Automated Calculation of Collisional Cross Sections for Synapt G2 data with a linear Drift Tube

By Christian Manz
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How to configure your PC:

1. Uninstall any versions of Python that are currently installed on your PC.
2. Restart PC.
3. Download current Python (x,y) version (free academic and development software with all needed libraries):
   https://python-xy.github.io
4. Install to default location, e.g. C:\Python27.
5. Restart PC.

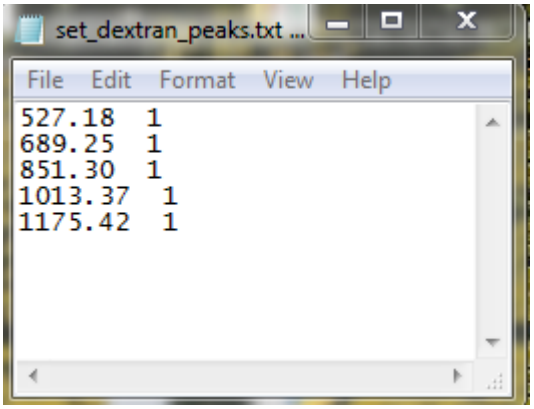
Step-by-step guide to automatically calculate CCS:

Place the folder with the script anywhere you want, e.g. your desktop or your data folder. To start the automatic calculation, you need to write a peaklist file to tell the program, which peaks you want to find in the data. You can simply do that by open an Editor file and writing the data in the format of two columns:

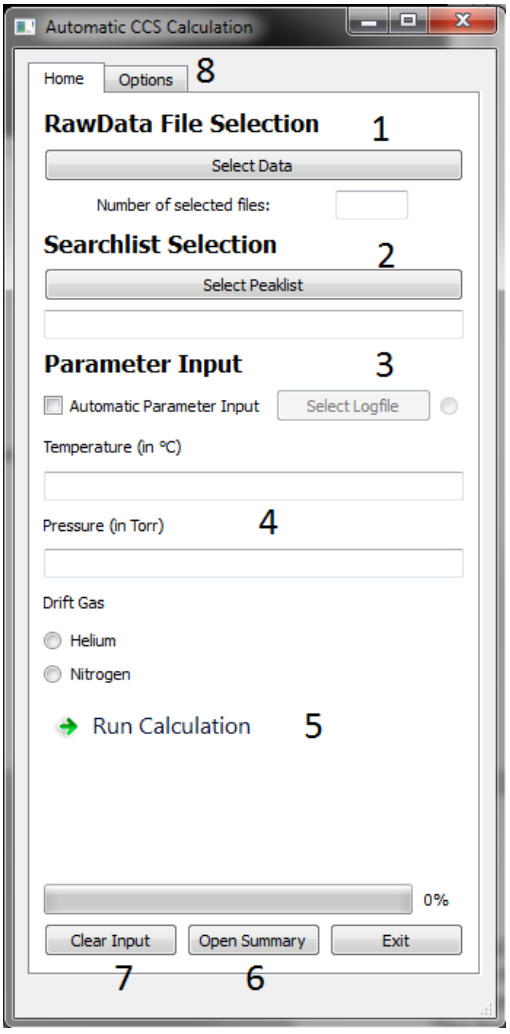
1) m/z of the peak (with at least two digit after comma)
Type in the accurate mass of the peaks you observe in MassLynx, not the calculated mass! This can lead to mismatches in peak finding!

2) Charge of the peak

It is important to let some space between the two columns (But it is not important how big the space is, it can be TAB, space or combination of that. Essentially it just needs two columns). Then save the file as "name_of_file.txt". The file can be saved anywhere you want, but it would be advantageous to save it next to your measured data, where you can easily find it again. The peaklist file should look like this:



Now you can start with the actual calculation. For this you simply double click on the python file “Aprid.py”. The program will start by opening a User Interface (first loading might take some time to compile the script and load libraries), which looks like this:



1) Select the data files you want to process and fit. Usually you would take up to 8 data files of one sample measured with eight different drift voltages.

2) Select the peaklist you created before.

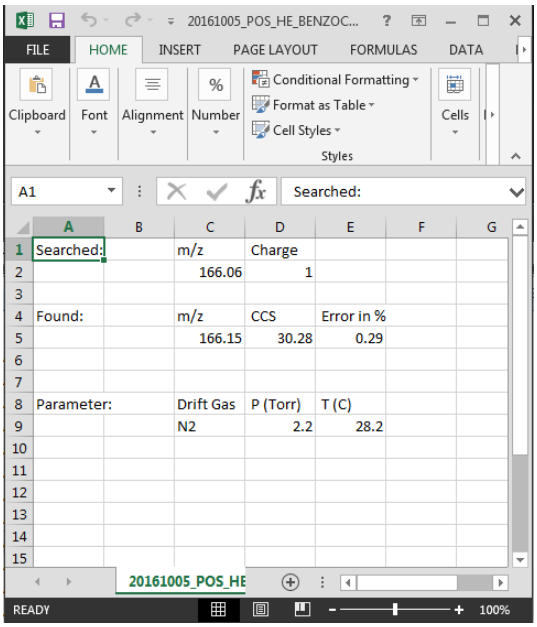
3) All relevant parameters are recorded at the measurement PC in a logfile. Now you can choose to put in all values by hand (follow point 4) or just select the logfile.

4) If you choose to put in values manually, you need to type in the temperature of your measurement (in °C), the pressure of your measurement (in Torr) and the used drift gas (helium or nitrogen)

.

5) Start calculation!

The script will go through your raw data files, convert them into text files and calculate the CCS from the now readable data. When the program is finished, the progress bar will show 100 %. Aprid will generate a results folder which contains a CSV file (can be opened by Excel or Editor) with a summary of all results. It contains a list of the searched peaks and a list of found peaks with their designated CCS in addition to all used parameters (temperature, pressure, drift gas). The name of the file is similar to the name of the measured data with the addition “name.summary.csv”. The result file will look like:



The results folder also contains an image file for each fit to control the accuracy.
For complex samples always have a look at the image files to check if the fit is accurate. The peak searching parameters do have an influence on this fits. If you search for lower masses (<1000 m/z) stay with the standard options. Otherwise try to adapt the options (point 8).

6) The summary file can be directly opened from Aprid by clicking on “Open Summary”.

7) “Clear Input” allows to delete all input data to start a new calculation.

8) The options contain peak sensitivity and peak search limit. For higher masses (>1000 m/z) always change it to sensitivity 0.6 and limit 0.3.

General Notes:

Due to the conversion of the raw data into text files and the process behind it, the m/z for single peaks can be shifted by 0.1 - 0.2 m/z in comparison to the displayed data in MassLynx. This has little to no effect on the calculation of the CCS!

For the error message:“option ‘—raw_file’ cannot be specified more than once”
→ This error shows up, when the path to your data file or the path to your peaklist contain spaces in between. To bypass this error, just rename the folder to a name without spaces, e.g. rename “data folder” to “data_folder” and the error should be gone.

If you have questions or trouble regarding the program, just contact me:

M.Sc. Christian Manz

Freie Universität Berlin
Institute of Chemistry and Biochemistry
Takustraße 3
14195 Berlin
Phone: +49 (0)30 838 55393
christian.manz@fu-berlin.de

Fritz Haber Institute of the Max Planck Society
Department of Molecular Physics
Faradayweg 4-6
14195 Berlin
Phone: +49 (0)30 8413 5686
cmanz@fhi-berlin.mpg.de