Instructions for the tutorial on least-squares spectral fitting using the *scanedit* program.

Windows VisualBasic Version Ed Berry 2017

The first tutorial (demo 1) involves fitting a set of spectra of purified mitochondrial cytochrome **bc1** complex obtained after adding different amounts of different reducing agents to reach different stages of partial reduction of the cytochromes. The second, demo2, involves fitting spectra of photosynthetic pigments in fractions eluting from a chromatography column. An extended version of this (demo3) involves setting up the standard basis spectra and introduces other features of the program.

Getting the program

Download the program and demos from sourceforge: https://sourceforge.net/projects/scanedit/files/openspectralworks-1.0/tutorials.zip

Unzip the file to a location on your hard drive or a flash drive (The size is about 6 MB, unpacks to 9MB). It unzips to a directory "SCANLSF" with the executable (scanedit.exe) and five subdirectories: speclib\, demo1\, demo2\, demo3\, doc\, and setup\. The doc folder contains this and other documentation files.

On many (most?) systems no setup or installation is required to run the tutorials: the program will run directly from the folder it is downloaded in. Test this by double-clicking scanedit.exe in the top folder SCANLSF. If you get an error message see setup.pdf in the docs folder.

To "uninstall" simply delete the directory scanlsf and all its contents (running the program from the scanlsf folder does not affect the registry or list of programs in start menu, or copy any files to your hard drive, outside of the working directory and %TEMP% directory).

If you will be using the program regularly, some further setup will make it more convenient. This includes a desktop icon, associating filetypes with the program, connecting with GhostScript for pdf output, and using environment variables to set some preferences. This is described in setup.doc. But this is not necessary to run the tutorial.

Getting your data in a format that can be read by the program https://sourceforge.net/projects/scanedit/files/openspectralworks-1.0/doc/dataimport.pdf

Getting Help

- (incomplete) manual scanman.pdf in the doc directory

-Forums at https://sourceforge.net/p/scanedit/discussion/

-Contact the programmer at:

eaberry at users.sourceforge.net,

eaberry1 at gmail.com

I would be glad to hear how you make out, and to help out if necessary.