BioSim2 User's Manual

Version 2.0.03

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A Program that Applies the Coefficient of Biotic Similarity, B, to Complex Data Matrices

by

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Notice

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Contents

Section Pag	ge
Noticei	iii
List of Figures	′ii
List of Tablesi	X
Acknowledgement	хi
Abstractxi	iii
Section 1 Introduction	1
Section 2 Use of This Manual	3
Section 3 Installing and Starting BioSim2	5
Section 4 Using BioSim2	7
4.1 Standard Menu Functions	8
4.1.1 "File" Drop-down Menu	8
4.1.2 "Actions" Drop-down Menu	1
4.1.3 "Print" Drop-down Menu2	0
4.1.4 "Edit" Drop-down Menu2	1
4.1.5 "Help" Drop-down Menu2	1
References	3
Appendix A	5

List of Figures

Numbe	r	Page
1	Opening Screen of BioSim2	8
2	Opening Screen with "File" Drop-down Menu Opened	9
3	Opening Screen with "Actions" Drop-down Menu Opened	12
4	Files Created and Saved Using the "Save Report" Option	13
5	Tab "B Matrices" Showing the Similarity Values (B) for Rows (top) and Columns (bottom)	14
6	Tab "Row Dendrogram" Showing the Dendrogram for Rows	15
7	Tab "Row Cophenetic Plot" Showing the Cophenetic Correlation Plot for Rows	16
8	Tab "Column Dendrogram" Showing the Dendrogram for Columns	17
9	Tab "Column Cophenetic Plot" Showing the Cophenetic Correlation Plot for Columns	18
10	Tab "Reordered Data" Showing the Data Reordered According to Both Row and Column Dendrograms	
11	Opening Screen with "Print" Drop-down Menu Opened	20
12	Opening Screen with "Edit" Drop-down Menu Opened	21

List of Tables

Number		
1	Example of CSV Spreadsheet as an Input File (partial data set <i>with</i> titles and options)	10
2	Example of CSV Spreadsheet as an Input File (partial data set <i>without</i> titles or user options)	11

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Abstract

The Pinkham-Pearson index of similarity has been evaluated by EPA as one of the more powerful tools for comparing community structure in its rapid bioassessment protocol. However, its use has been limited because the program that ran it, BioSim1, was only available in DOS format. A user-friendly version of BioSim2 is now available in a Java format that can run on Windows, Mac OS, Linux, or any computer operating system that supports Java v1.4 or higher.

Introduction

The index of similarity, *B* (Pinkham and Pearson, 1976), was proposed as a means for determining the impact of pollution on communities. Pinkham and Pearson showed that the index overcame many of the shortcomings inherent in other indexes used for the same purpose and was more versatile. Its use was coded in a DOS program (BioSim) (Pinkham *et al.*, 1975).

Since its publication, it has been widely used for diverse investigations. In 1989, Pfalkin *et al.* included it in EPA's rapid bioassessment protocols for use in streams and rivers. In 1990, it was identified by EPA as one of six commonly used community similarity indexes in a manual describing guidelines and standardized procedures for using benthic macroinvertebrates to evaluate the biological integrity of surface waters (Klemm *et al.*, 1990). At least one state, Vermont, has adopted *B* as a legal requirement for assessing surface water quality (Vermont Department of Environmental Conservation, 1990). Barbour *et al.* (1992), in a systematic comparison of the metrics proposed in EPA's rapid bioassessment protocol (Pfalkin *et al.*, 1989), concluded that *B* "may be the most appropriate metric to serve as a measure of community similarity."

In almost all published cases of its use, however, it was not being used to its full potential. Recognizing this, Pearson and Pinkham (1992) published a strategy for using it in an improved DOS version (BioSim1) (Gonzales *et al.*, 1993). However, this strategy also failed to encourage a widespread use of its full capabilities. It soon became apparent that the major reason for this shortcoming was the DOS platform of BioSim1. This manual describes the use of BioSim2, a Java program that finally overcomes that shortcoming.

Use of This Manual

It is assumed that users of this manual are familiar with the index of similarity, *B* (Pinkham and Pearson, 1976), and the use of dendrograms in the analysis of complex environmental data sets. If not, users should refer to previous publications on the topic (Bonham-Carter, 1967; Pinkham and Pearson, 1976; Kaesler, 1970; Klemm *et al.*, 1990; Pearson and Pinkham, 1992; and Gonzales *et al.*, 1993).

Installing and Starting BioSim2

Running BioSim2 requires that a Java Runtime Environment (JRE) of version 1.4.1 or higher be installed. Sun Microsystems, Inc. offers the Java Runtime Environment® for Windows®, Linux®, and Solaris®. Apple® offers Java® for the Mac OS. Links to download the appropriate JRE can be found at:

http://www.java.com

BioSim2 will run on most modern computers with Windows 98 SE or higher or Apple OS X or higher.

Once the JRE is installed, biosim2.jar is the only file needed to run BioSim2. The biosim2.jar file is a Java® archive which uses the same format as a compressed Zip file. To install, copy the biosim2.jar file to any convenient location or network directory. The most recent version of the program and its associated User's Manual are available at:

http://www2.norwich.edu/pinkhamc/

Start BioSim2 by double-clicking on the biosim2.jar file. The file menu at the top of the opening screen (see page 8) is used for most commands. The data are imported, or entered manually. The program is run using the "Process Data" command under the "Action" menu. Results are accessed through the various tabs at the bottom of the window.

Using BioSim2

BioSim2 was written with an entirely new appearance and a simpler approach while retaining most of the features discussed in Pearson and Pinkham (1992). A major change was to drop the agglomerative clustering method for forming dendrograms used in former versions of BioSim (Bonham-Carter, 1967) in favor of the simpler, average link method (Pankhurst, 1991). This method searches through each possible pair of unlinked parameters and an average B-value is calculated for the pair [see Pearson and Pinkham (1992) for a definition of these terms]. This average B-value is determined in three possible situations. 1) Both parameters are not found in any other cluster formed already. This normally happens toward the beginning of the process. In this case, the average is their single B-value. 2) One of these parameters is already part of another cluster. All B-values involving the unlinked parameter and every member of this other cluster are averaged. 3) Both parameters belong to existing clusters. All B-values between the two clusters are averaged. After searching the complete set of unlinked pairs, the pair with the highest average B-value is linked at that average value.

In addition to the above, the authors decided 1) to reduce the presentation of the program to a single screen that would sequentially display the original data and then the results; 2) to make the conditions of the original data matrix flexible enough that most presently used spreadsheet formats would be acceptable; 3) to provide a plot of the actual B-values used to calculate each average B-value found on the dendrogram, to visualize how well each joining branch of the dendrogram represents the actual distribution of B-values that formed the joining branch; 4) to reorient the dendrogram 180° so that the plot resulting from number 3, above, could be easily compared with the dendrogram; 5) to eliminate the matrix of cophenetic correlation coefficients (Kaesler, 1970) in favor of the simpler and more valuable cophenetic correlation coefficient for the entire dendrogram; 6) to enable BioSim2 to accept and analyze data matrices with missing data points (incomplete data matrices); and 7) to eliminate many of the choices that needed to be made in BioSim1 by making most options automatic in BioSim2.

Figure 1 represents the opening blank screen of BioSim2. The screen consists of four basic parts: a standard menu bar along the top; a data input / results display area; a message window near the bottom; and a series of "tabs" at the very bottom that provide access to panels for data input and, after running the program with data, to display results with a different array of "tabs."

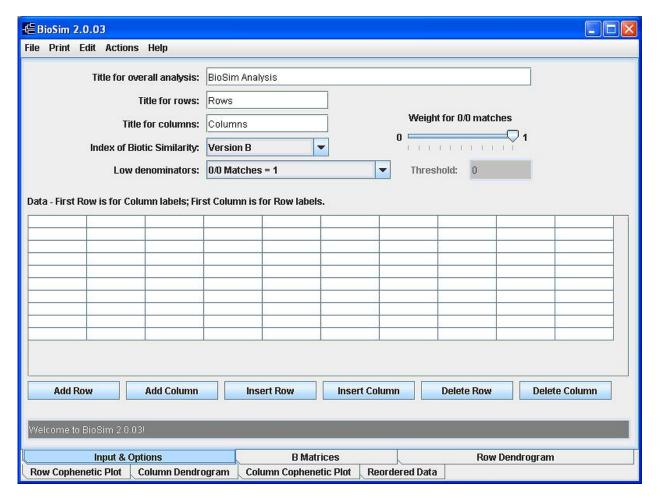


Figure 1. Opening Screen of BioSim2.

4.1 Standard Menu Functions

4.1.1 "File" Drop-down Menu

Figure 2 represents the opening screen with the "File" drop-down menu opened. This menu contains four options: New Data File, Open Data File, Save Data File, and Exit. The first three options are also available using the keyboard shortcut in the drop-down menu.

New Data File: If an existing file is open, the "New Data File" will clear the data in the spreadsheet portion of the screen. Currently, it does not clear the title data or the options selected. These data require manual entry.

Open Data File: The "Open Data File" option opens existing data files that are in CSV format (comma separated values; also referred to as comma delimited data). Most of the modern spreadsheet programs allow you to save files in this CSV format. Titles and options data may be entered manually using the *Input & Options* tab and its associated drop-down menus or by opening a CSV spreadsheet containing these data. When *importing all* of the data (titles,

options, and numerical data) from a spreadsheet file, the data must follow the format shown in Table 1 and must be saved as a CSV file.

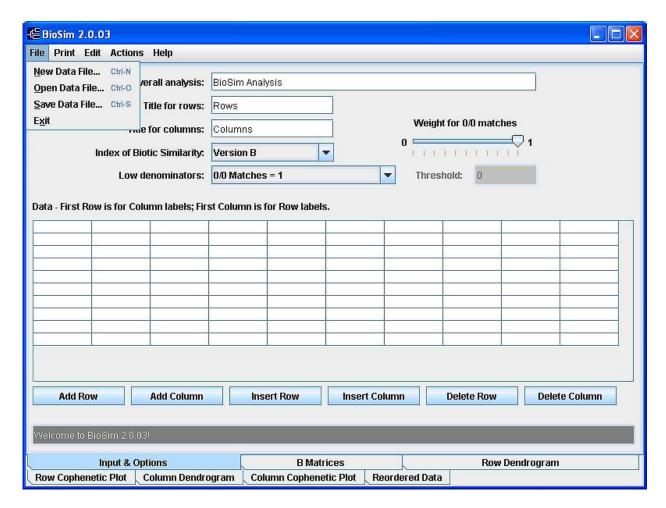


Figure 2. Opening Screen with "File" Drop-down Menu Opened.

The first five rows of an external spreadsheet must contain the input titles and program options data selected by the user. The sixth row must contain the titles to be used for the columns and the remaining rows contain the actual data set with the first column being the titles for the rows. The values in column A, rows 1-5 are fixed and must appear as in Table 1. The values in column B, rows 1-3 are user-entered titles and the values in rows 4 and 5 are options for calculating the similarity index (see Pearson and Pinkham (1992) for a complete explanation of these options). B is the standard similarity index and B1 is the same index, but the raw data values are converted to relative abundances. The "Low denominators" field allows the user to define how 0/0 matches and other matches with low denominators will be dealt with during the calculation of the similarity index. The 0/0 matches can be set to equal 1 (highest weight), 0 (lowest weight), any value between 0.0 and 1.0 (using the "Weight for 0/0 matches" slider bar), or ignored altogether in the calculations. Matches with low denominators can be ignored by setting the "threshold" to the value of the denominator at or below which matches should not be used in calculating B. This value is entered in the "Threshold" box on the opening screen.

Microsoft Excel - CPCTestData.csv File Edit View Insert Format Tools Data Window Help Type a question for help - A X · 10 · | B I U | 圖 圖 圖 | \$ | 準 | Ⅲ · 🔊 · 🗛 · f Data F Α C D E CPCRW-02 1 Title 2 Rows Sites 3 Columns Taxa 4 В Version B 5 0/0 Matches = 1 Low Denominators Data Tubific DCD-Diam DCD-Paga DCO-CrCo DCO-Euki CPC720R1 7 17 1 4 71 3 CPC720R2 16 3 3 53 8 27 2 9 CPC720R3 33 8 87 15 10 CC725R1 96 54 0 0 30 CC725R2 11 88 24 0 12 20 12 CC725R3 152 76 0 8 80 13 PC725R1 73 0 7 90 10 14 PC725R2 30 0 27 80 6 15 PC725R3 0 27 326 14 24 CPCTestData >

Table 1. Example of CSV Spreadsheet as an Input File (partial data set with titles and options).

Important: There must be a value in column A, row 6 (the word "Data" is written here by BioSim2 when saving the file).

As indicated above, the titles and options data may be entered directly on the screen accessed with the *Input & Options* tab. The maximum number of characters for these titles is 256, but long titles can cause some problems with the data displays. Data may also be entered directly using the table portion of this screen and the buttons (Add Row, Add Column, Insert Row, Insert Column, Delete Row, and Delete Column) directly below the data input table. You can also just import the data using the Open Data File option. This file must follow the format as shown in Table 2. The first row always contains the titles for the columns and the first column always contains the titles for the rows.

Important: There must be a value in column A, row 1 (the word "Data" is written here by BioSim2 when saving the file).

It is also possible to use the standard copy (Ctrl-C), cut (Ctrl-X), and paste (Ctrl-V) features of Windows to move data from a spreadsheet directly into the table on the *Input & Options* tab. When doing this, make sure that cell A-1 has something in it, otherwise, the column titles in row 1 shift to the left one column.

Save Data File: The "Save Data File" option saves all of the values contained in the spreadsheet under the *Input & Options* tab as a CSV file. The results look like the file in Table 1

when opened in Excel and contain the user input titles, options selected, and the numerical data in the table.

Exit: "Exit" option closes BioSim2. All data are lost if they have not been previously saved.

Microsoft Excel - CPCTestData.csv File Edit View Insert Format Tools Data Window Help Type a question for help - _ & × ▼ 10 ▼ | B I U | 臣 吾 吾 国 国 | \$ | 淳 | 田 ▼ 🍐 ▼ 🛕 ▼ 📲 🛅 🔩 🔩 🖸 🧖 🏷 | ラ 🌭 間 | W Reply with Changes... End Review. C F В D E Α DCD-Diam Tubific DCD-Paga DCO-CrCo DCO-Euki Data CPC720R1 CPC720R2 CPC720R3 CC725R1 CC725R2 12 CC725R3 13 PC725R1 14 PC725R2 15 PC725R3 CPCTestData >

Table 2. Example of CSV Spreadsheet as an Input File (partial data set without titles or user options).

4.1.2 "Actions" Drop-down Menu

Figure 3 represents the opening screen with all the data fields completed and the "Actions" drop-down menu opened.

Process Data: To run the program, select "Process Data" from the Actions menu or via the keyboard shortcut, "Ctrl-D." If the program executes properly, the following message will appear in green in the message window, "Data successfully processed" (see Figure 3). If the program does not execute properly, the message window will be red and an error message will appear to assist in trouble-shooting problems with the input data. Although the program processes small data sets almost instantaneously, data sets with 50 or more rows or columns take somewhat longer. When you select "Process Data," an hourglass appears to let you know that the program is running smoothly. You can maximize the performance of BioSim2 by minimizing the number of other applications running on your computer at the time you process the data.

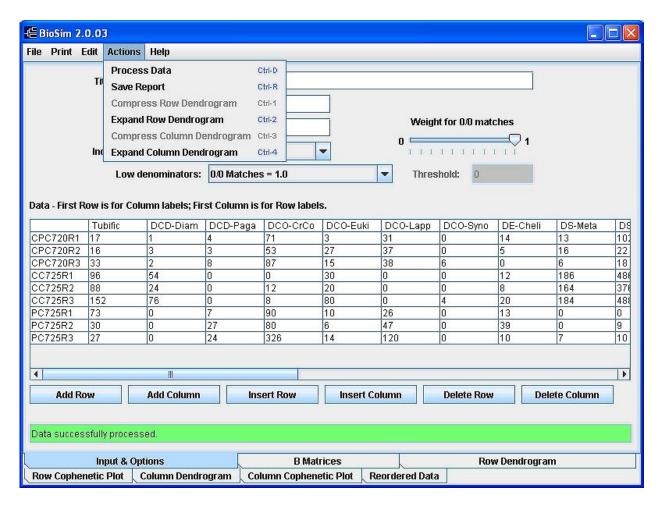


Figure 3. Opening Screen with "Actions" Drop-down Menu Opened.

Save Report: Selecting the "Save Report" option from the Actions menu gives the user the ability to identify or create a folder in which to save all of the program outputs using a standard Windows dialog box. This option is also available via the keyboard shortcut Ctrl-R. Figure 4 shows the files that are automatically created and saved to a folder when this option is selected. The dendrograms and the cophenetic correlation plots for both rows and columns are saved as .jpg files. All of the data matrices (original input data, matrices of matrix of similarity values (Bs), and the reordered and transposed data files) are saved as CSV files. An html file, index.html, is also created which allows the user to view the output from the program using any of the common Internet browsers. Depending on the size of the data matrix and the speed of the computer, this may take some time. During this time, the standard hourglass symbol will appear. Once the output files have been saved, you will get a green message in the message window that reads "Report saved."

Expand and Compress Row and Column Dendrograms: Selecting either the "Expand Row or Column Dendrogram" option from the Actions menu increases the size of the row or column dendrogram by 50 percent. This is useful when the matrix size is greater than 50 rows or columns. These options are also available via the keyboard shortcuts Ctrl-2 and Ctrl-4 (Figure 3). Once a dendrogram has been expanded, it can be compressed to its original size by

selecting either the "Compress Row or Column Dendrogram" option from the Actions menu. Again, these options are also available via the keyboard shortcuts Ctrl-1 and Ctrl-3 (Figure 3).

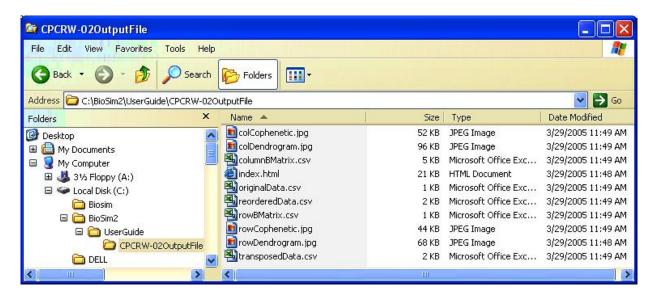


Figure 4. Files Created and Saved Using the "Save Report" Option.

Once you have successfully processed the data, you can view the results by selecting the various tabs at the very bottom of the screen. These are shown in Figures 5-10.

Examples of saved graphics files are shown in Appendix A.

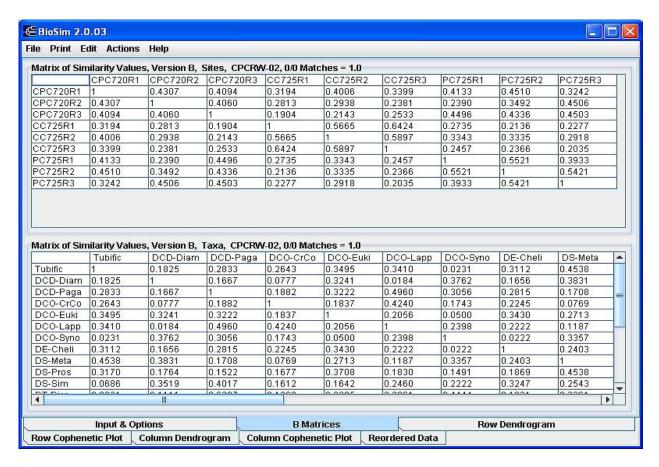


Figure 5. Tab "B Matrices" Showing the Similarity Values (B) for Rows (top) and Columns (bottom).

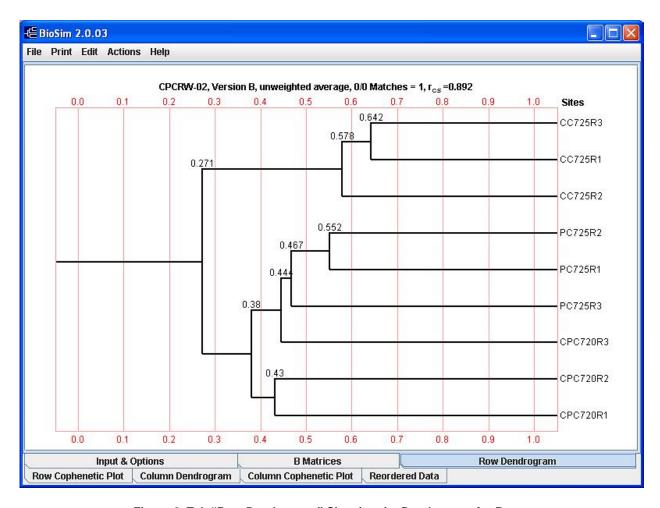


Figure 6. Tab "Row Dendrogram" Showing the Dendrogram for Rows.

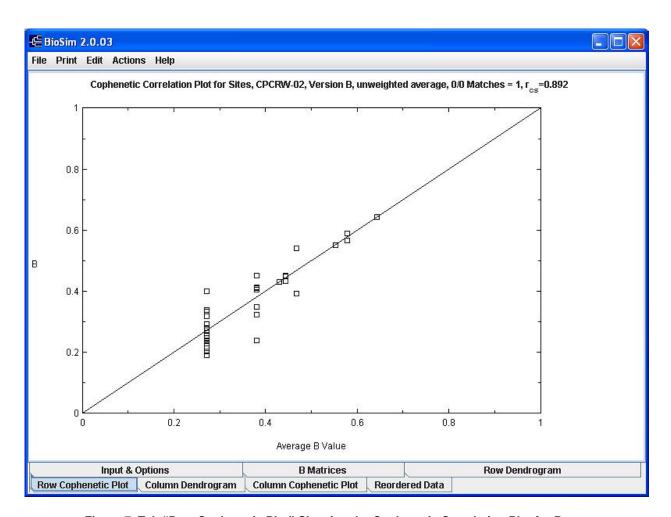


Figure 7. Tab "Row Cophenetic Plot" Showing the Cophenetic Correlation Plot for Rows.

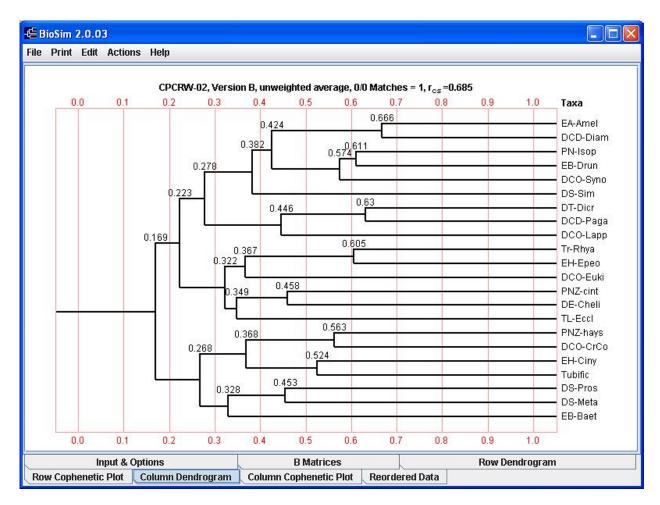


Figure 8. Tab "Column Dendrogram" Showing the Dendrogram for Columns.

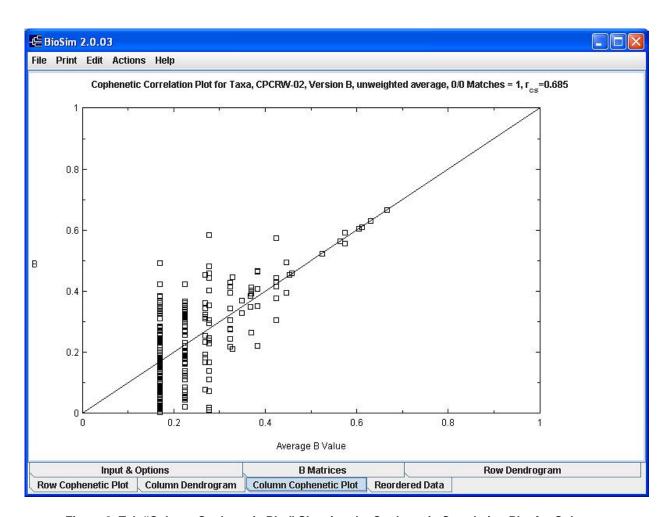


Figure 9. Tab "Column Cophenetic Plot" Showing the Cophenetic Correlation Plot for Columns.

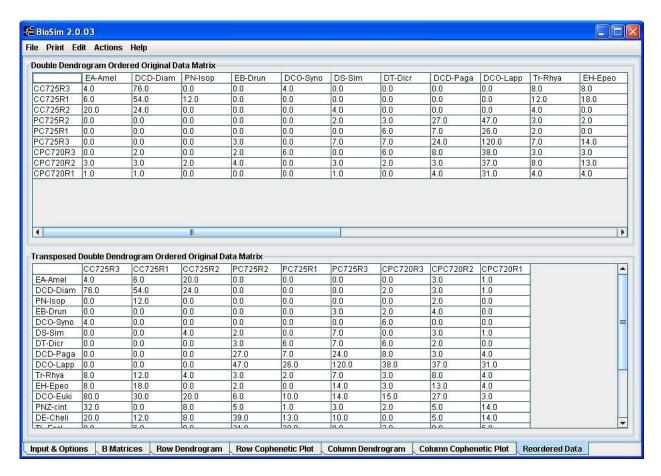


Figure 10.Tab "Reordered Data" Showing the Data Reordered According to Both Row and Column Dendrograms.

4.1.3 "Print" Drop-down Menu

Figure 11 represents the opening screen with the "Print" drop-down menu opened. From this menu, you can select and print any of the following outputs: Row Dendrogram, Column Dendrogram, Reordered Data, Transposed Reordered Data, Row B Matrix, Column B Matrix, Row Cophenetic Plot, or the Column Cophenetic Plot. You can also print all of these outputs by selecting "Print All" or the keyboard shortcut Ctrl-P.

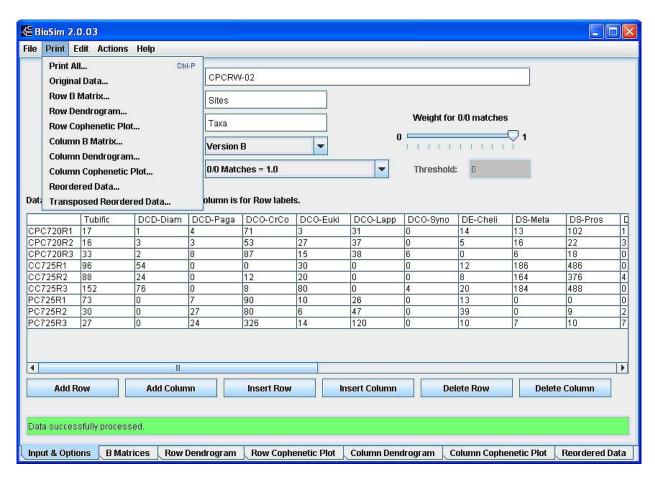


Figure 11. Opening Screen with "Print" Drop-down Menu Opened.

4.1.4 "Edit" Drop-down Menu

Figure 12 represents the opening screen with the "Edit" drop-down menu opened. From this menu, you can highlight any of the input data fields and use the standard cut, copy, or paste functions. The standard keyboard shortcuts (Ctrl-X, Ctrl-C, and Ctrl-V) also work for these functions.

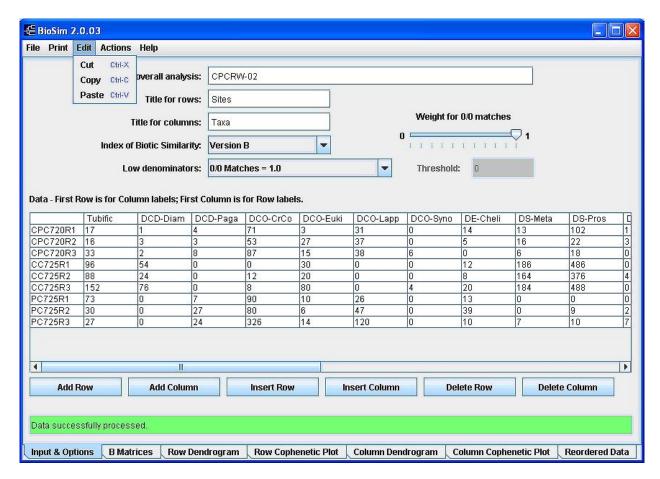


Figure 12. Opening Screen with "Edit" Drop-down Menu Opened.

4.1.5 "Help" Drop-down Menu

The "Help" menu has two options. The "About BioSim2" option provides information on the authors and the version number of BioSim2. At present, the "Help for BioSim2" provides access to an html version of this User's Manual.

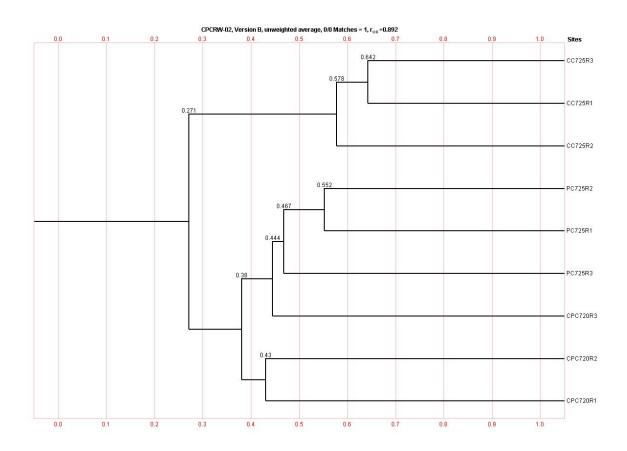
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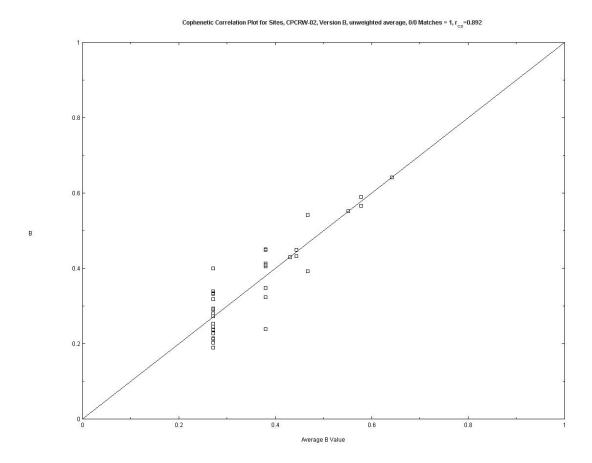
Appendix A

Samples of Saved Graphic Output Files

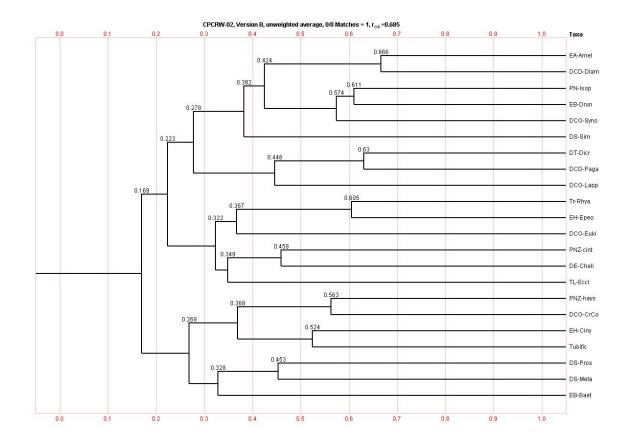
Row Dendrogram



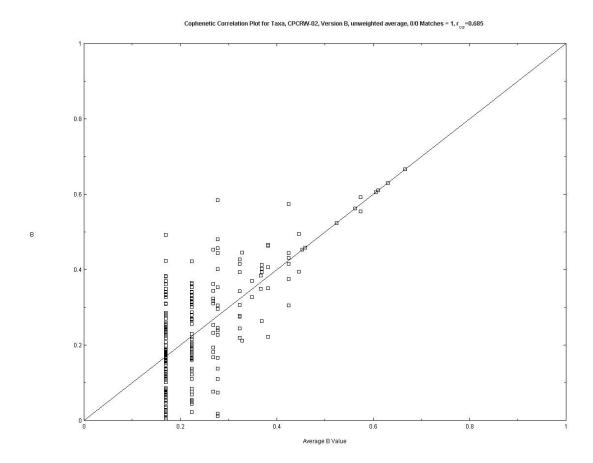
Row Cophenetic Correlation Plot



Column Dendrogram



Column Cophenetic Correlation Plot





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