

OECD QSAR Toolbox v.4.1

Examples illustrating customized
search (Query Tool) in Toolbox

Outlook

- **Background**
- Objectives
- Overview of Query tool
- Query tool window
- The exercise
- Workflow process
- Save QT searches

Background

- This is a step-by-step presentation designed to take the user through the functionalities of Query tool (QT) engine implemented in Toolbox

Outlook

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Objectives

This presentation demonstrates a number of functionalities of the Query tool (QT):

- Identifying chemicals with specified structural fragments
- Identifying chemicals answering specific structural fragment criteria combined with parametric ranges
- Identifying chemicals answering specific combination of data, structural fragments and parametric data

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Overview of Query tool

Goal: Searching for chemicals by structure, sub fragments, phys-chem properties and experimental data

- **Chemical identifier search**

- CAS
- Name
- Molecular structures

- **Parameter search**

- Calculated 2D parameters
- Calculated 3D parameters

- **Data search**

- Search for data and metadata within imported databases

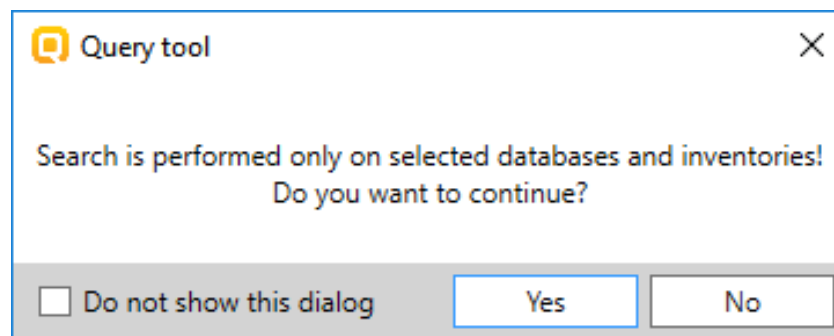
- **Extended search**

- Profiling
- Substructure
- Similarity

Overview of Query tool

Prerequisites

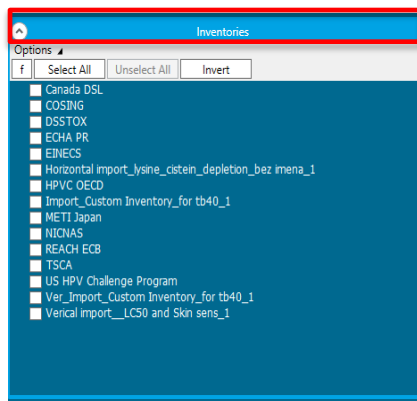
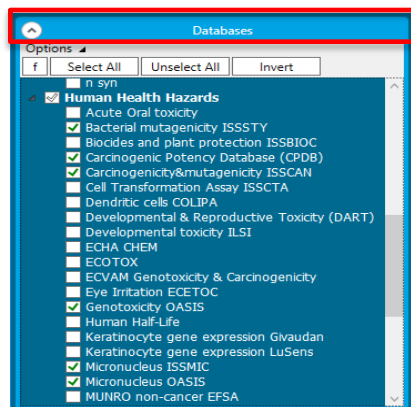
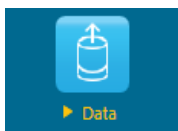
- The Query tool functionality search for single structures matching desired criteria.
- The Query tool functionality search for chemicals within the selected databases and inventories only



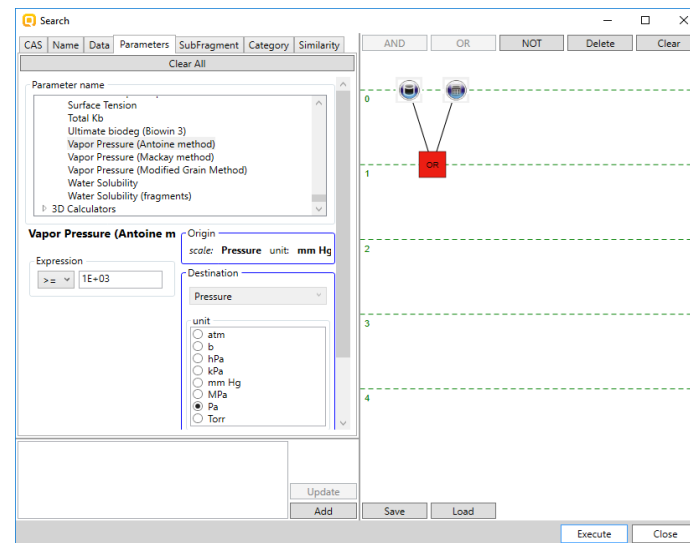
Overview of Query tool

Procedure for defining query

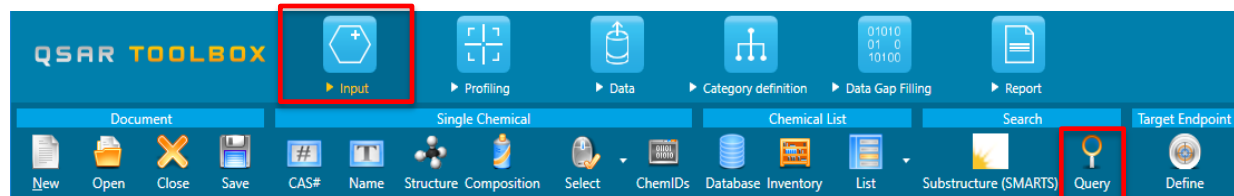
Step 1: Select databases/inventories of interest in the *Data* module



Step 3: Specify criteria for searching structures



Step 2: Click *Query* button

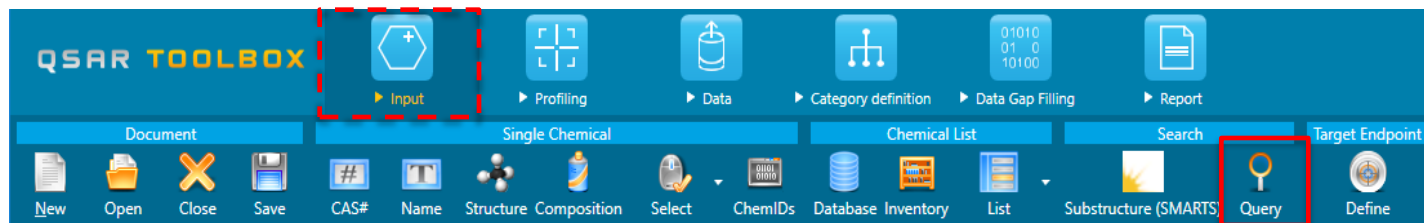


Outlook

- Background
- Objectives
- Overview of Query tool
- **Query tool window**
- The exercise
- Workflow process
- Save QT searches

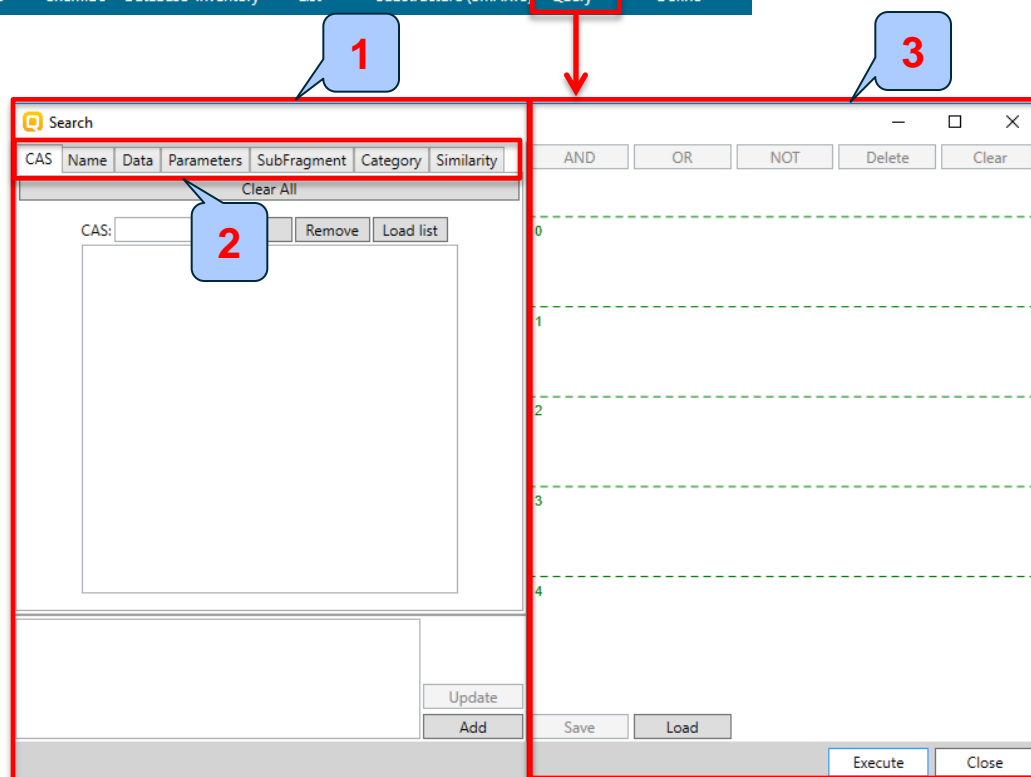
Query tool window

- The Query tool is easily accessible on the Toolbox input panel



The main components of Query tool include:

- Query edit panel (1)
 - search group panel (2)
- Query tree logic panel (3)



Outlook

- Background
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- Overview of Query tool
- Query tool window
- **The exercise**
- Workflow process
- Save QT searches

The Exercise

- In this exercise we will demonstrate the following queries:
 - Subfragment search for:
 - *Substituted diphenyl amine (Example 1)*
 - *Aliphatic halogens (Example 2)*
 - Combination of Environmental Data (BCF) and 3D parameters (*Dmax*) (*Example 3*)
 - Combination of predefined category (Aldehydes) and ecotox data ($LC_{50} < 1\text{mg/l}$) (*Example 4*)
 - Combination of positive Ames; positive Carcinogenicity data and Subfragment search (*Epoxides*) (*Example 5*)
 - Combination of Skin sensitization data (EC3) and predefined category (*Aldehydes*) (*Example 6*)

Outlook

- Background
- Objectives
- Overview of Query tool
- Query tool window
- The exercise
- **Workflow process**
- Save QT searches

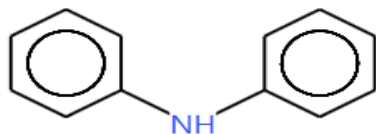
Subfragment search for identifying chemicals

Substituted diphenyl amine

Example 1

Search for structures that meet the structural requirements:

- *Substituted diphenyl amine*



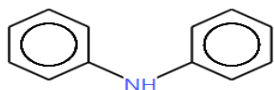
N(c1ccccc1)c1ccccc1

Subfragment search for identifying chemicals

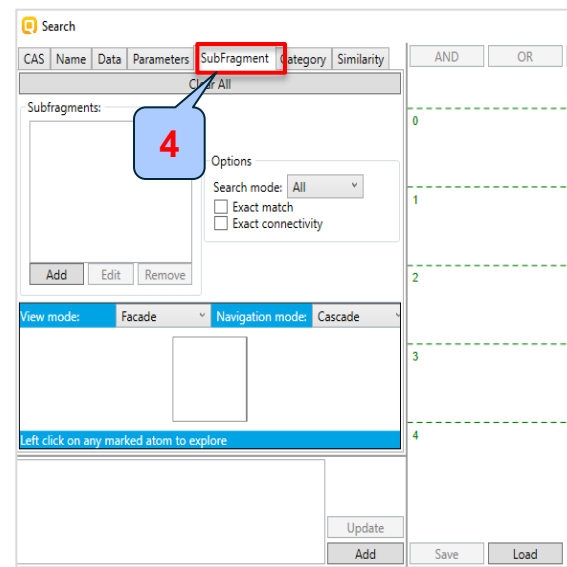
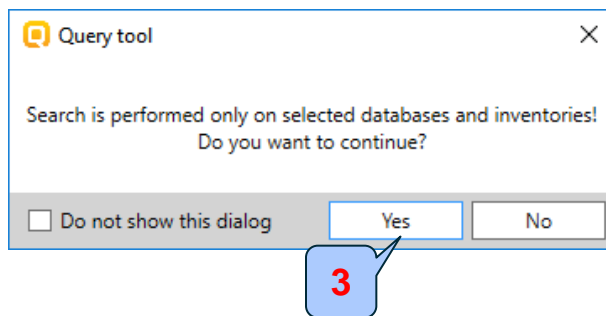
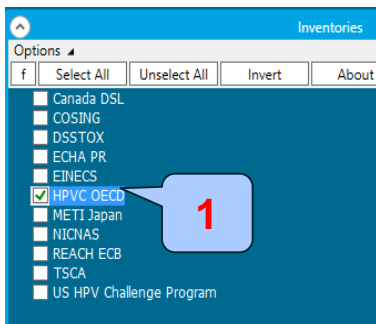
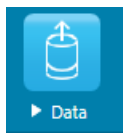
Procedure for defining

Example 1

Substituted diphenyl amine



N(c1ccccc1)c1ccccc1



QT procedure starts with selecting databases/inventories used for searching the desired criteria:

1. **Select** HPVC OECD inventory located under Data section. No databases have been selected in this exercise;
2. Click **Query** button located under **Input** section; The message informs the user that search will be performed on selected databases or inventories only
3. Click **Yes**;
4. Query panel appears;
5. Select **SubFragment** panel;

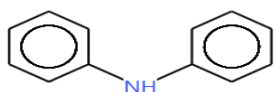
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Subfragment search for identifying chemicals

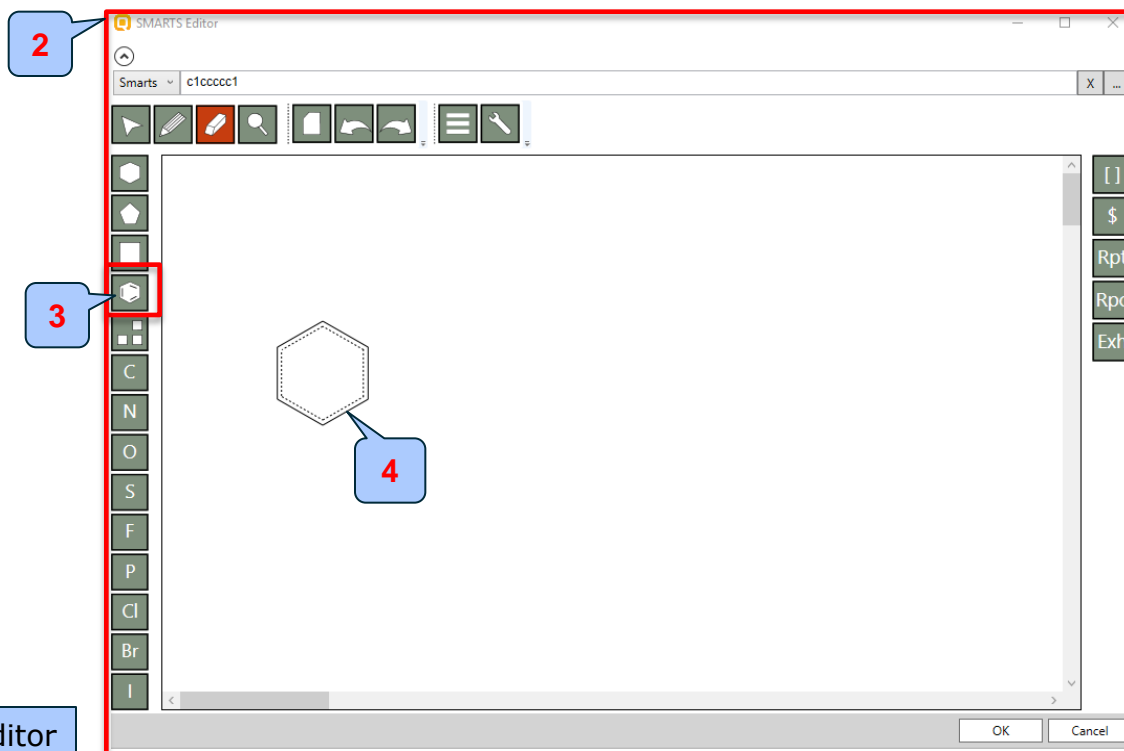
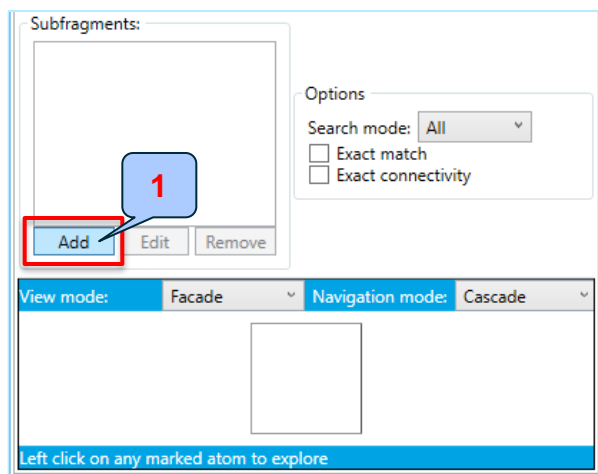
Procedure for defining

Example 1

Substituted diphenyl amine



N(c1ccccc1)c1ccccc1



1. Click **Add** button; 2. The SMARTS Editor window appears; 3. Perform **left click** on the benzene ring from the Template panel 4. **Left click** on the blank plot in order to put benzene fragment;

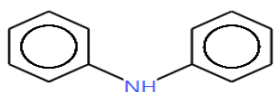
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Subfragment search for identifying chemicals

Procedure for defining

Example 1

Substituted diphenyl amine



N(c1ccccc1)c1ccccc1

Subfragments:

Options

Search mode: All

Exact match

Exact connectivity

Add Edit Remove

View mode: Facade

Navigation mode: Cascade

Left click on any marked atom to explore

5. Click the pencil button to draw a single bond; 6. Click near to one of the C atom from the benzene ring to draw a single bond; 7. Click **N** atom from the templates; 8. Put the selected N atom over the C atom from the single bond; 9. Repeat step 5 and draw a single bond to the N atom from NH2 group;

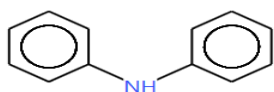
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Subfragment search for identifying chemicals

Procedure for defining

Example 1

Substituted diphenyl amine



N(c1ccccc1)c1ccccc1

Subfragments:

Options

Search mode: All

Exact match

Exact connectivity

Add Edit Remove

View mode: Facade Navigation mode: Cascade

Left click on any marked atom to explore

SMARTS Editor

Smarts: c1ccc(cc1)NC

10

11

12

OK Cancel

10. Left click over benzene ring from the template in order to take benzene ring 11. Left click over the C atom in order to define second benzene ring to the NH group 12. Click **OK**.

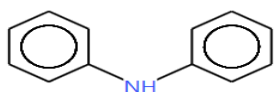
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Subfragment search for identifying chemicals

Procedure for defining

Example 1

Substituted diphenyl amine



N(c1ccccc1)c1ccccc1

1. Click **Add** button; 2. The defined query appears on logic panel; 3. Double click over the query or click **Execute** button to execute it.

The screenshot shows the 'Search' window with the following components:

- Subfragments:** A list containing the query c1ccc(cc1)Nc1ccccc1. Below the list are 'Add', 'Edit', and 'Remove' buttons.
- Options:** A section with 'Search mode: All' and checkboxes for 'Exact match' and 'Exact connectivity'.
- Logic Panel:** A vertical stack of slots (0-4). Slot 0 contains the query c1ccc(cc1)Nc1ccccc1, which is highlighted with a red box and callout '2'.
- Buttons:** At the bottom, the 'Add' button is highlighted with a red box and callout '1', and the 'Execute' button is highlighted with a red box and callout '3'.

Subfragment search for identifying chemicals

Procedure for defining

Example 1

Substituted diphenyl amine

The screenshot shows the QSAR Toolbox software interface. The main workspace displays a table of search results for substituted diphenyl amines. The table has 7 columns, each containing a chemical structure. A red box highlights the entire table. A red arrow points from a 'Structural criteria' box (containing a diphenyl amine structure) to a 'Filter endpoint tree...' box (containing a complex chemical structure). A red box also highlights the 'Filter endpoint tree...' box. A red box with the number '1' is in the top left corner of the interface.

1. The Query tool (QT) identified 26 chemicals matching the desired criteria

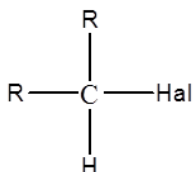
Subfragment search for identifying chemicals

Aliphatic halogens

Example 2

Search for structures that meet the structural requirements:

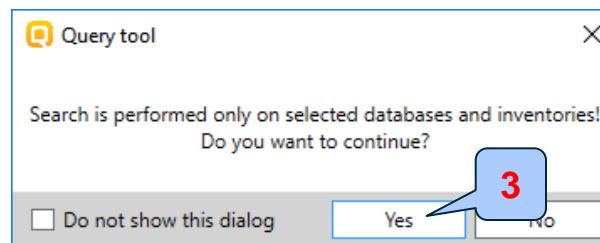
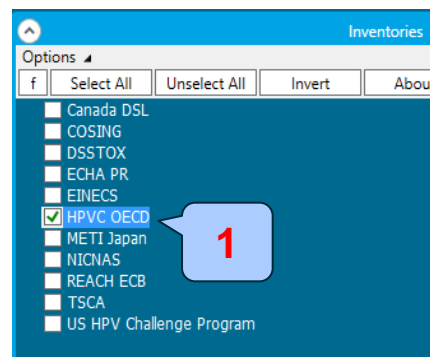
- *Aliphatic halogens*



R – Any atom except H

Hal – Cl, Br, I

- **HPVC OECD** inventory has been selected
- Search for discrete chemicals



1. Select the **HPVC OECD** inventory (no database has been selected in this case, only HPVC OECD) located under *Data* section; 2. Click **Query** button under *Input* section; 3. Click **Yes**

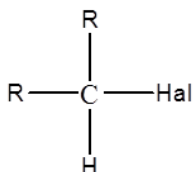
Subfragment search for identifying chemicals

Aliphatic halogens

Example 2

Search for structures that meet the structural requirements:

- *Aliphatic halogens*



R – Any atom except H

Hal – Cl, Br, I

- **HPVC OECD** inventory has been selected
- Search for discrete chemicals

1. Query panel appears; 2. **Go** to SubFragment panel; 3. **Click** "Add" button; 4. "SMARTS Editor" window appears;

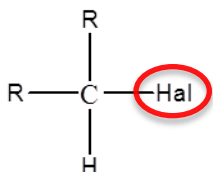
Subfragment search for identifying chemicals

Aliphatic halogens

Example 2

Search for structures that meet the structural requirements:

- *Aliphatic halogens*



R – Any atom except H

Hal – Cl, Br, I

- Define **Enumeration** fragment with three members (halogen atoms)

1. Left click the **C** symbol from the template and then left click in the drawing panel;
2. Left click the **pencil** button and draw a single bond;
3. Select the “[]” (enumeration) button;
4. Click over one of the carbon atoms;

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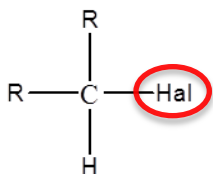
Subfragment search for identifying chemicals

Aliphatic halogens

Example 2

Search for structures that meet the structural requirements:

- Aliphatic halogens



R – Any atom except H

Hal – Cl, Br, I

- Define **Enumeration** fragment with three members (halogen atoms)

5. Click the **selection tool**; 6. Click the new object; 7. *Object explorer* panel appears; 8. Right click over the **OR** expression node and select **Add child**;

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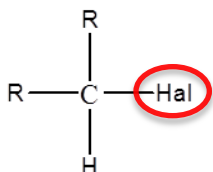
Subfragment search for identifying chemicals

Aliphatic halogens

Example 2

Search for structures that meet the structural requirements:

- Aliphatic halogens



R – Any atom except H
Hal – Cl, Br, I

- Define **Enumeration** fragment with three members (halogen atoms)

The screenshot shows the SMARTS Editor window with the following elements:

- Callout 9:** Points to the 'OR' operator in the SMARTS fragment editor.
- Callout 10:** Points to the 'Element' dropdown menu in the Object Explorer, which is set to 'C'.
- Callout 11:** Points to the 'Element' dropdown menu in the Object Explorer, which is set to 'Cl'.
- Callout 12:** Points to a carbon atom in the workspace that is highlighted in green.
- Callout 13:** Points to the 'OR' operator in the SMARTS fragment editor, indicating the addition of more elements.

9. Click the first element which corresponds to the first "child" query; 10. The panel with the atom characteristics appears; 11. Select "Cl" from the *Element* drop-down menu; 12. The part of the SMARTS fragment corresponding to the first element have colored in green. 13. Select "Br" and "I" in the same way for the rest two elements , successively.

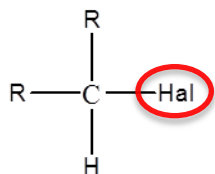
Subfragment search for identifying chemicals

Aliphatic halogens

Example 2

Search for structures that meet the structural requirements:

- *Aliphatic halogens*



R – Any atom except H

Hal – Cl, Br, I

- Define **Enumeration** fragment with three members (halogen atoms)

The screenshot shows the SMARTS Editor interface. The main window displays a central carbon atom (C) with a selection box. The Object Explorer on the right shows an enumeration fragment defined as 'OR' with three members: 'Element: Cl', 'Element: Br', and 'Element: I'. The enumeration is represented by a blue box with the number '1' and a red bracket. Below the Object Explorer, a diagram shows the 'OR' fragment branching into three circles labeled 'Cl', 'Br', and 'I', which are enclosed in a red dashed oval.

Hal substituent is ready when all elements are selected (1). Now we can continue with defining of the rest substituents of the carbon atom (see the general structure above).

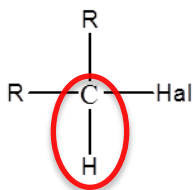
Subfragment search for identifying chemicals

Aliphatic halogens

Example 2

Search for structures that meet the structural requirements:

- Aliphatic halogens



R – Any atom except H

Hal – Cl, Br, I

- Define the number of hydrogens bonded to **C atom**

1. Click *Selection tool*; 2. Click *C atom*; 3. Define this carbon atom to be bonded with total one H atom from the *Total hydrogens* drop-down menu

The screenshot shows the SMARTS Editor interface. The main window displays the SMARTS expression C[Cl,Br,I]. A blue callout '1' points to the Selection tool icon in the toolbar. The Object Explorer on the right shows the configuration for the selected Carbon atom (C):

- Element: C
- Aromatic or aliphatic: Aliphatic
- Explicit connections (D): undefined
- Total hydrogens (H): undefined (highlighted with a red dashed box and callout '3')
- Implicit hydrogens (h): undefined
- Ring membership (R): 0
- Ring size: 2 (highlighted with a blue callout '2')
- Valence: 3
- Total connections (c): 4
- Ring atom connections (x): 5
- Charge (+/-): 7
- Atomic number (#): 8
- Chirality (@): undefined
- Atomic mass:
- Radical: undefined

At the bottom of the Object Explorer, there are OK and Cancel buttons.

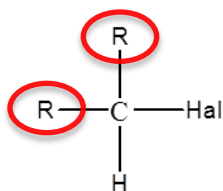
Subfragment search for identifying chemicals

Aliphatic halogens

Example 2

Search for structures that meet the structural requirements:

- *Aliphatic halogens*



R – Any atom except H

Hal – Cl, Br, I

- Define fragment R including any type atom except H atom

1. Select the pencil button; 2. Draw two single bonds to the C atom;

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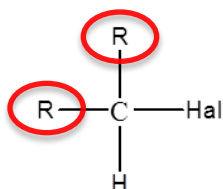
Subfragment search for identifying chemicals

Aliphatic halogens

Example 2

Search for structures that meet the structural requirements:

- Aliphatic halogens



R – Any atom except H

Hal – Cl, Br, I

- Define fragment R including any type atom except H atom

3. Click *Selection tool*; 4. Select C atom;
5. Select "**Any atom**" from the *Element* drop-down menu;

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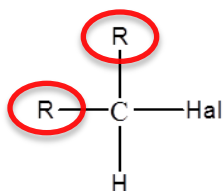
Subfragment search for identifying chemicals

Aliphatic halogens

Example 2

Search for structures that meet the structural requirements:

- Aliphatic halogens



R – Any atom except H

Hal – Cl, Br, I

- Define fragment R including any type atom except H atom

6. Select **Any** from the *Aromatic or aliphatic* drop-down menu; 7. Repeat the steps from 3 to 6 for the second carbon atom

SMARTS Editor

Smarts [Cl,Br,I][CH](C)[A]

Rectangle Make first Expression

Object explorer

Element: any atom

1

Element:	AnyAtom	<input type="checkbox"/>
Aromatic or aliphatic:	Aliphatic	<input type="checkbox"/>
Explicit connections (D):	Any	<input type="checkbox"/>
Total hydrogens (H):	Aromatic	<input type="checkbox"/>
Implicit hydrogens (I):	Aliphatic	<input type="checkbox"/>
Implicit hydrogens (I):	undefined	<input type="checkbox"/>
Ring membership (R):	undefined	<input type="checkbox"/>
Ring size (r):	undefined	<input type="checkbox"/>
Valence (v):	undefined	<input type="checkbox"/>
Total connections (X):	undefined	<input type="checkbox"/>
Ring atom connections (X):	undefined	<input type="checkbox"/>
Charge (+/-):	unspecified	<input type="checkbox"/>
Atomic number (#):		
Chirality (@):	undefined	<input type="checkbox"/>
Atomic mass:		
Radical:	undefined	<input type="checkbox"/>

OK Cancel

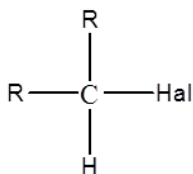
Subfragment search for identifying chemicals

Aliphatic halogens

Example 2

Search for structures that meet the structural requirements:

- *Aliphatic halogens*



R – Any atom except H
Hal – Cl, Br, I

- Define skeleton of target compound

SMARTS Editor

Smarts [Cl,Br,I][CH]([*])[*]

Rectangle Make first Expression C

Object explorer

Atom: AnyAtom

1

Element:	AnyAtom	<input type="checkbox"/>
Aromatic or aliphatic:	Any	<input type="checkbox"/>
Explicit connections (D)	undefined	<input type="checkbox"/>
Total hydrogens (H)	undefined	<input type="checkbox"/>
Implicit hydrogens (h)	undefined	<input type="checkbox"/>
Ring membership (R)	undefined	<input type="checkbox"/>
Ring size (r)	undefined	<input type="checkbox"/>
Valence (v)	undefined	<input type="checkbox"/>
Total connections (X)	undefined	<input type="checkbox"/>
Ring atom connections (x)	undefined	<input type="checkbox"/>
Charge (+/-)	unspecified	<input type="checkbox"/>
Atomic number (#)		<input type="checkbox"/>
Chirality (@)		<input type="checkbox"/>
Atom mass:	1	<input type="checkbox"/>

OK Cancel

When all substituents of the carbon atom are defined (Hal, H, R) click on **OK** (1).

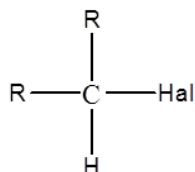
Subfragment search for identifying chemicals

Aliphatic halogens

Example 2

Search for structures that meet the structural requirements:

- *Aliphatic halogens*



R – Any atom except H

Hal – Cl, Br, I

- Define skeleton of target compound

The screenshot shows the 'Search' window in the QSAR Toolbox. The 'Subfragment' tab is active, displaying a search query: [Cl,Br,I][CH]([*])([*]). The 'Options' section shows 'Search mode' set to 'All', with 'Exact match' and 'Exact connectivity' checkboxes. A chemical structure plot shows a central carbon atom bonded to three other atoms, with a callout '1' pointing to it. Below the plot, the 'Add' button is highlighted with a callout '2'. On the right side, a search tree is visible with a callout '3' pointing to the root node.

1. The defined general structure of the aliphatic halogens appears on the separate plot; 2. Click **Add** button; 3. Double click the query to perform the search

Subfragment search for identifying chemicals

Aliphatic halogens

Example 2

- Aliphatic halogens

The screenshot displays the QSAR Toolbox software interface. The top menu bar includes options like Document, Single Chemical, Chemical List, Search, and Target Endpoint. The toolbar contains icons for various functions such as New, Open, Close, Save, and CAS#. The main workspace is divided into several panes. On the left, a 'Documents' pane shows 'Document 1' and 'Query tool: 44' with a red callout box containing the number '1'. The central pane is titled 'Filter endpoint tree...' and contains a 'Structure' field. Below this, there are expandable sections for 'Structure info', 'Parameters', 'Physical Chemical Properties', 'Environmental Fate and Transport', 'Ecotoxicological Information', and 'Human Health Hazards'. The right pane shows a grid of 9 chemical structures, each in a separate cell. A red box highlights this grid. Below the grid, a diagram illustrates the search criteria. It shows a general structure: $\begin{matrix} R \\ | \\ R-C-Hal \\ | \\ H \end{matrix}$. A red arrow points to a specific example: $\begin{matrix} H_3C & & Cl \\ & \diagdown & / \\ & C & \\ & / & \diagdown \\ CH_3 & & \end{matrix}$. A red box highlights this diagram.

1. The Query tool (QT) identified 44 chemicals matching the desired criteria.

Subfragment search for identifying chemicals

BCF and (Dmax)

Example 3

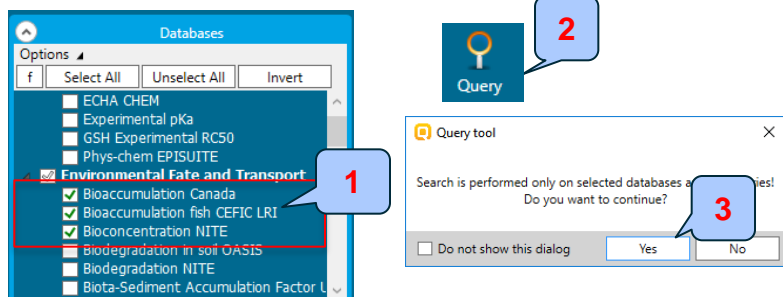
- Structures search criteria
 - Endpoint is $BCF \geq 10$ L/kg bdwt
 - 3D parameter – minimum value of Diameter maximum $>15 \text{ \AA}$

Subfragment search for identifying chemicals

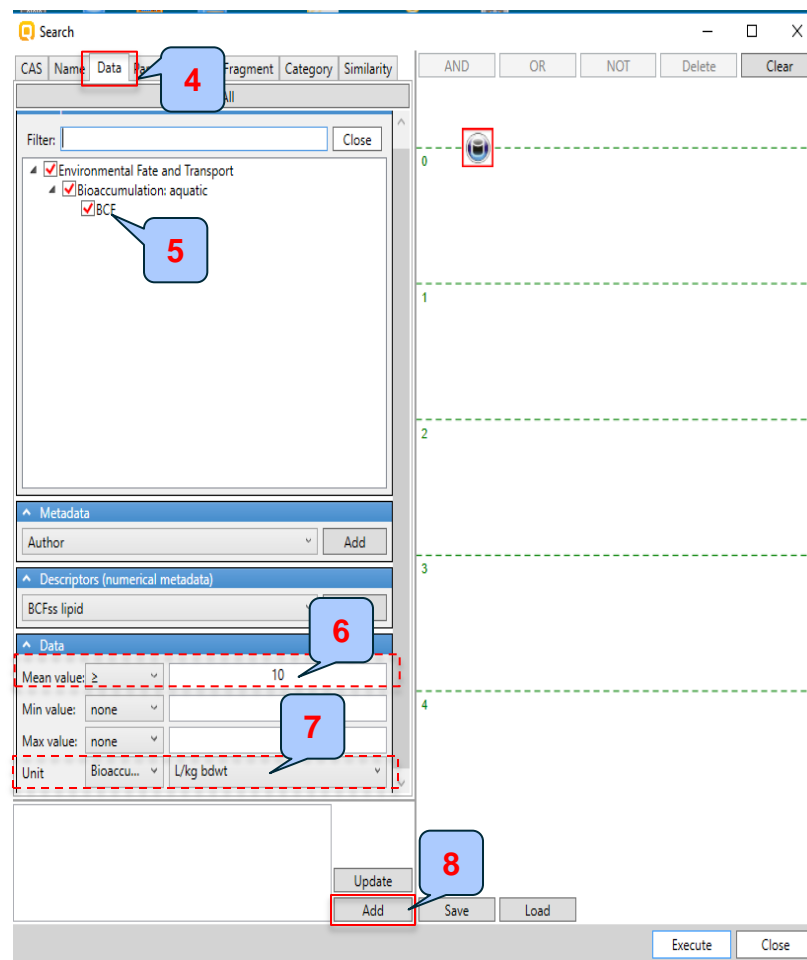
BCF and (*D*_{max})

Example 3

- Structures search criteria
 - Endpoint is $BCF \geq 10$ L/kg bdwt
 - 3D parameter – minimum value of Diameter maximum $> 15 \text{ \AA}$



- Select databases including BCF data (Bioaccumulation Canada; Bioaccumulation fish CEFIC LRI and Bioconcentration NITE). No inventory has been selected in this exercise;
- Click **Query** button;
- Confirm that the searches perform on selected databases and inventories;
- Go to **Data** panel;
- Expand the endpoint tree and select BCF;
- Specify qualifier " \geq " 10 in the *Mean value* field;
- Define the scale "**Bioaccumulation**" and appropriate unit (**L/kg bdwt**) ;
- Click **Add** button;



Subfragment search for identifying chemicals

BCF and (*D*_{max})

Example 3

- Structures search criteria
 - Endpoint is BCF \geq 10 L/kg bdwt
 - 3D parameter – minimum value of Diameter maximum > 15 Å

1. Open Parameters panel;
2. Select **Diameter maximum** from the pop-up list;
3. Specify qualifier " \geq " **15** in the *Expression* field;
4. Click **Add** button;

The screenshot shows the 'Search' window in the QSAR Toolbox. The 'Parameters' tab is active, and a list of parameters is displayed. 'Diameter maximum' is selected and highlighted. The 'Expression' field is set to '>= 15'. The 'Origin' is 'Unknown' and the 'unit' is 'Å'. The 'Destination' is also 'Unknown'. The 'Add' button is highlighted, indicating the final step in adding the search criterion to the search list.

Subfragment search for identifying chemicals

BCF and (*D*_{max})

Example 3

- Structures search criteria
 - Endpoint is BCF ≥ 10 L/kg bdwt
 - 3D parameter – minimum value of Diameter maximum >15 Å

Both queries should be linked together by logical **AND**. For this purpose both queries should be selected first. How to do this:

1. **Right click** over the first query to select it (the selected boundary should become orange colored);



Selected query



Not selected query

2. When the both queries are selected, **click "AND"** button;

3. The two queries are combined by logical "AND";

4. Double click "AND" query or click "Execute" button to execute the search;

The screenshots illustrate the process of combining two queries:

- Step 1:** The first query is selected, indicated by an orange border around its icon in the search history.
- Step 2:** The "AND" button in the logical operator menu is highlighted with a red box.
- Step 3:** The "AND" operator is placed between the two query icons in the search history.
- Step 4:** The "Execute" button at the bottom right is highlighted with a red box.

Subfragment search for identifying chemicals

BCF and (D_{max})

Example 3

The screenshot displays the QSAR Toolbox software interface. The top menu bar includes options for Document, Single Chemical, Chemical List, Search, and Target Endpoint. Below the menu bar, there are various tool icons for file operations (New, Open, Close, Save), search (CAS#, Name, Structure, Composition, Select), and data management (ChemIDs, Database, Inventory, List, Substructure (SMARTS), Query, Define). The main workspace is divided into a left sidebar and a central table. The sidebar shows 'Document 2' with a 'Query Tool: 107' notification. The central table has a 'Filter endpoint tree...' section on the left and a grid of chemical structures on the right. The grid has 7 columns and 107 rows. A red box highlights the first row of chemical structures.

The Query tool (QT) identified 107 chemicals matching the desired criteria. The list of identified chemicals appear automatically on data matrix. Number of found chemicals is marked in the name of the document (1). In order to check the correctness of the performed query search, the user should calculate D_{\max} for the list of chemicals and to gather BCF data for them. The last two steps are presented on the next two slides.

Subfragment search for identifying chemicals

BCF and (D_{max})

Example 3

1. Expand the **Parameters** node of the endpoint tree;
2. Expand the **3D** node;
3. Right click over the row corresponding to the **Diameter maximum** parameter;
4. Select **Calculate Diameter maximum for all chemicals** from the appeared menu;
5. Once the values are calculated right click over the Diameter maximum row and select **Sort** values by **Ascending** order.

The screenshot displays the QSAR Toolbox interface. On the left, the 'Filter endpoint tree...' panel shows the 'Parameters' node expanded, with the '3D' sub-node also expanded. A red dashed box highlights the 'Diameter maximum' parameter. A callout '1' points to the 'Parameters' node, '2' to the '3D' node, and '3' to the 'Diameter maximum' row. A context menu is open over this row, with a red dashed box highlighting the option 'Calculate/extract "Diameter maximum" for all chemicals'. Callout '4' points to this option. Below, the data table shows the 'Diameter maximum' row highlighted in blue. A callout '5' points to the 'Sort' option in the context menu, which is set to 'Ascending'. The table columns include parameters like 'Diameter maximum', 'Diameter minimum', 'Dipole moment', etc., and their values for various chemical structures.

Parameter	15.8 (16+16) Å	16.9 (23.7+23.7) Å	16.2 (17.3+17.3) Å	16.4 (18.5+18.5) Å	17.4 (20.2+20.2) Å	17.6 (19.7+19.7) Å	15.7
Diameter maximum	15.8 (16+16) Å	16.9 (23.7+23.7) Å	16.2 (17.3+17.3) Å	16.4 (18.5+18.5) Å	17.4 (20.2+20.2) Å	17.6 (19.7+19.7) Å	15.7
Diameter minimum	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not.
Dipole moment	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not.
Electronegativity	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not.
GAP Energy	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not.
Geometric info Wenier index	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not.
Geometric Wenier index	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not.
HOMO Energy	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not.
LUMO Energy	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not.
Maximum distance	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not.
Maximum donor delocalizability	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not.
Planarity	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not.
Planarity conjugated	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not.
VdW surface	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not.
VdW surface DPSA1	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not.
VdW surface DPSA2	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not calculated	Not.

Subfragment search for identifying chemicals

BCF and (D_{max})

Example 3

The screenshot shows the QSAR Toolbox software interface. The top menu bar includes 'Data', 'Category definition', 'Data Gap Filling', and 'Report'. The left sidebar shows a tree view of databases, with 'Environmental Fate and Transport' expanded to show 'Bioaccumulation: aquatic' selected. A central data matrix table displays BCF values for 107 chemicals. Numbered callouts (1-6) indicate the steps: 1. Clicking the 'Data' icon; 2. Clicking the 'Gather' button; 3. Clicking 'OK' in the 'Read data?' dialog; 4. Clicking 'OK' in the '424 points added across 107 chemicals' dialog; 5. The data appearing in the matrix; 6. The 'Bioaccumulation: aquatic' row being highlighted in red.

1. Go to the *Data* module;
2. The databases are already selected, click **Gather** data;
3. Click **OK**;
4. Click **OK**;
5. Data appear on data matrix;
6. All 107 chemicals have BCF data;

Subfragment search for identifying chemicals

LC 50 and predefined category (Aldehydes)

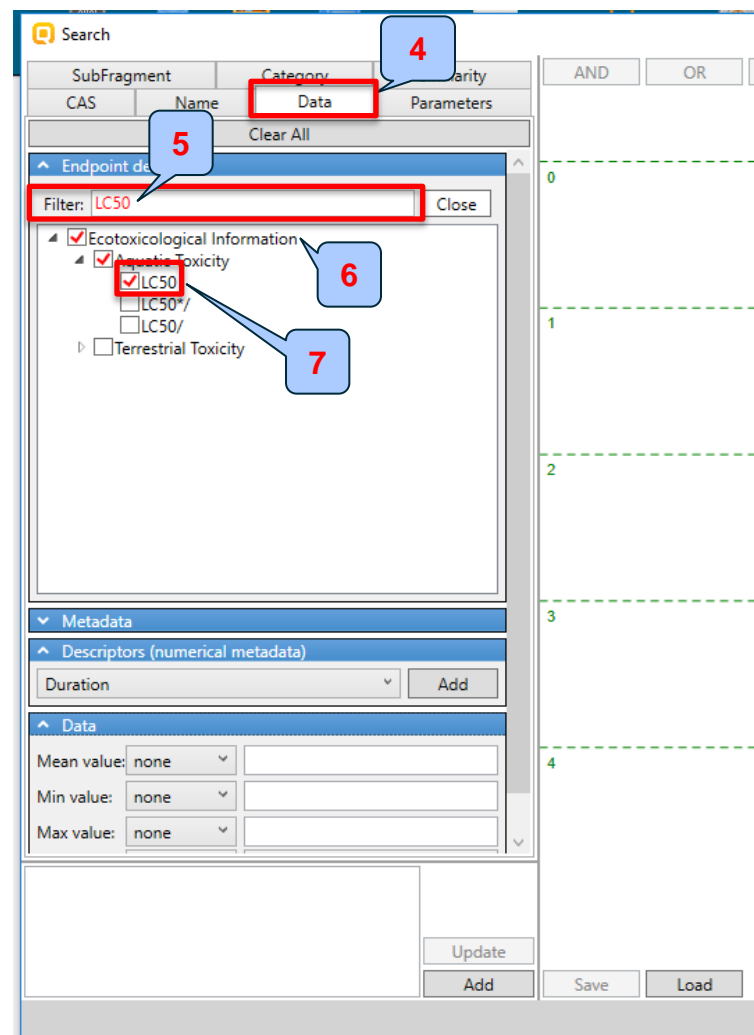
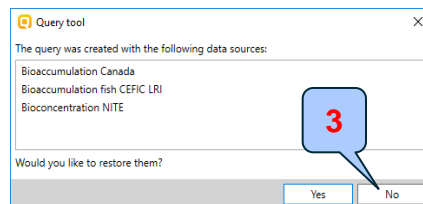
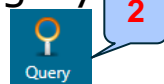
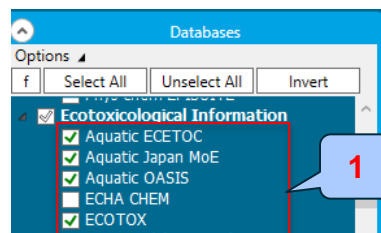
Example 4

- Structures search criteria
 - Endpoint: LC 50 <1 mg/l
 - Fish: *P.promelas*
 - Effect: *Mortality*
 - Predefined category:
aldehydes

Subfragment search for identifying chemicals LC 50 and predefined category (Aldehydes)

Example 4

- Structures search criteria
 - Endpoint: LC 50 <1 mg/l
 - Fish: *P.promelas*
 - Effect: Mortality
 - Predefined category *aldehydes*



- Select databases related to LC50 data (Aquatic ECETOC; aquatic Japan MoE; Aquatic OASIS; ECOTOX). No inventories has been selected in this case;
- Click **Query** tool button;
- Select **"No"**;
- Go to **Data** panel;
- Type in filter the name of searched endpoint (**LC50**);
- Select **Aquatic Toxicity** and expand the endpoint tab;
- Check **LC50**

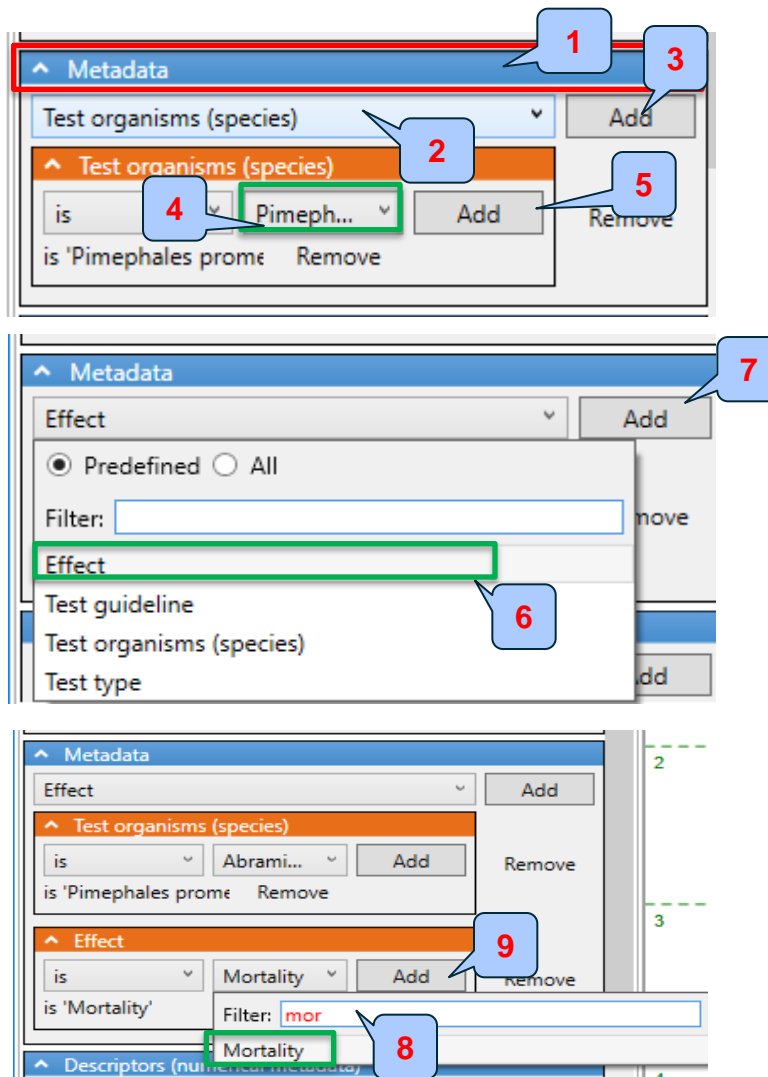
Subfragment search for identifying chemicals

LC 50 and predefined category (Aldehydes)

Example 4

- Structures search criteria
 - Endpoint: LC 50 <1 mg/l
 - Fish: *P.promelas*
 - Effect: *Mortality*
 - Predefined category: *aldehydes*

1. Open **Metadata** field
2. Select “**Test organism (species)**” from the drop-down menu;
3. Click **Add**;
4. Select ***Pimephales promelas*** from the drop-down menu;
5. Click **Add**;
6. Go back to **Metadata** field and select **Effect** from the drop-down menu;
7. Click **Add**;
8. Use filter to find “**Mortality**” from the appeared drop-down menu;
9. Click **Add**



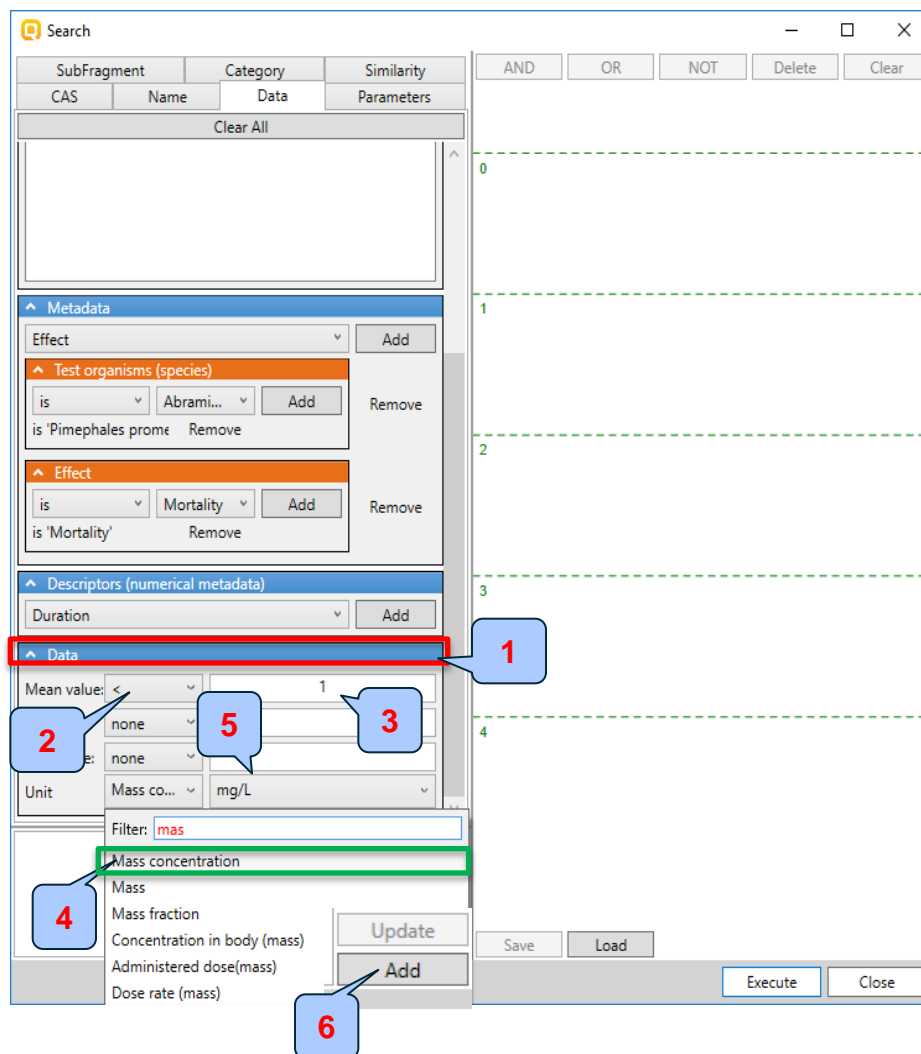
Subfragment search for identifying chemicals

LC 50 and predefined category (Aldehydes)

Example 4

- Structures search criteria
 - Endpoint: LC 50 <1 mg/l
 - Fish: *P.promelas*
 - Effect: *Mortality*
 - Predefined category: *aldehydes*

- Open **Data** panel;
- Open qualifiers from Mean value and select "<";
- Type "1" in the blank field;
- Use Filter to find "**Mass concentration**";
- Select "**mg/l**" from the list with units;
- Click **Add**;



Subfragment search for identifying chemicals

LC 50 and predefined category (Aldehydes)

Example 4

- Structures search criteria
 - Endpoint: LC 50 <1 mg/l
 - Fish: *P.promelas*
 - Effect: *Mortality*
 - Predefined category: *aldehydes*

1. Open **Category** panel;
2. Use *Filter* to find **Organic functional groups** profiler from the list with profilers;
3. Find **"Aldehyde"**;
4. Click **"Up"** to move the selected category from panel *"Profilers"* to the panel *"Target"*
5. The selected category appears in the panel *"Target"*

The screenshot shows the 'Search' window in the QSAR Toolbox. The 'Category' panel is open, and 'Aldehyde' is selected in the 'Profilers' list. The 'Target' panel shows 'Aldehyde' as the selected category. The 'Up' button is highlighted, indicating the action to move the selected category to the target panel. The 'Combine profiles' section shows 'AND' selected. The 'EndpointPath/EndpointDefinition' section shows 'Ecotoxicological Information' selected. The 'Textual Metadata' section shows 'Text metadata: Test organisms (species) is' and 'Text metadata: Effect is 'Mortality'' selected. The 'Numerical Metadata' section shows 'Numerical Metadata: Not defined'.

Subfragment search for identifying chemicals

LC 50 and predefined category (Aldehydes)

Example 4

- Structures search criteria
 - Endpoint: LC 50 <1 mg/l
 - Fish: *P.promelas*
 - Effect: *Mortality*
 - Predefined category: *aldehydes*

- Click **Add** button;
 - The query with predefined category appears on the logic panel.
- The both queries should be combined by logical "AND". Follow the steps explained on slide # 39
- Right click over the both queries to highlight them;
 - Click **AND** button;
 - The two queries are combined by logical "AND";
 - Click **Execute** button in order to execute the Query

The screenshot shows the 'Search' window in the QSAR Toolbox. The interface is divided into several sections:

- Search Criteria Table:** A table with columns 'CAS', 'Name', 'Data', and 'Parameters'. The 'SubFragment' and 'Category' columns are highlighted.
- Profile Selection:** A dropdown menu set to 'Organic functional groups' and a 'Target' field containing 'Aldehyde'.
- Logic Panel:** A visual representation of the search query. It shows two query nodes (represented by beaker icons) connected to a central 'AND' operator node. Callouts 2, 3, 4, and 5 point to these elements.
- Profiles List:** A scrollable list of chemical categories including Acrylic acids, Acyl halide, Acylal, Acyloin, Alcohol, Aldehyde, Aldimine, Aldoxime derivatives, and Aliphatic amine, primary.
- Combine Profiles:** Radio buttons for 'AND' (selected), 'OR', and 'Strict', along with an 'Invert' checkbox.
- Execution Panel:** Buttons for 'Update', 'Add' (highlighted with callout 1), 'Load', 'Execute' (highlighted with callout 6), and 'Close'.

Subfragment search for identifying chemicals

LC 50 and predefined category (Aldehydes)

Example 4

1	2	3	4	5	6

The Query tool (QT) identified 6 chemicals matching the desired criteria. The list of identified chemicals appear automatically on the data matrix. Number of found chemicals is marked in the name of the node (1). In order to check the correctness of the performed query search the user should gather ecotox data and profile according to OFG Profiler. The last two steps are presented on the next two slides.

Subfragment search for identifying chemicals LC 50 and predefined category (Aldehydes)

Example 4

1. Go to the **Data** module
2. Databases are already selected, click gather data;
3. Click **OK** to read all data;
4. Confirm the number of gathered data:
5. Data appear on data matrix answering the following criterias:
LC50 < 1mg/l
Effect: Mortality
Test species: P.promelas
Aldehydes by OFG

Subfragment search for identifying chemicals LC 50 and predefined category (Aldehydes)

Example 4

The screenshot shows the QSAR Toolbox interface. The top toolbar has icons for Input, Profiling (highlighted with a red dashed box and callout 1), Data, Category definition, Data Gap Filling, and Report. Below the toolbar is a 'Custom profile' section with 'Apply' (callout 3), 'View', 'New', and 'Delete' buttons. The main workspace is divided into several panels: 'Documents' on the left, 'Filter endpoint tree...' in the middle-left, and a grid of chemical structures and their properties on the right. A red box highlights the 'Organic functional groups' section in the 'Filter endpoint tree...' panel, which lists 'Aldehyde' as a common group for all six chemicals. Numbered callouts (1-4) indicate the steps: 1. Profiling module selected; 2. Organic functional groups profile checked; 3. Apply button clicked; 4. Aldehyde group identified in the results table.

Structure	1	2	3	4	5	6
Structure						
Structure info						
Parameters						
Physical Chemical Properties						
Environmental Fate and Transport						
Ecotoxicological Information						
Human Health Hazards						
Profile						
Empiric						
Organic functional groups	Aldehyde Alkyl (hetero)arenes Alkyl-, alkenyl- and al Aryl Ether tert-Butyl	Aldehyde Aryl Aryl halide Ether	Aldehyde Alkyl halide Aryl	Aldehyde Aryl Aryl halide Phenol	Aldehyde Aryl Aryl halide Phenol	Aldehyde Aryl Ether

1. Go to the *Profiling* module;
2. Check **Organic functional group** profile;
3. Click **Apply**;
4. All 6 chemicals have "Aldehyde" fragment within its structure;

Subfragment search for identifying chemicals

Chemicals with Ames and Carcinogenicity positive data including Epoxide fragment

Example 5

- Structures search criteria
 - Endpoint: Gene mutation
 - Species: *S.thyphimurium*
 - Data: *Positive*

AND

- Endpoint: *Summary carcinogenicity*
- Species: *Rat*
- Route: *gavage*
- Data: *Positive*
- Predefined category: *Epoxides*

Subfragment search for identifying chemicals

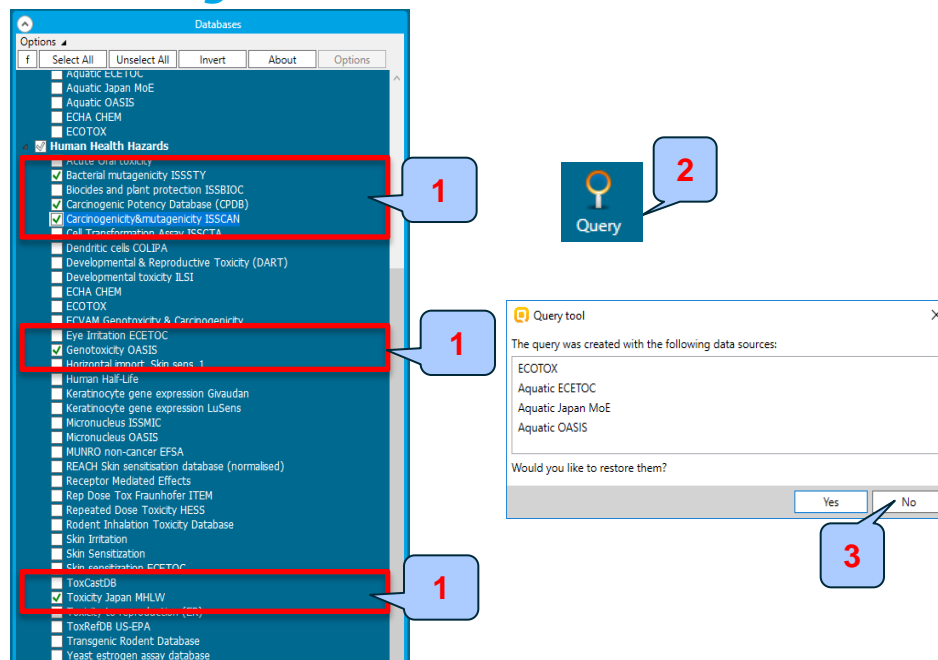
Chemicals with Ames and Carcinogenicity positive data including Epoxide fragment

Example 5

- Structures search criteria
 - Endpoint: Gene mutation
 - Species: *S.thyphimurium*
 - Data: *Positive*

AND

- Endpoint: *Summary carcinogenicity*
- Species: *Rat*
- Route: *gavage*
- Data: *Positive*
- Predefined category: *Epoxides*



Before application of Query tool, the user should select databases which includes required data. Inventories are not selected in this particular case.

- Select the following databases:
 - Bacterial mutagenicity ISSSTY
 - Carcinogenicity potency Database (CPDB)
 - Carcinogenicity&mutagenicity ISSCAN
 - Genotoxicity OASIS
 - Toxicity Japan MHLW
- Click **Query** button;
- Select **No** to not restore the databases used in the previous example.

Subfragment search for identifying chemicals

Chemicals with Ames and Carcinogenicity positive data including Epoxide fragment

Example 5

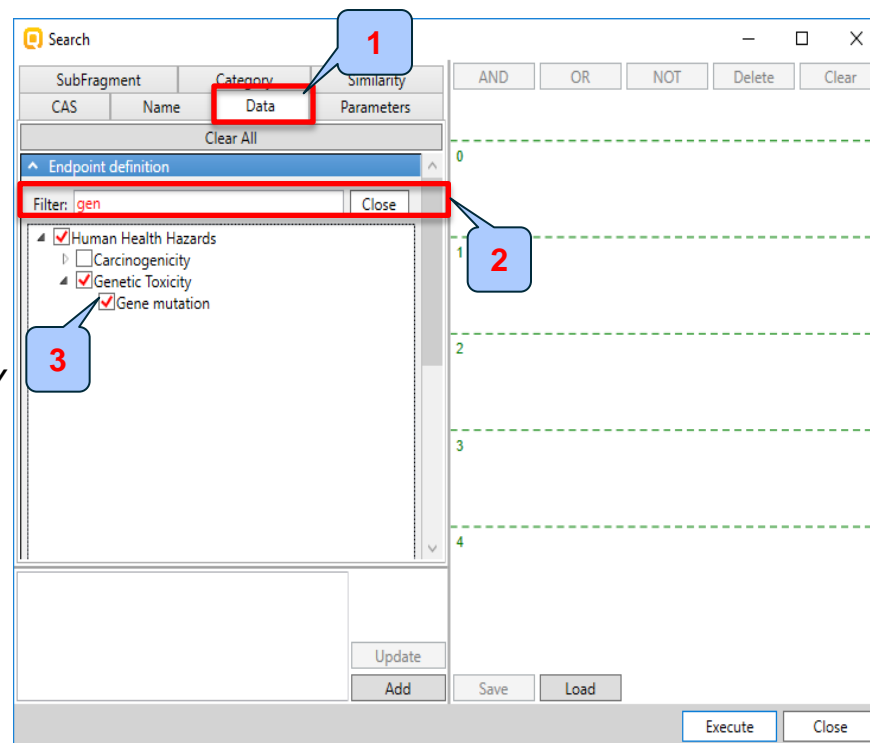
•Structures search criteria

- Endpoint: Gene mutation
- Species: *S.thyphimurium*
- Data: *Positive*

AND

- Endpoint: *Summary carcinogenicity*
- Species: *Rat*
- Route: *gavage*
- Data: *Positive*
- Predefined category: *Epoxides*

1. Click on the **Data** panel;
2. Use filter to find searched endpoint;
3. Select **Gene mutation**;



Subfragment search for identifying chemicals

Chemicals with Ames and Carcinogenicity positive data including Epoxide fragment

Example 5

- Structures search criteria
 - Endpoint: Gene mutation
 - Species: *S.thyphimurium*
 - Data: *Positive*
 - Endpoint: *Summary carcinogenicity*
 - Species: *Rat*
 - Route: gavage
 - Predefined category: *Epoxides*

The screenshot shows the 'Search' window in the QSAR Toolbox. The 'Endpoint definition' panel is open, showing 'Filter: gen' and checked options for 'Human Health Hazards', 'Genetic Toxicity', and 'Gene mutation'. The 'Test organisms (species)' pop-up menu is open, with 'Test organisms (species)' selected. The 'Metadata' panel shows 'Test organisms (species)' with 'Salmonella typ...' selected. The 'Data' panel shows 'Gene m...' selected in the 'Unit' dropdown. The 'Filter' dropdown in the 'Data' panel is open, showing 'Positive' selected. The 'Add' button is highlighted.

1. Open Metadata panel;
2. Select **Test organism (species)** from the pop-up menu;
3. Click "Add";
4. Select **S.thyphimurium** from the pop-up-menu
5. Click **Add**;
6. Open **Data** panel;
7. Select **Gene mutation I** scale (belonging to the Mutagenicity family) from the *Units* drop-down menu;
8. Select **Positive** from the list with scale members;
9. Click **Add** button;

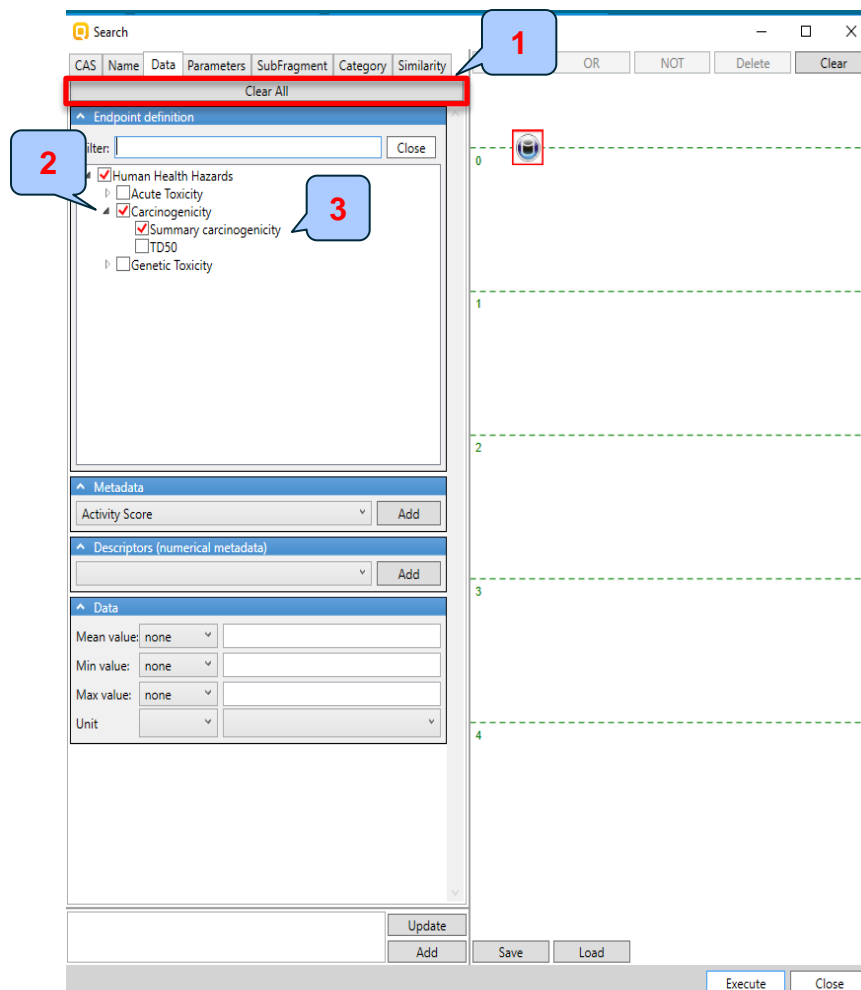
Subfragment search for identifying chemicals

Chemicals with Ames and Carcinogenicity positive data including Epoxide fragment

Example 5

- Structures search criteria
 - Endpoint: Gene mutation
 - Species: *S.thyphimurium*
 - Data: *Positive*
 - Endpoint: *Summary carcinogenicity*
 - Species: *Rat*
 - Route: gavage
 - Predefined category: *Epoxides*

1. Before defining the second query click **Clear All** button;
2. Open endpoint path and select *Carcinogenicity* node;
3. Select **Summary carcinogenicity**;



Subfragment search for identifying chemicals

Chemicals with Ames and Carcinogenicity positive data including Epoxide fragment

Example 5

•Structures search criteria

- Endpoint: Gene mutation
- Species: *S.thyphimurium*
- Data: *Positive*
- Endpoint: *Summary carcinogenicity*
- Species: *Rat*
- Route: *gavage*
- Predefined category: *Epoxides*

1. Open *Metadata* panel;
2. Select **Route of administration** from pop-up menu;
3. Click **Add** button;
4. Select **Gavage** from the list. Click **Add** button;
5. Go back to *Metadata* panel and select **Test organism (species)** from the pop-up menu. Click **Add** button;
6. Select **Rat** from the list. Click **Add** button;
7. Open *Data* panel
8. Select scale **Carcinogenicity I (ISSCAN)**;
9. Select **Positive**;
10. Click **Add** button;
11. The query appears on the logic panel.

The screenshot shows the QSAR Toolbox search interface. The 'Search' window is open, displaying various panels and a logic panel on the right. The 'Endpoint definition' panel is expanded, showing 'Human Health Hazards' with 'Carcinogenicity' checked. The 'Metadata' panel is open, showing 'Route of administration' and 'Test organisms (species)'. The 'Data' panel is also open, showing 'Carcinogenicity I (ISSCAN)' with 'Positive' selected. The logic panel on the right shows the query structure with a red box around the 'AND' operator and a callout '11' pointing to the query.

Subfragment search for identifying chemicals

Chemicals with Ames and Carcinogenicity positive data including Epoxide fragment

Example 5

- Structures search criteria
 - Endpoint: Gene mutation
 - Species: *S.thyphimurium*
 - Data: Positive
 - Endpoint: Summary carcinogenicity
 - Species: Rat
 - Route: gavage
 - Predefined category: Epoxides

1. Click *Category* panel;
2. Select **Carcinogenicity (genotox and nongenotox) alerts by ISS**;
3. Select category **Epoxides and aziridines (Genotox)**;
4. Click **Up** to move the selected category to the panel *Target*;
5. Click **Add** button;
6. The query appears on the logic panel;

Subfragment search for identifying chemicals

Chemicals with Ames and Carcinogenicity positive data including Epoxide fragment

Example 5

- Structures search criteria
 - Endpoint: Gene mutation
 - Species: *S.thyphimurium*
 - Data: Positive
 - Endpoint: Summary carcinogenicity
 - Species: Rat
 - Route: gavage
 - Predefined category: Epoxides

- Right click over the three queries (see slide # 39);
- Click **AND** button;
- The three queries are combined by logical "AND";
- Click **Execute** button;

The screenshot displays the QSAR Toolbox search interface. On the left, the 'Search' panel is open, showing the 'Endpoint definition' section with 'Genetic Toxicity' checked under 'Human Health Hazards'. The 'Test organisms (species)' section is set to 'is Salmonella typhimurium'. The 'Data' section is set to 'Positive'. On the right, a query tree is shown with three queries being combined using an 'AND' operator. Callouts 1-4 indicate the steps: 1. Right-clicking the queries, 2. Clicking the AND button, 3. The queries being combined, and 4. Clicking the Execute button.

Subfragment search for identifying chemicals

Chemicals with Ames and Carcinogenicity positive data including Epoxide fragment

Example 5

The screenshot shows the QSAR Toolbox software interface. The top menu bar includes options like Document, Single Chemical, Chemical List, Search, and Target Endpoint. Below the menu is a toolbar with icons for New, Open, Close, Save, CAS#, Name, Structure, Composition, Select, ChemIDs, Database, Inventory, List, Substructure (SMARTS), Query, and Define. The main window is divided into several panes. On the left, there is a 'Documents' pane showing 'Document 1' and 'Query Tool: 6'. The central pane is titled 'Filter endpoint tree...' and contains a 'Structure' section. Below this, there are expandable sections for 'Structure info', 'Parameters', 'Physical Chemical Properties', 'Environmental Fate and Transport', 'Ecotoxicological Information', and 'Human Health Hazards'. The rightmost pane displays a table with 6 columns, numbered 1 to 6. Each column contains a chemical structure. The structures are: 1. 2-hydroxyethyl epoxide, 2. 2-chloroethyl epoxide, 3. benzene ring with an epoxide group, 4. a complex organic structure with an epoxide ring, 5. a simple epoxide ring, and 6. methyl epoxide (H₃C-epoxide). The entire table area is highlighted with a red border.

The Query tool (QT) identified 6 chemicals matching the desired criteria. In order to check the correctness of the query the user should gather experimental data for Ames and Carcinogenicity and profile the identified chemicals according to applied Carcinogenicity profiler. The last two steps are presented on the next two slides.

Subfragment search for identifying chemicals

Chemicals with Ames and Carcinogenicity positive data including Epoxide fragment

Example 5

176 points added across 6 chemicals.

Endpoint	Chemical 1	Chemical 2	Chemical 3	Chemical 4	Chemical 5	Chemical 6
Summary carcinogenicity (gavage, rat)	M: Positive	M: Positive	M: Positive	M: Positive	M: Positive	M: Positive
Salmonella typhimurium	M: Positive	M: Positive	M: Positive	M: Positive	M: Positive	M: Positive

1. Go to the *Data* module;
 2. Databases are already selected, click **Gather** data;
 3. Click **OK**;
 4. Click **OK**;
- Data appear on data matrix answering the following criteria:
- Ames mutagenicity (*S. thuphimurium*): Positive (5)
 - Summary carcinogenicity (gavage, rat): Positive (6)

Subfragment search for identifying chemicals

Chemicals with Ames and Carcinogenicity positive data including Epoxide fragment

Example 5

Filter endpoint tree...	1	2	3	4	5	6
Structure						
Structure info						
Parameters						
Physical Chemical Properties						
Environmental Fate and Transport						
Ecotoxicological Information						
Human Health Hazards	(6/176)					
Profile	M: 34.7 mg/kg bdwt	M: 2.96 mg/kg bdwt	M: 118 mg/kg bdwt	M: 24.3 mg/kg bdwt	M: 21.3 mg/kg bdwt	M: 74.4 mg/kg bdwt
Predefined						
Substance type	Discrete chemical	Discrete chemical	Discrete chemical	Discrete chemical	Discrete chemical	Discrete chemical
Endpoint Specific	Epoxides and aziridines Structural alert for gen	Aliphatic halogens (Gen Epoxides and aziridines Structural alert for gen	Epoxides and aziridines Structural alert for gen	Epoxides and aziridines Structural alert for gen	Epoxides and aziridines Structural alert for gen	Epoxides and aziridines Structural alert for gen
Carcinogenicity (genotox and nongenotox) al ...						

1. Go to *Profiling*;
2. Click **Unselect All**;
3. Use filter and select *Carcinogenicity (genotox and nongenotox) alerts by ISS*;
4. Click **Apply**;
5. All 6 chemicals have "Epoxides and Aziridines" fragment within its structure.

Subfragment search for identifying chemicals

Chemicals with Skin sensitization positive data including Aldehyde fragment

Example 6

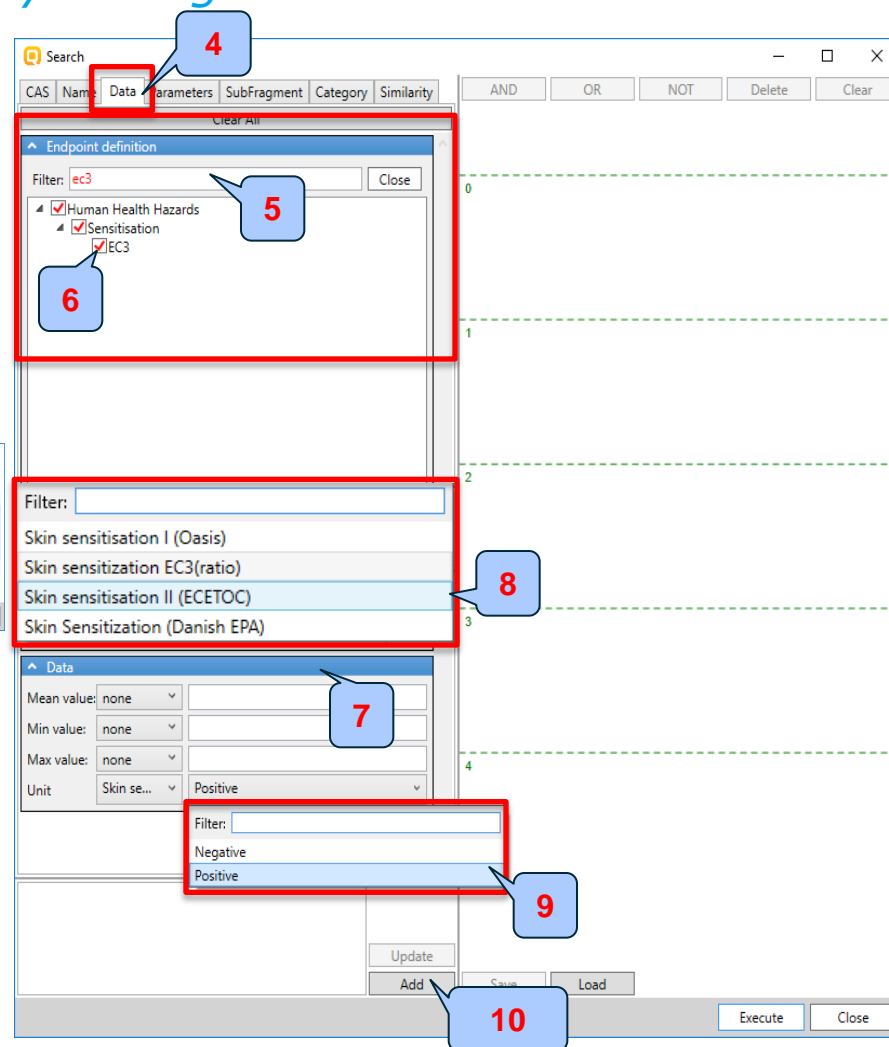
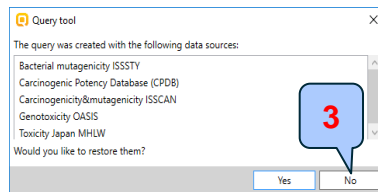
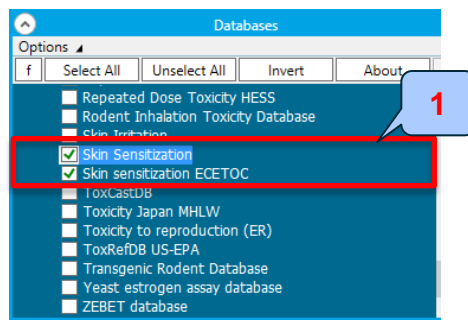
- Structures search criteria
 - Endpoint: *EC3*
 - Data: *Positive*
 - Predefined category: alpha, beta-unsaturated aldehydes

Subfragment search for identifying chemicals

Chemicals with Skin sensitization positive data including Aldehyde fragment

Example 6

- Structures search criteria
 - Endpoint: *EC3*
 - Data: *Positive*
 - Predefined category: alpha, beta-unsaturated aldehydes



- Select databases including skin sensitization data. No inventories has been selected in this case;
- Click **Query tool** button;
- Select **No** to confirm that the databases in previous example not be used;
- Click on *Data* panel;
- Use filter to find searched endpoint;
- Check **EC3**;
- Go to *Data* panel;
- Select scale **Skin sensitization II (ECETOC)**;
- Select **Positive**;
- Click **Add** button;

Subfragment search for identifying chemicals

Chemicals with Skin sensitization positive data including Aldehyde fragment

Example 6

- Structures search criteria
 - Endpoint: *EC3*
 - Data: *Positive*
 - Predefined category: alpha, beta-unsaturated aldehydes

- Click *Category* panel;
- Type in *Filter* to find the profile "**Protein binding alerts for skin sensitization by OASIS**";
- Select category *Michael addition >>alpha, beta-Unsaturated carbonyl compounds>>alpha, beta-Aldehydes* and move the selected category to the panel *Target*;
- Click **Add** button;
- The query appears on the logic panel.

The screenshot displays the QSAR Toolbox search interface. The 'Category' panel is highlighted with a red box and labeled '1'. The 'Filter' field contains the text 'prote', and a dropdown menu is open, showing a list of profiles. The profile 'Protein binding alerts for skin sensitization by OASIS' is highlighted in blue and labeled '2'. The 'Target' panel shows the selected category 'Michael Addition >> Michael addition on alpha,beta-Unsaturated carbonyl compounds >> alpha,beta-Aldehydes' highlighted with a red box and labeled '3'. The 'Add' button is highlighted with a blue box and labeled '4'. The logic panel on the right shows the query 'Michael Addition >> Michael addition on alpha,beta-Unsaturated carbonyl compounds >> alpha,beta-Aldehydes' highlighted with a blue box and labeled '5'.

Subfragment search for identifying chemicals

Chemicals with Skin sensitization positive data including Aldehyde fragment

Example 6

- Structures search criteria
 - Endpoint: *EC3*
 - Data: *Positive*
 - Predefined category: alpha, beta-unsaturated aldehydes

The screenshot shows the 'Search' window in the QSAR Toolbox. The 'Endpoint definition' panel is open, showing a tree view where 'Human Health Hazards' is expanded to 'Sensitisation', and 'EC3' is selected. The 'Data' panel shows 'Unit' set to 'Skin se...' and 'Positive'. The main workspace shows a logical query tree with two nodes connected by an 'AND' operator. Callout 1 points to a right-click on the first node, callout 2 points to the 'AND' button, callout 3 points to the 'AND' node in the tree, and callout 4 points to the 'Execute' button at the bottom right.

- Right click over the queries in order to select them;
- Click **AND** button;
- The two queries are combined together by logical "AND";
- Click **Execute** button or double click *And*;

Subfragment search for identifying chemicals

Chemicals with Skin sensitization positive data including Aldehyde fragment

Example 6

The screenshot shows the QSAR Toolbox interface. The top menu bar includes 'Input', 'Profiling', 'Data', 'Category definition', 'Data Gap Filling', and 'Report'. Below this are 'Data', 'Import', and 'Export' tabs. The 'Documents' panel on the left shows 'Document 1' with 'Query Tool 14'. The 'Databases' panel on the left lists various toxicity endpoints, with 'Skin Sensitization' and 'Skin sensitization ECETOC' checked. The main area displays a 'Filter endpoint tree...' on the left and a grid of 9 chemical structures on the right. A red box highlights the 'Structure' row in the grid. A blue callout bubble with the number '1' points to the 9th structure in the grid. Below the grid is a list of toxicity endpoints, with 'Sensitisation' highlighted in blue and 'AW SW AOP' written next to it.

The Query tool (QT) identified 14 chemicals matching the desired criteria. In order to check the correctness of the query the user should gather experimental data for skin sensitization and profile the identified chemicals according to the "Protein binding alerts for skin by OASIS" profiler used in the query boundary. The last two steps are presented on the next two slides.

Subfragment search for identifying chemicals

Chemicals with Skin sensitization positive data including Aldehyde fragment

Example 6

1. Go to the *Data* module;

2. Databases are already selected, click **Gather** data;

3. Click **OK**;

4. Click **OK**;

5. Data appear on data matrix answering the following criteria:
EC3: Positive

Human Health Hazards									
Acute Toxicity									
Bioaccumulation									
Carcinogenicity									
Developmental Toxicity / Teratogenicity									
Genetic Toxicity									
Immunotoxicity									
Irritation / Corrosion									
Neurotoxicity									
Photoinduced toxicity									
Repeated Dose Toxicity									
Sensitisation									
Skin									
in Vivo									
GPMT	(2/2)				M: Positive				
HRIPT	(6/8)				M: 1.2E+03 µg/cm2	M: Positive	M: Positive		M: Negative
LLNA									
EC3	(14/15)	M: Positive	M: Positive	M: Positive	M: Positive	M: Positive	M: Positive	M: Positive	M: Positive
Miscellaneous	(3/3)				M: Positive				M: Negative
Undefined Assay	(2/2)				M: Positive				
ToxCast									

Subfragment search for identifying chemicals

Chemicals with Skin sensitization positive data including Aldehyde fragment

Example 6

1. Go to *Profiling*;

2. Click **Unselect All**;

3. Select the profile *Protein binding alerts for skin sensitization by OASIS*;

4. Click **Apply**;

5. Perform right click over the *Protein binding alerts for skin sensitization by OASIS* and select "Profile statistic";

6. Check the box next to *Group by category*.

7. All 14 chemicals are alpha-beta aldehydes according to Protein binding alerts for skin sensitization profiler.

#	Category	Count	%
1	Michael Addition	14	28.57
2	Michael Addition >> Michael addition on alpha,beta-	14	28.57
3	Michael Addition >> Michael addition on alpha,beta-	14	28.57
4	Michael Addition >> Michael addition on conjugated	2	4.08
5	Michael Addition >> Michael addition on conjugated	2	4.08
6	Schiff base formation	1	2.04
7	Schiff base formation >> Schiff base formation with c1	2.04	
8	Schiff base formation >> Schiff base formation with c1	2.04	

Profile Statistic

Michael Addition >> Michael addition on alpha,beta-Unsaturated carbonyl compounds >> alpha,beta-Aldehydes

Save to smi | Print | Add in new doc

1 142-83-6

2 5910-85-0

3 104-55-2

4 6728-26-3

5 3913-71-1

6 101-39-3

7 22418-66-2

8 14371-10-9

9 101-86-0

Protein binding alerts for skin sensitization by OASIS

Count

10

5

Outlook

- Background
- Objectives
- Overview of Query tool
- Query tool window
- The exercise
- Workflow process
- **Save QT searches**

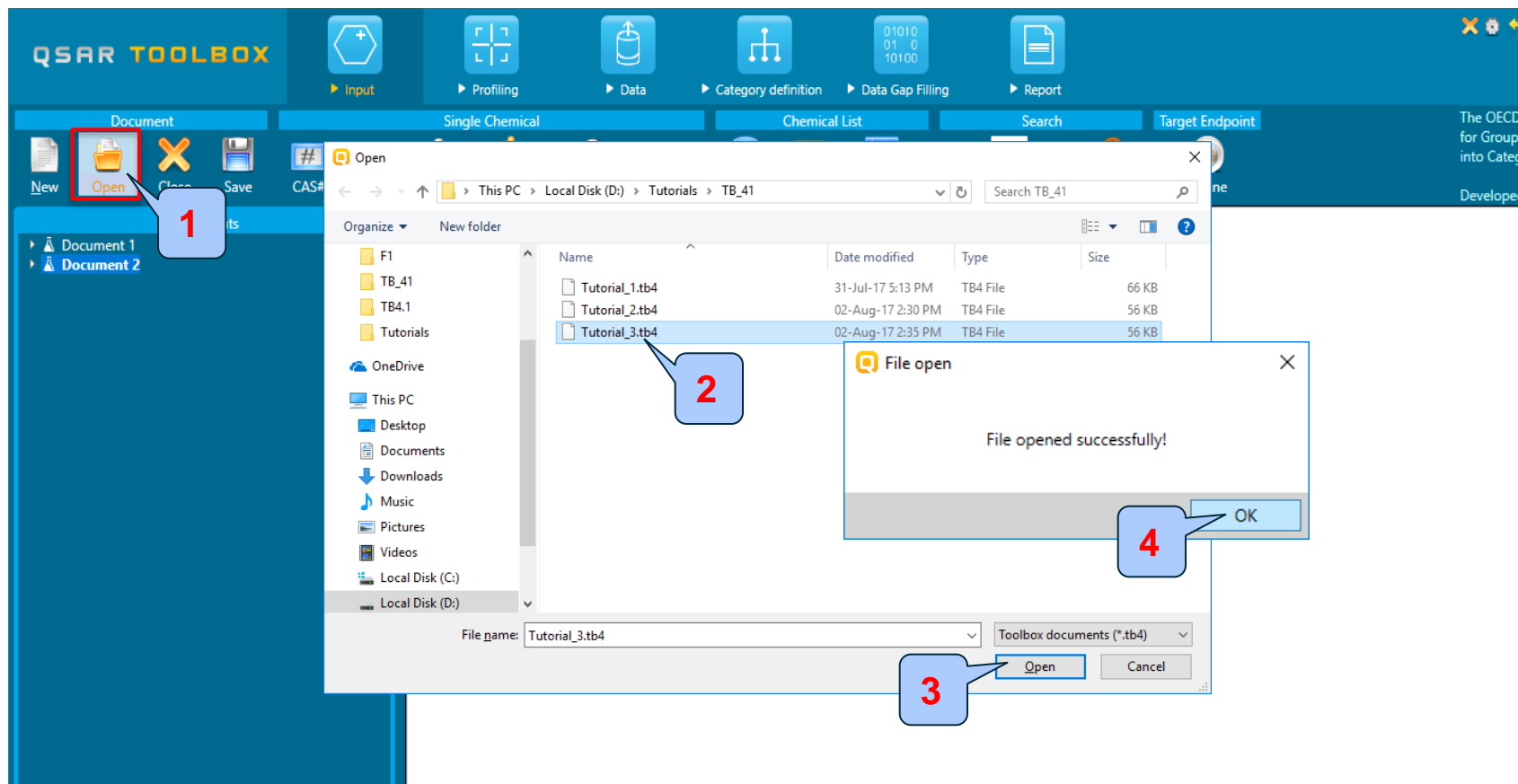
Saving the prediction result

- This functionality allows storing/restoring the current state of Toolbox documents including loaded chemicals, experimental data, profiles, predictions etc., on the same computer. The functionality is implemented based on saving the sequence of actions that led to the current state of the Toolbox document and later executing these actions in the same sequence in order to get the same result(s).
- Saving/Loading the file with TB prediction is shown on the next screenshots

Saving the QT requests

1. Go to the *Input* module; 2. Click **Save** button; 3. Select **Yes** to confirm the operation; 4. Define name of the file; 5. Click **Save** the file; 6. A message informs that the document is saved successfully, click **Ok**.

Open saved file



Once the file has been saved: 1. Click **Open** button within the Input module; 2. Find and select the file; 3. Click **Open**; 4. A message informs that the document is opened successfully, click **Ok**.