

# SemantX Panoramix doku

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## Panoramix Portal

### Login

To login into the Panoramix web portal complete the following steps:

1. Open a browser and enter the uniform resource locator (URL) for the Panoramix web portal login window.

URL= [https://ssl.biomax.de/panoramix/cgi/login\\_token\\_2fa.cgi](https://ssl.biomax.de/panoramix/cgi/login_token_2fa.cgi)

The login page will be displayed.

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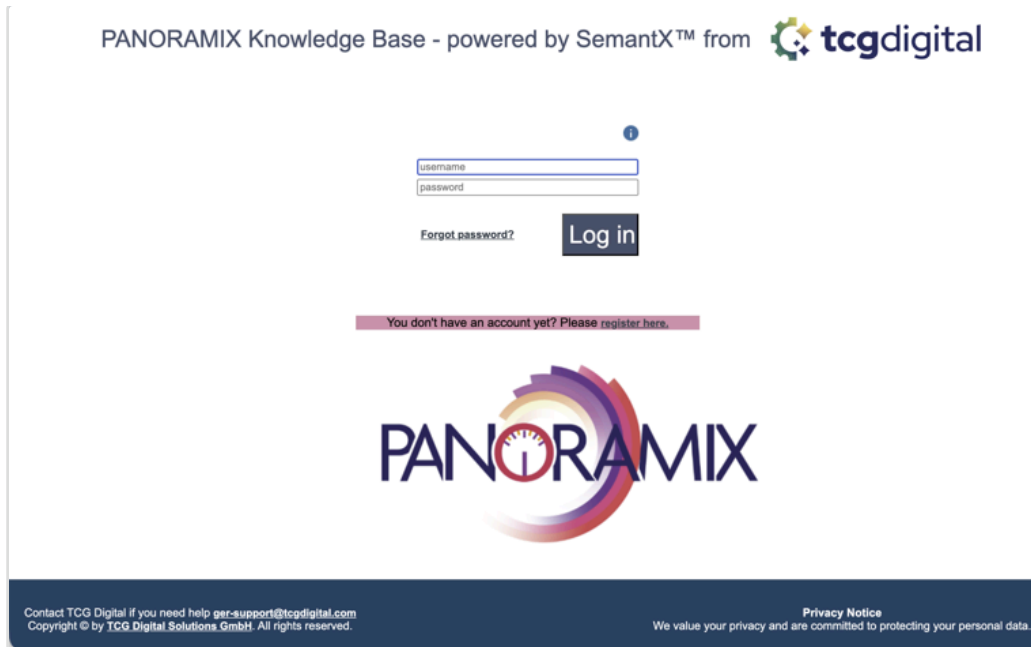


Figure 1: Login page of the Panoramix Project

2. Enter your user name and password, then click the **Login** button. You will be directed to the token page (Figure 2.), where you are required to enter the token sent to your registered e-mail address associated with your portal access.

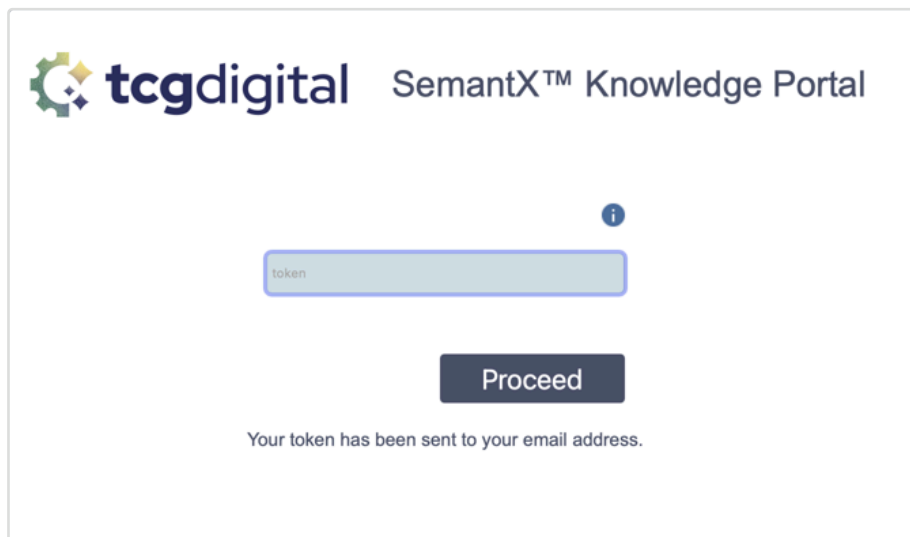


Figure 2: Token Page

Enter the token and click the **Proceed** button to access the Panoramix web portal **WebHome (Figure 4)**

3. If a user does not have account credentials, they can use the highlighted link below the Log in button to send an email request to the administrator, who can grant access to the portal.

My e-mail address \*

First name \*

Last name \*

Company/institution \*

Phone

By pressing "Register" your request will be sent to our account managers.

\* Required entries

**Register**

#### Privacy Notice

We value your privacy and are committed to protecting your personal data.  
The personal data you provide on the request and the login page (such as your username, email address, and password) will be collected and processed solely for the purpose of enabling secure login and granting access to the system.  
Your data will not be used for any other purposes, shared with third parties, or stored longer than necessary to maintain your access and ensure system security, unless required by applicable law.  
By logging in, you acknowledge and agree to the processing of your personal data for these purposes.

Figure 3: Request for access page

3. Enter the token and click the **Proceed** button to access the Panoramix web portal **WebHome**.

# Homepage

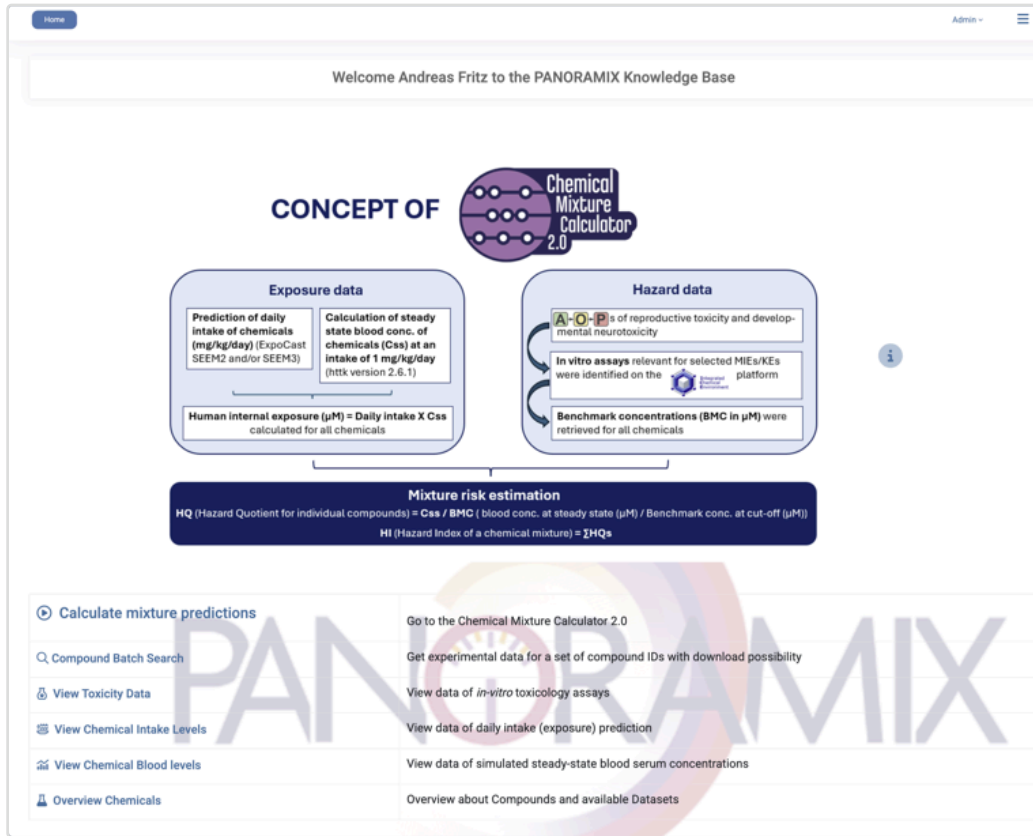


Figure 4: Homepage of the CMC

## Navigation

Navigation Bar with **Home** button, Admin menu and SideBar



The **Home** button allows users to return to the start page at any time. The **Admin** menu is displayed only for users with administrative privileges. Navigation within the system is provided via the expandable menu on the right-hand side, in addition to the three sections presented as tiles.

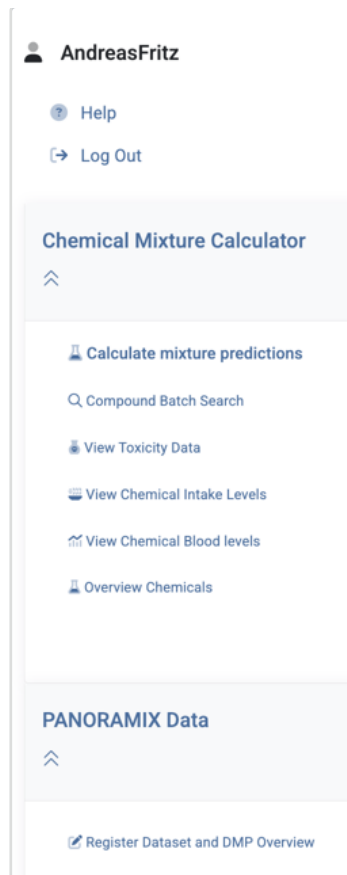


Figure 5: WebSide Bar for Navigation

## Breadcrumbs

Breadcrumbs represent your interaction trail, showing the concepts selected during refinement or filtering steps. Each time a concept is selected in a refiner, a new breadcrumb is added to the trail.

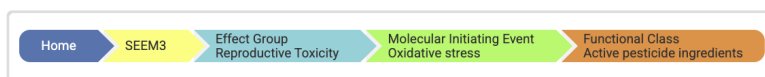


Figure 6: Example of the Bread Crumb Navigation Bar

## Functionality:

- To restart a search at any step, select that step in the Breadcrumb.

- Select the last breadcrumb to view your complete journey, or select an earlier step to view its corresponding results.

## Content

### Chemical Mixture Calculator

After clicking the CMC icon on the Home page, you will be taken to the overview page. The upper section explains the operating principle of the CMC (see Figure: xxx). Various options for searching within the system are available, including:

1. Calculate mixture predictions
2. Compound Batch Search
3. View Toxicity Data
4. View Chemical Intake levels
5. View Chemical Blood levels
6. Overview Chemicals

The info button on the right-hand side opens a modal window that provides information about the calculations and the datasets used.

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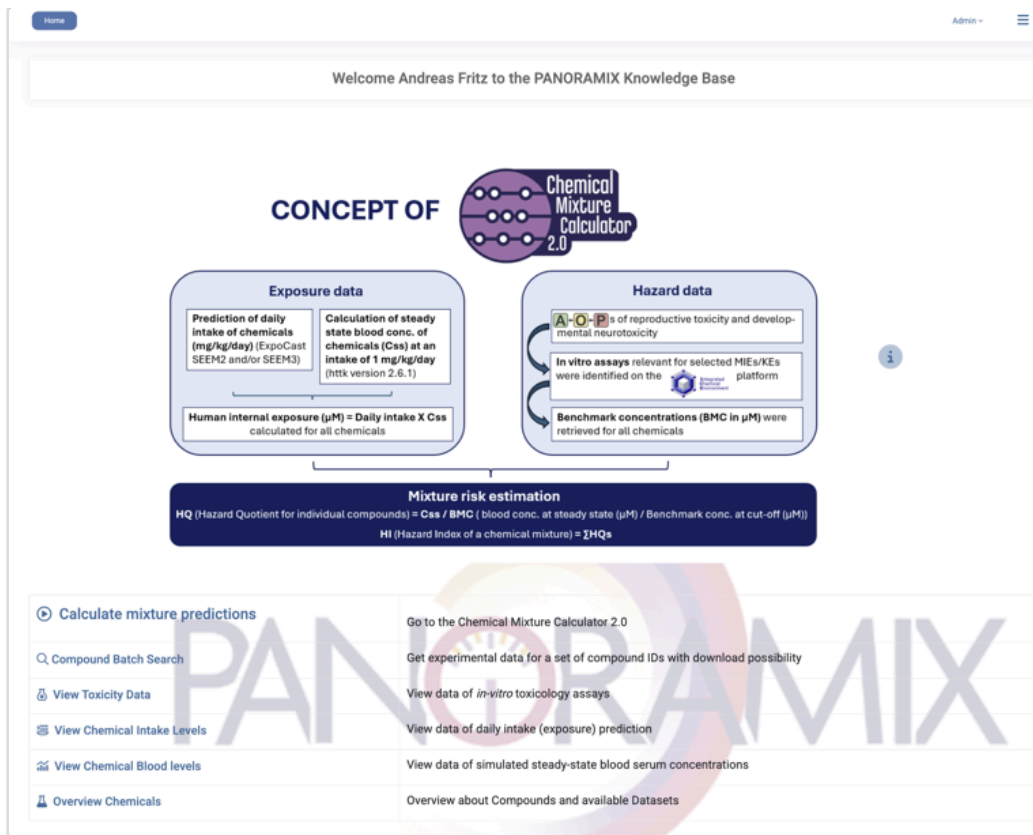


Figure 7: CMC Entry Page

## Calculate mixture predictions

### Exposure settings

By clicking the **Chemical Mixture Predictions** link, you will be directed to the CMC exposure settings. A description of the datasets is available via the **More Information** link and the information displayed on the left hand side. After selecting a setting you will be directed to the CMC calculation page.

Home > CMC2.0 > Exposure Settings

## Chemical Mixture Calculator 2.0

Go to CMC 2.0 calculations by selecting DI and CS quantiles [More information...](#)

- FF High DI - High CS
- ↑ Mean DI - High CS (default settings)
- TJ High DI - Mean CS
- ↓ Mean DI - Mean CS

**Why Quantiles?**

Mean or High quantiles of DI prediction can be used in any combination with Mean or High quantiles of C<sub>ss</sub> Simulation to produce a C<sub>ss</sub> value for the given population group.

Based on the distribution patterns, it was judged that for DI prediction, where values for the High quantile are very far from the Median, the latter would give a better representation of the population. On the other hand, C<sub>ss</sub> simulations with a lesser discrepancy between Median and High quantile, invite to choose the latter as to minimize the risk of hazard under-estimation (and also partly to compensate the choice of Median for DI prediction).

Therefore, the "Mean DI - High CS" combination should in most cases be used as default.

For populations with a known or suspected exposure above average, it might be useful to choose the High DI prediction instead. For populations with a known robust constitution it might be safe to assume the Mean C<sub>ss</sub> simulation as default.

Figure 8: Exposure Settings Page

## Chemical Mixture Calculator 2.0

The calculator layout consists of several sections. In the top row, you can select the population for which the calculations are performed. Below this, an overview of the main three sections is provided, along with the actual calculation results, which are generated automatically.

The left panel contains the refiners, which act as filters to narrow down and further specify the dataset. The middle panel displays the compounds available for calculation that can be performed. The right panel is initially empty and is populated as compounds are selected. These selected compounds are then used for the calculation, and the results are displayed above in the middle panel.

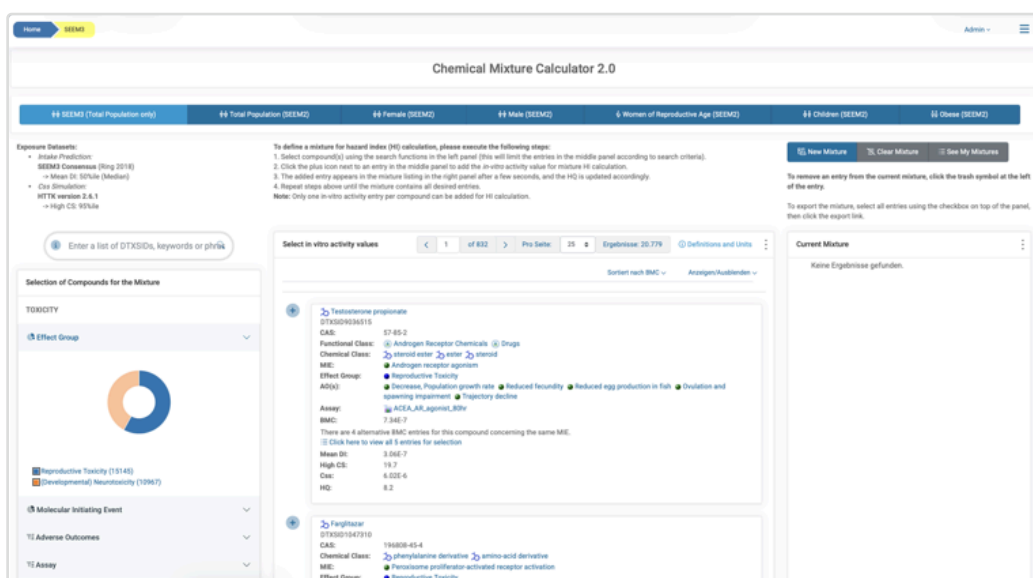


Figure 9: CMC 2.0 Page for Refinement and Mixture selection

### Description of How to Perform a Calculation

To define a mixture for Hazard Index (HI) calculation, please follow these steps:

1. Use the search functions in the left panel to select the desired compound(s).  
This will filter the entries displayed in the middle panel according to your search criteria.
2. In the middle panel, click the **plus icon** next to a compound to add its *in vitro* activity value to the mixture.
3. The selected entry will appear in the mixture list in the right panel after a few seconds.
4. Repeat the steps above until all desired compounds have been added to the mixture.
5. Click the link to [Calculate and display the Hazard Index](#) to perform the calculation.

**Note:** Only one *in-vitro* activity entry per compound can be added for HI calculation.

By clicking the link “[calculate and display the Hazard Index](#)“ the calculation is performed.

Once the calculation is executed, the results will be displayed as shown in the figure below.

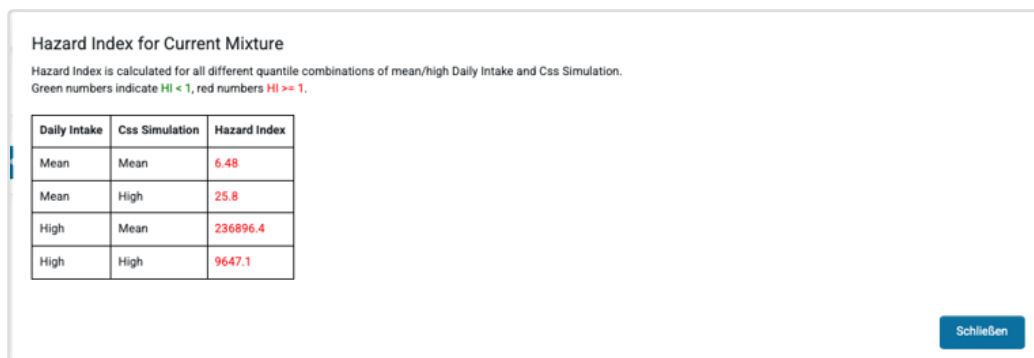


Figure 10: Modal window with results of a calculation

#### Left Panel - Refiners

Within the Panoramix Project, the following refiners are available. They can be used individually or in combination:

- Search Box (supports DTX IDs, CAS numbers in quotes, phrases and keywords)
- Toxicity
  - Effect groups (e.g. Reproductive Toxicity, Developmental Neurotoxicity)
  - Molecular Initiation Event
  - Adverse Outcomes
  - Assay
- Compound Classification
- ChEBI Ontology Classification
- Compound Data
- Hazard Data

The different types of refiners are described below, along with guidance on how to use them effectively.

Keyword/batch search

Graphical representation

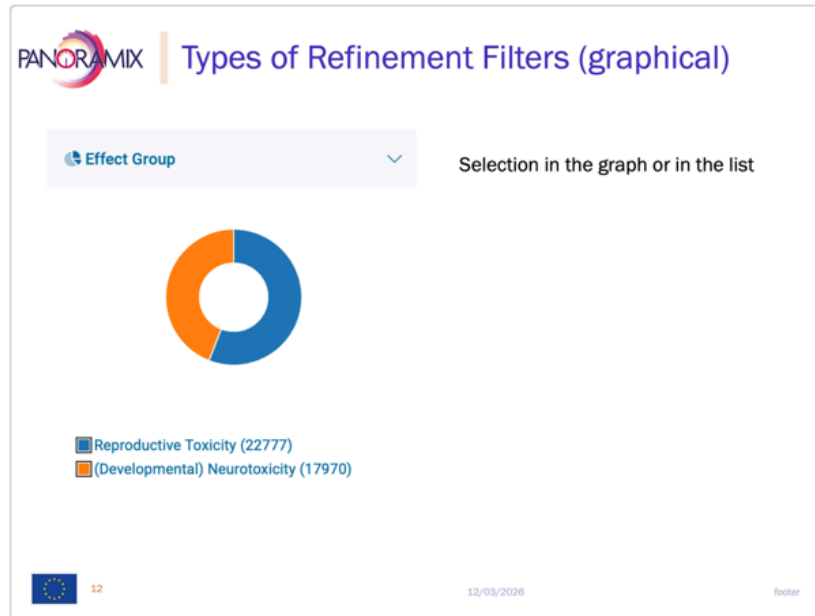


Figure 11: Graphical Filter example

Categorical Filters

Categorical filters allow users to select **specific categories or groups**. A search box can be used to quickly locate items in the list. Selections are made using checkboxes, and multiple items can be selected at once. After making your selections, click **Apply** to execute the search. Use the **down arrow** to navigate through the list.

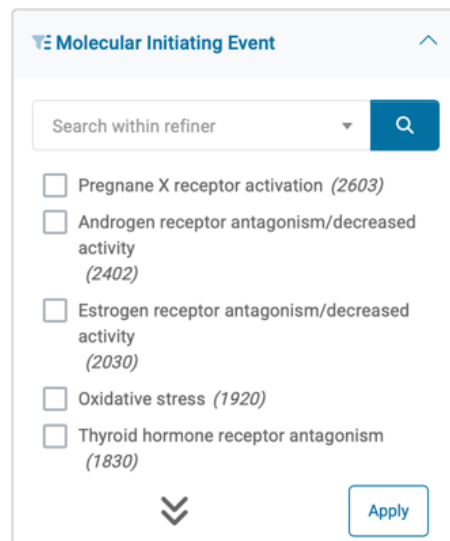


Figure 12: List Filter example

A **Sunburst diagram** is a **radial, hierarchical data visualization** used to display how categories are structured within larger categories. It represents hierarchical relationships using **concentric rings**, where each ring corresponds to a level in the hierarchy.



Figure 13: Sunburst Filter example

- Structure

- + The **center circle** represents the **root node** (the top level of the hierarchy).
- + Each **outer ring** represents a deeper level of the hierarchy.
- + **Segments (arcs)** within each ring represent categories or nodes.
- + The **size of each segment** is typically proportional to a quantitative value (e.g., count, weight, or percentage).
- + Parent segments contain their **child segments** in the next outer ring.

- Navigation Possibilities

Sunburst diagrams are often **interactive**, enabling several navigation techniques:

1. **Drill-Down (Zoom-In)**

Clicking on a segment focuses on that node, moving it to the center and displaying its children as new outer rings.

This helps users explore deeper levels of the hierarchy.

2. **Drill-Up (Zoom-Out)**

Users can return to higher levels by clicking the center node, a breadcrumb trail, or a “back” control.

## Range Filter

Range Filters are used to select **numeric or continuous values**. They include slider controls, minimum–maximum input fields, and a range selector. After setting the desired range, click the **Apply** button to perform the search.

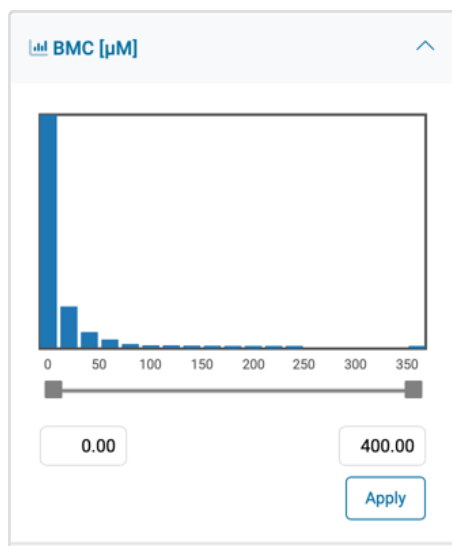


Figure 14: Range Filter example

## Middle Panel

In the middle panel of the **Chemical Mixture Calculator**, displays the *in vitro* assay data for chemicals with available experimental results. Navigation through the results is provided via the pagination controls at the top of the panel, and the total number of results is shown to give an overview of the dataset.

## Panel Navigation and Display

Results are presented across multiple pages. Use the pagination controls at the top of the panel to move between pages.

Users can customize the displayed information using the **show/hide** function. This option allows specific categories or variables to be shown or hidden depending on the user's preference.

Each result is presented in a structured display within the panel, enabling easy comparison and review of the available information.

The number of visible results and their arrangement may vary depending on active filters and sorting settings.

Select in vitro activity values

1 of 1.283 Pro Seite: 25 Ergebnisse: 32.073 Definitions and Units

Sortieren nach Anzeigen/Ausblenden

**Ritanserin**  
DTXSID9042594  
CAS: 87051-43-2

**Functional Class:** [Drugs](#) [serotonergic antagonist](#) [anxiolytic drug](#) [antipsychotic agent](#) [dopaminergic antagonist](#) [antidepressant](#) [EC 3.4.21.26 \(prolyl oligopeptidase\) inhibitor](#) [psychotropic drug](#) [antagonist](#) [dopaminergic agent](#) [serotonergic drug](#) [tranquilizing drug](#) [EC 3.4.21.\\* \(serine](#)  
[Show more...](#)

**Chemical Class:** [organofluorine compound](#) [thiazolopyrimidine](#) [piperidines](#) [fluorine molecular entity](#) [organic heterobicyclic compound](#) [organic heteromonocyclic compound](#) [organohalogen compound](#) [organonitrogen heterocyclic compound](#) [organosulfur](#)  
[Show more...](#)

**MIE:** [Germ layer developmental toxicity](#)

**Effect Group:** [Reproductive Toxicity](#)

**Assay:** [CCTE\\_Deisenroth\\_DEVTOX-GLR\\_legacy\\_Bra](#)

**BMC:** 2.11E-8

There are 10 alternative BMC entries for this compound concerning the same MIE.  
[Click here to view all 11 entries for selection](#)

**Mean DI:** 1.02E-7  
**High CS:** 1.36  
**Cas:** 1.39E-7  
**HQ:** 6.58

**Cyclopamine**  
DTXSID6043709  
CAS: 4449-51-8

**Functional Class:** [glioma-associated oncogene inhibitor](#) [inhibitor](#)

**Chemical Class:** [piperidines](#) [organic heteromonocyclic compound](#) [organonitrogen heterocyclic compound](#)

**MIE:** [Germ layer developmental toxicity](#)

**Effect Group:** [Reproductive Toxicity](#)

**Assay:** [CCTE\\_Deisenroth\\_DEVTOX-GLR\\_legacy\\_Bra](#)

**BMC:** 2.42E-8  
**Mean DI:** 4.16E-8  
**High CS:** 0.251  
**Cas:** 1.04E-8  
**HQ:** 0.432

Figure 15: Middle Panel example with in vitro assay data for compounds.

A link provides access to the definitions of the terms and units used.

For each individual *in vitro* experiment, a card is displayed containing information on the chemical's classifications, its ontology assignment, and the corresponding experimental data and calculations:

The result list can be sorted according their defined variables:

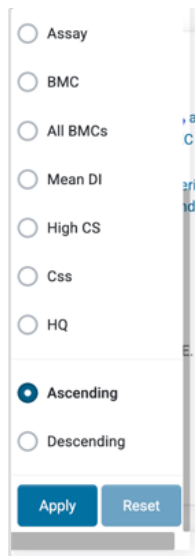


Figure 16: Sorting Function in the pagination area of the Middle Panel

By clicking the **plus sign** on the left side of the card, the chemical is added from the middle panel to the Chemical Mixture and displayed in the right panel.

The display of categories and variables depends on the selected settings, which can be adjusted using the **show/hide** menu.

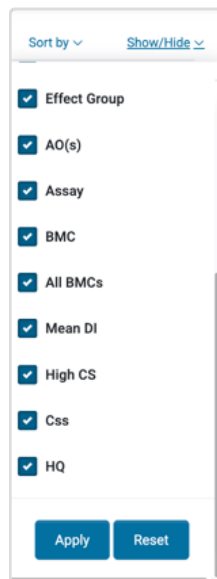


Figure 17: Show/Hide Function in the pagination area of the Middle Panel

The number of results depends on the filter functions in the left panel as well as on the selected sorting.

### Right Panel

In the right panel, the current selection used for calculating the Hazard Index is listed. Three tabs allow the user to display the current selection, delete it, or view previously saved selections. An export function is also available.

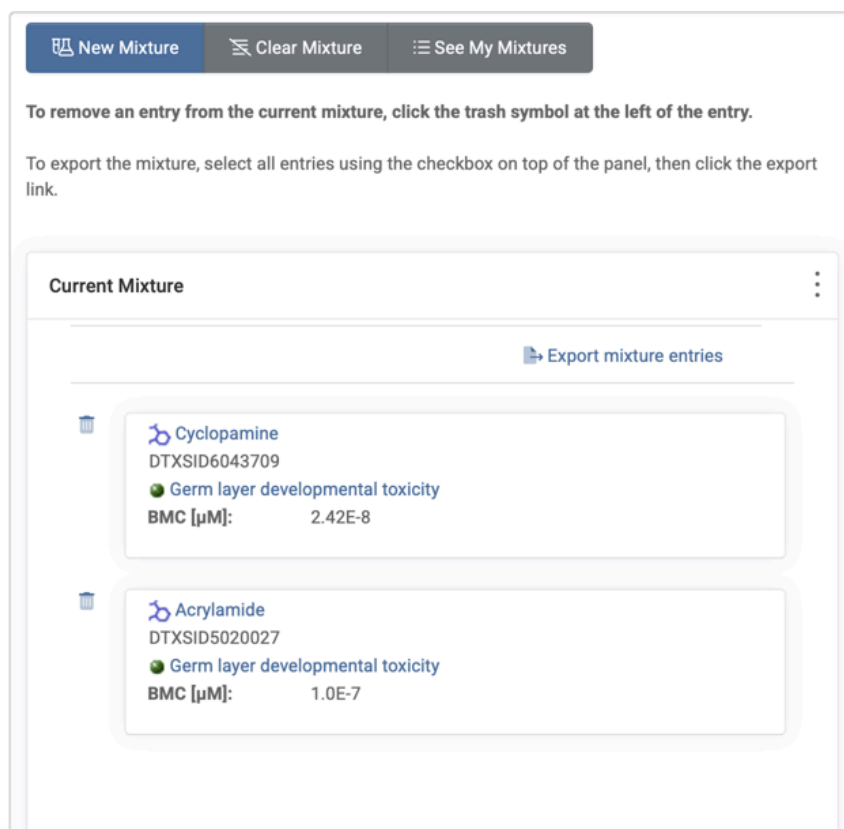


Figure 18: Right Panel with a selected chemical Mixture

### How to: My saved selections

- Go to the “**See my mixtures**” tab.
- Select an entry from the list by clicking the **check mark**, or remove it by clicking the **x**.

**My Mixtures**

A previously stored mixture can be used as current mixture for calculation of Hazard Index (compounds can be added to or removed from current mixture). Click the check symbol in the **Current** column of the table to make the corresponding mixture current (Status= "new").

Current	Delete	Mixture from (date-time)	Status	# Compound BMC entries	Associated MIEs
<input checked="" type="checkbox"/>	<input type="checkbox"/>	Feb 3, 2026, 8:38:42 AM	stored	2	<ul style="list-style-type: none"> <li>Androgen receptor agonism</li> <li>Estrogen receptor binding</li> </ul>
<input checked="" type="checkbox"/>	<input type="checkbox"/>	Feb 5, 2026, 7:47:18 AM	stored	1	<ul style="list-style-type: none"> <li>Androgen receptor agonism</li> </ul>
<input checked="" type="checkbox"/>	<input type="checkbox"/>	Feb 5, 2026, 8:01:25 AM	stored	2	<ul style="list-style-type: none"> <li>Androgen receptor antagonism/decreased activity</li> </ul>
<input checked="" type="checkbox"/>	<input type="checkbox"/>	Feb 5, 2026, 9:39:34 AM	stored	3	<ul style="list-style-type: none"> <li>Androgen receptor antagonism/decreased activity</li> <li>Aryl hydrocarbon receptor agonism/activation</li> </ul>
<input checked="" type="checkbox"/>	<input type="checkbox"/>	Feb 5, 2026, 12:59:27 PM	stored	1	<ul style="list-style-type: none"> <li>Peroxisome proliferator-activated receptor activation</li> </ul>
<input checked="" type="checkbox"/>	<input type="checkbox"/>	Feb 7, 2026, 7:48:59 AM	stored	1	<ul style="list-style-type: none"> <li>Germ layer developmental toxicity</li> </ul>
<input checked="" type="checkbox"/>	<input type="checkbox"/>	Feb 9, 2026, 8:09:37 AM	stored	2	<ul style="list-style-type: none"> <li>Germ layer developmental toxicity</li> <li>Androgen receptor agonism</li> </ul>
<input checked="" type="checkbox"/>	<input type="checkbox"/>	Feb 9, 2026, 9:07:57 AM	stored	3	<ul style="list-style-type: none"> <li>Estrogen receptor antagonism/decreased activity</li> </ul>
<input checked="" type="checkbox"/>	<input type="checkbox"/>	Feb 13, 2026, 8:28:08 AM	stored	3	<ul style="list-style-type: none"> <li>Androgen receptor antagonism/decreased activity</li> </ul>
<input checked="" type="checkbox"/>	<input type="checkbox"/>	Feb 15, 2026, 7:23:15 AM	stored	3	<ul style="list-style-type: none"> <li>Synapse Assembly</li> <li>Estrogen receptor antagonism/decreased activity</li> <li>Androgen receptor antagonism/decreased activity</li> </ul>
<input checked="" type="checkbox"/>	<input type="checkbox"/>	Feb 16, 2026, 8:56:12 AM	stored	3	<ul style="list-style-type: none"> <li>Androgen receptor antagonism/decreased activity</li> </ul>
<input checked="" type="checkbox"/>	<input type="checkbox"/>	Feb 16, 2026, 9:38:44 AM	stored	3	<ul style="list-style-type: none"> <li>Retinoic acid (RAR)/retinoid (RXR) receptor modulation</li> </ul>
<input checked="" type="checkbox"/>	<input type="checkbox"/>	Feb 16, 2026, 4:14:02 PM	stored	3	<ul style="list-style-type: none"> <li>Retinoic acid (RAR)/retinoid (RXR) receptor modulation</li> </ul>
<input checked="" type="checkbox"/>	<input type="checkbox"/>	Feb 17, 2026, 9:16:37 AM	stored	1	<ul style="list-style-type: none"> <li>Germ layer developmental toxicity</li> </ul>
<input checked="" type="checkbox"/>	<input type="checkbox"/>	Feb 17, 2026, 11:19:30 AM	stored	1	<ul style="list-style-type: none"> <li>Germ layer developmental toxicity</li> </ul>

[Schließen](#)

Figure 19: See My Mixtures Tab with a history of used mixtures

## How to: Export

- Press the **export link**.
- A modal window will appear showing the progress of the process.
- A message will appear in the modal window when the process is finished.
- Download the file.
- Open it in **Excel**.



Figure 20: Example of the Export Modal Window which appears after pressing the export link

## Compound Batch Search

The compound batch search allows users to query multiple compounds at once by submitting a list of identifiers, either CAS numbers or DTXS IDs. For demonstration purposes, two predefined ID lists are available: one containing DTXS IDs and one with CAS numbers. Mixed lists containing both types of types are also supported.

To perform a batch search, paste the identifier list into the batch search input field and click **Search**.

Search results are displayed in a table view. The full result set can be exported, or a subset by selecting individual entries using the corresponding checkboxes.

Additional information for a specific compound can be accessed by clicking the **+ icon** to expand a panel displaying detailed compound data. The table layout can be customized by showing or hiding columns. Columns support sorting, and column-specific search functionality is available.

To export data, select the desired entries and click the **Export** button located in the toolbar above the table. An export status dialog is displayed to indicate progress. Once the export process is complete, the generated file can be downloaded to the local machine.

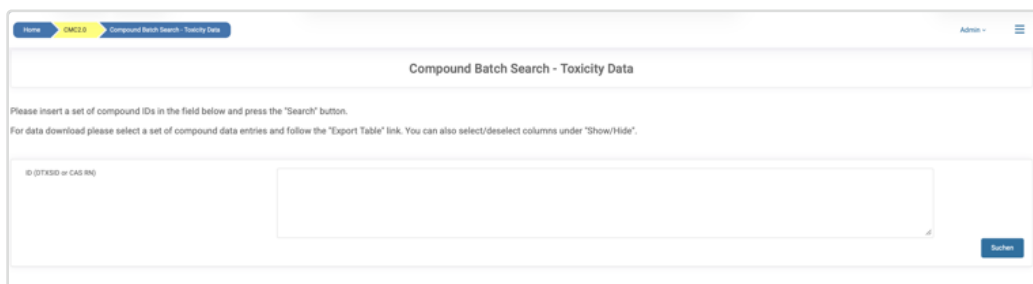


Figure 21: Compound batch Page

Examples of a batch search for

## a) CAS numbers

101-61-1

101-77-9

10161-33-8

102-50-1

102676-31-3

103-56-0

## b) DTOXS IDs

DTXSID6025513

DTXSID1045083

DTXSID1045085

DTXSID9040130

## View Toxicity Data

Toxicity Data														
Assay Component Name														
Selected items: 0														
Target Gene														
Assay Component Name	Assay Name	Assay Description	Assay Function Type	Mechanistic Target	Target Gene	EntrezGene ID	Symbol	Organism	Organism	Cell Format	Cell Short Name	MIE	AO(s)	# Compounds
<input type="checkbox"/>	ACEA_ER_80hr											● Estrogen receptor agonism/increased activity	● Altered, Larval development ● Impaired development of, Reproductive organs ● Show more...	282
<input type="checkbox"/>	APL_HepG2_StressKinase_1hr											● Oxidative stress	● Decreased Cognitive Function ● Decreased sperm quantity or quality in the adult ● Show more...	19
<input type="checkbox"/>	APL_HepG2_StressKinase_24hr											● Oxidative stress	● Decreased Cognitive Function ● Decreased sperm quantity or quality in the adult ● Show more...	63
<input type="checkbox"/>	APL_HepG2_StressKinase_72hr											● Oxidative stress	● Decreased Cognitive Function ● Decreased sperm quantity or quality in the adult ● Show more...	99

Figure 22: Results Page with a list view after a batch search



## View Chemical Blood Levels

The list provides steady state concentrations for selected compounds. The dataset can be **searched**, **sorted** and **customized** by selecting or deselecting variables to show or hide them in the list view.

The **HTTK R package** calculates simulated serum steady-state concentration (**C<sub>ss</sub>**) values [ $\mu\text{M}$ ], based on an exposure of **1mg/kg body weight per day** of the corresponding substance.

The version **2.3.0** of the simulation covers several different population groups (corresponding table headers):

- Total Population (Total-v.2.3.0)
- Females (Female-v2.3.0)
- Males (Male-v2.3.0)
- Women of Reproductive Age (WomenRA-v2.3.0)
- Children (Children-v2.3.0)
- Obese (Obese-v2.3.0)

The dataset includes both the **median (50% quantile)** and the **upper limit of the 90% confidence interval (95% quantile)** for each group.

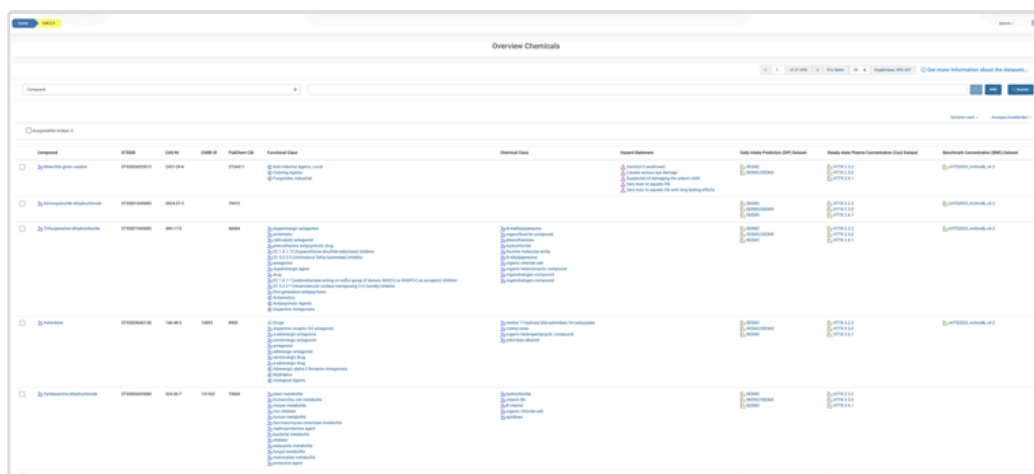
The screenshot displays the 'CSS Simulation Data: HTTK v2.3.0' interface. It features a search bar at the top and a table of simulation results. The table has columns for 'Substance', 'CAS', 'IUPAC Name', 'Chemical Class', 'Hazard Statement', and a series of columns for 'Upper-0.95', 'Median-0.50', and 'Lower-0.05' for each of the six population groups: Total, Female, Male, WomenRA, Children, and Obese. The substances listed include 'Acetaminophen', 'Aspirin', 'Ibuprofen', 'Paracetamol', 'Salicylic acid', and 'Tylenol'. Each row contains numerical values representing the simulated steady-state concentrations in  $\mu\text{M}$ .

Substance	CAS	IUPAC Name	Chemical Class	Hazard Statement	Total		Female		Male		WomenRA		Children		Obese	
					Upper-0.95	Median-0.50	Upper-0.95	Median-0.50	Upper-0.95	Median-0.50	Upper-0.95	Median-0.50	Upper-0.95	Median-0.50	Upper-0.95	Median-0.50
Acetaminophen	103-90-2	N-(4-aminophenyl)acetamide	Amide	H302, H312, H332, H400, H410	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007
Aspirin	50-81-7	Acetylsalicylic acid	Carboxylic acid	H302, H312, H332, H400, H410	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007
Ibuprofen	1568-87-5	(S)-2-(4-(2-(4-carboxyphenyl)butyl)phenyl)propanoic acid	Carboxylic acid	H302, H312, H332, H400, H410	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007
Paracetamol	103-90-2	N-(4-aminophenyl)acetamide	Amide	H302, H312, H332, H400, H410	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007
Salicylic acid	75-30-9	2-Hydroxybenzoic acid	Carboxylic acid	H302, H312, H332, H400, H410	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007
Tylenol	103-90-2	N-(4-aminophenyl)acetamide	Amide	H302, H312, H332, H400, H410	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007	0.0015	0.0007

Figure 24: Blood Levels for chemicals

## Overview - Chemicals

This is a list view containing DTX data for approximately **700,000 compounds**, including population information and hazard data. The dataset can be **searched, sorted, and customized** by selecting or hiding specific variables using the **show/hide** function.



The screenshot displays a web application interface titled "Overview Chemicals". It features a search bar at the top, a table of chemical entries, and a "show/hide" function for columns. The table has the following columns: "General", "CAS No.", "SMILES", "PubChem CID", "Hazardous", "General Data", "Hazard Statement", "Only Under Pressure (GHS Label)", "Ready for Transport (Classification) (GHS Label)", and "Relevant Concentration (GHS Label)". The table contains several rows of data, each representing a chemical compound with its corresponding identifiers and hazard information.

Figure 25: DTX Data for Chemical in List View

## Panoramix Data

Register Dataset and DMP Overview

