United States Environmental Protection Agency

CompTox Chemicals Dashboard Virtual Training

Breakout Group Worksheet
Topic: General

This worksheet was developed for the Breakout Group session of the CompTox Chemicals Dashboard Virtual Training, hosted by the U.S. Environmental Protection Agency's Center for Computational Toxicology and Exposure on October 18, 2022.

For more information about the CompTox Chemicals Dashboard tool, visit the CompTox Chemicals Dashboard at comptox.epa.gov/dashboard. Users also are welcome to review the Help page (epa.gov/chemical-research/comptox-chemicals-dashboard-help) and Release Notes (comptox.epa.gov/dashboard/releasenotes). Starting from the CompTox Chemicals Dashboard, click on the About drop-down menu. The Help page link is third from the top, and the link for Release Notes is at the bottom.

Goal

To identify a general variety of information and tools for a chemical of interest.

Directions

This session is for beginner users or those who wish to work through examples that use a wide range of tabs in the Dashboard. The suggested example chemical is Bisphenol A (CAS RN 80-05-7), but we encourage you to explore the Dashboard.

Basic Search

1. Enter a chemical name or CASRN in the main search bar and select the chemical of interest from the automatically populated options that appear under the search bar. For this exercise, facilitators will be using Bisphenol A (BPA) (CAS RN 80-05-7).

    a. Using the navigation tabs in the toolbar on the left-hand side, what is another valid synonym for your chemical?

2. In a basic search, how do you identify a set of related chemicals, rather than retrieve results for a single chemical?

Properties

3. Navigate to the Properties tab. How many experimental studies are included in the melting point data?

4. Click “Melting Point” and locate OPERA. Then, click the link under “Calculation Details.” How many nearest neighbors were included in the OPERA model melting point prediction?

Hazard

5. From the Hazard tab, what are some of the Sources and Risk Assessment types for the available Exposure Limits?

6. How can one download metadata about each row in the Hazard table?

ADME > IVIVE

7. *In vitro* assays that measure the clearance (removal) of chemicals by hepatocytes (the primary cell of the liver) are used to estimate how fast a chemical is metabolized by the body. What is the human intrinsic hepatic clearance of the chemical?

    a. What is the source of the clearance data?

8. What is the predicted steady-state plasma concentration of the chemical for the 3 compartment model? What is the value for 95% percentile prediction?

9. Where can you find more information about the prediction model used? (Hint: Icon on the ADME-IVIVE page.)

Bioactivity

10. From the Bioactivity tab, select the ToxCast: Summary option. What is the cytotoxic lower bound and cytotoxic median concentrations?

a. How many assay endpoints are active at an AC50 below the cytotoxic lower bound concentration? (Note: If the ToxCast: Summary menu item is unavailable for your searched compound, try a searching for a different compound.)

11. Click the Bioactivity tab again and navigate to the Toxcast: Conc. Response Data page. How many **active** assay endpoints (active hit calls) include PPARg in the endpoint name?

12. Where can the tissue or cell type be viewed for various assay endpoints? What cell types were used for the PPARg assay endpoints? (Hint: Remove "active" filter if you used it to answer the previous question.)

Chemical Lists

13. Click the Lists tab in the toolbar at the top of the Dashboard. Using the Chemicals Lists option from the drop-down menu, locate and navigate to the ATSDRMRLS list (ATSDR: Minimal Risk Levels (MRLs) for Hazardous Substances). Toggle to "Grid View" from the "Preferred View" drop-down menu on the right side. Filter to show all chemicals that are active in ≥30% of ToxCast assays, then export using the "Send To Batch Search" button. Click "Choose Export Options," then "Choose Export Format" and add the following to the export:
    - Metadata: IRIS and PPRTV
    - Enhanced Data Sheets: ToxValDB Details

    a. Within the exported file—

        i. How many chemicals have IRIS data? PPRTV data?

        ii. How many rows of data are available for the hazard component (Toxval Details tab)?

About the CompTox Chemicals Dashboard

14. Click the About tab in the top toolbar of the Dashboard. Navigate to the About page. How should the CompTox Chemicals Dashboard be cited if it's used as a general source of information or data? How should it be cited for referencing a specific chemical?

15. From the About drop-down, navigate to the "Release Notes" page. What is one resolved issue from the Fall 2022 release?

16. From the About drop-down, navigate to the News page. When was the first News update published?

Advanced and Batch Search

17. Click the Search tab in the toolbar at the top of the Dashboard, and choose “Advanced Search” from the drop-down menu. Notice that batch search is also available in this menu. In Advanced Search, input a random mass or molecular formula and search. What file types can be downloaded from the advanced search results page?

Reflection

1. In what case example from your work environment would CompTox be useful?
2. What have you learned about the process and workflow used to find information in CompTox?
3. What challenges did you encounter, and how did you solve them?

CompTox Chemicals Dashboard Virtual Training

Breakout Group Worksheet—Answers
Topic: General

This worksheet was developed for the Breakout Group session of the CompTox Chemicals Dashboard Virtual Training, hosted by the U.S. Environmental Protection Agency's Center for Computational Toxicology and Exposure on October 18, 2022.

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Goal

To identify a general variety of information and tools for a chemical of interest.

Directions

This session is for beginner users or those who wish to work through examples that use a wide range of tabs in the Dashboard. The suggested example chemical is Bisphenol A (CAS RN 80-05-7), but we encourage you to explore the Dashboard.

Basic Search

1. Enter a chemical name or CASRN in the main search bar and select the chemical of interest from the automatically populated options that appear under the search bar. For this exercise, facilitators will be using Bisphenol A (BPA) (CAS RN 80-05-7).

   Bisphenol A

   a. Using the navigation tabs in the toolbar on the left-hand side, what is another valid synonym for your chemical?

      Navigate to the Synonyms tab on the left-hand side of the page, and choose a synonym labeled "Valid" in the Quality column. For Bisphenol A, one valid synonym is BPA.

2. In a basic search, how do you identify a set of related chemicals, rather than retrieve results for a single chemical?

   From the home page, you can select "Identifier substring search" in the checkbox under the basic Chemicals search. Or, from the searched chemical, select the Related Substances tab.

Properties

3. Navigate to the Properties tab. How many experimental studies are included in the melting point data?

   7 studies. From Properties, you have two options: Under Experimental Average, see the number in parentheses. Or, click the Melting Point drop-down, then count the rows in the Experimental table.

4. Click Melting Point and locate OPERA. Then, click the link under "Calculation Details." How many nearest neighbors were included in the OPERA model melting point prediction?

   From Properties, click Melting Point, then locate OPERA under Predicted. Click calculation details. For BPA, there are 4 nearest neighbors, and BPA itself is listed for a total of 5 structures.

Hazard

5. From the Hazard tab, what are some of the Sources and Risk Assessment types for the available Exposure Limits?

   FDA CEDI, EFSA, DOE PAC. Select Exposure Limit from the drop-down menu.

6. How can one download metadata about each row in the Hazard table?

   In the More column on the left-hand side of the Hazard table, hover over the paper icon to see the chemical ID, then click on the paper icon to see a pop-up of the row summary with a .CSV download option.

ADME > IVIVE

7. *In vitro* assays that measure the clearance (removal) of chemicals by hepatocytes (the primary cell of the liver) are used to estimate how fast a chemical is metabolized by the body. What is the human intrinsic hepatic clearance of the chemical?

   Navigate to ADME > IVIVE, then review data in the provided table.

   a. What is the source of the clearance data?

      For BPA: data source species is human, reference is Wambaugh 2019. View table data.

8. What is the predicted steady-state plasma concentration of the chemical for the 3 compartment model? What is the value for 95% percentile prediction?

   For BPA: 3.19 mg/L predicted for 95% (50% not available). In ADME > IVIVE, view table data in the Predicted column.

9. Where can you find more information about the prediction model used? (Hint: Icon on the ADME-IVIVE page.)

   Hover over the "i" at the top of the page next to ADME - IVIVE, then click the link to the httk info page.

Bioactivity

10. From the Bioactivity tab, select the ToxCast: Summary option. What is the cytotoxic lower bound and cytotoxic median concentrations?

    Cytotoxic lower bound concentration = 9.509. Cytotoxic median concentration = 53.511.

    a. How many assay endpoints are active at an AC50 below the cytotoxic lower bound concentration? (Note: If the ToxCast: Summary menu item is unavailable for your searched compound, try a searching for a different compound.)

       View the graphic to identify the cytotoxic concentrations. Enter the Cytotox lower bound concentration (9.509 for BPA) into the AC50 field, assign the filter to "less than," and scroll to bottom of the table to see the number of rows: 92.

       Note that the Dashboard will default to only showing active Hit Call assay endpoints and filtering out "background" assays. The number 92 assumes those defaults were not changed.

11. Click the Bioactivity tab again and navigate to the Toxcast: Conc. Response Data page. How many **active** assay endpoints (active hit calls) include PPARg in the endpoint name?

    Enter *PPARg* in the Endpoint Name filter (the answer is 2 for BPA). Filter to Active.

12. Where can the tissue or cell type be viewed for various assay endpoints? What cell types were used for the PPARg assay endpoints? (Hint: Remove "active" filter if you used it to answer the previous question.)

    View the Cell Line column. For PPARg, the Cell Line types are liver, kidney, and NA.

Chemical Lists

13. Click the Lists tab in the toolbar at the top of the Dashboard. Using the Chemicals Lists option from the drop-down menu, locate and navigate to the ATSDRMRLS list (ATSDR: Minimal Risk Levels (MRLs) for Hazardous Substances). Toggle to "Grid View" from the "Preferred View" drop-down menu on the right side. Filter to show all chemicals that are active in ≥30% of ToxCast assays, then export using the "Send To Batch Search" button. Click "Choose Export Options," then "Choose Export Format" and add the following to the export:
    - Metadata: IRIS and PPRTV
    - Enhanced Data Sheets: ToxValDB Details

      Filter the table by the % Active column, selecting the "Greater than or equals" option for the filter and typing 30. This results in 21 chemicals. Once in the Export screen, click the Choose Export Options button, then the Choose Export Format button to display all options in the Customize Export Results screen.

    a. Within the exported file—

       i. How many chemicals have IRIS data? PPRTV data?

          IRIS data: 11. PPRTV data: 2.

ii. How many rows of data are available for the hazard component (Toxval Details tab)?

8627 rows of data.

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    Click the About drop-down menu, and select the About page option. Should you use the CompTox Chemicals Dashboard to source information and data of value, please cite the app using the URL https://comptox.epa.gov/dashboard/ and refer to the publication "The CompTox Chemistry Dashboard: a community data resource for environmental chemistry." For referencing a particular chemical, the specific citation can be obtained on the Details page under the Record Information tab.

15. From the About drop-down, navigate to the "Release Notes" page. What is one resolved issue from the Fall 2022 release?

    Click the About drop-down menu, and select the Release Notes page option. Any of the bulleted resolved issues are potential answers.

16. From the About drop-down, navigate to the News page. When was the first News update published?

    August 23, 2016. Click the About drop-down menu, and select the News page option. Sort by date to see the oldest items first.

Advanced and Batch Search

17. Click the Search tab in the toolbar at the top of the Dashboard, and choose "Advanced Search" from the drop-down menu. Notice that batch search is also available in this menu. In Advanced Search, input a random mass or molecular formula and search. What file types can be downloaded from the advanced search results page?

    CSV, Excel, SDF. Options can be found by clicking on the Export button.

Reflection

1. In what case example from your work environment would CompTox be useful?

2. What have you learned about the process and workflow used to find information in CompTox?

3. What challenges did you encounter, and how did you solve them?