


Graphical user interface is made with streamlit package - <https://streamlit.io/>

Underlying code is python

*Caution: program can be RAM intensive depending on the files you load. 16GB is safe amount, it can work with 8GB but your experience may be suboptimal*

side bar / pages  
(sequential)

main window



1. Read and process data

1.1 Wavenumbers per file

1.2 Unique wavenumbers

1.3 Experiment parameters

2. Baseline correction


2.1 Baseline correction - full range

3. Data analysis

4. Miscellaneous


4.1 Mega sum

Deploy



## 1. Read and process data

Select HDF5 files to read (adds files to existing list, click x to remove)




Drag and drop files here  
Limit 4GB per file • H5

Browse files

Enter file directory where data is saved. All outputs will be saved here.

Enter the step size of your scans. (not yet working)

 click this button to import, read, and process the H5 files. Wait for a prompt that files have been loaded to memory.

Note:

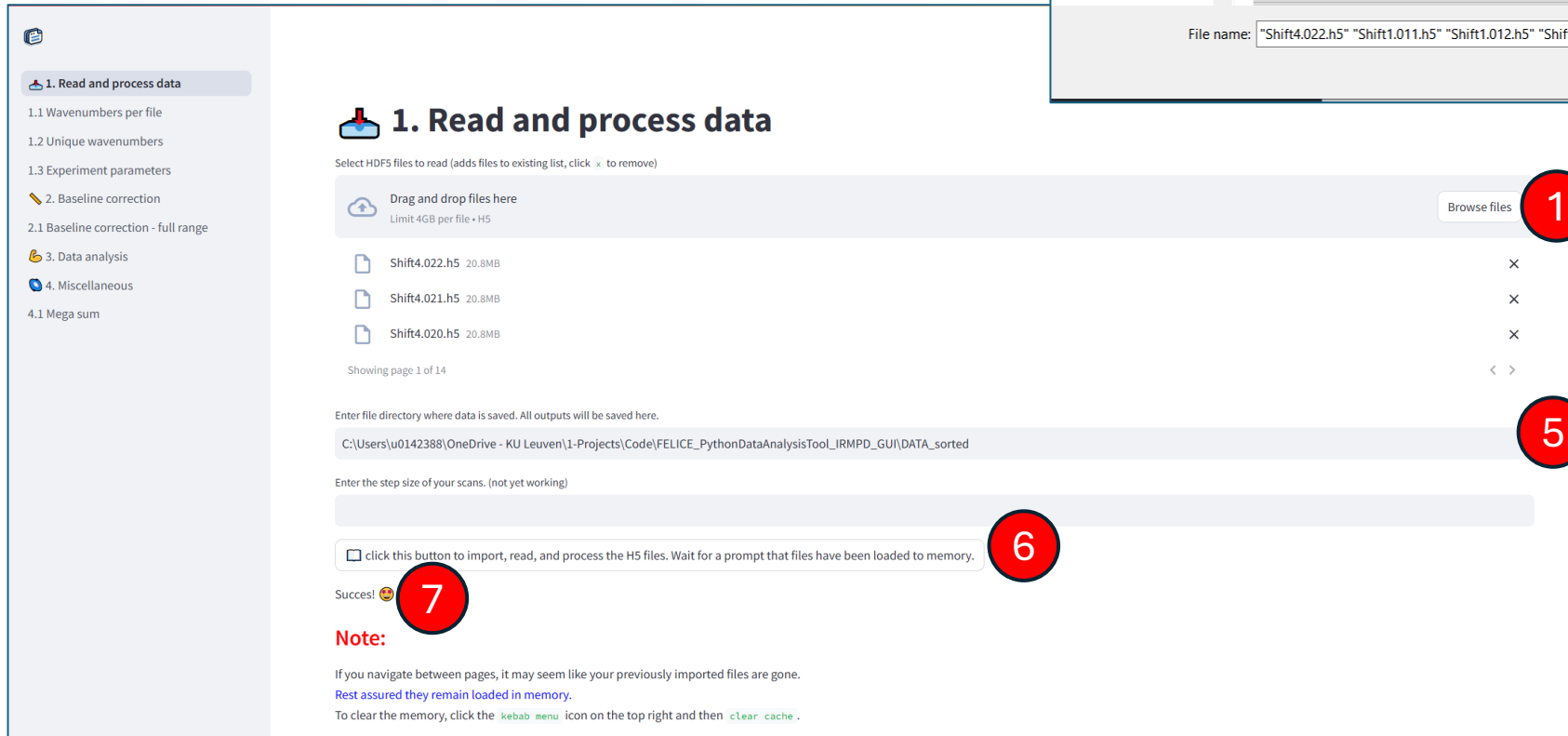
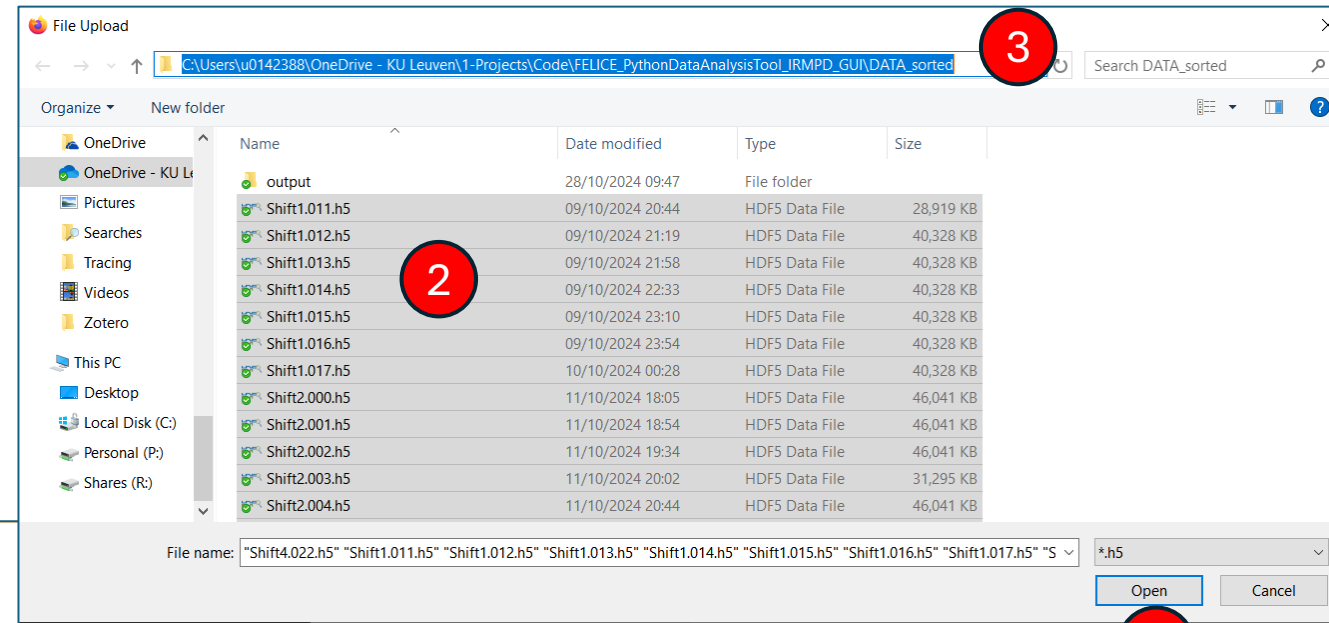
If you navigate between pages, it may seem like your previously imported files are gone.  
Rest assured they remain loaded in memory.

To clear the memory, click the kebab menu icon on the top right and then clear cache.

## Loading files

1. Click browse files
2. Select files (selection of multiple files possible)
3. Copy directory
4. Click open
5. Paste directory
6. Click import
7. Completion prompt

(output folder must be made manually)





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Inspect wavenumbers per file,  
Can load partial scans

## 1.1 Wavenumbers per file

1.010	Shift2.011	Shift3.002	Shift3.003	Shift3.004	Shift3.005	Shift3.006	Shift3.007	Shift3.009	Shift3.010	Shift3.011
10000	399.900000	220.000000	220.000000	220.000000	220.000000	180.000000	220.000000	220.000000	220.000000	220.000000
0000	397.500000	217.500000	217.500000	217.500000	217.500000	177.500000	217.500000	217.500000	217.500000	217.500000
10000	395.000000	215.000000	215.000000	215.000000	215.000000	175.000000	215.000000	215.000000	215.000000	215.000000
0000	392.500000	212.500000	212.500000	212.500000	212.500000	172.500000	212.500000	212.500000	212.500000	212.500000
10000	390.000000	210.000000	210.000000	210.000000	210.000000	170.000000	210.000000	210.000000	210.000000	210.000000
0000	387.500000	207.500000	207.500000	207.500000	207.500000	167.500000	207.500000	207.500000	207.500000	207.500000
10000	385.000000	205.000000	205.000000	205.000000	205.000000	165.000000	205.000000	205.000000	205.000000	205.000000
0000	382.500000	202.500000	202.500000	202.500000	202.500000	162.500000	202.500000	202.500000	202.500000	202.500000
10000	380.000000	200.000000	200.000000	200.000000	200.000000	160.000000	200.000000	200.000000	200.000000	200.000000
0000	377.500000	197.500000	197.500000	197.500000	197.500000	157.500000	197.500000	197.500000	197.500000	197.500000
10000	375.000000	195.000000	195.000000	195.000000	195.000000	155.000000	195.000000	195.000000	195.000000	195.000000
0000	372.500000	192.500000	192.500000	192.500000	192.500000	152.500000	192.500000	192.500000	192.500000	192.500000
10000	370.000000	190.000000	190.000000	190.000000	190.000000	150.000000	190.000000	190.000000	190.000000	190.000000
0000	367.500000	187.500000	187.500000	187.500000	187.500000	147.500000	187.500000	187.500000	187.500000	187.500000
10000	365.000000	185.000000	185.000000	185.000000	185.000000	145.000000	185.000000	185.000000	185.000000	185.000000
0000	362.500000	182.500000	182.500000	182.500000	182.500000	142.500000	182.500000	182.500000	182.500000	182.500000
10000	360.000000	180.000000	180.000000	180.000000	180.000000	140.000000	180.000000	180.000000	180.000000	180.000000
0000	357.500000	177.500000	177.500000	177.500000	177.500000	137.500000	177.500000	177.500000	177.500000	177.500000
10000	355.000000	175.000000	175.000000	175.000000	175.000000	135.000000	175.000000	175.000000	175.000000	175.000000
0000	352.500000	172.500000	172.500000	172.500000	nan	132.500000	172.500000	172.500000	172.500000	172.500000
10000	350.000000	170.000000	170.000000	170.000000	nan	130.000000	170.000000	170.000000	170.000000	170.000000
0000	347.500000	167.500000	167.500000	167.500000	nan	127.500000	167.500000	167.500000	167.500000	167.500000
10000	345.000000	165.000000	165.000000	165.000000	nan	125.000000	165.000000	165.000000	165.000000	165.000000
0000	342.500000	162.500000	162.500000	162.500000	nan	122.500000	162.500000	162.500000	162.500000	162.500000
10000	340.000000	160.000000	160.000000	160.000000	nan	120.000000	160.000000	160.000000	160.000000	160.000000
0000	337.500000	157.500000	157.500000	157.500000	nan	117.500000	157.500000	157.500000	157.500000	157.500000
10000	335.000000	155.000000	155.000000	nan	nan	115.000000	155.000000	155.000000	155.000000	155.000000
0000	332.500000	152.500000	152.500000	nan	nan	112.500000	152.500000	152.500000	152.500000	152.500000
10000	330.000000	150.000000	150.000000	nan	nan	110.000000	150.000000	150.000000	150.000000	150.000000



## 1. Read and process data

### 1.1 Wavenumbers per file

### 1.2 Unique wavenumbers

### 1.3 Experiment parameters

## 2. Baseline correction

### 2.1 Baseline correction - full range

## 3. Data analysis

## 4. Miscellaneous

### 4.1 Mega sum

# 1.2 Unique wavenumbers

Unique Wavenumbers	
0	110.000000
1	112.500000
2	115.000000
3	117.500000
4	120.000000
5	122.500000
6	125.000000
7	127.500000
8	130.000000
9	132.500000
10	135.000000
11	137.500000
12	140.000000
13	142.500000
14	145.000000
15	147.500000
16	150.000000
17	152.500000
18	155.000000
19	157.500000
20	160.000000
21	162.500000
22	165.000000
23	167.500000
24	170.000000
25	172.500000
26	175.000000
27	177.500000
28	180.000000
29	182.500000

List of unique wavenumbers,  
The program iterates over this list.

It makes a python dictionary on a per  
wavenumber basis.

For example:

key: 110.0

value: scan1 | scan2 | scan3 | scan4

key: 112.5

value: scan1 | scan2 | scan3 | scan4

key: 115.0

value: scan1 | scan1 | scan3 | scan4

*columns are separated by “|” in this  
illustration.*

It is possible that certain files can skip or have  
doubly measured wavenumbers like [115.0].  
But this seems to be from FELIX’s side i.e. not  
caused by rounding errors

Here you may define experimental conditions

1. Read and process data

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### 1.3 Experiment parameters

Species parameters

Main element

Fe

Mass of main element in amu

55.845

Charge state

+

Messenger species

Ar

Mass of messenger species in amu

39.948

Register inputs

Inputs registered! 😊

Calibration parameters

t\_off

72

alpha

1.0408e-06

length of dataset in the time axis

60000

completion prompt

Output style: Fe5(+)-Ar1

Modified for PAHs

### 1.3 Experiment parameters

Species	Parameters	Calibration parameters
Element 1	Mass of element1 in amu	t_off
C	12.0	58
Element 2	Mass of element2 in amu	alpha
H	1.007825	7.6987e-07
Element 3	Mass of element3 in amu	length of dataset in the time axis
Br	78.918336	60000
	Charge state	
	0	
<div><div> Register inputs</div></div>		

Output style: C14H10Br0(0)

1. Read and process data

1.1 Wavenumbers per file

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1.3 Experiment parameters

**2. Baseline correction**

2.1 Baseline correction - full range

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Baseline region =  
start position + width

## 2. Baseline correction

### Complex parameters

size of main element

5

-

+

size of messenger species

1

-

+

### Baseline parameters

start of baseline in amu

310.0

width of baseline in amu

5.0

[✦ Register parameters and make plot!](#)

### Plot parameters

Wavenumber to check plots

400.0

Maximum y-value for top plot

0.1

Maximum y-value for bottom plot

0.01

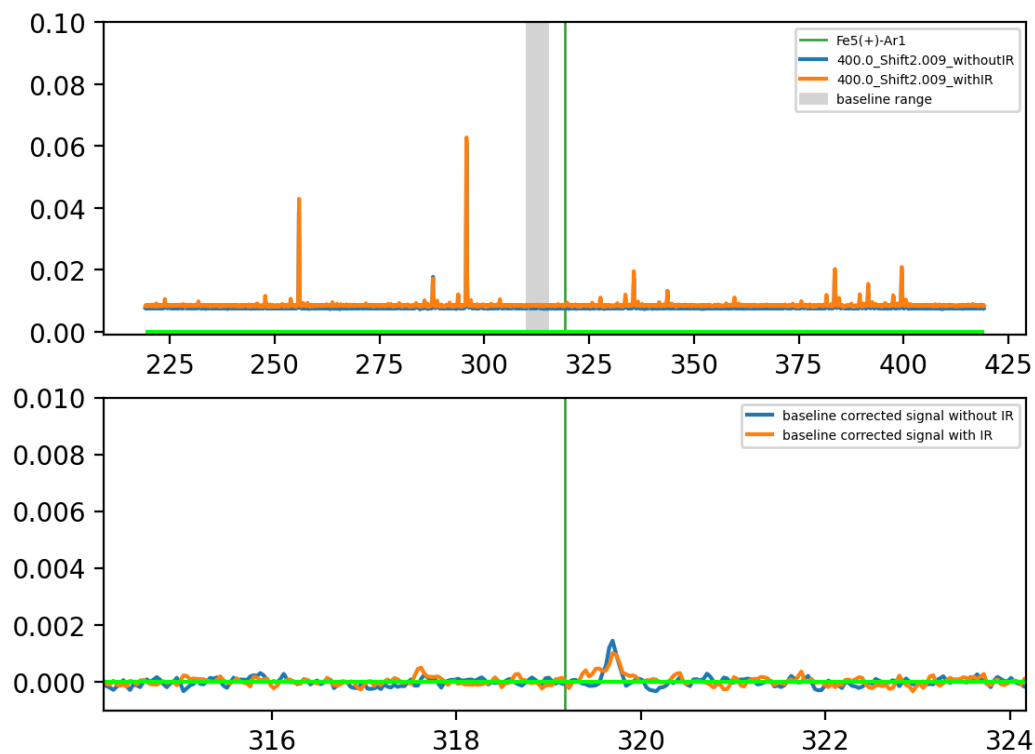
Column index for signal without IR irradiation

-2

Column index for signal with IR irradiation


-1

Tune plot parameters for  
better presentation



1. Click button
2. Completion prompt
3. Here you may check if the sums are done correctly


The program sums all the mass spectra first, and then does baseline correction based on user defined parameters (previous page)

1. Read and process data


1.1 Wavenumbers per file


1.2 Unique wavenumbers

1.3 Experiment parameters

2. Baseline correction

**2.1 Baseline correction - full range**


3. Data analysis


4. Miscellaneous

4.1 Mega sum

Deploy

## 2.1 Baseline correction - full range

#1  Perform baseline correction - full range

Success! 

	withoutIR	400.0_Shift2.008_withIR	400.0_Shift2.009_withoutIR	400.0_Shift2.009_withIR	sum_400.0_withoutIR	sum_400.0_withIR	sum_baseline_corrected_400.0_withoutIR	sum_baseline_corrected_400.0_withIR
0	0.0224	0.0223	0.0225	0.0232	0.3171	0.3165	0.2067	
1	0.0212	0.0207	0.0207	0.0211	0.2928	0.2928	0.1824	
2	0.0117	0.0113	0.0112	0.0115	0.158	0.1589	0.0476	
3	0.0057	0.0057	0.0058	0.0062	0.0836	0.0834	-0.0267	
4	0.0051	0.0048	0.005	0.0054	0.075	0.0747	-0.0354	

### Plot parameters

Wavenumber to check plots

400.0

Minimum x-value

0.0

Column index for signal without IR irradiation

-2

Maximum y-value


0.2

Maximum x-value

1300.0

Column index for signal with IR irradiation

-1

#2  Plot full range data

- 1. Click button
- 2. Navigation buttons for interactive plot

## 2.1 Baseline correction - full range

#1 ✨ Perform baseline correction - full range

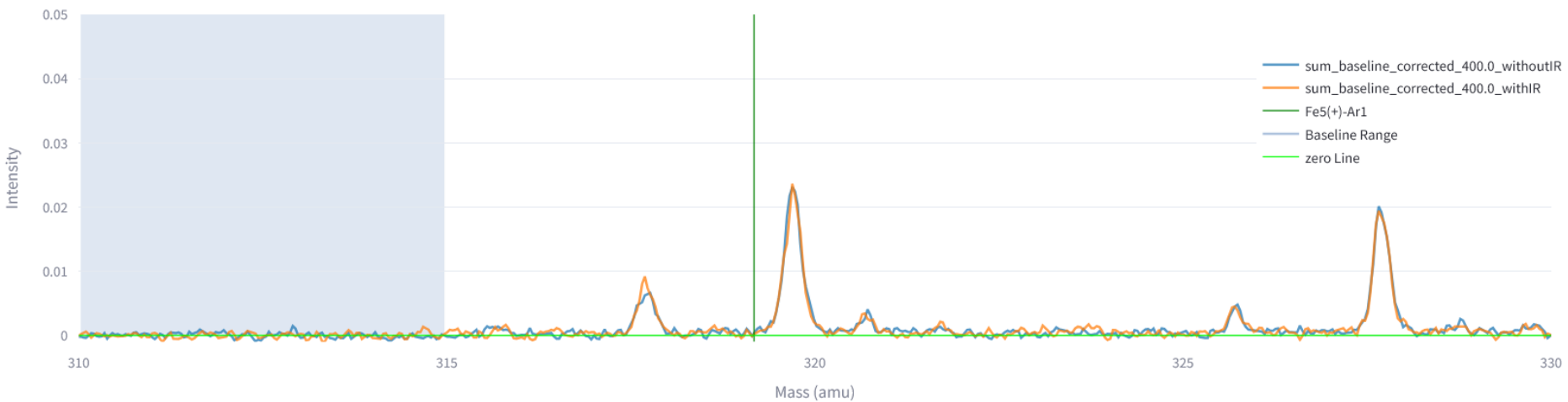
### Plot parameters

Wavenumber to check plots	Minimum x-value	Column index for signal without IR irradiation
400.0	310.0	-2
Maximum y-value	Maximum x-value	Column index for signal with IR irradiation
0.05	330.0	-1

#2 🚀 Plot full range data

1

Fe5(+)-Ar1



2



### 3. Data analysis

#### Integration parameters

Enter mass peaks, comma separated

- ☐ Average mass  
☒ Custom input

319.6, 317.6, 320.7

Input history

Active mass peak(s):

319.6, 317.6, 320.7

Integration width per peak in a

0.3

Save output

#### Plot parameters

Column index for signal without IR irradiation

-2

Column index for signal with IR irradiation

-1

Wavenumber to check plots

400.0

Mass Spectra: minimum x-value

310.0

Mass Spectra: maximum x-value

330.0

Mass Spectra: maximum y-value

0.05

Depletion: minimum y-value

-0.1

Depletion: maximum y-value

1.5

-ln(depletion): minimum y-value

-0.1

-ln(depletion): maximum y-value

0.5

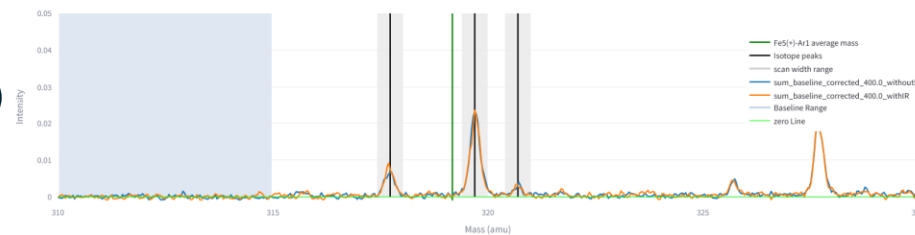
Analyze!

Output saved @ C:\Users\u0142388\OneDrive - KU Leuven\I-Projects\Code\FELICE\_PythonDataAnalysisTool\_IRMPD\_GUI\DATA\_sorted\output\fullrange\_depletion\_data\_Fe5(+)-Ar1\_400-110.csv

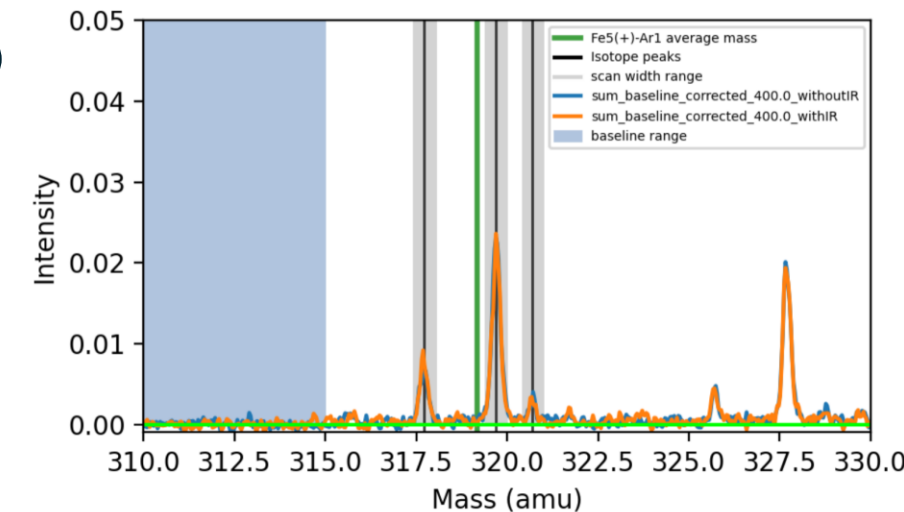
Mass spectra - specified wavenumber Depletion - full range -ln(depletion) - full range

Interactive plot with plotly

Fe5(+)-Ar1



Static plot with matplotlib



1. Enter the mass peaks separated by commas
2. Show the mass peaks the program is going to use
3. Option to save output (yes by default)
4. Click button to do calculations and make plots + completion prompt
  - Program automatically finds the maximum data point within the given scan width
5. Tabs for different plots (mass spectra, depletion, -ln(depletion))
6. Interactive plot with hover feature to read data points
7. Static plot for easier copy and paste
8. Adjust peak scan width
9. Tweak plot parameters for better visualization
10. Output of the program, you can check if the operation is done correctly (if save is on, this table will be exported as a csv file in the output folder)

310.0 312.5 315.0 317.5 320.0 322.5 325.0 327.5 330.0  
Mass (amu)

Full range depletion data Fe5(+)-Ar1:

	wavenumber	sum_withoutIR	sum_withIR	depletion	-ln(depletion)
0	110.0000	0.0062	0.0016	0.2574	1.3571
0	112.5000	0.0030	-0.0034	-1.1562	<NA>
0	115.0000	0.0154	0.0117	0.7634	0.2699
0	117.5000	0.0683	0.0810	1.1858	-0.1704

### 3. Data analysis

#### Integration parameters

Enter mass peaks, comma separated

- ☐ Average mass  
☒ Custom input

319.6, 317.6, 320.7

Input history ▾

Active mass peak(s):

319.6, 317.6, 320.7

Integration width per peak in amu

0.3

Save output

#### Plot parameters

Column index for signal without IR irradiation

-2

Column index for signal with IR irradiation

-1

Wavenumber to check plots

400.0

Mass Spectra: minimum x-value

310.0

Mass Spectra: maximum x-value

330.0

Mass Spectra: maximum y-value

0.05

Depletion: minimum y-value

-0.1

Depletion: maximum y-value

5.0

-ln(depletion): minimum y-value

-0.1

-ln(depletion): maximum y-value

0.5

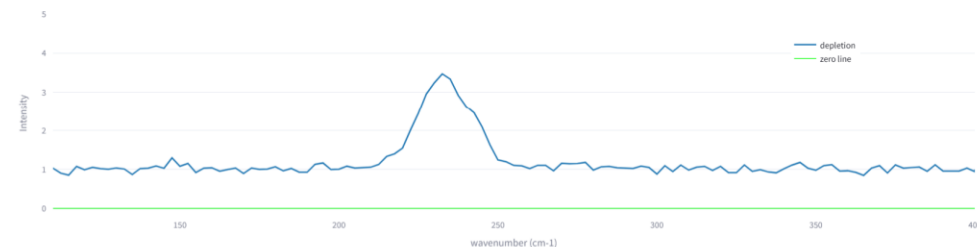


Note: save output is currently off.

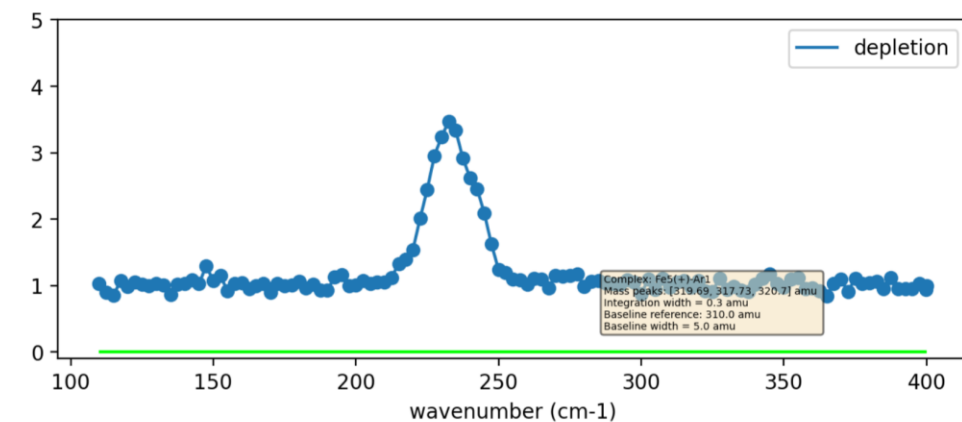
☒ Mass spectra - specified wavenumber 
 ☒ Depletion - full range 
 ☒ -ln(depletion) - full range

Interactive plot with plotly

depletion Fe5(+)-Ar1



Static plot with matplotlib



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4.1 Mega sum

### 3. Data analysis

#### Integration parameters

Enter mass peaks, comma separated

- ☐ Average mass  
☒ Custom input

319.6, 317.6, 320.7

Input history ▾

Active mass peak(s):

319.6, 317.6, 320.7

Integration width per peak in amu

0.3

Save output

#### Plot parameters

Column index for signal without IR irradiation

-2

Column index for signal with IR irradiation

-1

Wavenumber to check plots

400.0

Mass Spectra: minimum x-value

310.0

Mass Spectra: maximum x-value

330.0

Mass Spectra: maximum y-value

0.05

Depletion: minimum y-value

-0.1

Depletion: maximum y-value

5.0

-ln(depletion): minimum y-value

-1.5

-ln(depletion): maximum y-value

0.5

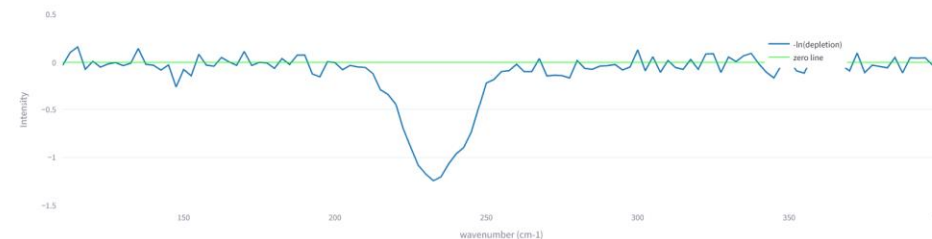


Note: save output is currently off.

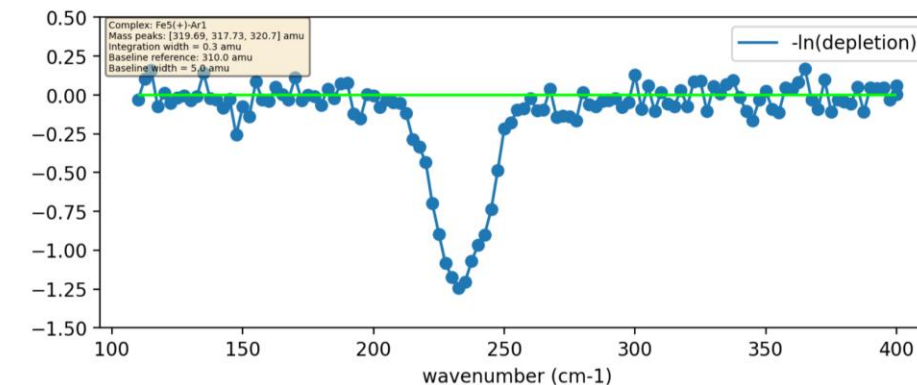
☒ Mass spectra - specified wavenumber 
 ☒ Depletion - full range 
 ☒ -ln(depletion) - full range

Interactive plot with plotly

-ln(depletion) Fe5(+)-Ar1



Static plot with matplotlib

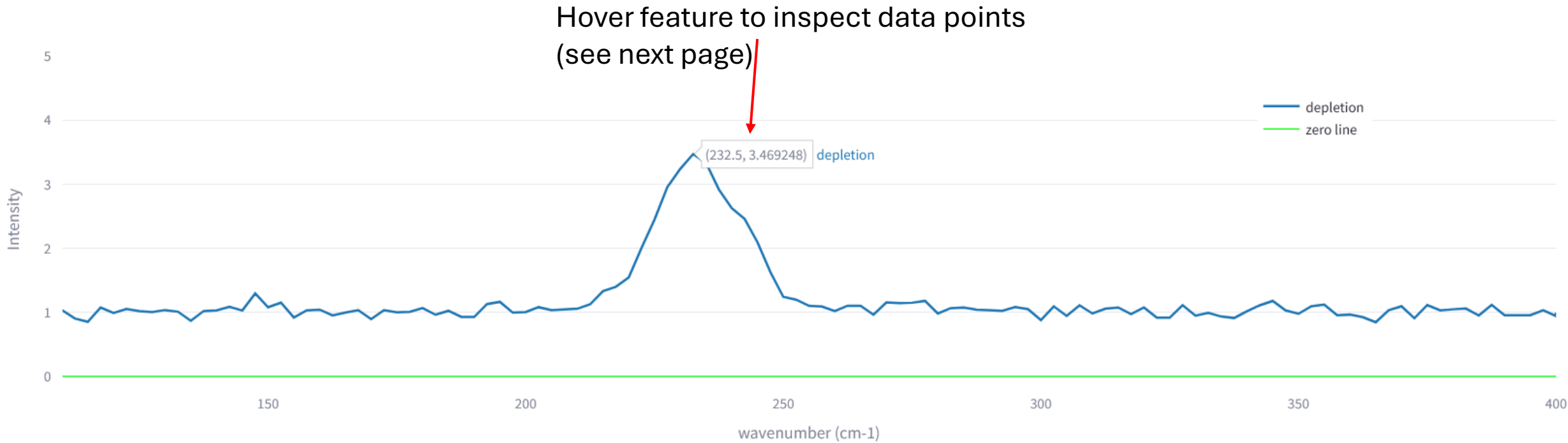


Full range depletion data Fe5(+)-Ar1:

 Mass spectra - specified wavenumber  Depletion - full range  -ln(depletion) - full range

Interactive plot with plotly

depletion Fe5(+)-Ar1



Input history ▾

☐ Save output

-1-+Wavenumber to check plots232.51

Mass Spectra: maximum y-value0.05

-ln(depletion): minimum y-value-1.5

-ln(depletion): maximum y-value0.5

Analyze! 2

Note: save output is currently off.

3

☒ Mass spectra - specified wavenumber ☒ Depletion - full range ☒ -ln(depletion) - full range

Interactive plot with plotly

1. Change wavenumber
2. Click button
3. Prompt if save output is turned off
4. Mass spectra at 232.5 cm<sup>-1</sup> (previously it was at 400 cm<sup>-1</sup>)

Fe5(+)-Ar1

