PEPICO_Elettra_VG – Data Analysis in Python

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Software Structure

Main program:

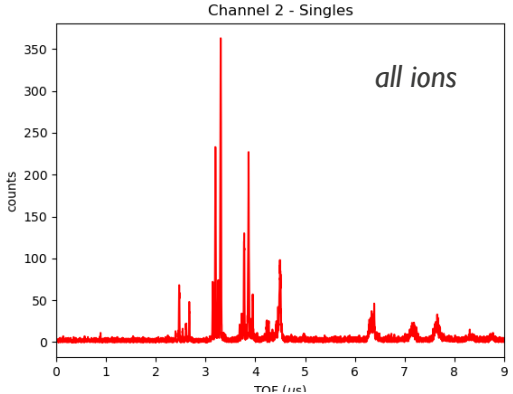
- main.py — runs the code with the parameters provided in the input section
  new in v1.1: a TOF background region must be selected so that the factor for the subtraction of the randoms is determined automatically (line 35)

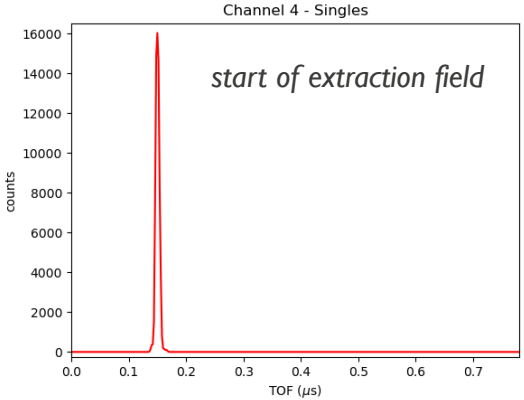
Classes:

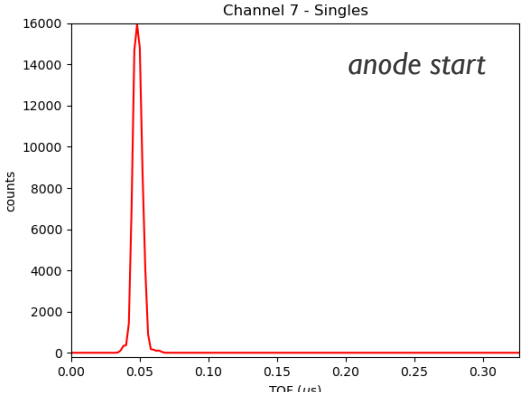
- VG_tof.py — reads in the raw files and creates lists with electron coordinates, ion stop times, start times, and assigns corresponding events
- VG_tof_only.py — ion TOF spectra started by anode or random trigger
- VG_figures.py — plots histograms, images, spectra
- VG_Movie_Tof.py — produces electron energy selected TOF spectra and subtracts weighted TOF spectrum of randoms

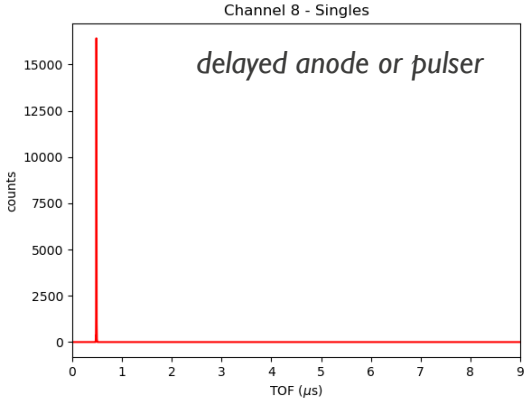
Output: channel histograms

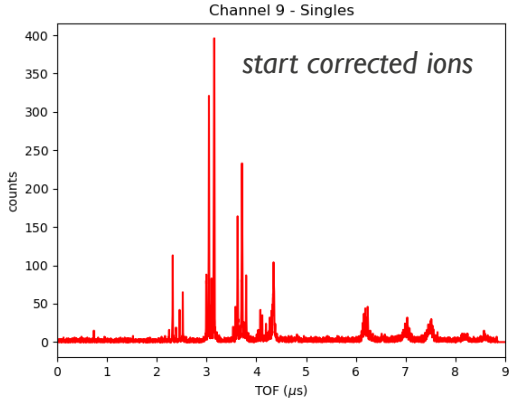
Channel stops in coincidence with a complete electron event



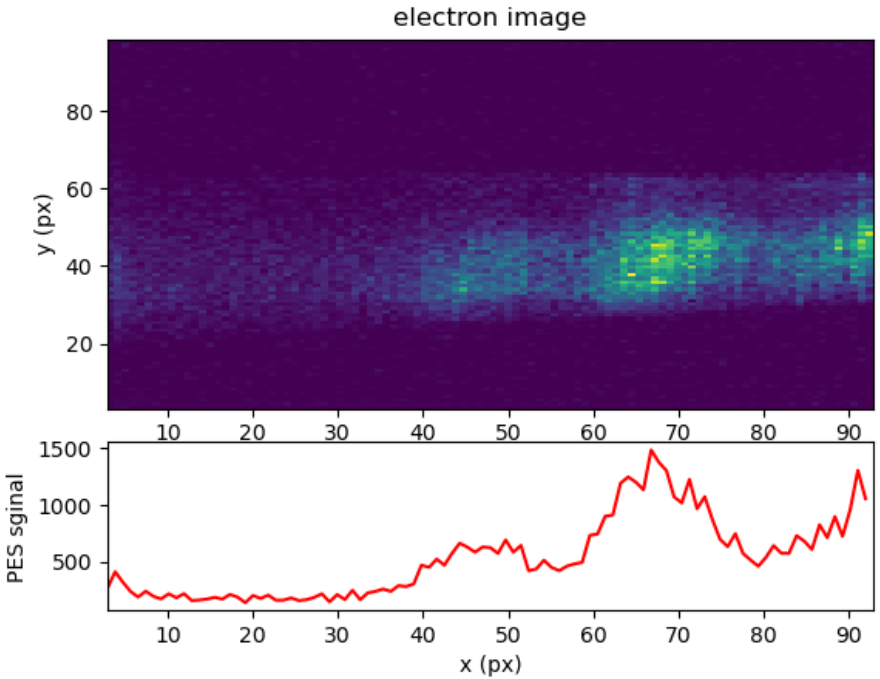








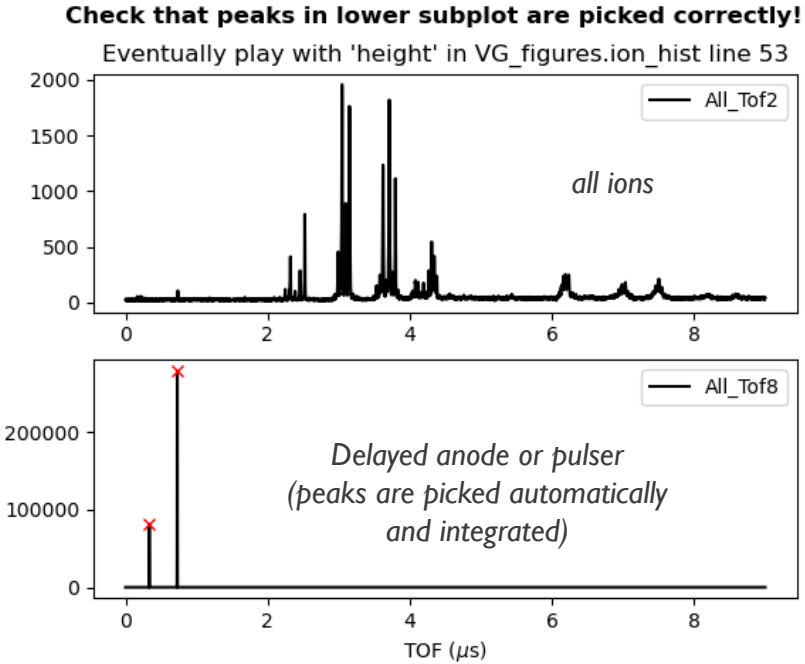
Output: electron image

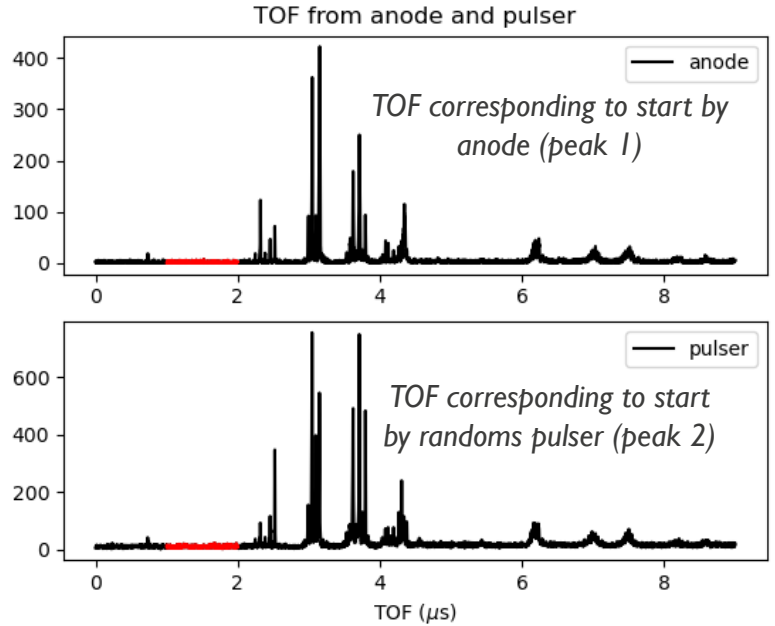


electron image in px

Projection on x-axis corresponding to electron energy

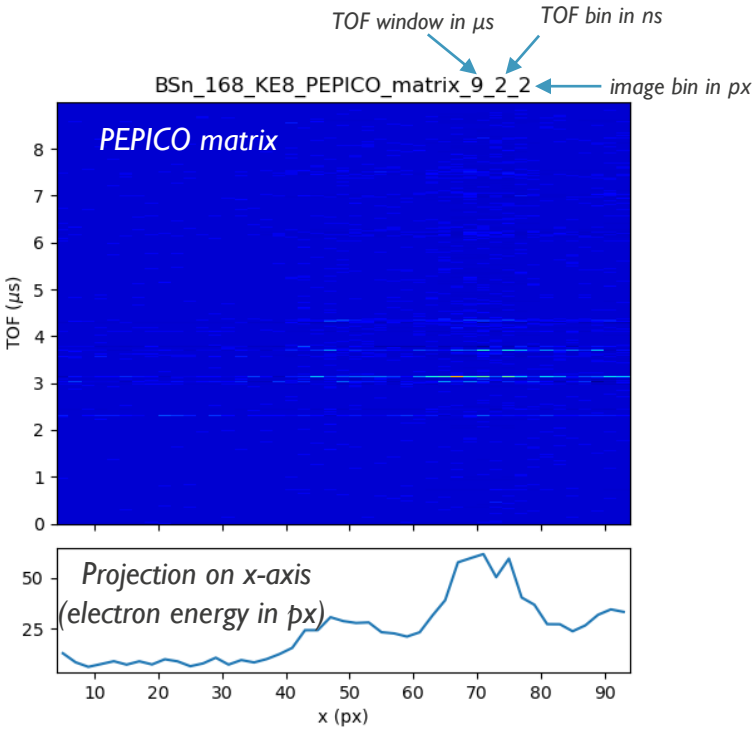
Output: TOF spectra (no coincidences)

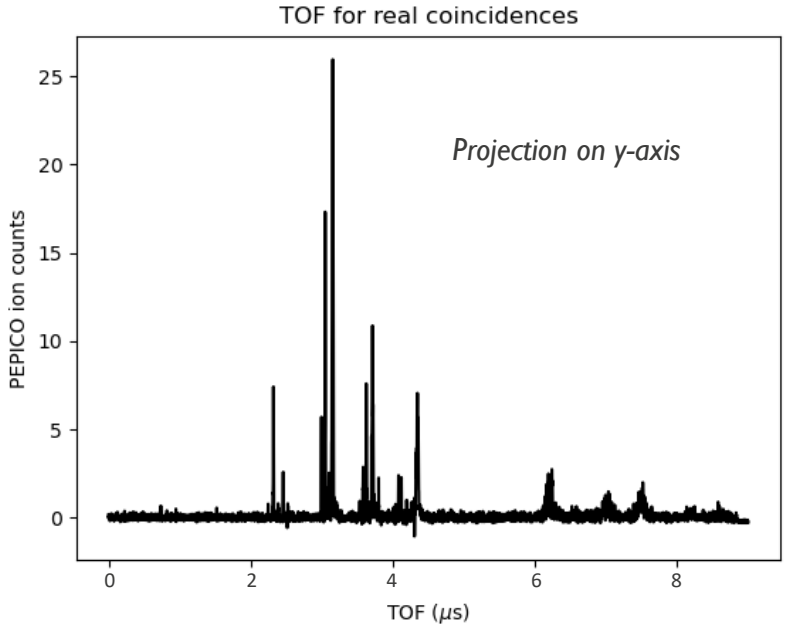




The background region for the correct subtraction is shown in red. If peaks lie in that region, uncomment line 221 to manually adjust the selection.

Output: PEPICO matrix (final result)





Output: Files

- *_PEPICO_matrix*.dat — text file containing the final PEPICO matrix (columns = TOF, rows = electron energy)
- *_PEPICO_matrix*.png — .png image of the PEPICO matrix figure

The 3 numbers at the end of the file name give the TOF upper limit in µs, the binning of the TOF spectrum in ns, and the binning of the electron image energy axis in px.

_9_2_2.dat contains therefore a (45,4500) matrix, for which the energy axis runs from 0 to 90 px in steps of 2 px, and the TOF axis runs from 0 to 9 µs in steps of 2 ns.

Putting together the kinetic energy groups

PEPICO_complete_sp.py

Puts together the PEPICO matrices for the different energy regions to obtain the complete matrix (overlapping regions are averaged)

Input needed in the first section

path to folder containing the input matrices

identifier of the mesurement

parameters used in the previous analysis

work function

path and file to a reference PES

energy calibration factor for PEPICO

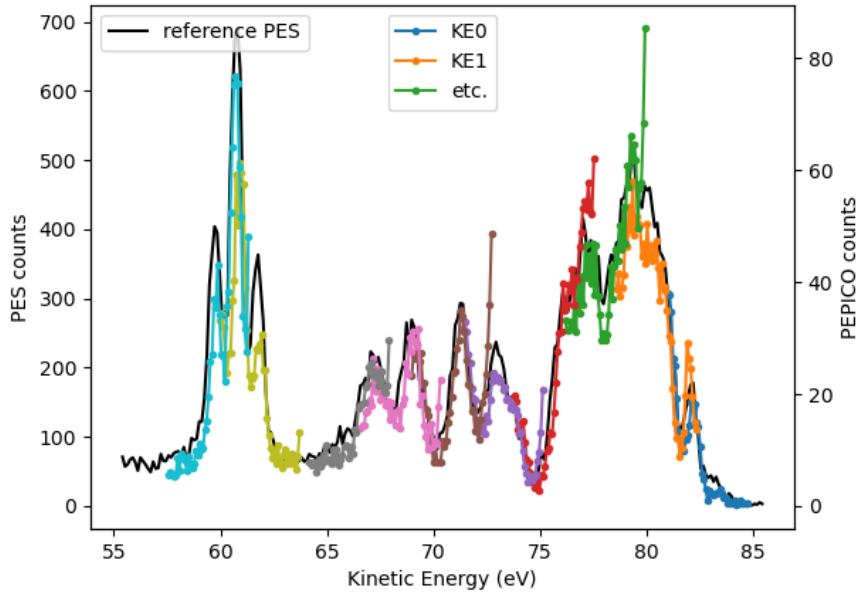
central energies of the different regions are retrieved automatically from the Energy .txt file

```
# -*- coding: utf-8 -*-
"""
Created on Fri Jan  7 09:32:27 2022

@author: holzme33
"""
import numpy as np
import os
import matplotlib.pyplot as plt
from matplotlib.gridspec import GridSpec
import time

# PATH = "B:\\analysis\\BSn\\PEPICO\\BSn_168\\"
PATH = "B:\\analysis\\BSn\\PEPICO\\BSn_168_fac0.65\\"
# PATH = "B:\\analysis\\tBMA\\PEPICO\\TBMA_088_tot\\"

ide = 'BSn_168'
MaxTof = '9'
tof_bin = '2'
x_step = '2'

# work function in eV
wf = 4.1

# reference PES (no coincidences)
path_ref = "B:\\VG\\rawdata\\"
file_ref = "BSn_165Sum"
DT_on = 1           # was the reference PES recorded with drift tube on?

px2eV = 0.85        # calibration factor px to eV
DT_shift = 0.6      # energy shift with drift tube on (eV)


# kinetic energies at which the measurement was done (eV) are retrieved automatically
path_en = "B:\\PEPICO\\rawdata\\"
file_en = "Energy_"+ide+".txt"
energy = np.loadtxt(path_en+file_en, skiprows=1, usecols=(2))
central_en = np.flip(np.unique(energy))


#**********************************************************************
# no need to change anything below this line
#**********************************************************************

files = []
# get the filenames of the raw data saved as .mat
for file in os.listdir(PATH):
```

Check parameters, calibration, etc.

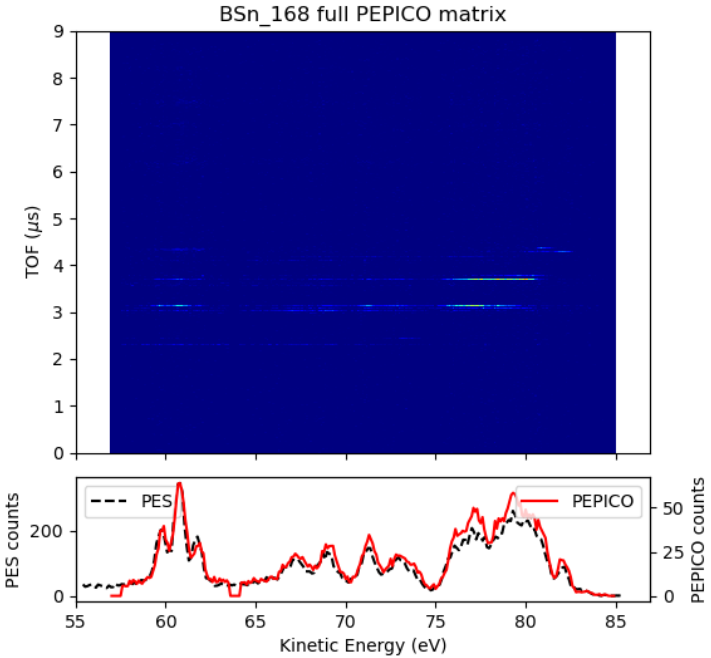
Compares the mass-integrated electron spectra for the individual energy regions to the pure photoelectron spectrum.

- Adjust drift tube shift if needed
- Adjust px2eV calibration parameter if needed



Combined PEPICO matrix

- Plots the combined PEPICO matrix and compares the mass-integrated electron spectrum to the reference PES
- Saves the figure as .png
- Saves the matrix and the kinetic energy axis, and the TOF axis in .txt files
- ‘cut’ (line 85) specifies how many points are dismissed for each energy region at the high energy side
- ‘z_max’ (line 88) defines the upper limit of the z axis (lower limit is by default 0)



Mass-selected photoelectron spectra (1)

Automatic peak picking – 'ms_PES.py'

Input:

- Output files from 'PEPICO_complete_sp.py', i.e., the PEPICO matrix, the TOF array, and the energy array
- Mass calibration in 2nd cell: TOFs and corresponding m/z for two points determined previously
- Threshold value for minimum peak height for automatic peak picking (line 50)

The program picks automatically the peaks in the mass spectrum and fits them with a Gaussian curve.

The integration limits for the mass-selected photoelectron spectrum corresponds to ± three standard deviations from the peak center

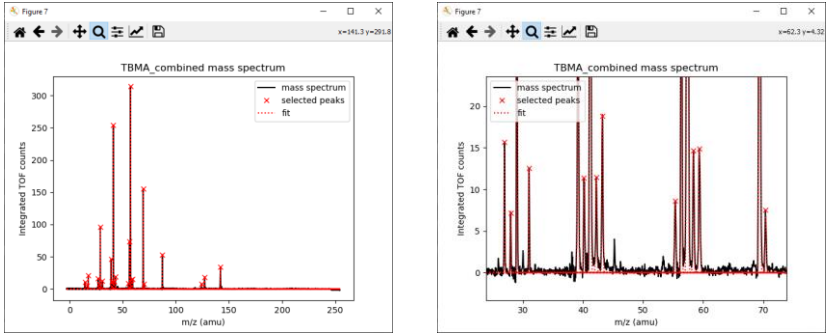
Mass-selected photoelectron spectra (1)

Automatic peak picking – 'ms_PES.py'

Output:

- *_ms_PES.out: contains for each selected mass peak a column with the ms-PES as a function of the binding energy
- *_binding_en.out: binding energy in eV
- *_masses.out: list of picked mass peaks

Figure of the mass spectrum for checking the peak picking



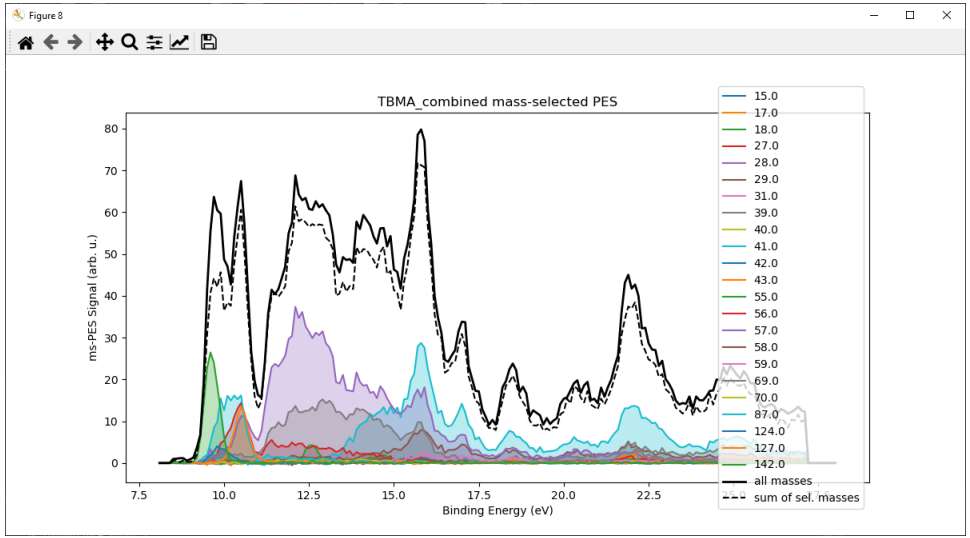


Figure with the final result for all masses
("all masses" means integration over the whole PEPICO matrix)

Mass-selected photoelectron spectra (2)

User interface for manual peak picking - 'msPES_GUI'

This GUI is useful when the integration limits for the peaks are not well defined for automatic peak fitting, e.g., when several peaks should be picked at once (isotopes) or when the peak shape is not Gaussian.

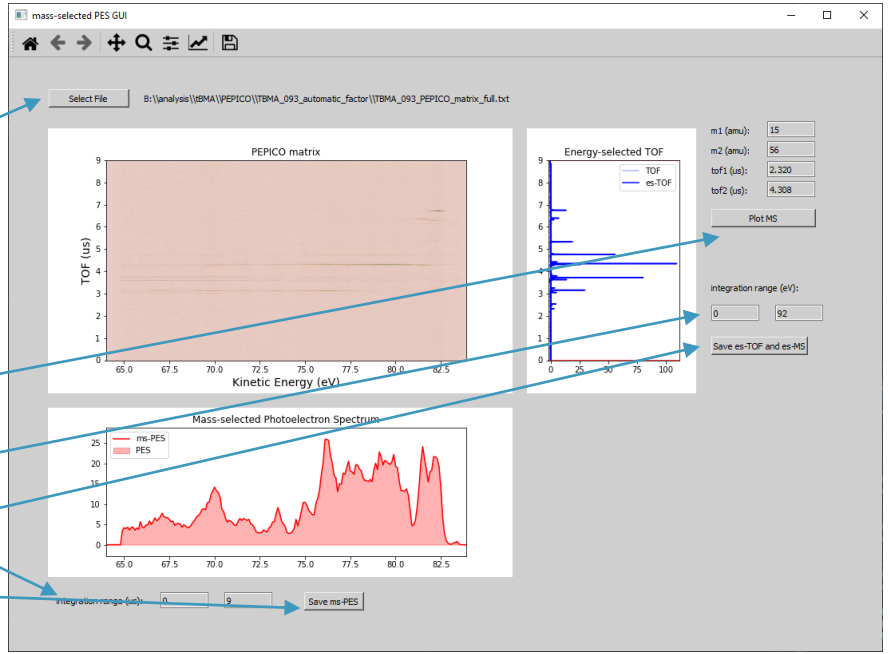
In Spyder the graphics backend must be "Inline" for PyQt GUIs to run well (Tools/Preferences/Ipython console/Graphics/)

Select the PEPICO matrix (loads slowly)

Toggle between TOF and m/z axis (using the calibration parameters)

Select integration range (figures are updated live)

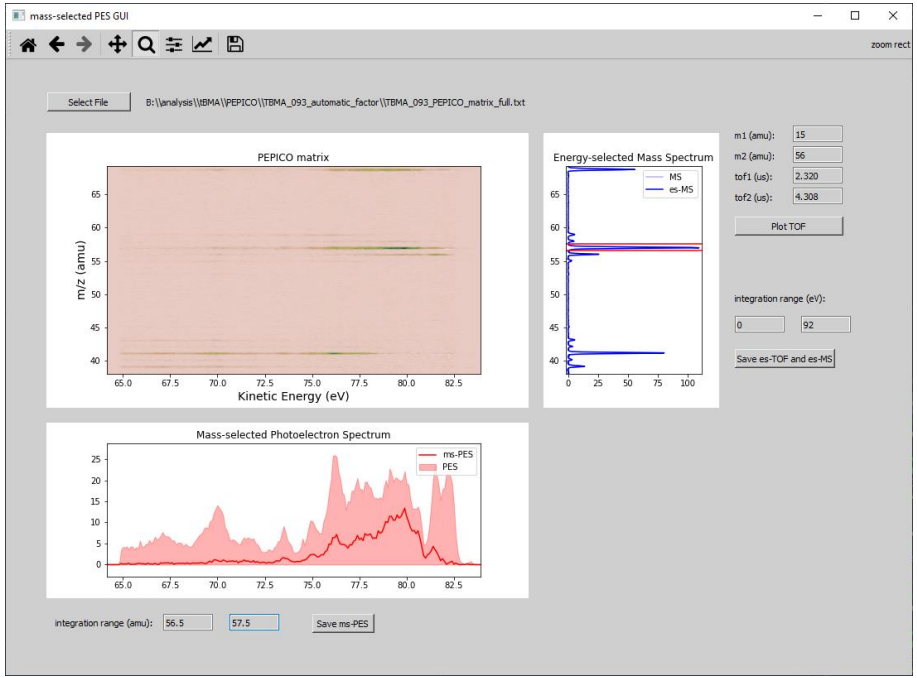
Save ms-PES or es-TOF/MS



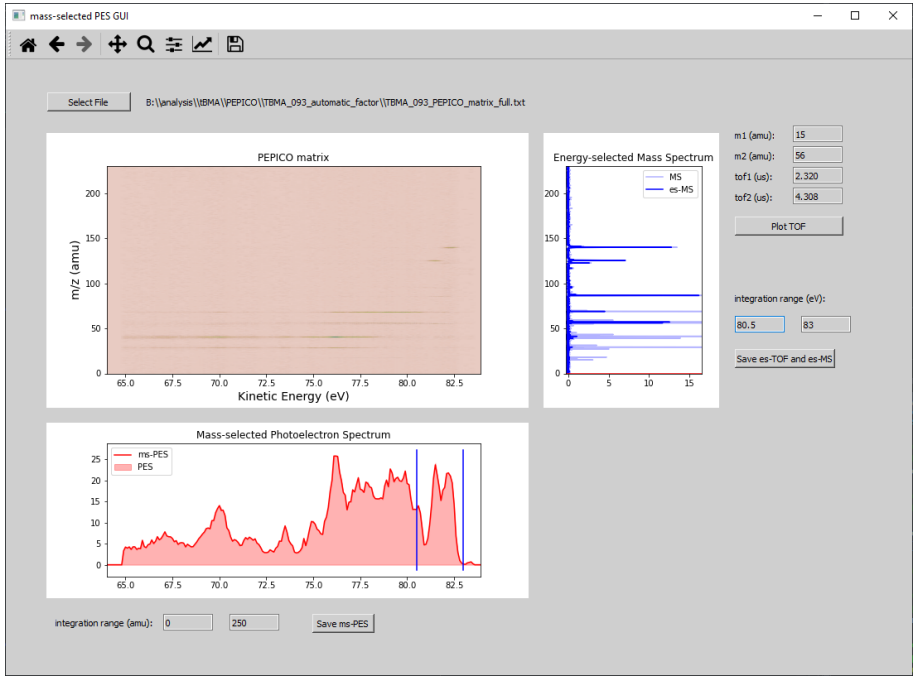
Mass-selected photoelectron spectra (2)

User interface for manual peak picking - ‘msPES_GUI’

Example for ms-PES



Example for es-MS



The spectra are saved as .txt in the parent directory with automatic file names containing the integration limits.

Contact

Address questions, suggestions for extension, bug reports etc. to:

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