OCD Analysis Software (v 1.0)

Nick Charron - Huang Biophysics Lab

Rice University. 2017.

This software is designed to plot and process spectra obtained from the J-810 Jasco CD spectrometer in the Huang lab. All measurement files must be in ASCII format (*.txt files). This format can be chosen when saving the measured spectra in the Spectra Manager software provided by Jasco. File reading routines are currently optimized for J-810 ASCII output, though these can be modifed to read any consistent text-based spectral data file.

The software is designed to work as a collection of tools, so that it may be used interactively. To start an interactive python session, type the following command at your shell or command prompt:

```
>_ python
Python 3.6.3 (default, Oct  4 2017, 06:09:15)
[GCC 4.2.1 Compatible Apple LLVM 9.0.0 (clang-900.0.37)] on darwin
Type "help", "copyright", "credits" or "license" for more
information.
>>>_
```

Depending on your distribution and machine details, the output above may not be exactly the same (This output was generated on a 2015 Apple MPB with a brew install of python 3.6). Next, the tools must be imported:

```
>>> from ocd import *
```

This also imports the following python modules: *numpy* as np, *matplotlib.pyplot* as plt, *os*, and *sys*. Loading a spectrum is done through the creation of a instance of the class ocd_spec. Providing a filename loads the corresponding spectral information (wavelength and CD signal). Optionally the class may be called without a filename to create an empty spectrum (no spectral information):

```
>>> myspec = ocd_spec("scan_01.txt")  #class with filename
>>> emptyspec = ocd_spec()            #empty class
```

You can also use file dialogs to select the file from your current directory. On Windows systems, this functionality is supplied by the wxPython-Phoenix package, which interfaces with the system default file manager and pipes the selected filename to the creation of an ocd_spec instance. On Linux and OSX systems, the same process is acheived through the use of pycurses and its lightweight text user interface. Selecting multiple files will return a list of ocd_spec instances.

```
>>> myspec = fs()
```

Once a spectrum is loaded, you have access to the following functions and variables:

ocd_spec.wl : returns a 1D numpy array of wavelengths used in the scan.

ocd_spec.cd : returns a 1D numpy array of CD signals measured.

ocd_spec.load(string) : loads wl and cd data from specified filename.

ocd_spec.save(string) : saves wl and cd data in mock JASCO format for later loading.

ocd_spec.name : returns the name of the spectrum.

ocd_spec.graph() : produces a simple graph of the spectrum.

ocd_spec.renorm(float) : globally rescales the CD signal by specified factor.

ocd_spec.rm_baseline(float) : returns an instance of. ocd_spec with a constant baseline subtracted from the CD signal.

ocd_spec.trim(wl1, wl2) : returns an instance of ocd_spec trimmed to the wavelength range specified by wl1 and wl2.

ocd_spec.filter(beta, lwidths) : returns an instance of ocd_spec that has a Kaiser-filtered CD signal. Beta refers to the Kaiser-Bessel response paramter (by default it is set to 2.0).

avg_signal([spec1, spec2, ...]) : returns an ocd_spec class with an average CD signal from spec1,spec2, ... The spectra must be passed to this function as a python list.

mult_graph(specs, types, colors, lwidths, title, xlim) : produces a graph of multiple spectra with custom style options. Specs, types, and colors must all be lists of the same size. A legend will automatically be generated using the values of spec.name. Xlim is an iterable that calls plt.xlim().

graph_series(specs, title, cmap, lwidths, xlim) : produces a graph of a sequence of experiments - useful for showing spectral changes dependent on concentration. The color map can be chosen from the matplotlib package, though the default is Reds(). A legend will automatically be generated using the values of spec.name. Xlim is an iterable that calls plt.xlim().

In this way, multiple spectra can be graphed, rescaled, filtered, corrected, and analyzed interactively at the user's discretion. Custom graphs beyond the scope of the simple **mult_graph()** function (advanced color schemes, plotstyles, line types, etc.) can be made by directly calling functions from the pyplot module:

```
>>> fig = plt.figure("Custom Plot")
>>> plt.plot(myspec.wl, myspec.cd, 'b--',linewidth=2)
>>> plt.xlim(220,240)
>>> plt.title("230 nm Peak - A State")
>>> plt.ylabel("CD [mdeg]")
>>> plt.xlabel("Wavelength [nm]")
>>> plt.show()
```