

ECOTOX Knowledgebase Virtual Training

Breakout Group Worksheet: Advanced

This worksheet was developed for the Breakout Group session of the ECOTOX Knowledgebase Virtual Training, hosted by the U.S. Environmental Protection Agency's Center for Computational Toxicology and Exposure on February 7, 2023.

For more information about the ECOTOX Knowledgebase tool—

- Visit the ECOTOX Knowledgebase at www.epa.gov/ecotox.
- Contact ECOTOX support at ecotox.support@epa.gov or by calling 218-529-5225.
- Read more in Olker et al. 2022, <https://doi.org/10.1002/etc.5324>.

Goal

With a recent publication as an initial reference, use ECOTOX to provide biological relevance to the chemicals and concentrations detected in surface water samples with effects data from aquatic toxicity studies.

Scenario—Part 1

As a part of your work, you need to determine the scope of aquatic toxicity data available for the 11 chemicals that were detected in more than 25 of the surface water samples collected from the St. Louis River, St. Louis Bay, and Superior Bay sites in Minnesota and Wisconsin in 2010 (Christensen et al. 2012) by using the chemical identifiers provided (CAS Registry Numbers [CASRNs]) and comparing measured concentrations to concentrations producing potential effects.

Christensen et al. 2012, <https://pubs.usgs.gov/sir/2012/5184/>: This worksheet can be completed by reading the abstract for this report and using the below information.

CAS Registry Numbers for the 11 chemicals detected in more than 25% of the samples from Christensen et al. 2012, Figure 4.
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58-08-2
78-51-3
119-61-9
134-62-3
53-16-7
57-88-5
298-46-4
206-44-0
129-00-0
1222-05-5
486-56-6

Directions

After reviewing the reference abstract above, use ECOTOX to explore and document answers to the following questions:

1. Does ECOTOX contain data for all 11 chemicals? *[Hint: Use the 11 above CASRNs in the Explore Chemicals option under Custom Group.]*
2. Describe the scope of the aquatic data available relative to this chemical list (scope of species, number of records, number of publications, etc.). *[Hint: First, limit the data to the "Aquatic" habitat option on the top left-hand side. Group Summary shows the number of records and publications for each chemical and can be exported as .csv file. Scope of species can be seen for the entire group by looking at the "Species Group" and "Species" query filters on the left-hand side. Scope of species for an individual chemical can be found by using the "Chemicals" filter to select each chemical and then looking at query filters on the left-hand side. The "Reset All" button on the bottom left-hand side will bring you back to the original custom group of 11 chemicals.]*
3. N,N-diethyl-meta-toluamide (DEET) was found in 100% of the surface water samples (Christensen et al. 2012, Figure 4). Create a custom plot view for only DEET. How would you describe the testing concentrations for most of the studies included in this plot view? *[Hint: Select DEET in the "Chemicals" query filter OR click the green arrow at the far-right in the DEET row on the Group Summary page. Then move to Plot View and select Custom Plot.]*
4. Figure 5E in Christensen et al. 2012 shows concentrations of DEET measured in water samples at study sites. The maximum on Figure 5E is ~0.15 micrograms per liter, which is equivalent to 0.00015 ppm. How do the concentrations for DEET records in ECOTOX compare to the water sample data? *[Hint: The y-axis shows exposure concentration standardized to ppm, and each point on the plot represents a data record in ECOTOX. Concentrations for specific records can be seen by hovering over the point on the plot or looking in the table below the plot.]*

5. Limit the plot results to the lowest observed effects concentration (LOEC). What effects are reported within 10 times the concentration of DEET reported in the water sample data? *[Hint: Select LOEC and LOEL under the “Endpoints” query filter. Then, Display Concentration line at: 0.0015 (option below the plot).]*

Scenario—Part 2

After seeing the available ECOTOX data, you realize you want to focus on reviewing available literature on mortality effects in short-term studies in fish for the list of 11 chemicals measured at these sites.

6. How can you use your current investigation to arrive at this set of literature? *[Hint: The “Reset All” button at the bottom of the left-hand side will bring you back to original custom group of 11 chemicals in Explore. Then, select Fish under the “Species Group” query filter.]*
 - a. Then, “Send Query Filters to Search” (green button at top-right) and continue your investigation in the Search module. *[Hint: Remember to click the green “Update Search” button in Search.]*
7. Limit the search to mortality effects in studies that were 2 days or less in duration. Review each study for acceptable quality and note what you find. *[Hint: Select “Mortality” in Effects and limit Duration in Test Conditions. Use the green “Customize Output Fields” at the top-right of the screen to add additional data fields to your table—such as Control—to use to review for acceptable quality and review for acceptability. Use options in “Test Conditions” to limit based on some acceptability criteria, such as “Concurrent Control” and “Measured Chemical Analysis.”]*
8. Identify a set of studies that meets the above criteria. Conduct a new search for all records from these studies for this set of 11 chemicals and export the results to an Excel file. *[Hint: Use the References tab to Export a list of identified studies as .csv. Start a new Search (“Reset All” at the bottom-left or open a new ECOTOX Search window). Copy ECOREF numbers into the Ref Num(s) box in Publication Options and CASRNs into the search box in Chemicals. Customize Output Fields to include additional fields of interest, then Export as an Excel file (either Condensed or Full).]*

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Breakout Group Worksheet: Advanced **ANSWERS**

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Goal

With a recent publication as an initial reference, use ECOTOX to provide biological relevance to the chemicals and concentrations detected in surface water samples with effects data from aquatic toxicity studies.

Scenario—Part 1

As a part of your work, you need to determine the scope of aquatic toxicity data available for the 11 chemicals that were detected in more than 25% of the surface water samples collected from the St. Louis River, St. Louis Bay, and Superior Bay sites in Minnesota and Wisconsin in 2010 (Christensen et al. 2012) by using the chemical identifiers provided (CAS Registry Numbers [CASRNs]) and comparing measured concentrations to concentrations producing potential effects.

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298-46-4
206-44-0
129-00-0
1222-05-5
486-56-6

Directions

After reviewing the reference abstract above, use ECOTOX to explore and document answers to the following questions:

1. Does ECOTOX contain data for all 11 chemicals? *[Hint: Use the 11 above CASRN in the Explore Chemicals option under Custom Group.]*

Yes

2. Describe the scope of the aquatic data available relative to this chemical list (scope of species, number of records, number of publications, etc.). *[Hint: First, limit the data to the "Aquatic" habitat option on the top left-hand side. Group Summary shows the number of records and publications for each chemical and can be exported as .csv file. Scope of species can be seen for the entire group by looking at the "Species Group" and "Species" query filters on the left-hand side. Scope of species for an individual chemical can be found by using the "Chemicals" filter to select each chemical and then looking at query filters on the left-hand side. The "Reset All" button on the bottom left-hand side will bring you back to original custom group of 11 chemicals.]*

This chemical group contains 10 species groups, covering 217 species. There are 4,731 total records in 483 publications (found by adding the # of records/publications for each chemical). Cotinine has the least information, with only 20 records in 1 publication.

[Additional guidance: You may also derive this answer by entering Plot View, creating a Custom Plot with Species Group on the x-axis and Chemical as the Legend Category. You can then toggle chemicals on and off by clicking in the legend to allow you to see which species groups have data for each chemical.]

3. N,N-diethyl-meta-toluamide (DEET) was found in 100% of the surface water samples (Christensen et al. 2012, Figure 4). Create a custom plot view for only DEET. How would you describe the testing concentrations for most of the studies included in this plot view? *[Hint: Select DEET in the "Chemicals" query filter OR click the green arrow at the far-right in the DEET row on the Group Summary page. Then move to Plot View and select Custom Plot.]*

The range for DEET Aquatic records (without any other filters) is 0.0006 mg/L to 235 mg/L (from the high and low points on the plot OR the first and last record on the table below the plot).

[Additional guidance: You can sort on the Conc Mean (Std) column and expand the number of rows displayed in the table (if you change this option to 100 rows per page, you can see all the DEET records).]

4. Figure 5E in Christensen et al. 2012 shows concentrations of DEET measured in water samples at study sites. The maximum on Figure 5E is ~0.15 micrograms per liter, which is equivalent to 0.00015 ppm. How do the concentrations for DEET records in ECOTOX compare to the water sample data? *[Hint: The y-axis shows exposure concentration standardized to ppm, and each point on the plot represents a data record in ECOTOX. Concentrations for specific records can be seen by hovering over the point on the plot or looking in the table below the plot.]*

ECOTOX only offers concentrations higher than Christensen et al. 2012, with 0.0006 ppm being a LOEC endpoint.

5. Limit the plot results to the lowest observed effects concentration (LOEC). What effects are reported within 10 times the concentration of DEET reported in the water sample data? *[Hint: Select LOEC and LOEL under the “Endpoints” query filter. Then, Display Concentration line at: 0.0015 (option below the plot).]*

At 0.0006 ppm, genetic effect: androgen receptor mRNA; morphology effect: organ weight in relationship to body weight.

Scenario—Part 2

After seeing the available ECOTOX data, you realize you want to focus on reviewing available literature on mortality effects in short-term studies in fish for the list of 11 chemicals measured at these sites.

6. How can you use your current investigation to arrive at this set of literature? *[Hint: The “Reset All” button at the bottom of the left-hand side will bring you back to original custom group of 11 chemicals in Explore. Then, select Fish under the “Species Group” query filter.]*

Limiting the duration field recommended to be done in Search in Step 7 (within the Hint). Use Plot View to get a sense of how many studies are “short-term.” This can be in the Dur X Chem plot OR Custom Plot (changing y-axis to Duration and y-scale to linear).

Limiting to Effect Group “Mortality” can be done in either Explore or Search.

- a. Then, “Send Query Filters to Search” (green button at top-right) and continue your investigation in the Search module. *[Hint: Remember to click the green “Update Search” button in Search.]*
7. Limit the search to mortality effects in studies that were 2 days or less in duration. Review each study for acceptable quality and note what you find. *[Hint: Select “Mortality” in Effects and limit Duration in Test Conditions. Use the green “Customize Output Fields” at the top-right of the screen to add additional data fields to your table—such as Control—to use to review for acceptable quality and review for acceptability. Use options in “Test Conditions” to limit based on some acceptability criteria, such as “Concurrent Control” and “Measured Chemical Analysis.”]*

Using criteria from the hint, ECOTOX will offer 11 results.

8. Identify a set of studies that meets the above criteria. Conduct a new search for all records from these studies for this set of 11 chemicals and export the results to an Excel file. *[Hint: Use the References tab to Export a list of identified studies as .csv. Start a new Search (“Reset All” at the bottom-left or open a new ECOTOX Search window). Copy ECOREF numbers into the Ref Num(s) box in Publication Options and CASRNs into the search box in Chemicals. Customize Output Fields to include additional fields of interest, then Export as an Excel file (either Condensed or Full).]*

Applying the criteria from the hint in question 7, 5 references are identified:

71703, 19043, 12859, 9994, 20414

Using these 5 ECOREF #s in Publication Options and the 11 CASRNs in Chemicals yields 109 records in ECOTOX.

Reflection

1. What process did you follow in ECOTOX to explore the initial group of chemicals?

[Open response]

2. What challenges did you encounter? How did you solve them?

[Open response]

3. In what case example from your work environment would ECOTOX be useful?

[Open response]