OECD QSAR Toolbox v.4.4

Category elements for assessing category consistency
Outlook

• **Background**
• **Keywords**
• **Objectives**
• **Aim**
• **Category consistency**
• **Examples**
Background

• This is a step-by-step presentation designed to introduce to the user the category elements applicable for assessing category consistency

• Further to illustrate some simple examples of using category consistency elements targeting Fate and Human toxicity endpoints
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Keywords

TARGET CHEMICAL - chemical of interest

MODULE - a Toolbox module is a section dedicated to specific actions and options (e.g. Profiling)

WORKFLOW - the use, in combination, of the different modules (e.g. prediction workflow: from input to report)

PROFILER - algorithm (rule set) for the identification of specific features of the chemicals. Several types of profilers are available, such as structural (e.g. Organic functional groups), mechanistic (e.g. Protein binding by OECD) and endpoint-specific (e.g. in vitro in vitro mutagenicity (Ames test) alerts by ISS) profilers.

ALERT - the profilers consist of sets of rules or alerts. Each of the rules consists of a set of queries. The queries could be related to the chemical structure, physicochemical properties, experimental data, comparison with the target or list with substances and external queries from other predefined profilers (reference queries).

CATEGORY - “group” of substances sharing same characteristics (e.g. the same functional groups or mode of action). In a typical Toolbox workflow, it consists of the target chemical and its analogues gathered according to the selected profilers during Category definition process.

ENDPOINT TREE - Endpoints are structured in a branched scheme, from a broader level (Phys-Chem properties, Environmental Fate and transport, Ecotoxicology, Human health hazard) to a more detailed one (e.g. EC3 in LLNA test under Human health hazard-Skin sensitization)

DATA MATRIX - Table reporting the chemical(s) and data (experimental results, profilers outcomes, predictions). Each chemical is in a different column and each data in a different row
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Objectives

This presentation demonstrates a number of functionalities of the Toolbox:

• Including category elements in the process of category consistency assessment.

• Generation of the category report including category consistency elements.
Outlook

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Aim

• To introduce and make the user familiar with:
  • the similarity elements (physicochemical parameters, profilers) used in category consistency assessment;
  • the default settings of category consistency elements for reporting.
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    o Adopted concept
    o Elements of category consistency
    o Implementation in Toolbox
• Examples
Overview
What is a category?

• Based on REACH regulation [1]:

“Substances whose physicochemical, toxicological and ecotoxicological properties are likely to be similar or follow a regular pattern as a result of structural similarity may be considered as a group, or ‘category’ of substances.”

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Category consistency
Adopted concept

• The read-across methodology is based on the premise that similar chemical structures (forming the category) are expected to have similar biological/toxicological action with respect to the endpoint

• Category consistency is endpoint specific;

• Category consistency check (using category elements) can be applied to:
  • a list with chemicals with a defined target endpoint - there is no need to enter into the data gap filling (i.e. it could be done without accepted prediction)
  • analogues developed during the read-across workflow (in the data gap filling)
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Three layers of information are considered important in analyzing consistency of chemical categories:

- **Physicochemical similarity** (e.g. MW, VP, logKow etc.) and experimental data
- **Structural similarity** (e.g. Organic functional groups (OFG))
- **Mechanistic similarity** (e.g. Protein binding alerts for skin sensitization accounting for (a)biotic activation in case the target endpoint is skin sensitization)

The layers mentioned above are implemented as elements of the category consistency (see next few slides)
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  o Implementation in Toolbox
• Examples
Category consistency

Implementation in Toolbox

• New functionality related to Category consistency assessment has been implemented in version 4.2
• It is located in the “Category definition” module and provides default selection of category consistency elements as follows:
  • **Physicochemical similarity** – does not depend on the endpoint
    ▪ **Parameters** - Boiling point, logKow, Molecular weight, Vapor pressure, Water solubility
    ▪ **Physico-chemical exp. data** - Boiling point, logKow, Vapor pressure, Water solubility
  • **Structural similarity** – does not depend on the endpoint
    ▪ Organic functional groups
    ▪ Structure similarity
  • **Mechanistic similarity** – depends on the pre-defined target endpoint

The profilers and metabolism simulators highlighted as “suitable” for the target endpoint are selected by default (e.g. for target endpoint Skin sensitization/LLNA/EC3 all *Protein binding alerts for skin sensitization* profilers along with the simulators for *Autoxidation* and *Skin metabolism* are selected by default)

• **(Eco)toxicological experimental data** – depends on the pre-defined target endpoint
• Different selection of the category consistency elements than the default one is allowed
Category consistency
Implementation in Toolbox

• “Category consistency” is located in *Category definition* module
• It allows to filter and collect physico-chemical properties, structural similarity, profiling results accounting for metabolic activation and experimental data
• All selected category elements are automatically stored in the so-called "*Report basket*", which could be added later on in the report (overview of the Report basket is provided on next slide).
• Evaluation of category consistency is possible if the target endpoint is defined
Category consistency

**Report basket - background**

- The specific report items are collected during the workflow or from external modeling sources.
- All items are stored in the “Report basket” and can be used in the report to support or justify the consistency of a category.
# Category consistency

## Report basket – examples of the items stored here

<table>
<thead>
<tr>
<th>#</th>
<th>Specific report item</th>
<th>Related to:</th>
<th>Options</th>
<th>Actions which trigger saving results in the basket</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Target information</td>
<td>Target chemical</td>
<td>Target is defined</td>
<td>Depiction of chemical; CAS; Names; SMILES</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Purity/ Impurity</td>
<td>Target chemical; Category</td>
<td>Target or category members have compositions</td>
<td>Table with description of composition with depictions, quantities of each structure</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Category members</td>
<td>Category</td>
<td>Category is defined or a list with structures is loaded/ created</td>
<td>Table with depiction; CAS; Name; SMILES of all chemicals</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>Physical chemical similarity</td>
<td>Category</td>
<td>Select 2D parameters and/or physical chemical properties</td>
<td>Table with calculated 2D parameters; Table with experimental physical chemical properties</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>Structural similarity</td>
<td>Category</td>
<td>Adjust structure similarity options</td>
<td>Table with calculated similarity and variation of similarity with other chemicals</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>Mechanistic similarity</td>
<td>Category</td>
<td>Select metabolism and profiler; Add table; add summary chart; add individual charts</td>
<td>Tables with generated metabolites and their profiling result; Table summarizing number of metabolites and found alerts; Graphic with distribution of alerts across metabolites</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>Common product</td>
<td>Metabolism</td>
<td>Category is defined with accounting for metabolism with map similarity option “exact” metabolite</td>
<td>Depiction of common compound (defined in grouping options) and used simulator</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>Alert performance</td>
<td>Category</td>
<td>Calculation of alert performance</td>
<td>Alert performance table</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>Reliability/ adequacy</td>
<td>Data</td>
<td>Select which metadata to be reported</td>
<td>Table with analogues used for retrieving the prediction with their observed data</td>
<td></td>
</tr>
<tr>
<td>…</td>
<td>………………………….</td>
<td>………………..</td>
<td>…………………………</td>
<td>……………………….</td>
<td></td>
</tr>
</tbody>
</table>
Category consistency

Report basket – visualization

**Report basket:**

- The selected category elements are automatically stored in the so-called "Report basket" (the latter appears once click Add/Remove button included in the Reporting wizard).

- Additional report items (such as parameter variation for the closest analogues, text, pictures etc.) could be added via clicking on “Create new”.

Examples of the report items generated in the basket are given on the next slides.
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• Category consistency
• **Exercise**
Category consistency elements

Exercise

• Three examples will be illustrated addressing category consistency elements used in the read-across assessment of Fate and Human health endpoints:
  • *Fate endpoint* – BOD
  • *Ecotoxicity endpoint* – LC50
  • *Human health hazard* – skin sensitization (EC3)

• Illustrating of category consistency elements will be applied on a predefined lists with chemicals without entering into the data gap filling

* Predefined lists with chemicals are available in the Toolbox installation folder located at: C:\Program Files (x86)\Common Files\QSAR Toolbox 4.4\Config\Examples
Category consistency elements

Example 1 – *Fate endpoint*

- A list of 7 aromatic halogens is submitted as a category
- The target endpoint is: Ready Biodegradability/BOD/OECD 301C

1. Open the list with chemicals "Category_consistency_BOD_Aryl_chlorides.smi" from the example folder
2. Click Define, open Environmental Fate and Transport, Biodegradation level and select Ready Biodegradability, after that select Endpoint: BOD; Test guideline: OECD 301C
3. Click Finish
Category consistency elements

Example 1 – *Fate endpoint*

This wizard allows selection of properties in the data matrix relevant to the assessment of the category consistency. The selection could be used for an expert judgment considerations and it is also saved for the Category report. It works by filtering the endpoint tree according to the selected properties.

The endpoint tree elements are grouped as follow:

1. **Physicochemical similarity**: calculated and experimental physicochemical parameters.
2. **Structural similarity**: empirical profilers.
3. **Mechanistic similarity**: mechanistic and endpoint specific profilers, and metabolic simulators.
4. **(Eco)tox data**: experimental data from Toolbox databases

The Toolbox automatically highlights profilers and metabolic simulators relevant to the target endpoint.
Category consistency elements

Example 1 – *Fate endpoint*

Category element: **Physicochemical similarity**

Default selection of 2D parameters (calculated values and exp. data) are as follows:

- Boiling point
- logKow
- Molecular weight
- Vapor pressure
- Water solubility
Category consistency elements

Example 1 – *Fate endpoint*

Category element: **Physicochemical similarity**

The user can select other parameters or experimental phys-chem data for the analysis from the lists.

The default selections can be changed by clicking the **Add/Remove** button (1). In this example keep the default selections. Move to Structural similarity. The selections will be preserved (see next slide).
Category consistency elements

Example 1 – Fate endpoint

Category element: Structural similarity

1. Select Structural similarity section
2. Keep the default selections
3. Move to Mechanistic similarity

Default selection of profilers related to structural similarity includes:
- Organic functional groups
- Structure similarity

You can select other structure-based profilers from the list. The selections will be preserved and applied once the category elements are executed.
Category consistency elements

Example 1 – *Fate endpoint*

**Category element:** Mechanistic similarity

You can select other profilers or metabolic simulators from the plausible list for example. The profiling results will appear on data matrix application of the category consistency elements (see next slide).

1. Select **Mechanistic similarity** section
2. Select the plausible Biowin 5 and 6 along with Aquatic toxicity classification by ECOSAR profilers as these are relevant to the investigated endpoint (BOD)

Default selection of endpoint specific profilers and simulators depend on defined target endpoint. In this case the default selection includes:

- Biodegradation fragments (BioWIN MITI)
Category consistency elements

Example 1 – *Fate endpoint*

Category element: *(Eco)tox experimental data*

1. Select *(Eco)tox experimental data* section
2. Data related to biodegradation endpoint is selected by default
3. Click *Add* button to add additional experimental data
4. **Select** *Bioaccumulation: aquatic* node after that select BCF endpoint in order to add BCF data for the analogues if available
5. Click *Finish* button
6. Finally, click *OK* on Category consistency wizard window in order to execute the consistency elements

Additional experimental data to support the consistency of the category could be selected. The data for the analogues will appear on the data matrix (DM) later on if available.
Category consistency elements

Example 1 – *Fate endpoint*

Selected parameters and experimental data related to “Physicochemical similarity” (shown on slides #26-27) are calculated/extracted from databases and filtered* on the DM

* Filtering of DM is illustrated on the next slide. More details could be found in tutorial: Manipulation of data matrix and manual transferring of data to the target outside data gap filling module.
Category consistency elements

Example 1 – *Fate endpoint*

Filtering of DM

Button for filtering the endpoint tree

In this case given the fact that “category elements” are applied to the category members, data matrix is filtered respectively (only the nodes associated with default 2D parameters, exp. BOD data and related profilers are selected)

Click OK button to confirm the selection
Category consistency elements

Example 1 – *Fate endpoint*

Profiling results from the selected structure–based profilers appeared on DM (see slide #28)

Profiling results from the selected OFG profiler appeared on DM
Category consistency elements

Example 1 – *Fate endpoint*

Profiling results from the selected structure–based profilers appeared on DM (see slide #28)

Profiling results from the selected “Structure similarity” profiler appeared on DM. The similarity is estimated by analyzing variations of similarity values between category members (analogues).
Category consistency elements

Example 1 – *Fate endpoint*

Profiling results from the selected mechanism-based profilers appeared on DM (slide #29)

All the chemicals within the category are consistent with respect to the selected mechanism-based profilers
Category consistency elements

Example 1 – *Fate endpoint*

Experimental data related to the target endpoint and additionally added (slide #30) appeared on DM.

BOD and BCF data are filtered and appeared on DM if available.
Category consistency elements

Example 2 – Ecotox endpoint

- A list of 15 Aliphatic amines is submitted as a category
- The target endpoint is: Aquatic toxicity/LC50/96h/P.promelas/Mortality

1. Open the list with chemicals “Category consistency_Ecotox_Amines_LC50_96h_P.promelas.smi” from the example folder
2. Click Define and fill in the fields of the target endpoint as shown on the snapshot on the right
3. Click Finish
Category consistency elements

Example 2 – Ecotox endpoint

1. Go to **Category Definition** module
2. Click on **Category elements** button
3. The “Category consistency wizard” appears

The OECD QSAR Toolbox for Grouping Chemicals into Categories

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1. The only difference with the previous example is the default selection of **mechanism-based profilers**. The latter **depends on the defined target endpoint**

2. Keep the default selections of profilers and phys-chem parameters

3. Click **OK** button
### Category consistency elements

**Example 2 – Ecotox endpoint**

Selected data and profilers related to the specific Category elements appeared on DM

#### Calculated phys-chem values

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Log Kow</td>
<td>-1.13, -0.13, -0.03, 4.27, 4.76, 5.25, 3.29, 2.8, 1.62, 1.33, 3.70, 2.31, 0.35, 0.03</td>
</tr>
<tr>
<td>Molecular Weight</td>
<td>741 Da, 451 Da, 171 Da, 189 Da, 199 Da, 145 Da, 129 Da, 601 Da, 87.2 Da, 157 Da, 116 Da, 73.1 Da, 101 Da</td>
</tr>
<tr>
<td>Vapor Pressure</td>
<td>0.09 mm Hg, 0.0495 mm Hg, 0.000645 mm Hg, 0.00013 mm Hg, 0.035 mm Hg, 1.07 mm Hg, 19 mm Hg, 32.8 mm Hg, 0.136 mm Hg, 3.3 mm Hg, 0.215 mm Hg, 97.6 mm Hg, 9.49 mm Hg</td>
</tr>
<tr>
<td>Water Solubility</td>
<td>139 mg/L, 45.1 mg/L, 14.6 mg/L, 1266 ± 3 mg/L, 3.150 ± 3 mg/L, 15 ± 06 mg/L, 8.866 ± 04 mg/L, 423 mg/L, 1.750 ± 03 mg/L, 5.340 ± 05 mg/L, 2.006 ± 05 mg/L, 2.068 ± 04 mg/L</td>
</tr>
</tbody>
</table>

#### Exp. phys-chem data

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Partition Coefficient</td>
<td>M: 1.43, M: 0.27</td>
</tr>
<tr>
<td>Vapour pressure</td>
<td>M: 4.11 kPa, M: 990 kPa</td>
</tr>
<tr>
<td>Water solubility</td>
<td>M: 0.0079 mg/L, M: 0.278 mm Hg, M: 0.81 kPa, M: 12 mm Hg, M: 30 mm Hg, M: 0.1 mg Hg, M: 3.74 mg/L, M: 0.110 mg/L, M: 92.9 mg/L, M: 8.99 mg/L</td>
</tr>
</tbody>
</table>

#### Experimental endpoint data

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aquatic Toxicity</td>
<td>AW SW 15/56, M: 1.1, M: 0.13, M: 4.3, M: 0.48, M: 5.68, M: 3.3, M: 2.8, M: 1.6, M: 1.3, M: 3.8</td>
</tr>
</tbody>
</table>

#### Mechanistic and structure-based profiling results

<table>
<thead>
<tr>
<th>Profile</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Structure similarity</td>
<td>25.40% ± 0.39%, 18.2 ± 57.1%, 23.9 ± 96.3%, 22.2 ± 96.3%, 28.6 ± 95.2%, 30.8 ± 94.7%, 22.2 ± 0.99%, 40.92% ± 3.93%, 26.7 ± 95.7%, 33.3 ± 94.1%, 18.2 ± 76.9%, 44.4 ± 9.0%, 30.4 ± 9.3%</td>
</tr>
</tbody>
</table>
Category consistency elements

Example 3 – Human health hazard endpoint

- A list of four amines is submitted as a category
- The target endpoint is: EC3/LLNA/Skin sensitization

1. Open the list with 4 amines “Category_consistency_SS_list_of_amines.smi” from the example folder
2. Click on Define button and define the target endpoint as shown on the snapshot on the right
3. Click Finish
Category consistency elements

Example 3 – *Human health hazard endpoint*

1. Go to **Category Definition** module
2. Click **Category elements** button
3. The “**Category consistency wizard**” appears
1. As in the previous two examples, the default selection of 2D/3D parameters and structure-based profilers are the same and do not depend on the defined target endpoint, while the default selection of mechanism-based profilers are different in all the three examples. Moreover, it depends on the defined target endpoint. As can be seen, the mechanistic profilers could be combined with appropriate metabolism.

2. Keep the default selection of profilers, metabolic simulators, and phys-chem properties.

3. Click OK button.
Category consistency elements

Example 3 – Human health hazard endpoint

Selected data and profilers related to the specific Category elements appeared on DM

- Calculated phys-chem values
- Exp. phys-chem data
- Experimental data
- Mechanistic and structure-based profiling results
Category consistency elements

Report

A report can be obtained for:

1) A category (list of chemicals) with defined target endpoint without entering into data gap filling (1) OR
2) The prediction based on the analogues grouped during the read-across workflow (in the data gap filling) (2)

A report for a list of chemicals without entering into data gap filling will be illustrated in the next few slides (point 1)
Category consistency elements

Report

A report for the list of aliphatic amines associated with skin sensitization endpoint (Example 3) will be illustrated.

1. Click on the document for assessment category consistency of the list with aliphatic amines
2. Go to Report module
3. Click on Category report
4. The wizard window with sections of the category report appeared

Sections of the Category report
Category consistency elements

Report

Category part of the wizard has three sections:

- “Category definition and members” – include sections associated with the definition of the category and category members
- “Consistency check” - include sections associated with category consistency elements
- “Options” - include options for changing number of reported category members
Section “Category definition and members” includes three subsections:
- 1.1. Category definition
- 1.2. Category members
- 1.3. Profiles/Metabolisms
Sub-section “1.1. Category definition” includes fields related with:

- Category name which should be added manually by the user
- Target endpoint definition - automatically populated
- Hypothesis for defining the category – need to be added manually
Sub-sections “1.2. Category members” and “1.3. Profiles/metabolisms” includes fields related with:

- Information for the category members. A table with category members is automatically provided.
- Description why the category can be formed (e.g. common functional group(s), common precursor(s)/breakdown product(s), common mechanism(s) of action, trends in properties and/or activities).
- Purity/Impurity information should be added by the user.
- List of profilers/metabolisms used in category definition are provided.
Category consistency elements

Section “Consistency check” includes elements of the category consistency:

- 2.1. Physicochemical similarity
- 2.2. Structural similarity
- 2.3. Mechanistic similarity
- 2.4. Additional endpoints
Sub-section “2.1. Physicochemical similarity” includes fields related with:

- Collection of calculated physicochemical parameters already selected in the ‘Category consistency’ tool appear here
- A table with calculated physicochemical parameters selected in the ‘Category consistency’ tool appear here
- The experimental physicochemical parameters selected in the ‘Category consistency’ tool appear here. A table with phys-chem parameters for category members is automatically provided.

Text justifying the selected parameters should be added by user.
Sub-section “2.2. Structural similarity” includes fields related with:

- The profilers selected in the ‘Category consistency’ tool appear here
- Tables with profiling results based on the selected profilers for the chemicals from the category appear here
- Tables could be edited or previewed
- The order of appearance of the tables in the report could be changed

Text justifying the selected profilers should be added by user

Keep the default settings
Sub-section 2.3. Mechanistic similarity includes:

- The profilers and simulators selected in the ‘Category consistency’ wizard appear here

- Tables with profiling results for the category members appear here

Text justifying the selected profilers should be added by user

Keep the default settings
Sub-section 2.4. Additional endpoints includes fields related with:

- Details for the selected target endpoint is automatically listed here
- Tables with selected endpoint data is automatically generated

In this field user could add a summary of how the available experimental data verify that the category is robust (i.e. category hypothesis and consistency check)
“Report basket” stores automatically all category elements which have been applied by the user. It is visualized by clicking Add/Remove button. Some of the items are automatically selected and could be used directly for generating the report.

New items with external content can be also included by click on the Create New button.

Finally, Click Create report
Category consistency elements

Report

1. Select **Category report**
2. Click **Open**

Two files are generated:
- **Category report** - includes all the information related to the category in pdf format
- **Data matrix** – includes information for the category (as parameters, profilers, data) in excel (xlsx) format
1. **Category definition section:**

1.1. Category definition – includes:
- name of the category if provided by the user;
- Covered (target) endpoint(s) – automatically fulfilled
- Category hypothesis – information provided by the user

1.2. Category members
- a table with category members is provided;
- ranges of selected experimental and calculated physicochemical properties in table format;
- information for Purity/Impurity manually added by the user

1.3. Profiling/Metabolisms –
- additional profilers/metabolisms could be provided by the user
2. Consistency check section:

2.1. Physicochemical similarity – provides information for the selected physicochemical parameters (calculated values and exp data) for each member of the category.

2.2. Structural similarity – provides profiling results from the selected structure-based profilers – “Structural similarity” and “OFG” for each member of the category.
## Category consistency elements

### 2. Consistency check section (cond.):

#### 2.3. Mechanistic similarity

- Provides information for the selected profiles (assigned as suitable with respect to the target endpoint and/or manually added by the user to justify the consistency).

This section includes:

- Profiling results for all category members
- Tables for parents and generated metabolites (if any)
- Graphics with distribution of alerts across metabolites
- Tables summarizing the number of metabolites (including parent) with specific alerts
2. Consistency check section (cond.):  

2.4. Additional endpoints

Additional endpoints
- Human Health Hazards/Sensitisation: Skin
- Type of method: In Vivo
- Assay: LLNA
- Endpoint: EC3

Table with selected endpoint data values

<table>
<thead>
<tr>
<th>CAS #</th>
<th>H2N—NH—NH2</th>
<th>H2N—NH2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 56-18-8</td>
<td>0.882±0.9 % (x2)</td>
<td>2.2±2.7 % (x4)</td>
</tr>
<tr>
<td>2 107-15-3</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>CAS #</th>
<th>H2N—NH—NH2</th>
<th>H2N—NH2—OH</th>
</tr>
</thead>
<tbody>
<tr>
<td>3 111-40-0</td>
<td>1.85±5.8 % (x4)</td>
<td></td>
</tr>
<tr>
<td>4 111-41-1</td>
<td>15.2 %</td>
<td></td>
</tr>
</tbody>
</table>

Comments on additional endpoints
Not provided by the user

2. Consistency check section:

2.4. Additional endpoints – provides experimental data for all category members related to the additionally added endpoints
The number in brackets shows how many times the same experimental result is recorded
Category consistency elements

Data matrix

1. Select Data matrix report
2. Click Open
# Category consistency elements

## Data matrix report

### Parameters values and profilers used in the workflow

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Profilers accounting for metabolism if applied</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dosing route</td>
<td>Oral, Intravenous, Intraperitoneal</td>
</tr>
<tr>
<td>Route</td>
<td>Oral, Intravenous, Intraperitoneal</td>
</tr>
<tr>
<td>Species</td>
<td>Rat, Mouse, Human</td>
</tr>
<tr>
<td>Profilers</td>
<td>Fatty acid profile, Protein profile, mRNA expression profile</td>
</tr>
</tbody>
</table>

### Measured data for the chemicals in the category

<table>
<thead>
<tr>
<th>Chemical Identity</th>
<th>Structure</th>
<th>measured data for chemicals</th>
<th>profiled data for metabolism</th>
<th>calculated data for toxicity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemical #1</td>
<td><img src="image1" alt="Chemical #1 structure" /></td>
<td><img src="image2" alt="Measured data" /></td>
<td><img src="image3" alt="Profiled data" /></td>
<td><img src="image4" alt="Calculated data" /></td>
</tr>
<tr>
<td>Chemical #2</td>
<td><img src="image5" alt="Chemical #2 structure" /></td>
<td><img src="image6" alt="Measured data" /></td>
<td><img src="image7" alt="Profiled data" /></td>
<td><img src="image8" alt="Calculated data" /></td>
</tr>
<tr>
<td>Chemical #3</td>
<td><img src="image9" alt="Chemical #3 structure" /></td>
<td><img src="image10" alt="Measured data" /></td>
<td><img src="image11" alt="Profiled data" /></td>
<td><img src="image12" alt="Calculated data" /></td>
</tr>
</tbody>
</table>

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The OECD QSAR Toolbox for Grouping Chemicals into Categories

November, 2019
Congratulations!

• You have now been introduced to the defining of a target endpoint;
• You have now been introduced to the elements of the category consistency;
• You have now been introduced to the Report basket;
• Note, proficiency comes with practice!