

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

The screenshot shows a Streamlit application interface. On the left is a sidebar with a light gray background, containing a vertical list of steps:

- 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

The main window has a white background and displays the first step, "1. Read and process data". It features a large title "1. Read and process data" with a blue icon of a cloud with a lightning bolt. Below the title is a sub-instruction: "Select HDF5 files to read (adds files to existing list, click to remove)". There is a "Drag and drop files here" input field with a cloud icon, a "Limit 4GB per file • H5" note, and a "Browse files" button. Further down, there are three input fields with placeholder text: "Enter file directory where data is saved. All outputs will be saved here.", "Enter the step size of your scans. (not yet working)", and a large button labeled "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)

The screenshot shows the FELICE Python Data Analysis Tool interface. On the left, a sidebar lists categories: 1. Read and process data, 2. Baseline correction, 3. Data analysis, and 4. Miscellaneous. Under 'Read and process data', sub-options include 1.1 Wavenumbers per file, 1.2 Unique wavenumbers, 1.3 Experiment parameters, 2.1 Baseline correction - full range, 3.1 Data analysis, and 4.1 Mega sum.

The main window has a title '1. Read and process data'. It contains a section 'Select HDF5 files to read (adds files to existing list, click x to remove)' with a 'Drag and drop files here' area and a 'Browse files' button (circled 1). Below this, three files are listed: Shift4.022.h5, Shift4.021.h5, and Shift4.020.h5. A message at the bottom says 'Showing page 1 of 14'.

Below the file selection is a text input field 'Enter file directory where data is saved. All outputs will be saved here.' containing the path C:\Users\u0142388\OneDrive - KU Leuven\1-Projects\Code\FELICE_PythonDataAnalysisTool_IRMPD_GUI\DATA_sorted (circled 5).

Further down is a text input field 'Enter the step size of your scans. (not yet working)'.

A large button at the bottom is labeled 'click this button to import, read, and process the H5 files. Wait for a prompt that files have been loaded to memory.' (circled 6). Below it, a message says 'Succes! 😊' (circled 7).

File Upload Window:

Name	Date modified	Type	Size
output	28/10/2024 09:47	File folder	
Shift1.011.h5	09/10/2024 20:44	HDF5 Data File	28,919 KB
Shift1.012.h5	09/10/2024 21:19	HDF5 Data File	40,328 KB
Shift1.013.h5	09/10/2024 21:58	HDF5 Data File	40,328 KB
Shift1.014.h5	09/10/2024 22:33	HDF5 Data File	40,328 KB
Shift1.015.h5	09/10/2024 23:10	HDF5 Data File	40,328 KB
Shift1.016.h5	09/10/2024 23:54	HDF5 Data File	40,328 KB
Shift1.017.h5	10/10/2024 00:28	HDF5 Data File	40,328 KB
Shift2.000.h5	11/10/2024 18:05	HDF5 Data File	46,041 KB
Shift2.001.h5	11/10/2024 18:54	HDF5 Data File	46,041 KB
Shift2.002.h5	11/10/2024 19:34	HDF5 Data File	46,041 KB
Shift2.003.h5	11/10/2024 20:02	HDF5 Data File	31,295 KB
Shift2.004.h5	11/10/2024 20:44	HDF5 Data File	46,041 KB

At the top right of the file upload window, there is a search bar (circled 3) and an 'Open' button (circled 4).



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

Inspect wavenumbers per file,
Can load partial scans

1.1 Wavenumbers per file

Shift2.010	Shift2.011	Shift3.002	Shift3.003	Shift3.004	Shift3.005	Shift3.006	Shift3.007	Shift3.009	Shift3.010	Shift3.011
399.900000	399.900000	220.000000	220.000000	220.000000	220.000000	180.000000	220.000000	220.000000	220.000000	220.000000
397.500000	397.500000	217.500000	217.500000	217.500000	217.500000	177.500000	217.500000	217.500000	217.500000	217.500000
395.000000	395.000000	215.000000	215.000000	215.000000	215.000000	175.000000	215.000000	215.000000	215.000000	215.000000
392.500000	392.500000	212.500000	212.500000	212.500000	212.500000	172.500000	212.500000	212.500000	212.500000	212.500000
390.000000	390.000000	210.000000	210.000000	210.000000	210.000000	170.000000	210.000000	210.000000	210.000000	210.000000
387.500000	387.500000	207.500000	207.500000	207.500000	207.500000	167.500000	207.500000	207.500000	207.500000	207.500000
385.000000	385.000000	205.000000	205.000000	205.000000	205.000000	165.000000	205.000000	205.000000	205.000000	205.000000
382.500000	382.500000	202.500000	202.500000	202.500000	202.500000	162.500000	202.500000	202.500000	202.500000	202.500000
380.000000	380.000000	200.000000	200.000000	200.000000	200.000000	160.000000	200.000000	200.000000	200.000000	200.000000
377.500000	377.500000	197.500000	197.500000	197.500000	197.500000	157.500000	197.500000	197.500000	197.500000	197.500000
375.000000	375.000000	195.000000	195.000000	195.000000	195.000000	155.000000	195.000000	195.000000	195.000000	195.000000
372.500000	372.500000	192.500000	192.500000	192.500000	192.500000	152.500000	192.500000	192.500000	192.500000	192.500000
370.000000	370.000000	190.000000	190.000000	190.000000	190.000000	150.000000	190.000000	190.000000	190.000000	190.000000
367.500000	367.500000	187.500000	187.500000	187.500000	187.500000	147.500000	187.500000	187.500000	187.500000	187.500000
365.000000	365.000000	185.000000	185.000000	185.000000	185.000000	145.000000	185.000000	185.000000	185.000000	185.000000
362.500000	362.500000	182.500000	182.500000	182.500000	182.500000	142.500000	182.500000	182.500000	182.500000	182.500000
360.000000	360.000000	180.000000	180.000000	180.000000	180.000000	140.000000	180.000000	180.000000	180.000000	180.000000
357.500000	357.500000	177.500000	177.500000	177.500000	177.500000	137.500000	177.500000	177.500000	177.500000	177.500000
355.000000	355.000000	175.000000	175.000000	175.000000	175.000000	135.000000	175.000000	175.000000	175.000000	175.000000
352.500000	352.500000	172.500000	172.500000	172.500000	172.500000	nan	132.500000	172.500000	172.500000	172.500000
350.000000	350.000000	170.000000	170.000000	170.000000	170.000000	nan	130.000000	170.000000	170.000000	170.000000
347.500000	347.500000	167.500000	167.500000	167.500000	167.500000	nan	127.500000	167.500000	167.500000	167.500000
345.000000	345.000000	165.000000	165.000000	165.000000	165.000000	nan	125.000000	165.000000	165.000000	165.000000
342.500000	342.500000	162.500000	162.500000	162.500000	162.500000	nan	122.500000	162.500000	162.500000	162.500000
340.000000	340.000000	160.000000	160.000000	160.000000	160.000000	nan	120.000000	160.000000	160.000000	160.000000
337.500000	337.500000	157.500000	157.500000	157.500000	157.500000	nan	117.500000	157.500000	157.500000	157.500000
335.000000	335.000000	155.000000	155.000000	155.000000	155.000000	nan	115.000000	155.000000	155.000000	155.000000
332.500000	332.500000	152.500000	152.500000	152.500000	152.500000	nan	112.500000	152.500000	152.500000	152.500000
330.000000	330.000000	150.000000	150.000000	150.000000	150.000000	nan	110.000000	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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4.1 Mega sum

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

Calibration parameters

t_off

72

alpha

1.0408e-06

length of dataset in the time axis

60000

Modified for PAHs

1.3 Experiment parameters

Species

Element 1

C

Mass of element1 in amu

12.0

Element 2

H

Mass of element2 in amu

1.007825

Element 3

Br

Mass of element3 in amu

78.918336

Calibration parameters

t_off

58

alpha

7.6987e-07

length of dataset in the time axis

60000

Charge state

0

Register inputs

completion prompt

Output style: Fe5(+) - Ar1

Output style: C14H10Br0(0)



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

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4. Miscellaneous

4.1 Mega sum

**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

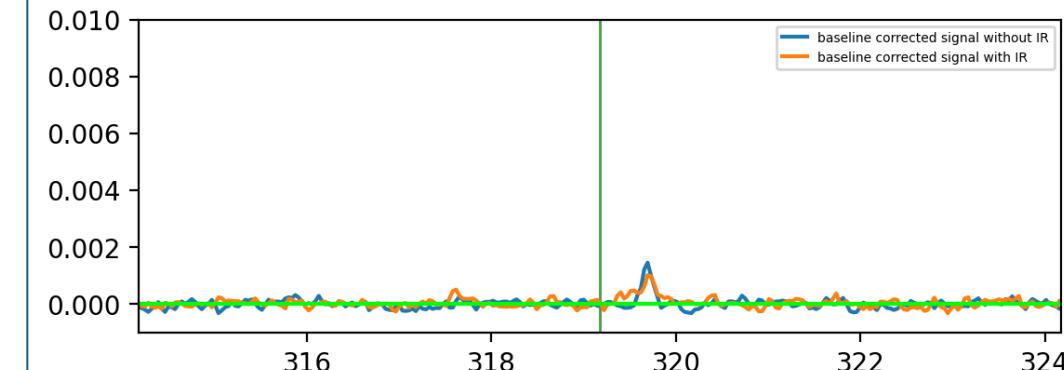
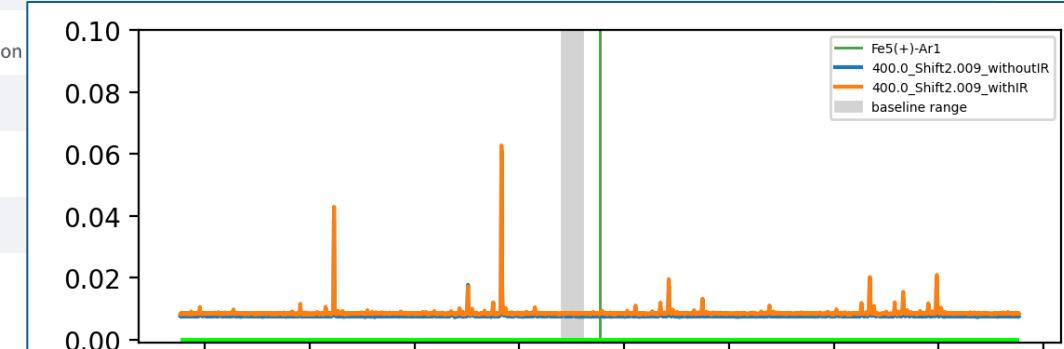
Maximum y-value for top plot

0.1

Maximum y-value for bottom plot

0.01

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)

Deploy

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**
- 2.2 Baseline correction - partial range

3. Data analysis

- 3.1 Peak detection
- 3.2 Spectrum comparison

4. Miscellaneous

- 4.1 Mega sum

5. Plotting

- 5.1 Full range plot
- 5.2 Partial range plot

6. Export

- 6.1 CSV export
- 6.2 JSON export

7. Help

- 7.1 Documentation
- 7.2 Support

2.1 Baseline correction - full range

#1 🚀 Perform baseline correction - full range
1

Success! 😊
2

3

	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

#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

400.0

Minimum x-value

310.0

Column index for signal without IR irradiation

-2

- +

Maximum y-value

0.05

Maximum x-value

330.0

Column index for signal with IR irradiation

-1

- +

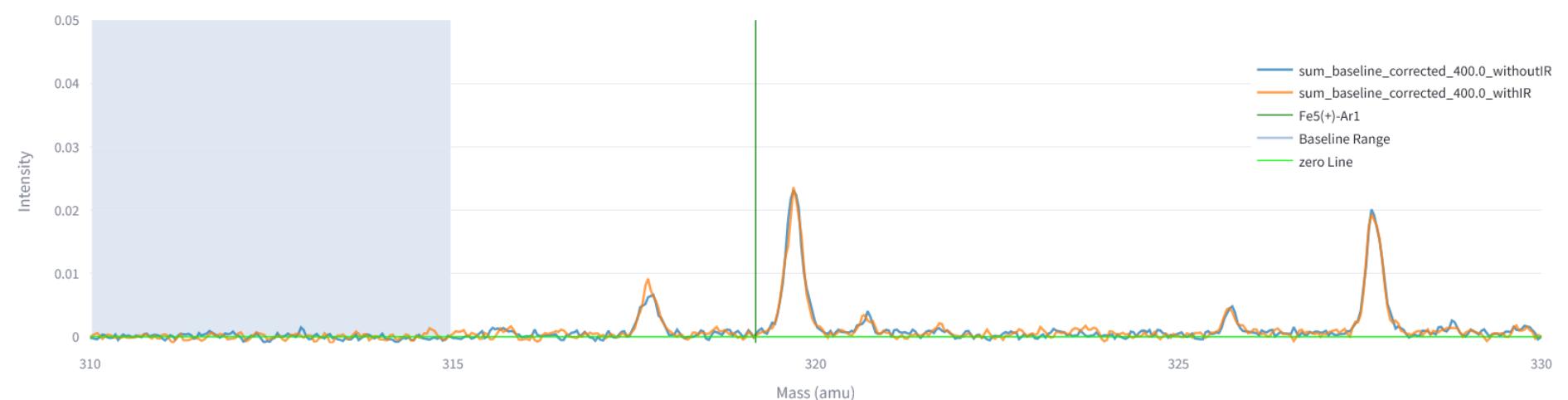
#2 🚀 Plot full range data

1

Fe5(+-)Ar1



2





- Enter the mass peaks separated by commas
- Show the mass peaks the program is going to use
- Option to save output (yes by default)
- Click button to do calculations and make plots + completion prompt
 - Program automatically finds the maximum data point within the given scan width
- Tabs for different plots (mass spectra, depletion, -ln(depletion))
- Interactive plot with hover feature to read data points
- Static plot for easier copy and paste
- Adjust peak scan width
- Tweak plot parameters for better visualization
- 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)

10

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)
110.0000	0.0062	0.0016	0.2574	1.3571
112.5000	0.0030	-0.0034	-1.1562	<NA>
115.0000	0.0154	0.0117	0.7634	0.2699
117.5000	0.0683	0.0810	1.1858	-0.1704

3. Data analysis

Integration parameters

Active mass peak(s):
 Average mass **Custom input**
 319.6, 317.6, 320.7
 Integration width per peak in amu
 0.3
 Input history
 Save output

Plot parameters

Column index for signal without IR irradiation	-2	Mass Spectra: minimum x-value	310.0	Depletion: minimum y-value	-0.1
Column index for signal with IR irradiation	-1	Mass Spectra: maximum x-value	330.0	Depletion: maximum y-value	5.0
		Mass Spectra: maximum y-value	-ln(depletion): minimum y-value		
		Wavenumber to check plots	0.05	-ln(depletion): maximum y-value	0.5
			400.0		

depletion

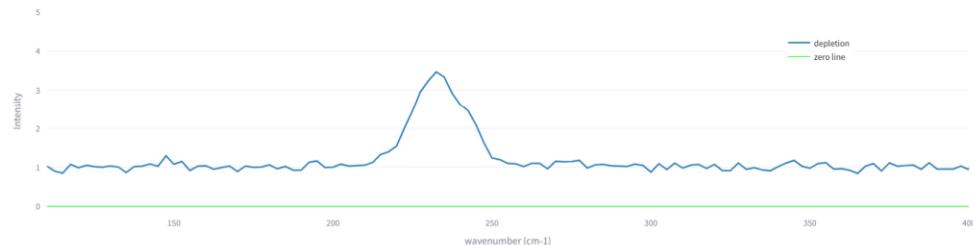
Analyze!

Note: save output is currently off.

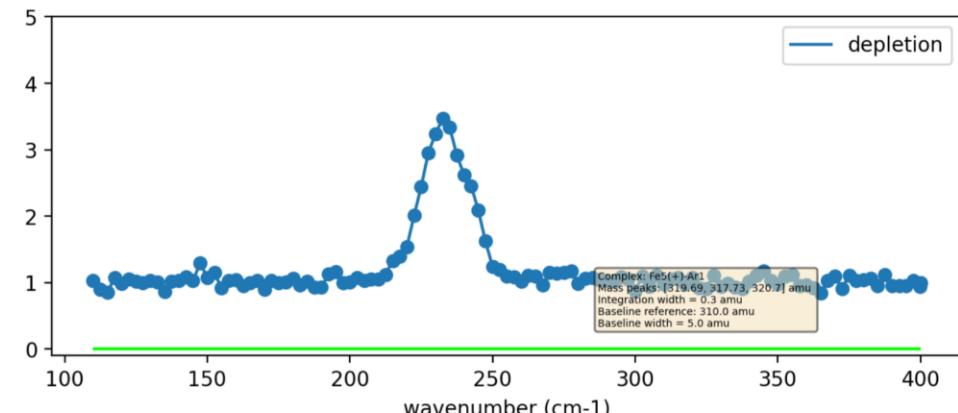
Mass spectra - specified wavenumber Depletion - full range -ln(depletion) - full range

Interactive plot with plotly

depletion Fe5(+)-Ar1



Static plot with matplotlib



3. Data analysis

Integration parameters

Active mass peak(s):
 Average mass **Custom input**
 319.6, 317.6, 320.7
 Integration width per peak in amu
 0.3
 Input history
 Save output

Plot parameters

Column index for signal without IR irradiation	-2	Mass Spectra: minimum x-value	310.0	Depletion: minimum y-value	-0.1
Column index for signal with IR irradiation	-1	Mass Spectra: maximum x-value	330.0	Depletion: maximum y-value	5.0
		Mass Spectra: maximum y-value	-ln(depletion): minimum y-value		
		Wavenumber to check plots	0.05	-ln(depletion): maximum y-value	0.5
			400.0		

-ln(depletion)

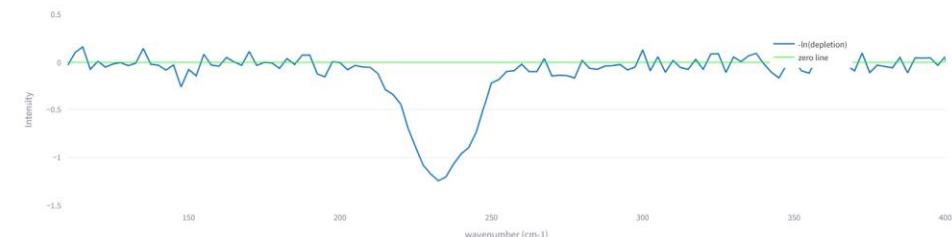
Analyze!

Note: save output is currently off.

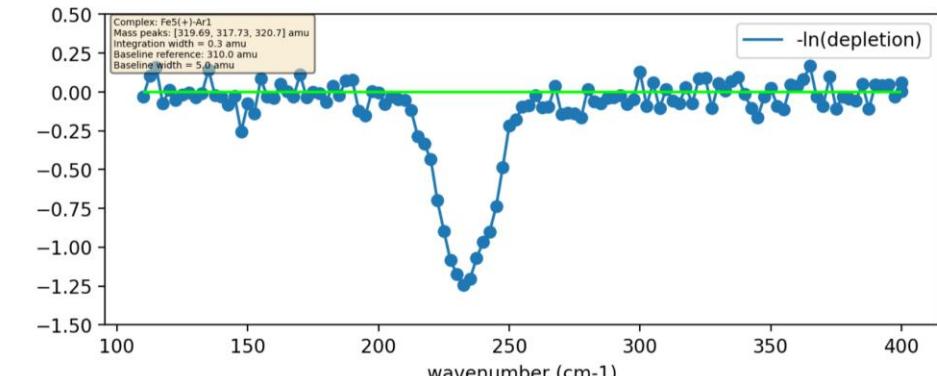
Mass spectra - specified wavenumber Depletion - full range -ln(depletion) - full range

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

Hover feature to inspect data points
(see next page)



The screenshot shows the VIBRANT software interface. At the top, there are input history, save output, and wavenumber selection dropdowns. The wavenumber dropdown is set to 232.5 and has a red circle with the number 1 over it. Below the dropdown is an 'Analyze!' button with a red circle containing the number 2. A note below the button says 'Note: save output is currently off.' with a red circle containing the number 3 over it. At the bottom, there are three checkboxes: 'Mass spectra - specified wavenumber' (unchecked), 'Depletion - full range' (unchecked), and '-ln(depletion) - full range' (unchecked).

1. Change wavenumber
2. Click button
3. Prompt if save output is turned off

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

