OECD QSAR Toolbox v.4.1

Tutorial of how to Import/Export a custom database and Import/Export IUCLID
Outlook

• **Aim**
• Definition of Database/Inventory
• Import
• Export
Aim

This is a step-by-step presentation designed to take the user of Toolbox through the process of importing/exporting of custom databases/inventories.
Outlook

- Aim
- **Definition of Database and Inventory**
- Import
- Export
Definition of database and inventory

• **A database** is a collection of structures accompanied with experimental data.

• **An inventory** is a collection of structures without experimental data.
Outlook

• Aim
• Definition of Database and Inventory
• Import:
  - Import of database
    - Vertical import
    - Horizontal import
  - Import of inventory
  - Import via IUCLID
• Export Data matrix
Import of database:
Types of import

• **Vertical import:**
  It is appropriate for a set of chemicals with consistent experimental data and the same supporting information (e.g. endpoint, test organism, test condition, author etc.).

• **Horizontal import:**
  It is appropriate for a set of chemicals with different types of experimental data accompanied with supporting information (endpoints, test condition, test organism, author etc).
Outlook

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• Import:
  ❖ Import of database
    ➢ Vertical import
    ➢ Horizontal import
  ❖ Import of inventory
  ❖ Import via IUCLID
• Export Data matrix
Import of database: Vertical import

- Vertical import layout contains two main sections: substance information (1) and experimental data (2);
- Each column (2) defines data points for a single experiment.
- The imported file can be in **xlsx** or **tsv** format.
Import of database: Vertical import

- In this tutorial an example of vertical import of a database containing experimental information about Biochemical oxygen demand (BOD) and Bacterial reversed mutation assay (Ames) is shown.
- The excel file (*Vertical import_ BOD and Ames.xlsx*) is depicted below and it could be found: C:\Program Files (x86)\Common Files\QSAR Toolbox 4\Config\Examples

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>CAS</td>
<td>NAME</td>
<td>Smiles</td>
<td>BOD</td>
<td>Ames</td>
</tr>
<tr>
<td>60-34-4</td>
<td>METHYLHYDRAZINE</td>
<td>CN</td>
<td>N</td>
<td>=O</td>
</tr>
<tr>
<td>50-29-3</td>
<td>DICHLORO DIPHENYL TRICHLOROETHANE</td>
<td>C1([Cl][Cl])[Cl][Cl][Cccl(C)cc(1)c1ccc(1)c1cc(1)]</td>
<td>7.1</td>
<td>Negative</td>
</tr>
<tr>
<td>50-32-8</td>
<td>BENZOPYRENE, 3,4, 5-trisubstituted</td>
<td>c12c3c4c5c6c7c8c9c10c11c12c13c14c15c16</td>
<td>60.7</td>
<td>Negative</td>
</tr>
<tr>
<td>50-33-9</td>
<td>PHENYL BUTAZONE</td>
<td>C1([C][C][C][C][C]=[O]N(c2ccc2)c2)</td>
<td>0.09</td>
<td>Negative</td>
</tr>
<tr>
<td>148-82-3</td>
<td>MELPHALAN</td>
<td>C==O</td>
<td>O</td>
<td>O(C(N)Cc1cc(N(C)(C)C))CCC</td>
</tr>
<tr>
<td>154-93-8</td>
<td>carmustine</td>
<td>C==O</td>
<td>N(C(C)(C))N-O</td>
<td>NCCC</td>
</tr>
<tr>
<td>61785-57-7</td>
<td>Benzo(furazan, 4-(1-aziridinyl)</td>
<td>C1(N==O)O</td>
<td>C2=C(C(N3CC3)==C)CCC</td>
<td>1.63</td>
</tr>
<tr>
<td>62-75-7</td>
<td>N-NITROSODIMETHYLAMINE</td>
<td>C1([C][C])N=O</td>
<td>80</td>
<td>Positive</td>
</tr>
<tr>
<td>91-59-8</td>
<td>2-NAPHTHYLAMINE</td>
<td>c12c3c4c5c6c7c8c9c10c11c12c13c14c15c16</td>
<td>25</td>
<td>Positive</td>
</tr>
<tr>
<td>96-09-3</td>
<td>STYRENE_OXIDE</td>
<td>c1Cc(CO2)c3ccc1</td>
<td>0.01</td>
<td>Positive</td>
</tr>
<tr>
<td>107-13-1</td>
<td>2-propenenitrile</td>
<td>C(#N)C=C</td>
<td>2</td>
<td>Positive</td>
</tr>
<tr>
<td>51-79-6</td>
<td>URETHANE</td>
<td>C(N)O=O</td>
<td>1.8</td>
<td>Negative</td>
</tr>
<tr>
<td>53-96-3</td>
<td>2-ACETYLAMINOFLUORENE</td>
<td>c12-c3-c4-c5-c6-c7-c1-c8-c9-c10-c11-c12-c13-c14-c15-c16</td>
<td>6.2</td>
<td>Negative</td>
</tr>
<tr>
<td>54-11-5</td>
<td>Pyridine_3-(1-methyl-2-pyryl)</td>
<td>c1Cc(CCN2Cc1)ccc1</td>
<td>75</td>
<td>Negative</td>
</tr>
<tr>
<td>54-42-2</td>
<td>idoxuridine</td>
<td>C1(=O)C(=O)=C=CCO=C=O</td>
<td>0.09</td>
<td>Negative</td>
</tr>
<tr>
<td>55-38-9</td>
<td>FENTHION</td>
<td>C1(CO)[Oc3-]=S[Oc1-]OCOC</td>
<td>1.8</td>
<td>Negative</td>
</tr>
<tr>
<td>55-48-1</td>
<td>atropine_sulphate</td>
<td>C(=O)</td>
<td>C(c1ccc1)CD(OC)CC2CCO</td>
<td>4.5</td>
</tr>
</tbody>
</table>
Import of database: Vertical import

1. Go to Data panel (1);
2. Click on Import (2);
3. Click on Open file (3);
4. Select the file (Vertical import_ BOD and Ames.xlsx)(4);
5. Click on Open (5).
Import of database: Vertical import

1. A preview of the imported file is shown (1); 2. The title of the imported file is also included; 3. Click on Next (2);
1. Select *Vertical* radio button (1).
2. Header row (2)
3. Define the relevant endpoints associated with BOD (Biological oxygen demand) and Ames (Bacterial reverse mutation assay) (2) by clicking individually on each *No endpoint* selected button under the endpoints names. (4)
For BOD:
Define endpoint window is displayed (1). Select Ready Biodegradability (2) from the endpoint tree, then select the family (Biodegradability %) (3) by using the filter options (4).
Import of database: Vertical import

For **BOD**: Then select the unit from the drop-down menu (% Biodegradability(%))(5) and then to press Next (6).
Import of database: Vertical import

For BOD: Select BOD endpoint (7) from the drop-down menu. Then from the drop-down menu associated with test guideline select OECD301C (8) and test organism (species): select Microorganisms (9).
Import of database: Vertical import

For BOD: Once all the data fields are filled, press Finish (10).
Import of database: Vertical import

For **BOD**: The edited fields are displayed in the main table (11).
Import of database: Vertical import

For *Ames*:
1. Click on *No endpoint selected* (1);
2. Expand the tree and select Genetic toxicity (2).
3. From the drop-down menu of Family (3) select Gene mutation I (4), which could be found by using the implemented filter.
4. Click on *Next* (5)
Import of database: Vertical import

For Ames:
1. Select Endpoint(6) – Gene mutation(7).
Import of database: Vertical import

For Ames:
From the drop-down menu of Type of method, select In vitro and from Test type filed select : Bacterial reverse Mutation assays (e.g. Ames test) (9).
For **Ames**: Select **Test organism (species)**: Salmonella typhimurium (10) and for **Metabolic activation** and click on Without S9 (11).
Import of database: Vertical import

For *Ames*:
Select Strain: TA 100 (12) for instance and then click Finish (13).
**Import of database: Vertical import**

For **Ames**: The edited fields are displayed in the main table (14). Finally, click on **Import** (15).
Import of database: Vertical import

- The import process could take a couple of minutes;
- An informative message is displayed when it is completed;
- Click on OK (1).
The new database is displayed in the Databases panel (1) in the *Environmental fate and transport* group and in the *Human health hazard group* (2).

- Right-click menu (3) is implemented where you can see the database statistics or delete the database.
Outlook

• Aim
• Definition of Database and Inventory
• **Import:**
  - **Import of database**
    - Vertical import
    - **Horizontal import**
  - Import of inventory
  - Import via IUCLID
• Export Data matrix
Import of database: Horizontal import

- In this tutorial an example of horizontal import of a database containing experimental information related to genotoxicity is shown.
- The excel file (Horizontal import_Genotoxicity.xlsx) is depicted below and it could be found: C:\Program Files (x86)\Common Files\QSAR Toolbox 4\Config\Examples
1. Go to Data panel (1);
2. Click on Import (2);
3. Type in the name of the database as you would want it to be displayed in Toolbox (3). Otherwise the name of the file will be used as the name of the database.
4. Click on Open file (4);
5. Select the file (Horizontal import_genotoxicity.xlsx)(5);
6. Click on Open (6).
Import of database: Horizontal import

1. A preview of the imported file is shown (1); 2. Click on Next (2);
Import of database: Horizontal import

- Select *Horizontal* radio button (1)
- When there are fields from the original file which cannot be mapped to the labels existing in Toolbox, burgundy colored messages are displayed on the top (2) and Undefined is written below the data which is not mapped (3).
Import of database: Horizontal import

1. Open the drop down menu (1), type in “end” in the filter (2), select EndpointPath (3).
2. The selected label has to correspond to the one in the original file and it also written in the top message (4).
Import of database: Horizontal import

1. Open the drop down menu (1), type in “data” in the filter (2), select Data.MeanValue (3).
2. The selected label has to correspond to the one in the original file and it also written in the top message (4).
Import of database: Horizontal import

- Once all fields are mapped (1), the messages on top disappear (2).
- You can use the scrollbar (3) to check all columns, their titles and content.
- Click on Import (4)
Import of database: Horizontal import

- The import process could take a couple of minutes;
- An informative message is displayed when it is completed;
- Click on OK (1).
Import of database: Horizontal import

- The new database is displayed in the Databases panel (1) in the *Human health hazard* group (2).
- Right-click menu (3) is implemented where you can see the database statistics or delete the database.
- The software automatically adds a numeration in the name (“1” in this example) in case the same database is imported for the second time.
Outlook

• Aim
• Definition of Database and Inventory
• **Import of database:**
  - Vertical import
  - Horizontal import
  - **Supporting information**
• Import of inventory
• Export Data matrix
Supporting information

• A table of the most important endpoints implemented in Toolbox could be found in *F1 Help: D.3.4.4. Supporting Information*.

• The information in the table aims to facilitate the users’ work when importing new databases.
Outlook

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• Definition of Database and Inventory
• **Import:**
  ❖ Import of database
    ➢ Vertical import
    ➢ Horizontal import
  ❖ **Import of inventory**
  ❖ Import via IUCLID
• Export Data matrix
Import of inventory

1. Go to **Data** panel (1);  
2. Click on **Import** (2); 
3. Type in the name of the inventory as you would want it to be displayed in Toolbox (3). Otherwise the name of the file will be used as the name of the inventory. 
4. Tick “Import as inventory” (4);  
5. Click on **Open file** (5);  
6. Select the file (Import_Custom Inventory.xlsx)(6); 
7. Click on **Open** (7).
1. A preview of the imported file is shown (1);
2. Click on Next (2);
1. On the second top row are displayed the chemical identifiers as they are going to be shown in Toolbox(1);
2. Click on Import(2);
Import of inventory

• The import process could take a couple of minutes;
• An informative message is displayed when it is completed;
• Click on OK (1).
Import of inventory

- The new inventory (1) is displayed in the Inventories panel (2).
- Right-click menu (3) is implemented where you can or delete the inventory.
- The software automatically adds a numeration in the name ("1" in this example) in case the same database is imported for the second time.
Outlook

• Aim
• Definition of Database and Inventory
• **Import:**
  - Import of database
    - Vertical import
    - Horizontal import
  - Import of inventory
  - **Import IUCLID**
• Export Data matrix
Import of IUCLID

1. Go to **Data** panel (1);
2. Click on **Import** (2);
3. Click on **IUCLID** (3);
4. Select **New database** (4);
5. Write the database name (5);
6. Click on **Next** (6).
Import IUCLID

1. Write **IUCLID Server name** (1);
2. Next Port (2);
3. Next Username (3);
4. Password (4);
5. Click on **Next** (5).
1. Get All Substances (1).
2. Select the substance (2)
3. Finish (3)

Import IUCLID
1. Import completed(1).
1. Load IUCLID database(1).
Outlook

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• Import:
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    ➢ Vertical import
    ➢ Horizontal import
  ❖ Import of inventory
  ❖ Import IUCLID
• Export Data matrix
Export data matrix: Type of export

- One type of export are available in Toolbox:
  - Horizontal
- Export IUCLID
Horizontal Export

Possibility to export chemicals with data and supporting information (e.g. profiling results, 2D/3D parameters, molecular formula, etc.) available on Data matrix in text format organized in a horizontal layout.

Two options of export:

- Export row from data matrix
- Export whole data matrix

In this tutorial only the export of the whole data matrix is shown as it encompasses the first option as well.
Horizontal Export: Collecting data

1. Go to **Input** (1);
2. Go to Select (2)
3. Select from Database (3);
4. Click on **Aquatic OASIS** (4);
5. Click on **OK** (5).
Horizontal Export: Collecting data

1. Select chemicals from the first row by holding Ctrl button and click over the chemicals (1);
2. Click on OK (2).
The following steps need to be executed to gather the experimental data for the chemicals loaded on data matrix:

1. Go to Data (1);
2. Select Aquatic OASIS (2);
3. Click on Gather (3);
4. Click on OK in the Read Data window (4).
5. Click on OK in the information window (5).
1. Select Acute aquatic toxicity MOA by OASIS and apply the profiler (1)
2. Perform right click over the data matrix and select Export data matrix (2)
1. Aquatic toxicity (1) is selected as the right click was next to that branch;
2. Expand the Profile level (2) and then select Acute aquatic toxicity MOA by OASIS(3);
3. Click on Export (5).
1. Type in the name (e.g. Horizontal_export) (1). The file is saved in csv format.
2. Click on Save (2).
3. Click OK in the information message (3).
The file can be opened in excel. It contains the following main sections: chemical identity of each chemical (red, 1), experimental data (pink, 2), endpoint (purple, 3), metadata (blue, 4), profiler results (green, 5). Here, if the chemical has several experimental data each one is listed on separate row (e.g. CAS 62-53-3).