***User Documentation for PRC\_GUI\_v2.xlsm***

This PRC\_GUI is a macro-enabled Excel Workbook. It must be installed along with a subfolder containing executable R software, which is provided with the GUI. R is an open-source statistical package widely used by statisticians and available for free on the internet. The Excel Workbook contains macros that enable the user to run R by clicking a button. A DOS window will appear on the screen while R processing takes place. After the DOS window closes, the results will be written back to the Excel workbook. All this processing is controlled by Excel, so the user does not have to issue any R commands.

***Note: no other Excel workbooks should be open while working with the PRC\_GUI. Multiple open workbooks can cause macros to malfunction.***

A note on significant figures entered into the ‘Measured PRC Fractional Equilibrium’ section of the Input Frame: there is no scientific limit to the number of significant figures that may be entered.  However, small differences in the calculated target contaminant fractional equilibrium values may occur with the same dataset if different significant figures are used in the Input Frame.  It is recommended that users of this GUI select a reasonable number of significant figures (e.g., 0.000, 0.0000) and apply that number consistently when entering data into the ‘Measured PRC Fraction Retained’ section of the Input Frame.

**Step-by-step Instructions:**

To use the PRC\_GUI software, open the Excel workbook PRC\_GUI\_v2.xlsm.

1. From the Intro worksheet, follow instructions to enable macros if prompted. You may also need to identify the workbook as “Trusted”.
2. Click the “RUN PRC\_GUI” button to bring up the GUI Form.
3. From the GUI Form:
4. In the Input Frame, enter the PRCs for the passive sampler deployment and the Fractions Lost (in decimal form). Up to 20 PRCs can be entered. The first two columns are required. The third column PRC Type can be used for descriptive information.

PRCs should be selected from a list provided by the “Select PRCs from List” button. Clicking this button brings up a window that allows you to select up to 20 PRCs from a list of possible PRCs. Use the “Remove Code” button to remove the “no selection” indicator. Use the “Add Code” button to add selections. Press “Continue” when codes are selected.

After PRCs are selected and pasted to the first column in the Input Frame, manually enter values for the second column (*Measured PRC Fraction Retained)*. Fraction values should be between 0.15 and 0.85.

Calculations performed by the GUI are based on PRC parameters associated with Target Properties.  To view these properties, click the “View Target Properties” button.  This will take you to the *Target Properties* sheet.  The current default target properties (i.e., DLDPE, DW, KLDPEW) are recommended for low density polyethylene polymer passive samplers.  The user should be aware that for selected PCB congeners, PAHs and DDT molecules, DLDPE was calculated based on Lohmann (2012) using molecular volume and DW was calculated by SPARC (<http://www.archemcalc.com/>).  For the remaining PCB, PAH and DDT molecules, DLDPE and DW were assigned based on structural similarities to PCBs, PAHs and DDTs for which properties had been calculated.  Values for KLPDEW were calculated using the linear free energy relationships reported in Ghosh et al. (2014). The use of estimated properties, especially DLDPE and DW, may result in some errors in the calculation of fractional equilibrium.  Use of this GUI with polyoxymethylene (POM) or polydimethylsiloxane (PDMS) is possible, but the target properties will need to be revised for those polymers.  On the *Target Properties* sheet, you can modify values in columns C, D and E for *Target PRCs*.  The PRC codes themselves cannot be modified.  Default values for columns C, D and E can be restored by clicking the “Restore Default Properties” button.

Click the “Return to PRC\_GUI” button leave the *Target Properties* sheet and return to the GUI Form.

1. After entering PRC data, enter the *Passive sampling duration* in days, and the *Passive* sampler thickness in microns (µm).
2. Select *Target Contaminant Class* for analysis by checking up to three check boxes.
3. Press the “Calculate” button to run analysis.
4. Analytic results are calculated in a DOS batch process that runs R scripts. While the R scripts are processing, a black DOS window will appear on the screen***. This will last for up to 15 seconds on most computers.*** Do not attempt to close the DOS window or click on any other form buttons before processing is complete.

After pressing “Calculate”, you will be prompted to press “OK” at the following two message boxes:

First: “Press OK and wait for DOS window to close”

(DOS window will then open and close)

Second: “Press OK to view output” (after DOS window closes.)

1. Viewing the Output: After completion of the batch processing, the results of the PRC analysis will be written to the Output Frame. The results are formatted to display significant digits out to three decimal places. Click the “Save Results to CSV” button to save raw results to disk. You will be prompted to provide a file name and locations, and to view the resulting file in Notepad. This CSV file is formatted for viewing in Excel after closing the PRC GUI.
2. To exit, first click “Exit PRC\_GUI”, then “EXIT EXCEL”. Your latest input data will be saved in the input frame. Results in the output frame are not saved on exit.

Troubleshooting:

* If the DOS window closes very quickly without producing output, the software may not be installed correctly. Refer to the installation guide*. Do not rename or relocate any files* after they are “unzipped” from the original zip file.
* The GUI provides some range checks on user input, but it is still possible to enter invalid data (such as missing PRC fractions.) If the calculation process does not provide two columns of results in the Output Frame, examine the values in the Input Frame carefully and try again. Make sure all required data elements are provided.
* Message boxes that require an “OK” may become hidden in the background while working in Excel. Clicking on the GUI frame should bring them to the foreground.
* **Be sure that the DOS window closes before attempting to view output**. Don’t click on any buttons while the DOS window is open.
* If other Excel files are open, the PRC\_GUI macros may not function properly. Close all other Excel files while using the PRC GUI.
* On a standard-sized single monitor, the Excel workbook will remain hidden behind the user form. This is by design. If the software is used on a dual monitor system, or with a large external monitor, the underlying Excel workbook may remain visible. Recommendation: move the Excel workbook so it is hidden behind the user form. Make sure DOS window closes before pressing OK buttons.
* Software will not run in a OneDrive folder. An address on the C:\ drive is recommended.
* Report technical problems with the GUI to [hbuffum@cox.net](mailto:hbuffum@cox.net) or burgess.robert@epa.gov

For information on the mathematical model used in the PRC\_GUI calculations, see :

* Apell et al. (2016). "Understanding the rates of nonpolar organic chemical accumulation into passive samplers deployed in the environment: Guidance for passive sampler deployments." Integrated Environmental Assessment and Management **12**(3): 486-492.
* Ghosh et al. (2014). “Passive sampling methods for contaminated sediments: Practical guidance for selection, calibration and implementation.” *Integrated Environmental Assessment and Management* **10**:210-223
* Lohmann (2012). “Critical review of low-density polyethylene’s partitioning and diffusion coefficients for trace organic contaminants and implications for its use as a passive sampler.” *Environmental Science and Technology* **46**:606–618.
* Thompson et al. (2015). "Modeling uptake of hydrophobic organic contaminants into polyethylene passive samplers." Environmental Science & Technology **49**(4): 2270-2277
* Tcaciuc et al. (2015). "Modeling the transport of organic chemicals between polyethylene passive samplers and water in finite and infinite bath conditions." Environmental Toxicology and Chemistry **34**(12): 2739-2749.