Atom Probe Microscopy

Mass Spectrum Workflow Generator

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# Use Cases

000 program run

Loading/saving files

101 load/save data file (POS or EPOS) (with monitoring)

102 load help/tutorial

Visualising data

201 interaction with plots/plot tools

202 visualising data

203 peak suggestion

204 auto peak detection and manual ranging

205 error alerts

Calculating new data

301 peak suggestions (based on various methods)

302 highlight un-ranged peaks

# GUI Features

f01 plot panel ranged mass spectrum

f02 plot panel working mass spectrum

f03 workspace: plot controls

f04 workspace: Peak ID controls

f05 Ranged data table

f06 Saxey-Plot

# Program Features

p01 data file reader/writer

p02 analysis run reader/writer

p02 xrng file writer

p03 workflow reader/writer

p04 calculation and removal of background

p05 FWTM calculation

p06 isotopic abundance fingerprinting

p07 overlapping peak identification

# 000 program run

GUI – what the program looks like to the user

data – what the ranges are and the workflow to get the ranges

### 000a program run general

1. System updates analysis states (GUI, data x n) (000c)
2. System creates a patch file for the change
3. System updates plots & tables (000b)

### 000b System updates plots and data

1. System reads analysis states (GUI, data x )
2. System updates available plots and tables

### 000c System updates analysis state

1. System updates analysis states (GUI, data)

# 101 load/save data file (POS/EPOS)

### 101a load file/workflow

1. User chooses to open file (either menu, hotkey, etc.)
2. System creates “file open” dialog
3. Choose file type (workflow, pos, epos, etc.)
4. User chooses file and presses “open”
5. Pop-up dialog opens choose either Auto or manual
6. User chooses preference and presses “ok”
7. Program run (000a)

### 101b save file

1. User chooses to save file (either menu, hotkey, etc.)
2. System creates “file save” dialog
3. User modifies properties, including filename
4. User select “Save” option
5. System saves file

### 101c save workflow

1. User selects to save workflow (either menu, hotkey, etc.)
2. System creates “data output” dialog
3. User modifies properties, including filename
4. System saves file

# 102 load help/tutorial

### 102a load help tutorial

1. User requests help (either hotkey, menu, etc.)
2. System displays help and tutorials

### 102b display element functionality

1. User hovers over element for longer than two seconds
2. System displays element functionality

# 201 interaction with plots/plot tools

### 201a interact with plot directly

1. User selects plot to make active
2. User interacts with plot (either mouse, hotkey, toolbar, etc.)
3. Program run (000b)

### 201b multiple plot view control

1. User chooses, which graphs to view and on which plots
2. User updates system
3. Program run (000b)

### 202c create Saxey-Plot

1. User chooses to create a Saxey-plot
2. Program run (000b)

# 202 visualising data

### 202a user selects ion display to be on or off

1. User selects desired ranges in the table
2. User selects to turn on or off
3. Program run (000b)

### 202b user deletes ion

1. User highlights desired ions
2. User selects to delete ions
3. Program run (000)

### 202c user sorts data

1. User clicks heading
2. Information is sorted based on the heading that was selected (first ascending, if ascending already selected, then sort descending)
3. Program run (000c)

### 202d apply/remove ranges to ranged mass spectrum

1. User selects desired ranges (if not choosing to apply all)
2. User selects to apply/remove these ranges to/from the final mass spectrum
   1. If ‘apply’ selected and system is in auto mode: dialog box displayed with choice of ‘FWTM’ or ‘background’
   2. If ‘apply’ selected and system is in manual mode: user is asked to draw range on graph, if happy press ok, if not happy redraw or enter values
3. Program run (000) (system highlights applied ranges)

(NEEDS TO BE ADAPTED FOR FULLY AUTOMATED)

### 202e zoom to selection

1. User selects a single range
2. User selects to zoom to this range
3. Program run (000b)

### 202f apply and move to next

# 203 peak suggestion

### 203a peak suggestion

1. User types in known elements
2. User selects maximum charge state
3. User requests suggestions
4. Program run (000c)
5. Suggested ions presented in list form

### 203b visualise selection

1. User selects a suggested ion
2. Program run (000b) (Peak ID is shown in the working mass spectrum)

### 203c remove ions from list

1. User selects ion/ions in list
2. User selects to remove from the list
3. Program run (000c)

### 203d add ions

1. User selects desired ions
2. User chooses to add ions to table
3. Program run (000)

# 204 Auto peak detection and manual ranging

### 204a change to manual ranging

1. User selects to switch to manual mode
2. Program run (000c)

### 204b draw and ID range

# 205 error alerts

### 205a check for overlapping ranges (only for manual mode)

1. System checks to see if any ranges overlap
2. System warns of invalid range
3. Range is reset

# 206 automated ranging of peaks

FWTM and background

# User Scenarios

## Scenarios:

1. 100% automated: AB
2. Auto + peak suggest: ABD
3. Auto + peak suggest + manual range: ABDC
4. Auto + manual range: ABC
5. Peak suggest + manual range: DC
6. manual range: C

### Rules:

1. If A then B
2. If D then C
3. If Automated then A and B
4. If Manual then (D and C) or C

### Scenario 1 (streamlined)

Quickest, most consistent scenario, where the entire ranging of the mass spectrum is completed by the program.

Below is the most streamlined version, but there is also the option to apply ranges with different ranging methods, i.e. FWTM vs background. These choices will be captured in the workflow.

: 100% automated - AB: [Auto peak detect/range][Auto peak ID]

|  |  |  |  |
| --- | --- | --- | --- |
| Open new file | 101a | Choose ‘pos’ ‘epos’ file  Choose auto | 5 user interactions |
| Apply all ID’s | 202d | Select either ‘FWTM’ or ‘Background’ | 2 user interactions |
| Save file | 101b | Enter filename | 3 user interactions |
|  |  |  | 2 interactions - not including file open and file save |

### Scenario 2 (streamlined)

Use this scenario when it is felt that the automatic version has not captured everything.

In this scenario there is the potential for the program to only suggest elements that are not already in the table. Potentially the auto program has already detected all possible combinations

: Automated + Peak suggest - ABD: [Auto peak detect/range][Auto peak ID][Suggest peak ID]

|  |  |  |  |
| --- | --- | --- | --- |
| Open new file | 101a | Choose ‘pos’ ‘epos’ file  Choose auto | 5 user interactions |
| Enter element and charge state information | 203a |  | 3 user interactions |
| Add suggested ions to table | 203d |  | 2 user interactions |
| User applies desired IDs | 202d | Select either ‘FWTM’ or ‘Background’ | 3 user interactions |
| Save file | 101b | Enter filename | 3 user interactions |
|  |  |  | 8 interactions - not including file open and file save |

### Scenario 3 (streamlined)

This scenario is used when scenario 2 still fails to detect all of the ranges observed by the user. It enables the user to draw the ranges of undetected peaks.

In this mode the user can also choose to change the ranges as allocated to the peaks by the auto mode. Ranges can be added using the peak suggest method or by first ranging in the working mass spectrum and then adding your own element ID.

: Auto + Peak suggest + Manual – ABDC: [Auto peak detect/range][Auto peak ID][Suggest peak ID][Manual peak range/ID]

|  |  |  |  |
| --- | --- | --- | --- |
| Open new file | 101a | Choose ‘pos’ ‘epos’ file  Choose auto | 5 user interactions |
| Enter element and charge state information | 203a |  | 3 user interactions |
| Add suggested ions to table | 203d |  | 2 user interactions |
| User chooses to switch to manual mode | 204a |  | 1 user interaction |
| User draws range and enters ID | 204b |  |  |
| User applies desired IDs | 202d | Select either ‘FWTM’ or ‘Background’ | 3 user interactions |
| Save file | 101b | Enter filename | 3 user interactions |
|  |  |  | ? interactions - not including file open and file save |

### Scenario 4 (streamlined)

This scenario is for those ions that have been missed by auto and user knows exactly what they want them to be.

If user has decided not to apply ranges of auto mode until after the switch to manual mode, these IDs will be identified by the fact that they do not have ranges marked in the table yet. If any of these ranges then overlap the manual ranges, the program will give the user a number of options for how they would like to deal with the overlapping ranges.

: Automated + Manual - ABC: [Auto peak detect/range][Auto peak ID][Manual peak range/ID]

|  |  |  |  |
| --- | --- | --- | --- |
| Open new file | 101a | Choose ‘pos’ ‘epos’ file  Choose auto | 5 user interactions |
| User chooses to switch to manual mode | 204a |  | 1 user interaction |
| User draws range and enters ID | 204b |  |  |
| User applies desired IDs | 202d | Select either ‘FWTM’ or ‘Background’ | 3 user interactions |
| Save file | 101b | Enter filename | 3 user interactions |
|  |  |  | ? interactions - not including file open and file save |

### Scenario 5 (streamlined)

If the user does not want to use the automated mode, then there is still the potential to have the peaks suggested and to then apply their own ranges. However, when applying these ranges to the final mass spectrum, the decisions for the range chosen must be justified.

: Peak suggest + Manual - DC: [Peak suggest][Manual peak range/ID]

|  |  |  |  |
| --- | --- | --- | --- |
| Open new file | 101a | Choose ‘pos’ ‘epos’ file  Choose manual | 5 user interactions |
| Enter element and charge state information | 203a |  | 3 user interactions |
| Add suggested ions to table | 203d |  | 2 user interactions |
| User draws range associated with ID or draws a range and adds an ID | 204b |  |  |
| User applies desired IDs | 202d | Select either ‘FWTM’ or ‘Background’ | 3 user interactions |
| Save file | 101b | Enter filename | 3 user interactions |
|  |  |  | ? interactions - not including file open and file save |
|  |  |  |  |

### Scenario 6 (streamlined)

|  |  |  |  |
| --- | --- | --- | --- |
| Open new file | 101a | Choose ‘pos’ ‘epos’ file  Choose manual | 5 user interactions |
| User draws range and enters ID | 204b |  |  |
| User applies desired IDs | 202d | Select either ‘FWTM’ or ‘Background’ | 3 user interactions |
| Save file | 101b | Enter filename | 3 user interactions |
|  |  |  | ? interactions - not including file open and file save |