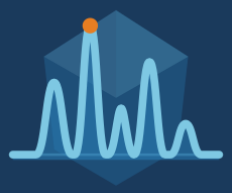

RamanNet

Raman Mineral Analysis

User Guide

Search-match identification of minerals from a 532 nm Raman spectrum, against the GeologyNet reference library of 2,464 spectra.

Version 1.0 · Windows, Android, iOS and macOS

Minserv Mineral Services · www.geologynet.com

Contents

This guide assumes you already work with Raman spectra. It covers how RamanNet processes a spectrum, how it ranks candidates, and — the part that matters most — how to judge whether a match is real.

1 · Quick start

From a cold start to a ranked identification takes about fifteen seconds.

1. Open the **Analyse Spectrum** page (the flyout menu, top left).
2. Tap **Open spectrum…** and choose your file. Any two-column text export works. If you have nothing to hand, tap **Demo** for a synthetic unknown.
3. The spectrum is baseline-corrected, normalised and its bands are picked automatically. Check the plot: the ticks above the curve are the bands that will be searched on.
4. Tap **Search-match**. The whole library is scored in under a second.
5. Tap a candidate. It is drawn mirrored below your spectrum so you can compare band for band — green ticks are bands the candidate accounts for.

> **Before you trust the top hit**
>
> Look at the overlay, not just the number. A high score with three matched bands in a crowded region is weaker evidence than a slightly lower score with eight bands spread across the range. Section 5 covers this.

What the four pages do

Page	Use it for
Analyse Spectrum	The main workflow. Import a measured spectrum, process it, search the library, compare candidates against it.
Peak Search	Identification when you have band positions but no file — a printed peak table, or numbers read off the instrument display.
Reference Library	Browse or text-search all 2,464 reference spectra by name, formula, locality or RRUFF ID.
About	Version, library size, and a summary of the scoring method.

2 · Getting your spectrum in

There is no single interchange format for Raman data, but nearly every vendor's ASCII export is the same thing underneath: two columns, wavenumber then intensity, with some header lines on top. RamanNet reads that directly — it does not ask you what instrument you have.

What the importer accepts

Aspect	Handling
Columns	Raman shift (cm^{-1}) first, intensity second. Extra columns are ignored.
Separators	Comma, tab, semicolon or space — detected per file.
Header lines	Any line that is not two numbers is skipped, as are lines starting with #, %, * or an apostrophe.
Direction	Files written high-to-low wavenumber are reversed automatically.
Extensions	.txt .csv .dat .asc .tsv .prn
Tested against	Renishaw, Horiba, Bruker, Thermo and RRUFF ASCII exports.

What it will not read

- Proprietary binary formats — Renishaw .wdf, Horiba .ngs, Thermo .spa. Export to text from the vendor software first.
- Spectral image or map files. Extract the single spectrum you want to identify.
- Files with fewer than eight data rows — the importer reports this rather than guessing.

> **Wavenumber, not wavelength**
>
> The first column must be Raman *shift* in cm^{-1}, not absolute wavelength in nm. Some instruments export wavelength by default. A spectrum in nm will import without complaint and then match nothing, because the whole library sits at 100–1400 cm^{-1} and your data will not.

3 · The Analyse page

Processing on import

Raman spectra sit on a broad fluorescence background that varies from sample to sample and can swamp the bands entirely. Three things happen the moment a file loads.

- **Baseline removal.** The background is smooth and always positive, so it is estimated by rolling minima and subtracted. Tick **Show fitted baseline** to see what was removed — worth doing once on any unfamiliar instrument.
- **Smoothing and normalisation.** A short moving average removes single-channel noise without visibly broadening a band, then the curve is scaled to 0–1000 so it is directly comparable with the library.
- **Band picking.** Bands are local maxima that stand a required height above their own surroundings. Judging a peak against its local neighbourhood rather than an absolute threshold is what stops noise spikes and shoulders being counted.

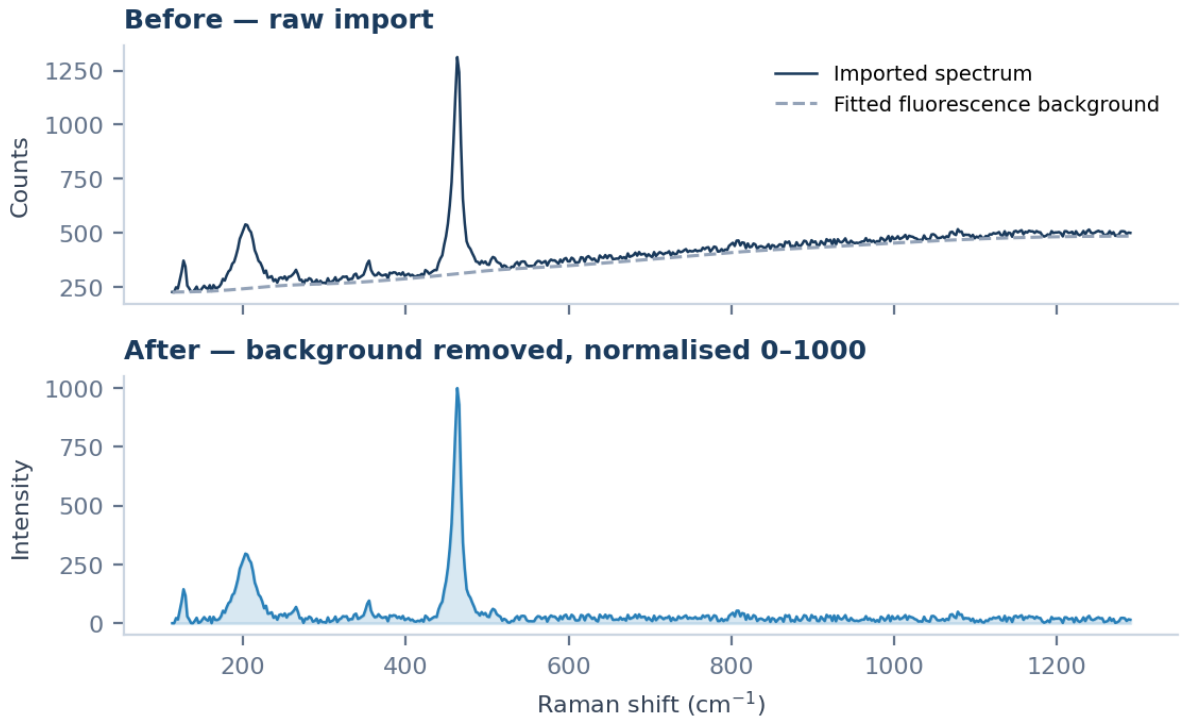

Figure 1 — A spectrum as imported, with the fitted fluorescence background (dashed), and the same spectrum after correction and normalisation. The weak bands below 400 cm^{-1} only become pickable after the background goes.

Band picking and the sensitivity control

Sensitivity sets how far a maximum must rise above its surroundings to count as a band. Low values keep only the unmistakable ones; high values reach into the noise.

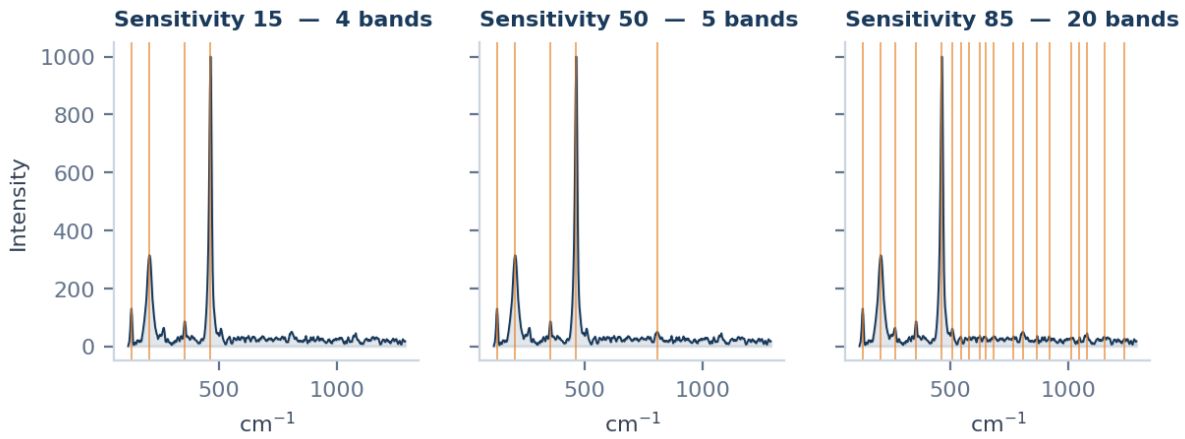

Figure 2 — The same spectrum picked at three sensitivities. At 15 the two weak low-wavenumber bands are missed; at 85 most of what is marked is noise. The default of 50 is where identification is most reliable.

> **More bands is not better**
>
> It is tempting to raise sensitivity so the search has more to work with. On a noisy spectrum it does the opposite: in testing, self-identification fell from 6 of 6 correct at sensitivity 50 to 3 of 6 at sensitivity 80, because the extra 'bands' were noise that matched nothing consistently.

4 · Controls reference

Control	Range	Default	What it does, and when to change it
Sensitivity	0–100	50	Band-picking threshold. Raise it only on a clean, high-signal spectrum where you can see weak bands the app has missed. Lower it on a noisy one.
Tolerance	±2–±25 cm^{-1}	±8	How far a reference band may sit from yours and still count as the same band. ±5–±8 suits a calibrated bench instrument; widen to ±12–±15 for a hand-held unit or an uncalibrated one.
Peak weight	0–100 %	60 %	Share of the score from band positions rather than overall curve shape. Raise it when your spectrum is noisy but the band positions are sound. Lower it when the band list is short but the profile is clean.
Remove baseline	on / off	on	Turn off only if your instrument software has already baseline-corrected the export. Correcting twice flattens real broad features.
Show fitted baseline	on / off	off	Draws the estimated background over the curve. Diagnostic — use it if a spectrum is picking oddly.

How the two score terms differ

The peak weight slider blends two independent lines of evidence. It helps to know what each one is good and bad at.

	Peak term (band positions)	Profile term (curve shape)
Measures	Whether the bands line up, weighted by intensity and by how close the match is.	Correlation of the two full curves over their overlapping range.
Strength	Explainable — you can point at which bands matched and by how much. Survives a noisy baseline.	Brings in relative band heights and overall shape, which a peak list throws away.
Weakness	A short band list in a crowded region matches too many minerals.	A strong fluorescence residue or a truncated range can wreck it.

The peak term is itself scored in both directions: how much of *your* band list the reference explains, and how many of the reference's strong bands *you* also show. Without that second direction, a mineral with a dense forest of bands would match almost anything by sheer coverage.

5 · Reading the result

Scores run 0 to 100. They are a ranking aid, not a probability — a score of 85 does not mean an 85 % chance of being right.

Score	Reading	What to do
80–100	**Confident match**	Accept if the overlay agrees band for band and the chemistry is plausible for the sample.
60–80	**Candidate**	Worth pursuing, not reporting. Check the next few candidates — if they are all the same mineral group, that group is your answer even if the exact species is not.
Below 60	**Family-level hint**	Treat as a direction to look in. Re-measure with longer integration, or check the spectrum for the problems in section 10.

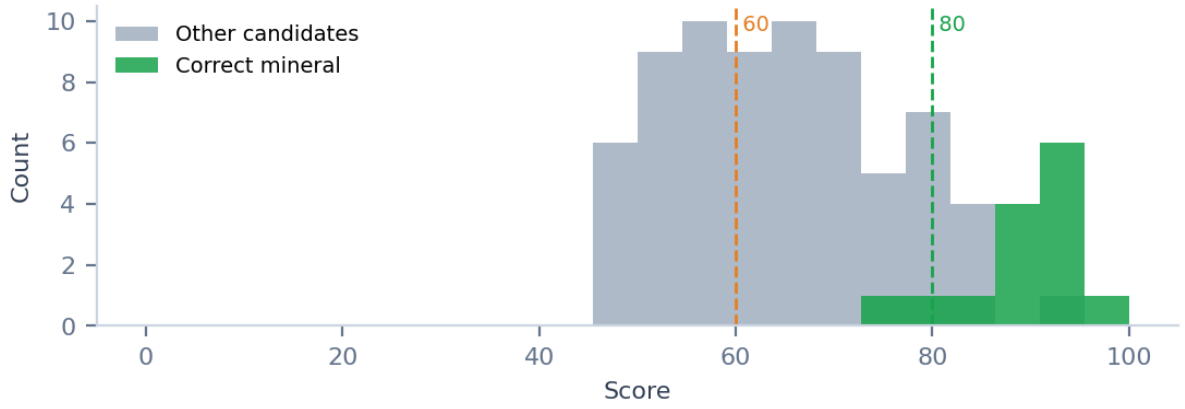

Figure 3 — Scores from 14 test identifications, each returning six candidates. The correct mineral (green) scored 74 or above every time, median 91.5. Wrong candidates (grey) had a median of 64, and 6 of 70 still passed 80 — which is precisely why the score alone is not enough.

Reading the overlay

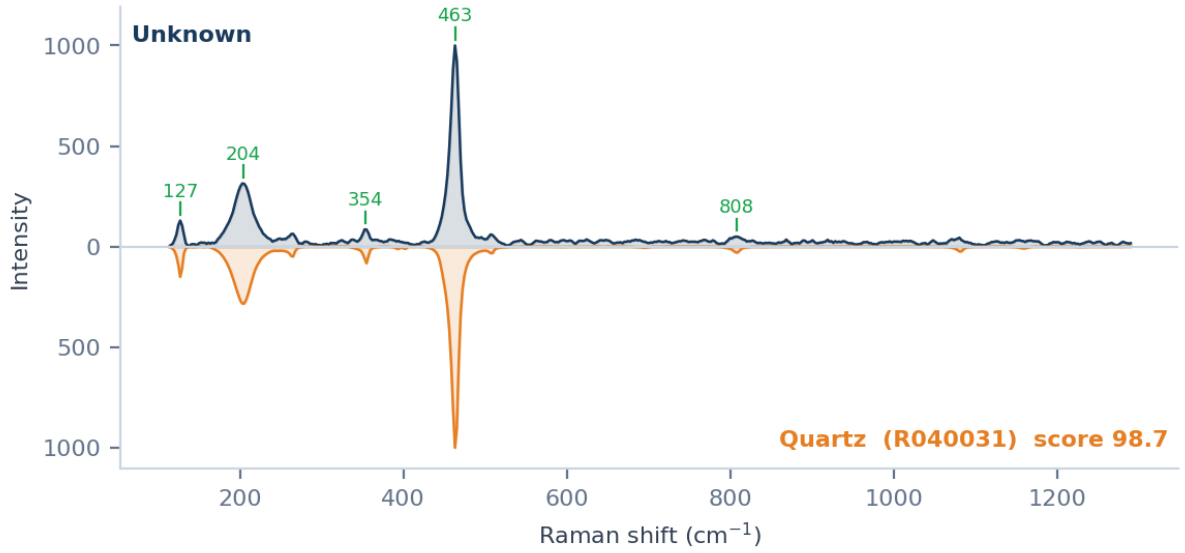

Figure 4 — The comparison plot. Your spectrum runs upward from the axis, the selected candidate downward. Green ticks mark bands the candidate accounts for within tolerance; grey ticks are bands it does not explain.

The mirrored layout is used rather than two overlaid curves because band-for-band agreement becomes a vertical line you can see at a glance. What to look for:

- **Grey ticks on strong bands.** A candidate that cannot explain one of your strongest bands is usually wrong, whatever it scored.
- **Reference bands with nothing above them.** Weak ones routinely vanish under noise and are forgivable. A strong one missing is not.
- **Spread.** Matches spread across the range are far stronger evidence than several in one crowded region.
- **Several samples of the same mineral in the top hits.** This is a good sign — the library holds multiple RRUFF samples per species, and agreement across them means the match is not an artefact of one particular specimen.

6 · Working the band list

The **Picked bands** panel lists every band found, strongest first. Tap any row to exclude it from the search; tap again to put it back. The count above the list shows how many are in use.

Bands worth excluding

- Substrate or mount bands — a glass slide contributes a broad feature near 1100 cm^{-1}, and epoxy or resin mounts contribute several.
- A cosmic ray spike: a single very narrow, very tall band that was not there on a repeat scan.
- Bands from a second phase in the field of view, once you have identified the first. Excluding the first mineral's bands and re-searching is the practical way to work through a mixture.

> **Exclude, do not re-measure**
>
> Excluded bands stay on the list greyed out rather than being deleted, so you can put one back if excluding it changes the answer. If it does change the answer, that is itself worth knowing — an identification resting on one band you were unsure about is not a safe identification.

Mixtures

RamanNet ranks single reference spectra; it does not fit combinations. For a two-phase sample the usual approach is: identify the dominant phase, exclude its bands, re-run the search on what is left. If the residual bands then give a sensible second mineral, you have a mixture. If they give nothing above 60, you probably have one mineral and some noise.

7 · Peak Search

For when you have band positions but no file. Type them in any of these forms:

Input	Meaning
464, 207, 1085	Three bands, all weighted equally.
464/100, 207/45, 1085/12	Bands with relative intensities, 1–100. Use this when you know the ranking — it materially improves the ordering.
One per line	Same thing; line breaks, commas, semicolons and spaces are all accepted as separators.

Scoring here uses band positions only — there is no curve to correlate. Expect lower scores and a longer shortlist than a full spectrum search, particularly with fewer than four bands. The optional name filter narrows the search to minerals whose name contains a string, which is useful when you already suspect a group: typing **calcite** or **feldspar** restricts the ranking to those.

8 · Reference Library

The full 532 nm collection, searchable by mineral name, chemical formula, locality or RRUFF sample ID. The list renders the first 500 matches — refine the search rather than scrolling. Opening an entry shows its curve full-frame with a table of every band detected in it, which is the quickest way to check what a mineral *should* look like before deciding whether your unknown resembles it.

Several entries share a mineral name: these are different RRUFF samples of the same species, from different localities. Comparing them shows how much a species' spectrum varies with composition and orientation — which is useful calibration for how closely you should expect your own spectrum to match.

9 · Reports and export

Print report

Every page has one. The report opens in your system browser, where Print or Save as PDF is one keystroke away. On Android use Print from the browser menu; on iOS and macOS the share sheet includes AirPrint and Save to Files.

Report	Contains
Analysis	The conclusion and its confidence, the comparison plot, the acquisition and processing settings, the observed band table with each band's nearest reference band and error, and the ranked candidate list.
Peak search	The bands you entered, the best match, and the ranking.
Reference	A single library spectrum with its full band table.

> **The analysis report follows your selection**
>
> It reports against the candidate you have *selected*, not automatically the top hit. If you have looked at the overlays and settled on the second-ranked mineral, select it before printing and that judgement is what reaches the page.

The processing settings are printed deliberately. Someone reading the report who was not at the instrument should be able to judge the identification rather than take it on trust — a match at ±20 cm^{-1} tolerance and sensitivity 90 means something different from one at the defaults, and the page should say so.

CSV export

Export CSV on the Analyse page writes out the wavenumber axis, the raw intensity as imported, the fitted baseline and the corrected curve, followed by the picked band list. Use it to take the processed spectrum into a plotting package, or to check the baseline fit against your own.

10 · Troubleshooting

Symptom	Likely cause	What to change
“No two-column spectral data found”	Binary vendor format, a single-column file, or a decimal comma in a comma-separated file.	Export as ASCII from the vendor software. If your locale writes 3,142 for 3.142, export with a point decimal or tab separators.
No candidates returned	Spectrum in nm rather than cm^{-1}, or a range too narrow to overlap the library.	Check the axis units. A candidate must share at least a quarter of your collected range to be scored at all.
Everything scores 40–60, nothing stands out	Fluorescence not fully removed, or too few real bands.	Tick Show fitted baseline and look at the fit. Re-measure with longer integration or photobleach the sample.
Top hits are all implausible minerals	Noise being picked as bands.	Lower sensitivity to 30–40 and re-run. Exclude any band you cannot see by eye in the plot.
Right mineral present but ranked fifth	Tolerance too tight for the instrument's calibration.	Widen tolerance to ±12–±15. If that fixes it, your wavenumber calibration is drifting — worth checking against a silicon standard.
Strong band in your spectrum matches nothing	Substrate, mount, or a second phase.	Exclude it and re-run. If the answer changes completely, treat both results as provisional.
Scores dropped after raising sensitivity	Working as intended — noise bands dilute the score.	Return sensitivity to 50.

Appendix A · About the reference data

The GeologyNet 532 nm Raman library holds 2,464 spectra derived from the RRUFF Project reference collection. Each record carries the mineral name, RRUFF sample ID, locality, chemical formula, and the measured spectrum resampled to 512 points and normalised 0–1000.

What the app derives from it

The source data publishes only the three strongest bands per spectrum, which is not enough to identify anything. RamanNet therefore extracts a full band list from each stored curve when the library loads — up to 40 bands per spectrum, down to 2 % of full scale. Checked against the published strongest band across 400 spectra, the derived list agreed in 397 cases (99.2 %).

Limits worth knowing

- **532 nm only.** Band positions are excitation-independent, so a spectrum collected at 785 nm can still be matched on position — but relative intensities differ, so lower the peak weight and treat the profile score with suspicion.
- **Coverage.** The library is broad but not exhaustive. A mineral that is absent cannot be found, and the search will confidently offer you its nearest structural relative instead.
- **Orientation.** Relative band intensities in a single-crystal spectrum depend on orientation. Positions do not. This is the main reason the default weighting leans on positions.
- **Single phases.** Scoring compares your spectrum against one reference at a time. Mixtures are handled by the manual approach in section 6.

> **A search-match result is a suggestion, not a determination**
>
> Confirm any identification against the sample's optical properties, chemistry and geological context before relying on it. The tool ranks candidates; the identification remains yours.

RamanNet is the Raman counterpart to XrdcalcNet and shares its approach: load an unknown pattern, pick its features, rank the reference library against it.