# SSHADE Users Newsletter – January 2025

## New tool: the Comparator

Dear SSHADE user,

The SSHADE team sends you its warmest wishes for the new year!

As we start this new chapter, we are thrilled to introduce two new tools to the SSHADE platform: **the user's spectrum import tool** and **the Comparator**.

### 〰 The user's spectrum import tool: import and manage your own spectra in your private space before comparing them with SSHADE spectra or band lists
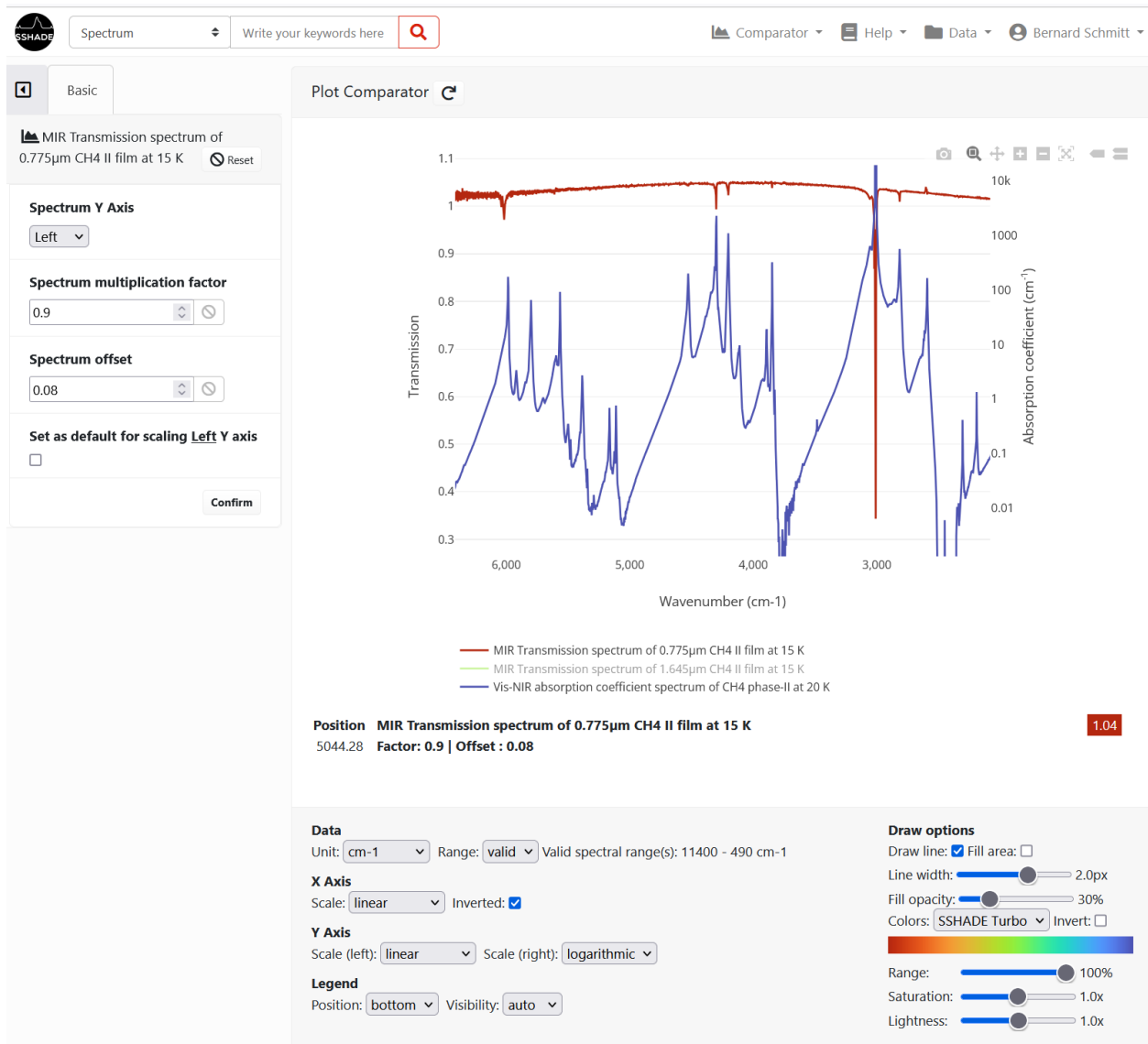
- First, go to the top right menu with your name, go to your "Dashboard" and select "Spectrum import"
- Upload your spectrum file (ascii/text only) in your private space and provide some information (spectrum type, number of header lines, wavelength, etc.)
- After adding the spectrum, you will see it in the table "My Spectra" where you can plot it and add it to the comparator

After comparison you can keep it (protected in your private space) or delete it.
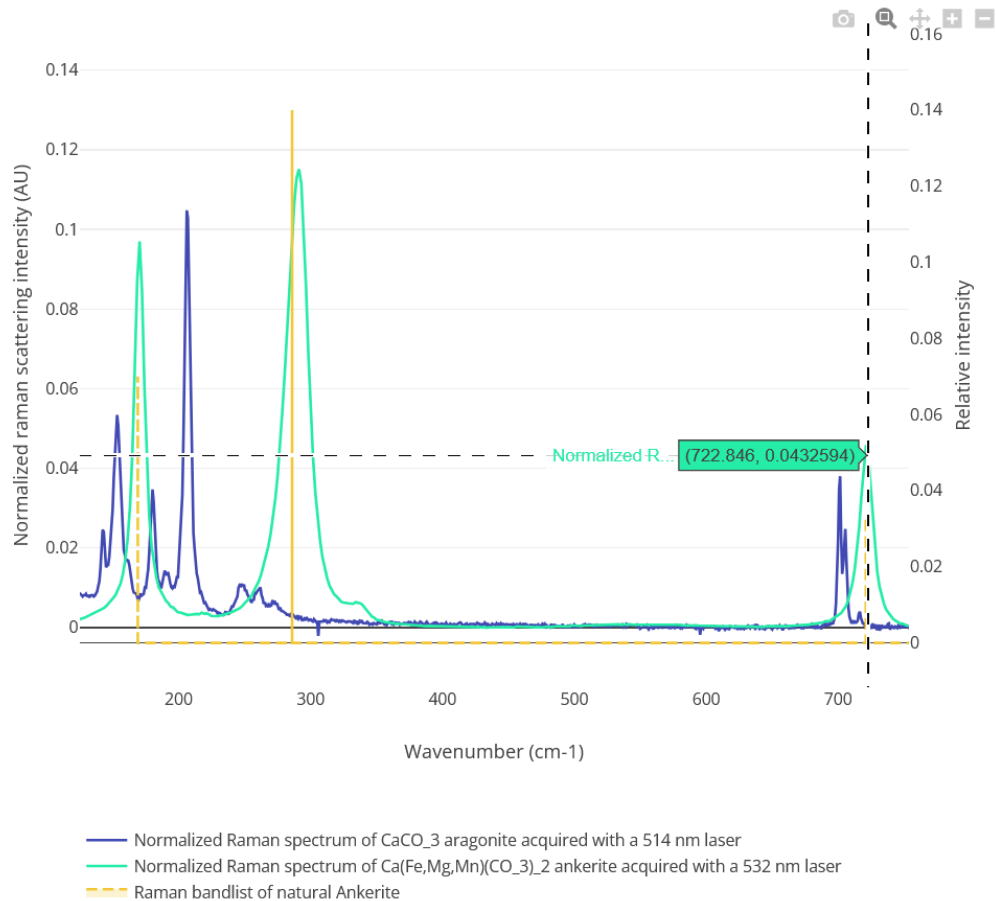
### 📈 What can the Comparator do for you?

- **Compare spectra across datasets**: dynamically plot spectra from different experiments, various solids, instruments or experimental conditions across the 30 databases hosted by SSHADE
  - Search for a spectrum, and click the " **+** " button to add it
  - Access the Comparator using "Comparator" → "Plot comparator" in the top menu
  - You will also find the " **+** " button at the top of each SSHADE spectrum page as well as in the list of your own spectra

- **Manage spectra:**
  - Add another spectrum with the " **+** " button
  - Remove a spectrum in the top menu of the Comparator. The plot should be automatically updated
  - You can also hide a spectrum in the plot by clicking on its legend

- **Perform basic operations on spectra**:
  - First, select a trace by clicking directly on a spectrum
  - Dynamically adjust its multiplication factor and offset in the left panel
  - Assign it to the Left or Right axis (need to "confirm") as needed
  - You can also set it as the "default spectrum" (+ "confirm") for scaling the axis when other spectra are assigned to the axis

o   Use the "Reset" button to return to the default settings



- **Overlay band lists of pure solids**: search carefully reviewed absorption and Raman band lists of more than 65 solids and add them to the Comparator just like spectra

- **Customize and export your plot**:
  o   Change spectral unit, range and scale (linear/log) of axes, customize line styles…
  o   Download your plot as PNG using the camera icon in the upper right of the plot

Plot legend:
— Normalized Raman spectrum of CaCO_3 aragonite acquired with a 514 nm laser
— Normalized Raman spectrum of Ca(Fe,Mg,Mn)(CO_3)_2 ankerite acquired with a 532 nm laser
‑ ‑ Raman bandlist of natural Ankerite

## ☀️ Incoming updates

This is a first release! We are working to enrich the Comparator in the upcoming months and years with advanced tools for spectroscopists, including:

- Normalization between spectra
- Transmission and absorbance conversion
- Spectral convolution to specific space instrument resolutions
- Denoising and baseline removal
- Spectral parameter computation
- …

Have a feature request or bug report? Don't hesitate to let us know via "Help" → "Contact".

## 🛠️ Behind the Tools

A huge thank to **Etienne Dode**, who developed the user's spectrum import and Comparator tools, to **Bernard Schmitt** and **Lucia Mandon**, who helped design and test these tools, and to **Damien Albert**, our head engineer, for continuous interface improvement and for keeping the SSHADE platform running smoothly!

## 🚀 Get Started Today!

The Comparator tool (beta version) is live and ready to use. Log in to your account: your spectral analysis using SSHADE just got easier.

Have fun with SSHADE data!

The SSHADE Team

All previous user newsletters are stored in the dedicated **'News' page** of the SSHADE Wiki.