Bayesian Network User Reference Guide

Upper San Francisco Estuary

Prepared for
Metropolitan Water District of Southern California

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ACRONYMS AND ABBREVIATIONS

AChE	acetylcholinesterase
BN	Bayesian Network
BN-RRM	Bayesian Network Relative Risk Model
CDFW	California Department of Fish and Wildlife
CDPR	California Department of Pesticide Regulation
CEDEN	California Environmental Data Exchange Network
CPT	conditional probability table
CPUE	catch per unit effort
CSV	comma-separated values
ECx	effective concentration
EC50	median effective concentration
IETC	Institute of Environmental Toxicology and Chemistry
Integral	Integral Consulting Inc.
SURF	surface water database
USEPA	U.S. Environmental Protection Agency
USFE	Upper San Francisco Estuary
WWU	Western Washington University

1 INTRODUCTION

A Bayesian Network Relative Risk Model (BN-RRM) was created by the Institute of Environmental Toxicology and Chemistry (IETC) at Western Washington University (WWU) (Landis et al. 2024) to calculate the risk of pesticide mixtures in the Upper San Francisco Estuary (USFE) to fish. The BN-RRM incorporates four pesticides and mercury and predicts their influence on fish survival and populations. This *Bayesian Network User Reference Guide* (Reference Guide) has been prepared by Integral Consulting Inc. (Integral), on behalf of the Metropolitan Water District of Southern California, to instruct users on how to run, update, and interpret results of the BN-RRM.

The report by Landis et al. (2024) provides full details on the development of BN-RRM. In brief, a Bayesian Network (BN) was created using input distributions for contaminant concentrations and fish abundance across six regions of the USFE using publicly available sources. A curve fitting process was applied to estimate exposure-response curves for each individual chemical as well as mixtures. For mixtures, the exposure-response models were normalized to specific effective concentration (ECx) values, optimizing the curve fitting for effects comparable to common threshold values. To combine the influence of different chemicals stressors on fish mortality, an expert judgment approach called "peg-the corners" was selected to maintain conservatism in the estimation of risk. A sensitivity analysis of BN-RRM using mutual information identified the most influential components the BN in determining toxicity. The two most critical pathways were the Malathion-Diazinon Mortality pathway and the Mercury Mortality pathway. For individual nodes, mercury, bifenthrin, and season were the key drivers. Landis et al. (2024) concluded with several important lessons learned and outlined next steps to enhance risk prediction and support adaptive management processes. Overall, the work demonstrated the potential for using BN to estimate risks associated with a variety of chemicals and other stressors affecting multiple management endpoints in the USFE.

This Reference Guide presents methods and instructions to acquire and process the underlying data used to construct the BN using a script-based workflow. Instructions are also provided on how to incorporate the processed data into the BN using the BN software Netica (Norsys 2024), and guidance is presented on the interpretation of results from the 2024 BN-RRM output. Finally, guidance is presented on how to conduct a sensitivity analysis on the resulting BN to identify the relative influence of nodes on model outcomes.

2 DATA ACQUISITION, PREPARATION, AND PROCESSING

In this section, we first provide an overview of the process of acquiring, preparing, and processing data for use in the BN-RRM described by Landis et al. (2024). Following the overview, instructions are provided to use a script-based workflow designed to carry out this process.

2.1 OVERVIEW

Data processing for the model is conducted in R (R Core Team 2024), using a series of R scripts that were developed by the IETC. The various scripting components are organized into the following sections:

1. CEDEN and SURF data download
2. Data aggregation and merging
3. BN input preparation
4. Dose-response modeling to be incorporated into the BN
5. Fish species abundance calculations to be incorporated into the BN.

2.1.1 CEDEN and SURF Data Download

This project integrates water quality, sediment quality, and toxicity data from the California Environmental Data Exchange Network (CEDEN), and the California Department of Pesticide Regulation (CDPR). CEDEN data, including a toxicity data set and a water quality dataset, can be downloaded from the CEDEN Advanced Query Tool (https://ceden.waterboards.ca.gov/Home/AqtTool) in TSV format. Surface Water Database (SURF) data, including a surface water chemistry dataset and sediment chemistry dataset, can be downloaded from the CDPR SURF database in CSV format (https://www.cdpr.ca.gov/docs/emon/surfwtr/surfcont.htm).

2.1.2 Data Aggregation and Merging

The downloaded CEDEN and SURF datasets undergo several processing steps to prepare for use in the BN. Entries in the CEDEN data with result quality codes indicating values that were not detected or not quantified are removed. The date range of the SURF data is aligned with the CEDEN data, and some data columns of the SURF data are renamed to align with analogous columns in the CEDEN database. The spatial datum from which the latitude/longitude coordinates of the SURF data are derived is transformed to NAD83 from WGS84 to align with the assumed spatial datum of the CEDEN data spatial coordinates. Using risk regions developed by the IETC (see Landis et al. [2024]) for details), the data in both datasets is

filtered to include only entries within the project's spatial boundaries. Finally, both datasets undergo a de-duplication step, and are merged into a combined CEDEN-SURF dataset.

2.1.3 Bayesian Network Input Preparation

The BN-RRM is based on the sources-stressors- habitats-effects-impacts conceptual model developed by the IETC, as described by Landis et al. (2024). The conceptual model includes multiple categories of stressors (e.g., metals, pesticides, etc.) identified as problematic for model fish species (i.e., Delta smelt), or individual stressors with concentrations that exceed U.S. Environmental Protection Agency (USEPA) Aquatic Life Benchmarks (see Figure 3 of Landis et al. [2024]). To construct the BN, concentration data for members of categories and individual chemicals of concern are extracted from the CEDEN-SURF dataset into a subset. Then, this subset is reduced and formatted to include only the columns required for use as case files by Netica.

2.1.4 Dose-Response Modeling

The following sections describe the dose-response models developed for parameterizing the conditional probability tables used by Netica as part of the BN. These models address chemical-induced effect pathways and include:

2.1.4.1 AChE Inhibition Mixture Model for Malathion and Diazinon

This model used experimental data to fit concentration-response curves for individual chemicals (malathion and diazinon) and mixtures of those chemicals to percent acetylcholinesterase (AChE) inhibition. Toxicity units were calculated based on median effective concentration (EC50) values, and a mixture model was fitted using summed toxicity units. The resulting equation was integrated into Netica under the node "AChE Activity (% Control)" with outputs discretized into bins, including values above 100%.

2.1.4.2 Model of Mortality from AChE Inhibition

Mortality was linked to % AChE activity using an inverse relationship equation from Mitchell et al. (2021). This model was incorporated into Netica under the node "Mixture Mortality 1 (%)" with output values discretized into predefined bins.

2.1.4.3 Mortality Mixture Model for Bifenthrin and Chlorpyrifos

Due to the absence of mixture experiment data, individual chemical models were created using EC20-normalized data. A combined model was developed using geometric means of parameters, assuming a maximum mortality of 100%. This equation was added to Netica, following similar discretization methods as the previous models.

2.1.4.4 Mercury Mortality Model

Based on Dillon et al. (2010), this model linked mercury concentration to fish mortality across species and age classes. The fitted equation was integrated into Netica under the node "Mixture Mortality 3 (%)" with output values discretized into bins ranging from 0% to 100%.

2.1.4.5 Overall Predicted Fish Mortality Model

The outputs from the three chemical-specific mortality models were combined using a "peg-the-corners" approach, a method based on expert judgment that defines minimum and maximum mortality values and specifies intermediate intervals systematically. The final node, "Predicted Fish Mortality (%)" in Netica, used discretized bins, with some values exceeding 100%.

These models collectively provide a framework for estimating fish mortality in response to chemical mixtures, supporting the development of risk assessment and management strategies.

2.1.5 Fish Species Abundance Calculations

Fish abundance data, as measured by catch per unit effort (CPUE) is used to link fish mortality predictions to predicted numbers of fish in the BN. This data is derived from the Fall Midwater Trawl dataset, which spans from 1967–2023, and is obtained from the California Department of Fish and Wildlife (CDFW) (https://filelib.wildlife.ca.gov/Public/TownetFallMidwaterTrawl/FMWT%20Data/).

Fish data is grouped into seasonal categories based on Delta seasonal classifications described by He (2022). Attributes including season and risk region are used to associate the fish data with other nodes of the BN. While Spring Kodiak Trawl data was evaluated, it was ultimately excluded from the analysis due to usability limitations. Further discussion on data relevance and usability can be found in Landis et al. (2024).

2.1.6 Dose-Response Equations

Using the processed input data, dose-response equations derived by the scripting process. These equations are then used in Netica to as part of the BN-RRM. Developed equations include:

1. A model linking AChE activity inhibition to diazanon and malathion concentrations:

$$AChEIn\ (Diazanon, Malathion) = 0 + \frac{99.25}{1 + exp^{10.18*(\log\left(\frac{Diazanon}{53.34}+\frac{Malathion}{83.29}\right)-\log(0.05))}}$$

2. A model predicting mortality from AChE inhibition:

$$Mortality_{AChE(Diazanon,Malathion)} = (-21.97 * \log(AChEIn)) + 100.49$$

3. A model predicting mortality from bifenthrin and chlorpyrifos concentrations:

$$Mortality_{Bifenthrin,Chlorpyrifos} = 0 + \frac{1}{1+exp^{-0.67*(\log\left(\frac{Bifenthrin}{0.000027}+\frac{Chlorpyrifos}{0.00032}\right)-\log(8.34))}}$$

4. A model predicting mortality from mercury concentration:

$$Mortality_{Mercury} = 0 + \frac{0.93}{1+exp^{-0.81*(\log(Mercury)-\log(97.10))}}$$

The equations shown above involving chemical mixtures are three parameter log logistic models with parameters derived using a model averaging process; see Landis et al. (2024) for more details.

2.2 DATA ACQUISITION, PREPARATION, AND PROCESSING INSTRUCTIONS

All components of this project, including the datasets, data processing scripts, and the BN model are hosted at https://github.com/IntegralEnvision/BayDelta_BNRRM. To reproduce these materials, we present instructions below for acquiring the raw datasets from online sources and processing them for use in the BN-RRM. These instructions assume the use of the file structure present in the git repository shown above for storing and processing datasets.

2.2.1 Data Acquisition

Input data necessary to run the BN-RRM can be acquired from three sources, CEDEN, SURF, and the CDFW.

2.2.1.1 CEDEN Data

CEDEN datasets can be downloaded from the CEDEN Advanced Query Tool (https://ceden.waterboards.ca.gov/AdvancedQueryTool). The model requires two datasets:

1. Water Quality (Chemistry)
2. Toxicity.

Steps to Download Data:

1. Use a browser to navigate to the CEDEN Query Tool (https://ceden.waterboards.ca.gov/AdvancedQueryTool).
2. Under **Category**, select **Water Quality (Chemistry)**.
3. Under **RegionBoard**, select **Central Valley** and **San Francisco Bay**.
4. Click **Submit**.
5. Click **Export to TSV** to download the file.
6. Save the file to the designated CEDEN data folder:
    a. **Water Quality (Chemistry):** .../Data/CEDEN_download/water_quality/.

For the **Toxicity** dataset, repeat the steps above, selecting **Toxicity** instead of **Water Quality (Chemistry)**, and save the dataset to a "toxicity" subfolder under the "CEDEN_download" folder. Note that the periods of record of the datasets exported from CEDEN and used to construct the BN-RRM was 10/01/2009-09/30/2019 for the Water Quality dataset, and 10/01/2009-09/26/2019 for the Toxicity dataset. Additional records beyond this time period may be available from the CEDEN database.

2.2.1.2 SURF DATA

SURF datasets can be downloaded from the CDPR SURF database (https://www.cdpr.ca.gov/environmental-monitoring/surface-water/). The model requires two datasets:

1. SURF Water Data 2023
2. SURF Sediment Data 2023.

Steps to Download Data:

1. Use a browser to navigate to the DPR SURF database (https://www.cdpr.ca.gov/environmental-monitoring/surface-water/).
2. Scroll down to the **Surface Water Reports: Surface Water Database (SURF)** section.
3. Download the **SURF Water Data 2023** and **SURF Sediment Data 2023** files.
4. Extract and save the files to the designated SURF data folders:
    a. **Water:** .../Data/SURF_download/water/
    b. **Sediment:** .../Data/SURF_download/sediment/.

2.2.1.3 CDFW DATA

Fish catch data can be downloaded from the CDFW file repository (https://filelib.wildlife.ca.gov/Public/TownetFallMidwaterTrawl/FMWT%20Data/).

Steps to Download Data:

1. Use a browser to navigate to the CDFW file repository (https://filelib.wildlife.ca.gov/Public/TownetFallMidwaterTrawl/FMWT%20Data/).
2. Download the **"FMWT 1967-2024 Catch Matrix updated.zip"** file.
3. Extract and save the contents of the downloaded file to the designated CDFW Fall Fish Data folder:
   a. .../Data/CDFW_Fall_Fish_Data/.

2.2.2 Data Processing using Script-based Workflow

2.2.2.1 Software Requirements

1. The R statistical environment (https://cran.r-project.org/bin/windows/base/). Scripts and packages are function with the most current version of R (as of this writing, v. 4.5.0). Scripts may work with earlier versions but were not tested.
2. RStudio Integrated Development Environment (https://posit.co/products/open-source/rstudio/). While R studio is not strictly required to run the scripts for this work, it is recommended as the scripts are designed to operate with an R project framework.

2.3 SCRIPTING WORKFLOW

R scripting is performed within the R project USFE_BNRRM_Data_Prep.Rproj, located in the R_project folder. Within this project, the USFE_BNRRM_Data_Prep.R script automates the processing of each data component (as developed by Landis et al. [2024]) and generates the necessary outputs for risk evaluation in Netica by sourcing a series of subordinate R scripts. Processed files are stored in the Output folder, categorized by designation.

The first few lines of the control script should automatically locate the data files within the project. If they do not (e.g., because they have been moved), the user may manually navigate to and specify the locations of the input data files using the “file.choose” command.

Following the specification of file pathways for input files, the remainder of the script calls other scripts that load needed packages and generate out all needed outputs.

2.3.1 User Instructions

To process the downloaded data and output the needed outputs, as described above, follow these steps:

1. Open the R project **USFE_BNRRM_Data_Prep.Rproj**, located in the **R_project** folder.
2. Open the **USFE_BNRRM_Data_Prep.R** script by selecting it from the **Files** panel in RStudio or manually opening it from Windows Explorer while the R project is active.
3. Ensure that the file pathways for the needed input data files (i.e., ceden_tox, ceden_wq, surf_sed, surf_wq, cdfw_updated, cdfw_updated_tidy) are correctly specified. Alternatively, the file.choose() command may be used to specify the file path of each file manually. Note that the data input file cdfw_updated_tidy requires formatting of the file cdfw_updated. For convenience, the processed file has been provided. However, the raw data in the file cdw_updated can be processed in the script "USFE CDFW Fish Abundance Data Prep and Analysis.R". See this script for more details.

Once file pathways for data inputs are specified, click **Source** to run the entire script or manually select and execute the code. This will produce all needed outputs in the Outputs folder.

3 BUILDING THE BAYESIAN NETWORK

The output files from the scripted workflow serve as inputs for various nodes within the BN (Figure 1). These outputs include data (analyte concentrations, fish abundance), and equations (e.g., AChE activity model, mortality models). The exported data are used as case learning files for select nodes in Netica, including analyte concentration and fish abundance nodes. The analyte concentration outputs include concentrations of malathion, diazinon, chlorpyrifos, bifenthrin, and mercury. The fish abundance outputs include fall delta smelt abundance, as indicated by CPUE. All outputs are specifically formatted to serve as inputs for Netica. Equation nodes use the data in the data nodes as parameters.

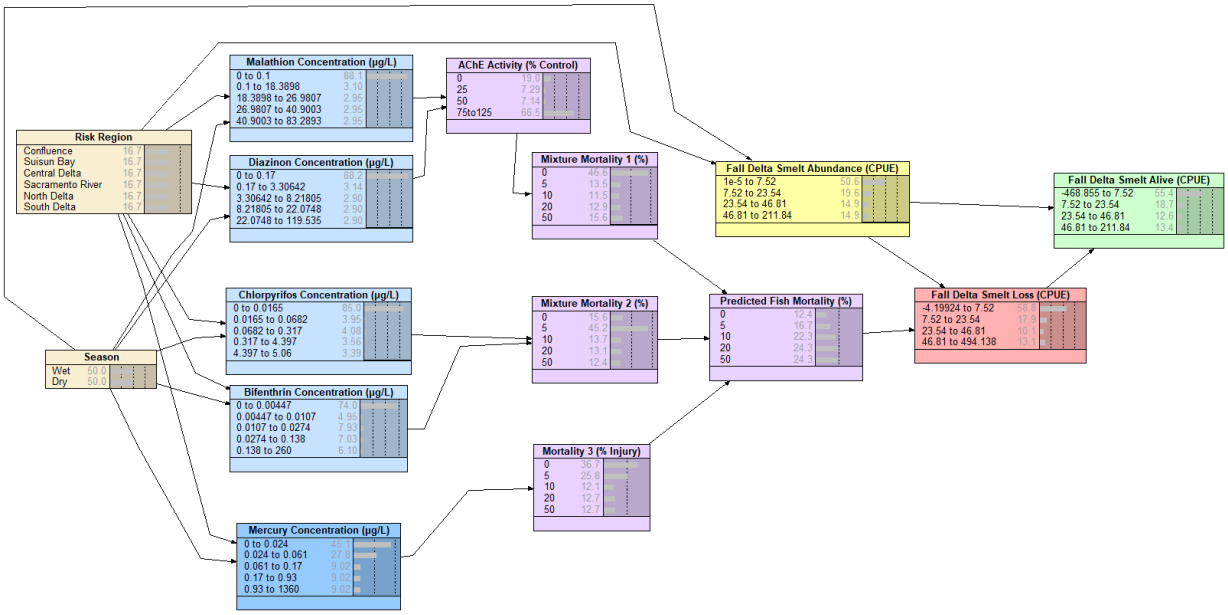


Figure 1. Landis et al. (2024) USFE Bayesian Network Relative Risk Model

4 BAYESIAN NETWORK INPUTS

The BN-RRM is constructed using Netica software. In this section, we present instructions for acquiring Netica software, entering the outputs from the scripting workflow into the software, and compiling the BN-RRM.

4.1 SOFTWARE

Netica (https://www.norsys.com/download.html). This software is freely downloadable, with a "Limited" version that allows for viewing and manipulating the existing BN created for this project. A paid license for this software is required to access full software functionality. Once the software is downloaded and installed, select "Limited" mode and open the model file included in the git repository (https://github.com/IntegralEnvision/BayDelta_BNRRM) associated with this project.

4.2 INCORPORATING DATA INTO NETICA

Nodes of the BN-RRM and their corresponding data sources output from processing workflow are listed in Table 1. All data types incorporated into the BN-RRM are discretized (i.e., categorical), and include case learning data, dose-response equations, categorical parameters (e.g., risk regions, season), or manually adjusted parameters (e.g., predicted fish mortality). Case learning data and dose-response equations may be updated if new or additional data becomes available. In that case, nodes of the BN-RRM can be updated and the model recompiled.

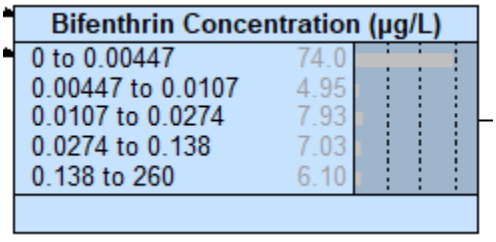
Table 1. Bayesian Network Node Data Sources

Node	Data Type	Input Source
Risk Region	Manual Discretization	GIS shapefile
Season	Manual Discretization	Categorical classification based on month
Malathion Concentration	Case Learning	USFE_Limited_Malathion_Water.csv
Diazinon Concentration	Case Learning	USFE_Limited_Diazinon_Water.csv
Chlorpyrifos Concentration	Case Learning	USFE_Limited_Chlorpyrifos_Water.csv
Bifenthrin Concentration	Case Learning	USFE_Limited_Bifenthrin_Water.csv
Mercury Concentration	Case Learning	USFE_Limited_Mercury_Water.csv
AChE Activity	Dose-Response Equation	dose_response_equations.csv
Mixture Mortality 1 (%)	Dose-Response Equation	dose_response_equations.csv
Mixture Mortality 2 (%)	Dose-Response Equation	dose_response_equations.csv
Mixture Mortality 3 (% Injury)	Dose-Response Equation	dose_response_equations.csv
Predicted Fish Mortality	Manual: Pin the Corners	Expert Judgement outlined in Tech Report
Fall Delta Smelt Abundance	Case Learning	USFE_CDFW_Fall_MWT_DeltaSmelt_No0s.csv

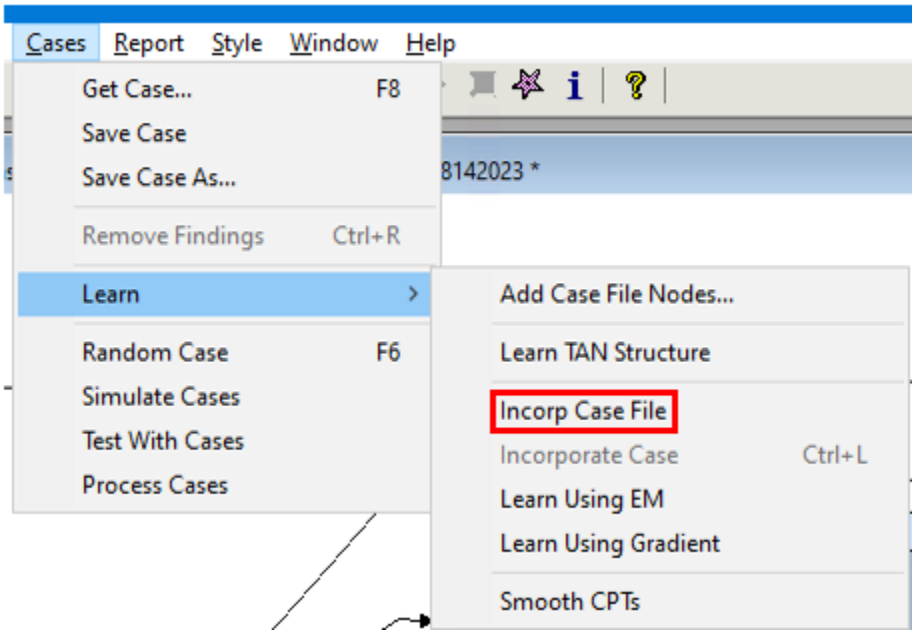
4.2.1 Case Learning Data

The processed data categorized as **Case Learning Data Types** in Table 1 are used to update the conditional probability tables (CPTs) in Netica. Follow these steps to incorporate this data:

1. In Netica, select the node to update (e.g., the bifenthrin concentration node).



2. In Netica, select **Cases → Learn → Incorp Case File** from the top ribbon.



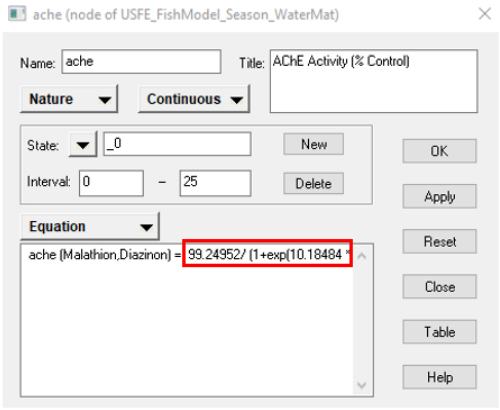
3. Navigate to the corresponding case file produced in the R processing steps (.../R_project/Output/Bifenthrin/USFE_Limited_Bifenthrin_Water.csv).
4. Select **YES** when prompted to remove existing node CPT and experience table.
5. Select **OK** when prompted to enter degree.

Repeat this process for the remaining analyte nodes and the Fall Delta Smelt Abundance node using the appropriate outputs found in the R outputs folder (.../R_project/Output).

4.2.2 Dose-Response Equations

For nodes classified as **Dose Response Equations**, follow these steps to incorporate the processed data:

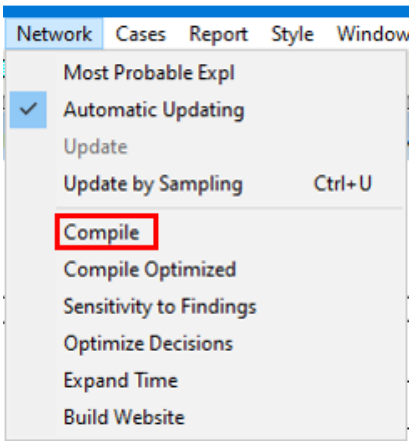
1. Right-click the applicable node and select properties. A window will open that allows the user to set the equation that will calculate the mortality based on the dose-response equation derived in R.
2. In the equation text box, paste the dose-response equation from the from the output .CSV file (.../R_project/Output/Dose Response Equations/ dose_response_equations.csv) for the specified equation after the equals sign. For example, to set the equation for the AChE Activity node, open the properties dialog box, and enter the equation listed for 'AChE_Activity' from the exported CSV file.



3. Continue this process for the remaining nodes in Table 1 listed as **Dose Response Equations.**

4.3 COMPILING THE BAYESIAN NETWORK

Once all the nodes have been updated with either dose-response equations or case learning files, the BN is ready for compilation. To compile the network, select **Network → Compile** from the top ribbon in Netica.



The BN is now compiled and calculating risk estimates based on the input parameters set in the above steps.

5 BAYESIAN NETWORK INTERPRETATIONS

5.1 RISK ESTIMATES

The BN allows users to interact with the parameters of the various nodes, facilitating comparisons across major categorical divisions in the data. For example, Figure 2 shows the BN-RRM that has been restricted to a specific region (e.g., Sacramento Risk Region) and season (e.g., the Wet season). Under this condition, the "Predicted Fish Mortality (%)" node shows that the mean mortality is predicted to be 42.8 ± 7.1%, and meeting or exceeding 50% mortality 17% of the time. Similarly, other combinations of risk regions and seasons can be evaluated.

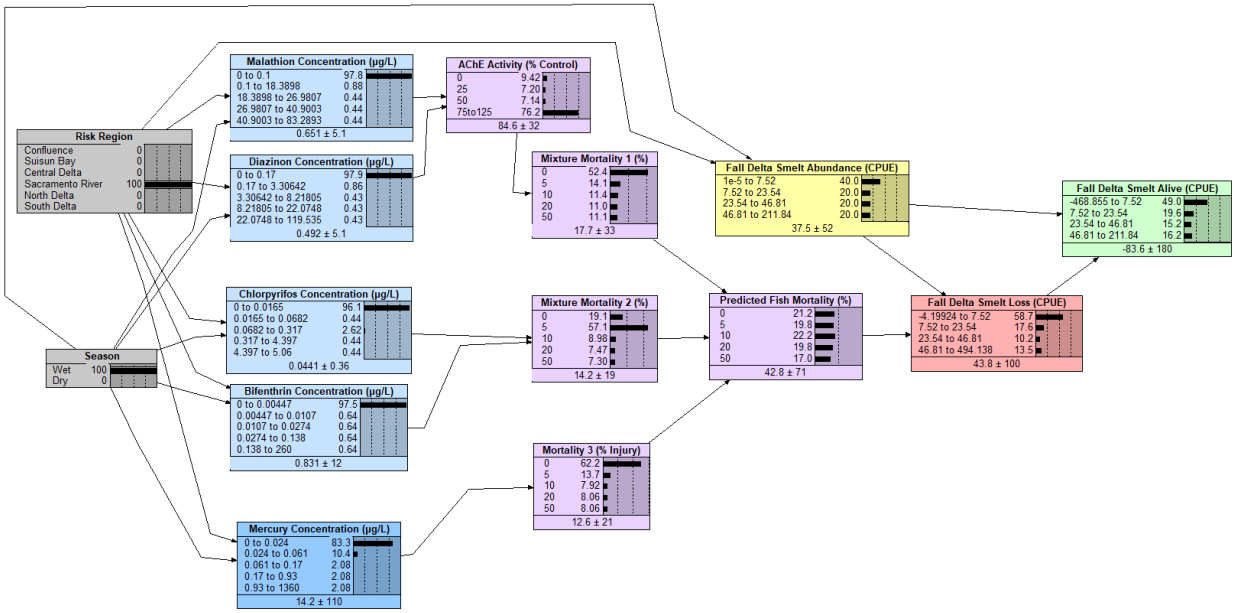
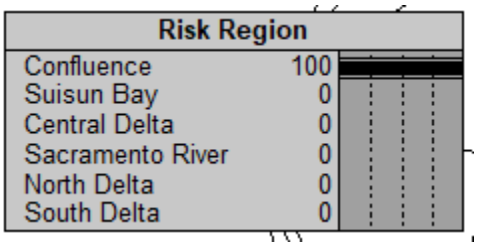


Figure 2. Expert Judgement Risk Estimates for Sacramento River Region and Wet Season. Note that the Risk Region and Season nodes have been restricted to only consider information for the Sacramento River and Wet season, instead of all risk regions and seasons (e.g., see Figure 1).

To set/restrict the values of nodes, simply click on the appropriate bin of the node of interest (e.g., the "Confluence" bin of the Risk Region node). This will set the value of that to bin to 100, and set the value of all other bins to 0:

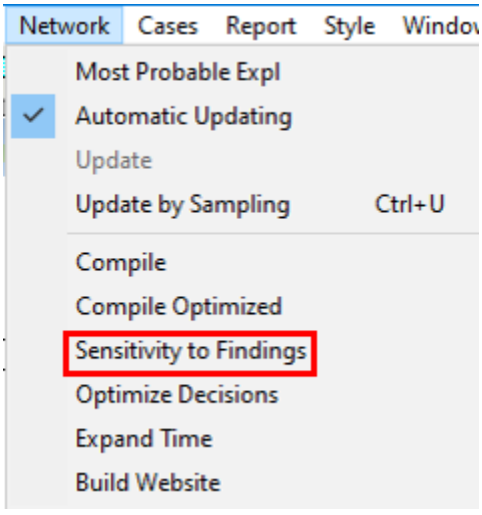


Clicking on the bin again will restore the previous distribution across the bins on the node. Bin values of nodes can also be manually adjusted by clicking and dragging each bar.

5.2 SENSITIVITY ANALYSIS

Netica provides robust utility-free sensitivity analysis capabilities, allowing users to evaluate how a target node's beliefs, mean values, or other parameters are influenced by individual findings from other nodes in the network (i.e., "findings nodes"). Sensitivity analysis ranks input nodes by their influence on a node of interest, calculated as shared mutual information. In general, the higher mutual information shared between nodes suggests a higher degree of sensitivity influencing the findings of the BN. This feature is invaluable for identifying which nodes most significantly influence outcomes in the BN, aiding in refining models and focusing further analysis on critical components.

This sensitivity analysis tool is accessed by first selecting the target node, and then clicking on **Sensitivity to Findings** under the Network option on the ribbon:



This produces a report under the "Messages" window that shows a comparative overview of degree of influence that each findings node exerts on the target node in terms of both variance reduction and mutual information (entropy). To facilitate comparison, these values are reported both in absolute terms and in cumulative percent reduction. In Figure 3, the output

from the sensitivity analysis tool was run with "Predicted Fish Mortality (%)" as the target node. Next to the target node itself (included for completeness), the Mixture Mortality 1 (%) node had the largest influence in terms of both variance reduction (13%) and entropy reduction (8.21%) on Predicted Fish Mortality (%) in the network.

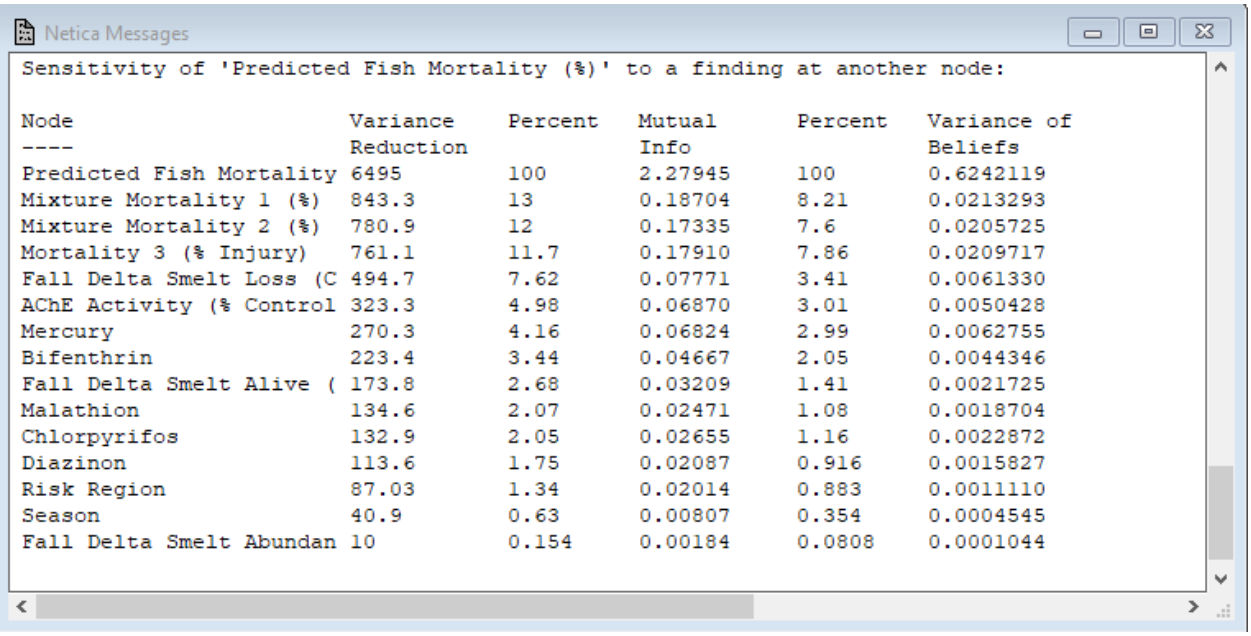


Figure 3. Sensitivity Analysis Output with "Predicted Fish Mortality (%)" as the Target Node

The analysis can also be customized to specific findings nodes by selecting nodes of interest using Ctrl + Click after selecting the target node. For example, Figure 4 shows an output from a sensitivity analysis in which the influence of chemical stressor nodes on the "Predicted Fish Mortality (%)" were selected. This output shows that mercury concentration has the highest relative influence on predicted fish mortality, followed by bifenthrin.

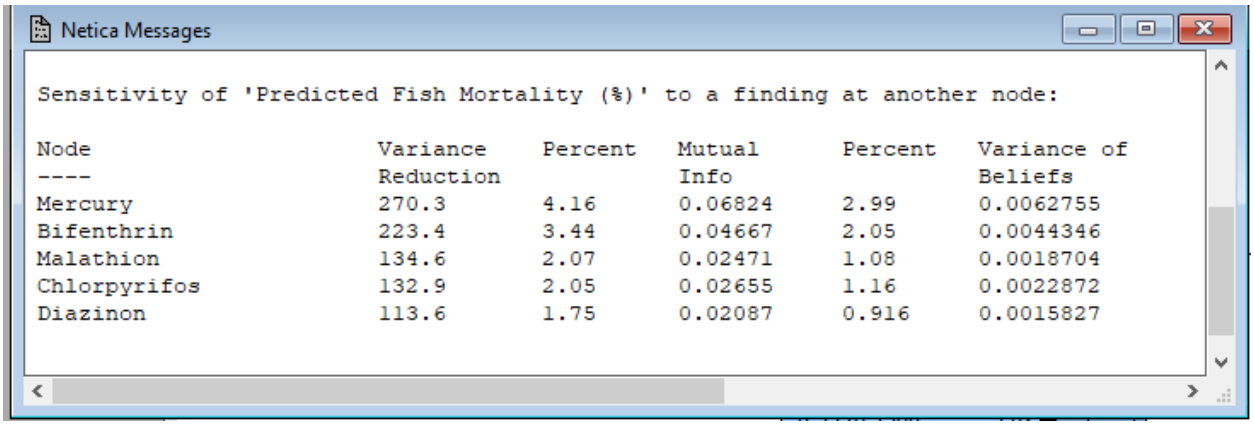


Figure 4. Sensitivity Analysis Output with "Predicted Fish Mortality (%)" as the Target Node and Only Pesticide and Mercury Nodes Selected as Findings Nodes.

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