CompTox Chemicals Dashboard Virtual Training

Breakout Group Worksheet
Topic: Chemistry

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 and review chemistry-focused data (e.g., physical chemistry properties – measured and predicted, environmental fate/transport, chemical structures, chemical lists) focusing on the Details, Physicochemical Properties, Environmental Fate/Transport, and Advanced Search tabs using case examples.

Directions

This session will focus on the Chemistry tab of the Dashboard using the suggested example chemical of Bisphenol A (CAS RN 80-05-7). When you finish, we encourage you to explore the Dashboard by redoing the worksheet with other chemicals of interest to you.

Individual Chemical 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).

Details

2. Navigate to the Details tab from the left-hand toolbar. How many other chemicals contain the same molecular formula?

3. Based on the Tanimoto Coefficient, how many compounds are similar to this chemical?

4. What are two ways to navigate to the list of similar compounds?

5. What is the level of confidence in the data associated with the chemical? (Hint: Click "Record Information" in the Details tab.)

6. Navigate to the Related Substances tab via the left-hand toolbar. How many transformation products are associated with the chemical?

Properties

7. What is the experimental and predicted median Viscosity of the chemical?

    a. What is the source of the viscosity data?

8. How many experimental studies are included in the melting point data?

9. How many nearest neighbors were included in the OPERA model melting point prediction? (Hint: Click OPERA hyperlink under *Calculation Details*.)

Environmental Fate/Transport

10. What is the experimental and predicted median Atmospheric hydroxylation rate of the chemical?

    a. What are similar chemicals from which the modeled data were predicted?

Batch Search

11. Using the Batch Search option under the Search tab in the top banner of the Dashboard, compare physical-chemical properties and environmental fate and transport data across several chemicals.
    - Select Batch Search from the drop-down Search menu.
    - Select Chemical Name from the Input Type options; list 3 or more chemicals by name. For example, enter the following three chemicals:
        - 1-Chlorododecane
        - 5-bromoundecane
        - 2,4-Dibromobenzene-1,3-diol
    - Select Choose Export Options.
    - Click the Choose Export Format button.
        - Choose the file type you wish to use. Excel or .csv is recommended.
        - From the options displayed, select all options in the Intrinsic and Predicted Properties section. Click the Download Export File button at the bottom of the page.

    a. Which chemical has the highest likelihood to accumulate in environmental media?

Chemical Lists

12. Using the Chemical Lists option under the Lists tab in the top banner of the Dashboard, locate and navigate to the DIOXINS list (LIST: Dioxins and dioxin-like compounds). Export the list using the "Send To Batch Search" button. Add the following to the export (some features are not available in .csv output, so choose Excel as the format type):
    - Intrinsic and Predicted Properties: Molecular Formula, Average Mass, Monoisotopic Mass
    - Enhanced Data Sheets: Physicochemical Property Values

    a. Within the exported file—

        i. What is the minimum and maximum average mass for the dioxin compounds list?

        ii. How many rows of data are available for the phys-chem component (Chemical Properties tab)?

Additional Items

Search

13. Does the CompTox Chemicals Dashboard have the capability to search by Mass and Molecular Formula? If so, where would you find that?

14. Does the CompTox Chemicals Dashboard have the capability to search by substring? If so, how would you do that?

Other Tabs

15. Can you predict toxicological properties and phys-chem properties using the Dashboard based on chemical structure? How?

16. Can you make generalized read-across predictions using the Dashboard? How?

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: Chemistry

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 and review chemistry-focused data (e.g., physical chemistry properties – measured and predicted, environmental fate/transport, chemical structures, chemical lists) focusing on the Details, Physicochemical Properties, Environmental Fate/Transport, and Advanced Search tabs using case examples.

Directions

This session will focus on the Chemistry tab of the Dashboard using the suggested example chemical of Bisphenol A (CAS RN 80-05-7). When you finish, we encourage you to explore the Dashboard by redoing the worksheet with other chemicals of interest to you.

Individual Chemical 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

Details

2. Navigate to the Details tab from the left-hand toolbar. How many other chemicals contain the same molecular formula?

   262 for BPA. Under the Intrinsic Properties section, next to Molecular Formula, "Find all chemicals."

3. Based on the Tanimoto Coefficient, how many compounds are similar to this chemical?

   428 for BPA. Shown under Linked Substances.

4. What are two ways to navigate to the list of similar compounds?

   Under Linked Substances on the Details page or via Similar Compounds in the left toolbar.

5. What is the level of confidence in the data associated with the chemical? (Hint: Click "Record Information" in the Details tab.)

   Level 1 for BPA. Under Record Information.

6. Navigate to the Related Substances tab via the left-hand toolbar. How many transformation products are associated with the chemical?

   15 for BPA. Click Related Substances, then filter relationship for transformation product.

Properties

7. What is the experimental and predicted median Viscosity of the chemical?

   Navigate to Properties, then review data in the Summary table.

   a. What is the source of the viscosity data?

      Navigate from Summary to Viscosity in the drop-down menu, then review data in the table(s) provided. For BPA, the answer is TEST.

8. How many experimental studies are included in the melting point data?

   7 studies. From Properties, click the Melting Point drop-down, then count the rows in the Experimental Studies table.

9. How many nearest neighbors were included in the OPERA model melting point prediction? (Hint: Click OPERA hyperlink under *Calculation Details*.)

   From Properties, click Melting Point, then locate OPERA under Predicted. Click the hyperlink under calculation details. For BPA, this link is titled "OPERA Calculation Report [Inside AD]." There are 4 nearest neighbors, and BPA itself listed for a total of 5 structures.

Environmental Fate/Transport

10. What is the experimental and predicted median Atmospheric hydroxylation rate of the chemical?

    Review data in the Summary table. For BPA: 1.64e-11 for predicted median; experimental median is not available.

    a. What are similar chemicals from which the modeled data were predicted?

       Navigate from Summary to Atmospheric hydroxylation rate in the drop-down menu, then click the hyperlink in the calculation details column. List Nearest Neighbors from the Training Set as displayed.

Batch Search

11. Using the Batch Search option under the Search tab in the top banner of the Dashboard, compare physical-chemical properties and environmental fate and transport data across several chemicals.
    - Select Batch Search from the drop-down Search menu.
    - Select Chemical Name from the Input Type options; list 3 or more chemicals by name. For example, enter the following three chemicals:
        - 1-Chlorododecane
        - 5-bromoundecane
        - 2,4-Dibromobenzene-1,3-diol
    - Select Choose Export Options.
    - Click the Choose Export Format button.
        - Choose the file type you wish to use. Excel or .csv is recommended.
        - From the options displayed, select all options in the Intrinsic and Predicted Properties section. Click the Download Export File button at the bottom of the page.

    a. Which chemical has the highest likelihood to accumulate in environmental media?

    Using BCF, 1-chlorododecane. *Additional information: Since the biodegradation factor is similar for both 1-chlorododecane and 2,4-dibromo and BCF is higher for 2-chlorfodecane, 1-chlordodecane is highly likely to accumulate.*

Chemical Lists

12. Using the Chemical Lists option under the Lists tab in the top banner of the Dashboard, locate and navigate to the DIOXINS list (LIST: Dioxins and dioxin-like compounds). Export the list using the "Send To Batch Search" button. Add the following to the export (some features are not available in .csv output, so choose Excel as the format type):
    - Intrinsic and Predicted Properties: Molecular Formula, Average Mass, Monoisotopic Mass
    - Enhanced Data Sheets: Physicochemical Property Values

    a. Within the exported file—

        i. What is the minimum and maximum average mass for the dioxin compounds list?

        Use filter functions to get values. Minimum: 291.98; maximum: 459.73.

        ii. How many rows of data are available for the phys-chem component (Chemical Properties tab)?

        926 rows of data.

Additional Items

Search

13. Does the CompTox Chemicals Dashboard have the capability to search by Mass and Molecular Formula? If so, where would you find that?

    Yes, Navigate to the Search > Advanced Search tab.

14. Does the CompTox Chemicals Dashboard have the capability to search by substring? If so, how would you do that?

    Yes, on the home page relating to the main search box, ensure that the Chemicals tab is selected and "Identifier substring search" is selected.

Other Tabs

15. Can you predict toxicological properties and phys-chem properties using the Dashboard based on chemical structure? How?

    Yes, Navigate to the Tools > Predictions tab. Here you can make predictions about the chemical based on systematic name, synonym, CAS number, DTXSID or InChIKey in the search box at the top of the page. Alternatively, you can search by chemical structure. Select the properties that you want to predict, and select the "calculate" button at the bottom of the page.

16. Can you make generalized read-across predictions using the Dashboard? How?

    Yes, you can find the GenRA (Generalized Read-Across) application in two ways. When you are in the Dashboard in the single chemical view, the GenRA tab is located on the left navigation. Alternatively, you can navigate to the GenRA application by selecting Tools > GenRA on the top menu bar.

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?