Using Jasco CD Spectra Manager Files with CDPro

CDPro software package consists of three of the popular programs for analyzing protein CD spectra for determining the secondary structure fractions (SELCON3, CDSSTR and CONTIN) and a program for determining tertiary structure class (CLUSTER). It is available free on the Internet courtesy of Sreerama and Woody at Colorado St. University:

http://lamar.colostate.edu/~sreeram/CDPro/main.html

What follows is an easy step by step method to successfully introduce Jasco CD data files into this program. In the following, it is assumed that you have already downloaded the CDPro zip file and unzipped it into a directory called “CDPro”.

1. Acquire your CD spectra at least within one of the following spectral ranges: 190-240 nm, 185-240 nm, 178-240 nm. These correspond to the spectral ranges of the 10 protein reference sets provided in CDPro. If your data exceeds the range of the reference set you want to use, you can edit it in one of the following steps.

2. Acquire your CD spectra with at least a 1 nm data interval (pitch, step size). If your data is in finer intervals (ie:0.2 nm, 0.1 nm, etc) you may edit the data in one of the following steps.

3. Using Spectra Manager /Spectra Analysis/Processing/CD Options/Optical Constants, create a new file with the spectral units expressed in Mean Residue Ellipticity. For this you need to enter the cell pathlength and the concentration in residue moles (as opposed to protein moles). (To get mean residue concentration you can either multiply the protein concentration times the # of residues per protein, or compute it directly from the mg/ml protein concentration using an estimated average residue molecular weight (such as 110). For instance, 0.2 mg/ml = 0.02% W/V=0.2g/L= 0.0018 Mole/L assuming an average residue weight of 110.

4. From the file created in 3), select Processing/Common Options, Data Dump. Use the “Thin Out” function to create a data interval of 1 nm, and select the range to be the same as one of the ones mentioned in 1) (generally use the largest range available).

5. After hitting OK in Data Dump, hit the “Copy” button to copy to the clipboard.

6. Open Excel (or other appropriate spread sheet) and paste the data into the spreadsheet. Use Excel functions to delete the text header and the “HT” column (3rd column) leaving only 2 columns containing wavelength and CD value respectively.

7. From Excel , save the result as a “Tab Delimited Text File” with an arbitrary name. You must save it directly into the “CDPro” directory (or else resurrect your DOS skills to designate another directory when you run the following DOS window).

8. Go to the CDPro directory and select and double click the file “CRDATA.EXE”; A DOS window will appear from which you will follow the prompts as follows: select “0” to create a new “INPUT” file: Enter the title of your choice: Enter “1” because your data is already at 1 nm data interval: Input appropriate “Initial” (long) wavelength: Input appropriate “Final” wavelength (short): Enter “1” indicating that the data is in molar ellipticity units: Enter the name of the ascii file you just saved from Excel: and finally hit Enter key. If it works properly, you will then be prompted to select a reference set (an appropriate one will be suggested). (A description of the various reference sets is included on the CDPro website)

9. A file named “INPUT” (no extension) will be generated (or overwritten if previously existing). You can check the contents of “INPUT” by opening it in “notepad” or another text editor.

10. You may now run any or all of the 4 estimation programs mentioned above (they all use the same “INPUT” file.

11. The output results are written (or overwritten if files already exist) to various output files which are described on the CDPro web page. For the 3 actual Secondary Structure Estimation programs, CDSSTR, SELCON and CONTINLL, the results are always appended to the file PROTSS.OUT which will save the basic results for all of you runs and which can be read by a text editor such as “Notepad”.