XRF Analyzer — User Guide

Fundamental Parameters Quantification of Amptek MCA Spectra

Version 39 · GeologyNet

---

1. Introduction

XRF Analyzer is a browser-based application for quantitative analysis of energy-dispersive X-ray fluorescence (EDXRF) spectra. It reads spectrum files produced by Amptek MCA hardware (DP5 / X-123 series and compatible instruments) and converts raw channel counts into elemental concentrations using the Fundamental Parameters (FP)

method — no calibration standards required.

The application runs entirely in your web browser. No data is uploaded to any server; all parsing, peak fitting, and quantification happen locally on your computer.

Key capabilities

- Direct import of Amptek `.mca` files, including embedded calibration and live-time metadata
- Automatic energy calibration from spectrum peaks when no calibration block is present
- Fundamental Parameters quantification with three iteration methods (De Jongh, Direct FP, Compton Normalization)
- K-line and L-line analysis with automatic line selection based on tube

voltage

- Spectral overlap detection, Kα/Kβ deconvolution, and automatic Lα→Lβ line switching
- Sample library presets for common applications (gold alloys, stainless steel, coins, whole-rock geochemistry, and more)
- Whole rock geochemistry mode with oxide conversion, LOI, and trace element reporting in ppm
- CSV export of results and a formatted print report with spectrum plot

---

2. Getting Started

2.1 Opening the application

Open the HTML file in any modern browser (Chrome, Edge, Firefox, or Safari). No installation is required.

On startup, the application loads a built-in **demo spectrum** (a brass alloy) so you can explore the workflow immediately. Click **Run FP Analysis** to process it, or load your own file to replace it.

2.2 The basic workflow

1. **Load** an Amptek `.mca` spectrum file (drag-and-drop or Browse)
2. **Verify** the energy calibration and instrument parameters
3. **Select** the elements to analyse (manually or via a Sample Library preset)
4. **Choose** the matrix type and iteration method
5. **Run FP Analysis** and review the quantitative results
6. **Export** to CSV or print a report

---

3. Loading Spectrum Files

3.1 Supported formats

Drag a file onto the drop zone, or click **Browse File**. Accepted extensions:

Extension	Description
`.mca`	Amptek MCA format (preferred)
`.txt`, `.csv`	Plain text — one count value per line, or whitespace/comma-separated counts
`.mps`, `.xrf`	Other text-based spectrum exports

Any file containing an Amptek `<<DATA>>` block is parsed as MCA regardless of extension. Files without a `<<DATA>>` block are parsed generically: the

application collects all numeric values as channel counts.

3.2 What is read from an Amptek MCA file

The parser recognises the standard Amptek sections and metadata keys:

- `<<DATA>>` … `<<END>>` — the channel counts (one integer per line)
- `<<CALIBRATION>>` — two-point (or multi-point) channel/energy calibration. The first and last points are used to derive a linear calibration (eV/channel slope and intercept), which is applied automatically.
- `LIVE_TIME` — copied into the Live Time field automatically
- `REAL_TIME` — used together with live time to compute and display **dead time %**

- `GAIN` and other key–value metadata — shown in the file information panel

Amptek files are read with Latin-1 encoding, so DPP status fields containing special characters (e.g. °C) are handled correctly.

3.3 Spectrum summary panel

After loading, the spectrum panel shows: number of channels, total counts, the energy and height of the tallest peak, and dead time. The spectrum is plotted with the top identified peaks labelled, and a **Peak Identification** table lists each detected peak with its channel, energy (keV), counts, FWHM, and the most likely element/line assignment.

---

4. Energy Calibration

Accurate energy calibration is the single most important input for correct element identification. The application sets it in one of three ways, indicated by the message below the calibration fields:

✔ **Cal from file** — the `.mca` file contained a `<<CALIBRATION>>` block. The slope (eV/channel) and intercept (eV at channel 0) are computed from the calibration points and applied automatically. This is the most reliable option.

⚡ **Auto-calibrated** — the file had no calibration block, so the application attempted calibration from the spectrum itself. It finds the statistically significant peaks (signal-to-noise ratio > 2 above local background), then tests peak-pair assignments against a database of known fluorescence lines (Ca Kα through Ag Kβ, including common tube scatter lines such as Rh Kα and W Lα). The

assignment that matches the most peaks within 60 eV wins. The status line reports how many peaks matched and the average residual. **Always verify auto-calibration before running analysis** — check that labelled peaks in the plot make sense for your sample.

⚠ **No calibration** — neither of the above succeeded. Enter the slope and intercept manually from your detector's calibration (e.g. from the Amptek DPPMCA software), then reload or proceed.

You can override the calibration at any time by editing the **Calibration Slope (eV/channel)** and **Calibration Intercept (eV at ch 0)** fields. The spectrum plot and peak identifications update on the next analysis.

---

5. Instrument Parameters

Set these to match the conditions under which the spectrum was acquired:

Parameter	Default	Notes
Tube Voltage (kV)	40	Determines which lines can be excited. Elements are only fitted if their Kα (or L3 edge, for L-line analysis) lies below ~90% of the tube voltage.
Tube Current (μA)	100	Acquisition tube current.
Tube Anode Material	Rh	Rh, Ag, Mo, W, Cu, Au, or Pd. Affects the modelled tube spectrum

Parameter	Default	Notes
		(bremsstrahlung + characteristic lines) used in FP sensitivity calculations.
Filter Material	None	Primary beam filter: Al 250 µm, Ti 50 µm, Cu 100 µm, or Pd 50 µm.
Live Time (s)	60	Auto-filled from the MCA file when present.
Detector FWHM at 5.9 keV (eV)	145	Detector energy resolution (Mn Kα reference). Affects peak integration windows and

Parameter	Default	Notes
		overlap detection.
Geometry / Incident Angle (°)	45	Angle of the primary beam to the sample surface.
Take-off Angle (°)	45	Angle of the detected fluorescence to the sample surface.

The incident and take-off angles enter the FP absorption path-length calculations, so set them to your actual instrument geometry if it differs from 45°/45°.

---

6. Selecting Elements

6.1 The element grid

The element grid lists all supported elements from Na (Z = 11) to Bi (Z = 83), covering the common rock-forming elements, transition metals, precious metals, and heavy elements (Pb, Hg, Bi, W, Ta, Hf, Ba, rare earths La/Ce, and more). Click an element to toggle it in or out of the analysis.

Select only the elements you genuinely expect in the sample. Including many implausible elements increases the chance of false positives from statistical noise and spectral overlaps.

6.2 Sample Library presets

The **Sample Library** dropdown provides one-click element selections (and a recommended tube voltage) for common applications:

Preset	Elements	kV
Gold Alloy (9–22ct)	Au, Ag, Cu, Zn, Ni, Pd, Fe, Sn, Pb	40
White Gold / Pd White Gold	Au, Ag, Cu, Ni, Pd, Pt, Zn	40
Silver Alloy (Sterling, Coin)	Ag, Cu, Zn, Au, Ni, Pb, Sn	30
Platinum Group Metals	Pt, Pd, Rh, Au, Ag, Cu	50
Coins / Numismatics	Au, Ag, Cu, Zn, Ni, Sn, Pb, Mn	40
Stainless Steel	Fe, Cr, Ni, Mo, Mn, Si, Ti, Cu, V	40
Brass / Bronze / Copper Alloy	Cu, Zn, Sn, Pb, Ni, Fe, Mn, As, Sb, Bi	40

Preset	Elements	kV
Solder / Brazing Alloy	Sn, Pb, Ag, Cu, Bi, Sb	40
Environmental / RoHS Screening	Pb, As, Cd, Cr, Cu, Mn, Ni, Zn, Fe, Ti, Ba, Sb	40
Whole Rock Geochemistry	Na, Mg, Al, Si, P, S, K, Ca, Ti, V, Cr, Mn, Fe, Ni, Cu, Zn, Rb, Sr, Zr, Ba, Pb	40

Choose a preset and click **Apply Preset**. You can then fine-tune the selection in the element grid.

6.3 K-lines vs L-lines

The application automatically decides which line series to use for each element. If an element's Kα cannot be efficiently excited at the current tube voltage (Kα

above ~85% of the tube kV), and the element's L3 absorption edge is excitable, the analysis switches to L-lines. In practice this means heavy elements — Au, Pt, Pb, Hg, Bi, W, Ta, Hf, Ba, La, Ce — are analysed on their Lα/Lβ lines with a typical 40 kV tube, while lighter elements use Kα.

The analysis log reports which elements ran in K-line mode and which in L-line mode for every run.

---

7. FP Analysis Settings

Matrix Type — Bulk/Infinite (default, for thick samples), Thin Film, Soil/Environmental, or Metal Alloy. Choose the one that best describes the physical sample.

Iteration Method

- **De Jongh (iterative)** — the default. Starts from an initial concentration estimate, then iteratively refines all concentrations, recalculating matrix absorption and enhancement effects each pass until convergence. Best general-purpose choice for alloys and unknown samples.
- **Direct FP** — a single-pass FP calculation without iterative matrix refinement. Faster; appropriate for screening or when matrix effects are minor.
- **Compton Normalization** — normalises to the Compton scatter peak of the tube anode line. Useful for light matrices (soils, powders) where scatter-based matrix correction outperforms pure FP.

Convergence Tolerance (%) — the iteration stops when the largest

concentration change between passes falls below this value (default 0.1%).

Max Iterations — safety limit (default 50). If the analysis reaches this limit without converging, treat the results with caution and check for mis-selected elements or a bad calibration.

---

8. Running the Analysis

Click ⚙ **Run FP Analysis**. The progress panel opens with a live log of every processing step:

1. **Excitability filter** — selected elements that cannot be excited at the current tube voltage are excluded.
2. **Overlap and noise suppression** — if two selected elements have peaks within one detector FWHM of each other, the statistically weaker one cannot be reliably quantified; it is

dropped and a warning is logged. L-line peaks use a wider (2× FWHM) exclusion window because of their broader tails. Elements whose net counts are indistinguishable from background noise are also suppressed.

3. **Automatic line switching** — if a heavy element's Lα line is contaminated by another element's Kα (e.g. Au Lα vs Zn Kα region), the analysis automatically switches that element to its Lβ1 line and logs the change.
4. **Kβ/Lβ deconvolution** — overlapping β lines from other selected elements are stripped from each peak's integration window.
5. **Net count extraction** — background-subtracted net peak areas for every element.

6. **FP sensitivities** — computed from the modelled tube spectrum (anode material, kV, filter), detector efficiency, fluorescence yields, and geometry.
7. **Iteration** — concentrations are refined until the convergence tolerance is met; the log reports the number of iterations and the final Δ.

Read the log after every run — it tells you exactly which elements were analysed, on which lines, what was suppressed and why, and whether the solution converged.

---

9. Interpreting the Results

9.1 Quantitative results table

Column	Meaning
Element / Z	Element symbol and atomic number

Column	Meaning
Line	The analytical line used (Kα, Lα1, Lβ1, …)
Net Counts	Background-subtracted peak area
Conc. (wt%)	Concentration in weight percent
Conc. (mg/kg)	The same concentration expressed in mg/kg (ppm)
Uncertainty (2σ)	Counting-statistics uncertainty at the 2-sigma (≈95%) confidence level

Column	Meaning
Detection	**Detected** if the concentration exceeds 3× the limit of detection; otherwise the value should be treated as a trace estimate near the noise floor

Below the table:

- **Σ wt%** — the sum of all reported concentrations. For a bulk metal sample this should approach 100%. A sum far below 100% usually means a major element is missing from the selection (or the sample contains light elements below Na that XRF cannot see, e.g. oxygen in oxide minerals). A sum far above 100% suggests a calibration or geometry problem.

- **Chi² / DoF** — goodness-of-fit statistic. Values near 1 indicate the model describes the spectrum well.

9.2 Analytical limitations to keep in mind

- Elements lighter than Na (Z < 11) are invisible to conventional EDXRF; oxygen, carbon, and hydrogen are never directly measured.
- Results are standardless FP estimates. For the highest accuracy (e.g. gold fineness certification), validate against a reference standard of similar composition.
- Very low concentrations near the detection limit carry large relative uncertainties — check the 2σ column and the Detection flag before quoting trace values.

---

10. Whole Rock Geochemistry Mode

When the element selection includes rock-forming elements (use the **Whole Rock Geochemistry** preset), a second results card converts elemental concentrations into standard oxide chemistry:

- The **ten standard major oxides** (SiO_2, TiO_2, Al_2O_3, Fe-oxide, MnO, MgO, CaO, Na_2O, K_2O, P_2O_5) are always listed, even when not analysed, so the report matches conventional whole-rock layouts.
- **Iron reporting** — choose **Fe_2O_3 (total)** or **FeO (total)** from the dropdown.
- **LOI (wt%)** — enter loss on ignition manually if measured; it is included in the analytical total.

- **Normalise to 100%** — optionally rescales the oxides so that oxides + LOI = 100%.
- **Trace elements** — any analysed element not reported as a major oxide (and minor oxides below 0.01 wt%) appears in a separate trace table in **ppm** with 2σ uncertainties and a Detected/Trace flag.

The card shows **Σ oxides** and **Total (oxides + LOI)**. For a good analysis of a silicate rock, the total should fall near 100% (98.5–101% is the conventional acceptance window in laboratory practice).

---

11. Exporting and Reporting

↓ Export Results (CSV) — saves the quantitative results table (element, Z, line, net counts, wt%, mg/kg, uncertainty,

detection status) as a CSV file for spreadsheets or LIMS import.

↓ **Export Whole Rock (CSV)** — saves the oxide table, LOI, sums, and the trace element table (ppm) as `xrf_whole_rock_chemistry.csv`.

🖨 **Print Report** — generates a formatted, print-ready report containing the analysis date, file name, a summary of instrument parameters, the spectrum plot (rendered as a clean print image), and the results tables. Use your browser's print dialog to print to paper or save as PDF.

---

12. Tips and Troubleshooting

"Could not parse file" — the file contained fewer than 10 readable count values. Confirm it is a text-format Amptek export

(not a binary format) and that it contains a `<<DATA>>` block or plain numeric counts.

Peaks are labelled with the wrong elements — the energy calibration is off. Prefer files with an embedded `<<CALIBRATION>>` block; otherwise enter the slope/intercept from your acquisition software manually. Even a few eV/channel of slope error shifts high-energy peaks by hundreds of eV.

An expected element is missing from the results — check the log. It was most likely (a) not excitable at the current tube voltage, (b) suppressed due to overlap with a stronger neighbouring peak, or (c) statistically indistinguishable from background. Raising the tube voltage, increasing acquisition time, or removing an interfering element from the selection may recover it.

Σ wt% is well below 100% on a metal — a major alloying element is probably missing from the selection. Look at the Peak Identification table for unassigned strong peaks.

Analysis doesn't converge — reduce the element list to plausible components, verify the calibration, and check that the matrix type matches the sample.

High dead time (> ~30%) — the spectrum was acquired at too high a count rate; peak shapes and ratios may be distorted. Re-acquire at lower tube current if possible.

Gold and heavy elements at 40 kV — these are quantified on L-lines. Watch the log for Lα→Lβ line switches when Cu/Zn/Ni are also present, as their Kα lines sit in the Au/Pt/Pb L-line region.

13. Privacy and Data

All processing is performed locally in the browser. Spectrum files are never transmitted anywhere, making the tool suitable for confidential assay work.

XRF Analyzer is developed by GeologyNet (geologynet.com). This guide corresponds to application version 39.