**Program for XMLD and XMCD spectra analysis**

**Technical documentation**

# Libraries and modules.

## Numpy.

Used for conversion of .txt file containing data to approachable to work with format of data.

## Os.

Used for file handling in the process of uploading and saving.

## Matplotlib.

Used for graphical visualization of data in the form of various plots.

## Re.

Used for searching the file to find individual measurements.

## CSV.

Used for writing results to file in a form enabling further analysis.

## Tkinter.

Used for creating a graphical user interface for the program.

# Upload tab.

## Uploading a file.

A standard data set is a .dat file that contains numbers of measurements. Every measurement consists of several columns proceded by several lines of comments describing measurement. Essential for analysis is the first line of comment which contain a number of measurement and its type and two columns of the data.

To load a file *select\_file()*  function is used. It opens File Explorer which allows for choosing a file. If the file is correct the program writes the file line by line to variable *Lines* and closes the file

To find all measurements existing in the whole data set the function *list of measurement()* is used.

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**Figure 1.** *List of measurement()* function.

There are two regular expressions used:

* pattern\_all – finding all measurements
* pattern\_rscan – finding only measurements made as a function of energy (subject of analysis)

Variable *total* is the number of all measurements in the data set and is used in the program for creating a list of available measurements (measurements are saved in the data set sequentially from the first to the last).

Measurement numbers made as a function of energy are saved in list *rscans*.

## Opening specific measurement.

For opening specific measurements for the purpose of plotting, for example, the function *search in file(nb)* is used.

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**Figure 2.** Regular expressions in *search in file* function.

There are two regular expressions used (Figure 2.):

* pattern\_first – the first line of commentary of a given measurement (*nb* – number of the measurement you are looking for)
* pattern\_last – the last line of data of a given measurement

To obtain the number of the first line of data of a given measurement, the number of comment lines is added to number of first line of commentary (Figure 3.).

Obraz zawierający tekst, zrzut ekranu, Czcionka, linia

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**Figure 3.** Searching for first line of data in *search in file* function.