELECTED TARGET

to data matrix -> metabolism mode...

②クリック

Load DB Load Inventory

Set target Add to post-targets list CAS# Chemical name Drawing RDT tests Database User List

My DB 17/07/0 Developed by LMC, Bulgaria ST 23

Detailed description: This is a screenshot of the 'Hazard Evaluation Support System' software interface. The window has a blue title bar and a main menu bar with 'Reset', 'Options', and 'Help' buttons. On the left is a vertical sidebar with buttons for 'Input', 'Profiling', 'RDT Data', 'Categories', 'Gap Filling', 'Report', and 'Metabolism'. The 'Input' button is highlighted with a red box and labeled '①選択'. The main area is divided into sections. The top section contains input fields for 'Chemical name:', 'CAS No', and 'SMILES', a 'NO SELECTED TARGET' status, and two buttons: 'to data matrix ->' and 'metabolism mode...'. A red annotation 'データベースをロードする。' (Load the database) is placed near the input fields. Below this is a toolbar with icons and labels for 'Set target', 'Add to post-targets list', 'CAS#', 'Chemical name', 'Drawing', 'RDT tests', 'Database', and 'User List'. The 'Load DB' button in this toolbar is highlighted with a red box and labeled '②クリック'. The bottom of the window shows a status bar with 'My DB', a date '17/07/0', 'Developed by LMC, Bulgaria', and a page number 'ST 23'.

Hazard Evaluation Support System

Reset Options Help

Input
Profiling
RDT Data
Categories
Gap Filling
Report
Metabolism

Chemical name:
CAS No
SMILES

NO SELECTED TARGET

to data matrix -> metabolism mode...

Set target Add to post-targets list CAS# Chemical name Drawing RDT tests Database User List

Load DB Load Inventory

Select database

- Biomarker DB
- COSMOS DB**
- HESS Repeated Dose Toxicity
- HESS Repeated Dose Toxicity (CSCL New Chemicals)
- My DB
- Parents in Rat Liver Metabolism DB
- ToxRef DB

① "COSMOS DB" を選択

OK Cancel

クリック

3 My DB Load database 10/17/00 Developed by LMC, Bulgaria 24

Input

Profiling

RDT Data

Categories

Gap Filling

Report

Metabolism

Chemical name:

CAS No

SMILES

to data matrix ->

metabolism mode...

NO SELECTED TARGET

Filter endpoint tree...

Structure

Delete Database

Select all

Unselect all

Invert selection

About

Import...

Reset

Options

Help

①右クリック

②"About"を選択

データベースの基本情報を表示させる。

Source About

Database Name

COSMOS DB

Short Description

The database contains repeated dose toxicity study data of 852 chemicals (2252 studies), which were extracted from COSMOS DB (<http://www.cosmostox.eu/home/welcome/>).

Study data in the following conditions were extracted from COSMOS DB

- species: RAT
- study_endpoint: Special Toxicology Study / Target organ toxicity
- study_duration: ≥28 day
- exposure_route: Oral

Extracted data were merged into the HESS database format. The study_ids in COSMOS DB and the original terminologies for toxicity effects in COSMOS DB are listed in the "summary" column in the "Data matrix" window.

Donators

This database was prepared as the result of data exchange between COSMOS DB and HESS (December 2013). The original data of COSMOS DB were provided from Altamira LLC. We would like to thank COSMOS project and Altamira LLC for the opportunity.

Disclaimer

Copyrights of the database are to be owned by NITE. Users are requested to comply with international conventions and rules related to copyrights. The commercial use of the database is prohibited. For example, it is prohibited to extract or to copy the contents of database, such as data

URL

| Available Data | |
|----------------------|------------|
| Number of chemicals | 852 |
| Number of data | 12852 |
| Number of endpoints | 2 |
| Name of endpoints | NOEL, LOEL |
| Version | |
| Adopted | Undefined |
| QA Chemical identity | |
| QA Data | |

OK

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