User Manual: Spectrometer Data Analysis Tool

1. Introduction

The Spectrometer Data Analysis Tool is a desktop application developed using Python and Tkinter. It is designed to assist users in performing standardized analysis and quality checks on spectrometer data, especially in laboratory environments handling multiple samples.

2. Getting Started

Before using the tool, please ensure the following prerequisites and preparation steps are completed as described in the application:

- Allow a 10-hour stabilization time after connecting power and argon.
- Prepare standards and samples using appropriate machines and materials.
- Clean all previous burn marks and ensure the sample surface is flat and uncontaminated.
- Follow routine maintenance such as spark chamber cleaning.
- Place burn spots accurately and avoid overlapping.
- Use 10 burns per standard and at least 7 CRM samples to proceed (or sample list for selected matrix).

3. Main Window

Follow these steps to use the tool effectively:

1. Step 1: Fill out user information on the first window:

- Username: Enter your name.
- Bench No.: Enter the bench number (e.g., 121).
- Last Standardization Date: Use the format DD-MM-YYYY.
- Base, Matrix, Model: Select from dropdowns.
- Checklist: Ensure all steps are ticked before proceeding.

2. Step 2: Click 'Next (Data Analysis)' to move to the analysis window.

4. Second Window

The second window displays the analysis results. It includes:

- User and session details (name, bench number, model, timestamp).
- List of samples analyzed.
- Grouped Accuracy Results by element:
  * Each group shows: Sample name, Certified Value, Mean, Deviation, Accuracy Limit, % Accuracy, and Result (pass/fail).

- Grouped Precision Results by element:
  * Each group shows: Sample name, Certified Value, Mean, SD, Precision Limit, % Accuracy, and Result (pass/fail).
- Number of Samples: Shown at the bottom, auto-filled.
- Buttons:
  * Analyze: Runs the calculation and analysis.
  * Export to PDF: Generates a printable/exportable report.

5. Main Window & second window

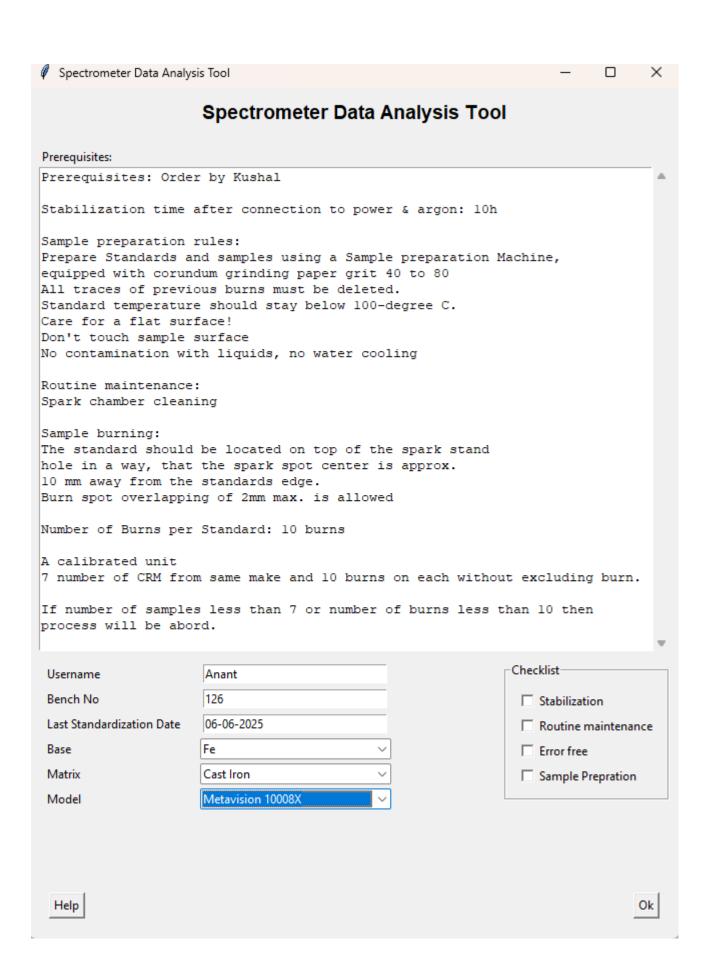Below are screenshots of the application interface:

Spectrometer Data Analysis Tool

Prerequisites:

```
Prerequisites: Order by Kushal

Stabilization time after connection to power & argon: 10h

Sample preparation rules:
Prepare Standards and samples using a Sample preparation Machine,
equipped with corundum grinding paper grit 40 to 80
All traces of previous burns must be deleted.
Standard temperature should stay below 100-degree C.
Care for a flat surface!
Don't touch sample surface
No contamination with liquids, no water cooling

Routine maintenance:
Spark chamber cleaning

Sample burning:
The standard should be located on top of the spark stand
hole in a way, that the spark spot center is approx.
10 mm away from the standards edge.
Burn spot overlapping of 2mm max. is allowed

Number of Burns per Standard: 10 burns

A calibrated unit
7 number of CRM from same make and 10 burns on each without excluding burn.

If number of samples less than 7 or number of burns less than 10 then
process will be abord.
```

		Checklist
Username	Anant	☐ Stabilization
Bench No	126	☐ Routine maintenance
Last Standardization Date	06-06-2025	☐ Error free
Base	Fe	☐ Sample Prepration
Matrix	Cast Iron	
Model	Metavision 10008X	

Help   Ok

Figure 1: Main Window (User Information and Checklist)

Data Analysis Page

Spectrometer Quality Test

```
Username              : Anant
Bench No.             : 126
Model                 : Metavision 10008X
Last Standardization Date : 06-06-2025
Timestamp             : 20-06-2025 11:42:13

Samples from base: 'Fe' and matrix: 'Cast Iron':
 - 667_13_Fe_BAS
 - 672_1_Fe_BAS
 - 673_1_Fe_BAS
 - 675_Fe_BAS
 - 670_22_Fe_BAS
 - 666_12_Fe_BAS
 - 668_13_Fe_BAS

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##### ACCURACY (A) RESULTS (Grouped by Element) #####

================================================================

--- Element: Al  ---
    Sample Name Cert. Val.    Mean      DEV  A_Limit     %A A_Result
  11XC1_R_Fe_MBH      0.02    0.02      0.0    0.008   0.00      pass
  11XC4_S_Fe_MBH     0.006   0.0065  0.0005    0.005  10.00      pass
  11XC5_Y_Fe_MBH      0.06    0.058   0.002    0.033   6.06      pass
  11XC9_D_Fe_MBH     0.051    0.053   0.002    0.033   6.06      pass
 11XC10_D_Fe_MBH     0.025    0.024   0.001    0.008  12.50      pass
     672#1_Fe_BAS      0.01   0.0099  0.0001    0.005   2.00      pass
     673#1_Fe_BAS     0.029    0.029     0.0    0.008   0.00      pass

================================================================

--- Element: As  ---
    Sample Name Cert. Val.    Mean      DEV  A_Limit     %A A_Result
  11XC1_R_Fe_MBH     0.014    0.014     0.0    0.003   0.00      pass
  11XC4_S_Fe_MBH     0.023    0.025   0.002    0.003  66.67      pass
  11XC5_Y_Fe_MBH      0.02     0.02     0.0    0.003   0.00      pass
  11XC9_D_Fe_MBH     0.068    0.067   0.001    0.010  10.00      pass
```

Number of Samples: 7

import report

Export to PDF

Figure 2: Data Analysis Window (Accuracy Results Displayed)

6. Troubleshooting

- If the 'Analyze' button doesn't respond, check that all user inputs and checklist items are filled.
- Ensure the sample list Excel file is in the correct format and path.