PHASE IDENTIFICATION PROGRAM AND DATABASE

DIFFRAC+® Version 6 (Bruker) / ICDD Release 2000

Search is normally performed on the whole profile after background suppression.
« Normal » phase identification procedure:

- Background suppression
- Choice of the database (Inorganic or Organic) (Master or Mineral or Zeolite or…)
- Choice of criterions
- Choice of requested quality for the candidate phases (*, C, I, D, ….)

RESULTS

Sample 1 - Mineral sample from a geologist

The normal procedure was applied to the data after background subtraction, and no satisfying solution was found, except Quartz.
From the positions of Quartz lines, a displacement error was estimated (0.28 mm) and data were corrected.
Then a new search was performed and following phases appears among the 20 first candidates.

- **Quartz** SiO2 **ICDD 46-1045**
- **Siderite** FeCO3 **ICDD 29-0696**
- **Hydroxyl Apatite** (or other from Apatite group) for instance **ICDD 82-1429**
- **Souzalite** (Mg,Fe)3(Al,Fe)4(PO4)4(OH)6,2H2O **ICDD 33-0863**

Some of the small unidentified peaks could correspond to **Lepidocrocite** FeOOH **ICDD 44-1415**. This phase was intuited from our experience, and from a mineral common phases table from the Brindley's Clay xxxxxx book.
Other minor peaks not identified.

See figure 1 for screen copy of the result in DIFFRAC+.

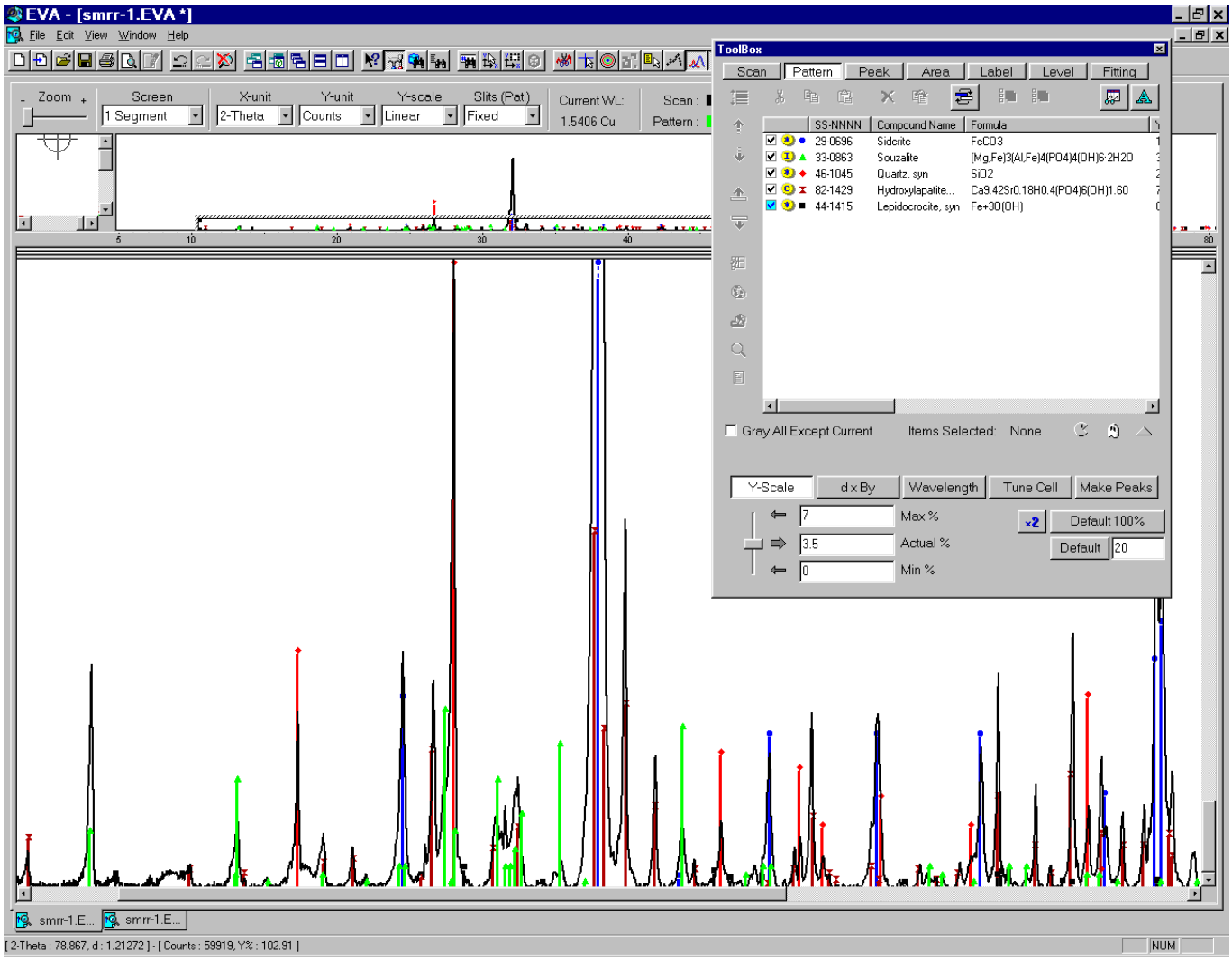

Figure 1: Mineral sample from a geologist

Sample 2 - Synthesis from a laboratory chemist

For this sample, the “normal” procedure didn’t give any result again. So we made a peak position search and performed the phase search on the d/I file, with a rather wide peak position window of 0.8°2θ.

ICDD 48-0475 reference data (Silicon Oxide Quinuclidine Octadecasil) correspond to the sample diffractogram, with a large discrepancy on the cell parameters. Experimental cell was roughly estimated to a=9.14Å and c=13.5Å whereas the ICDD reference has a=9.19Å and c=13.4Å.

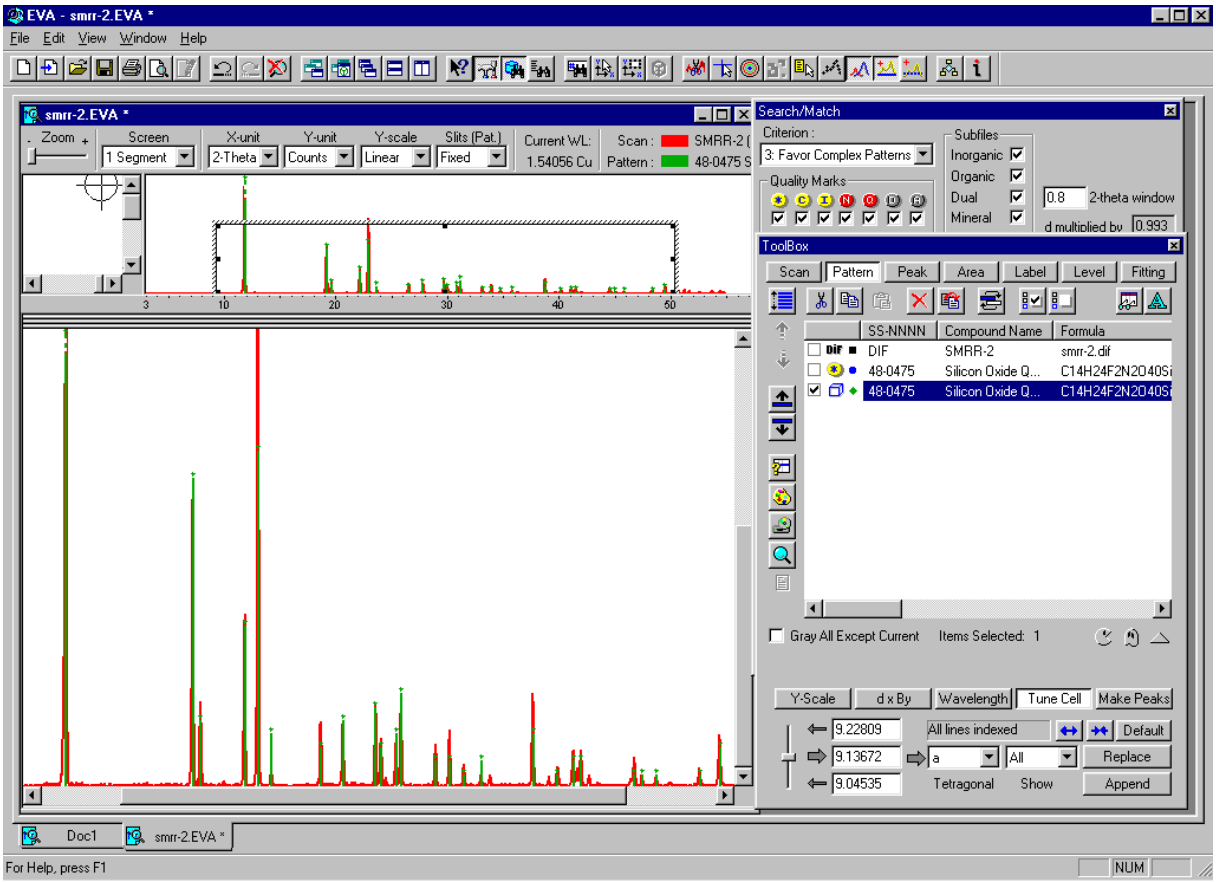

Figure 2 :Synthesis from a laboratory chemist

Sample 3 - Organic from a pharmaceutical engineer

The phase identification of this sample was difficult for us, probably because of the lack of experience in pharmaceuticals (we mainly deal with catalysts and zeolites…).
One phase matched correctly part of the data **(ICDD 19-1946, Thalidomide)**, and most of the lines remained unassigned.
A line position shift is suspected again.

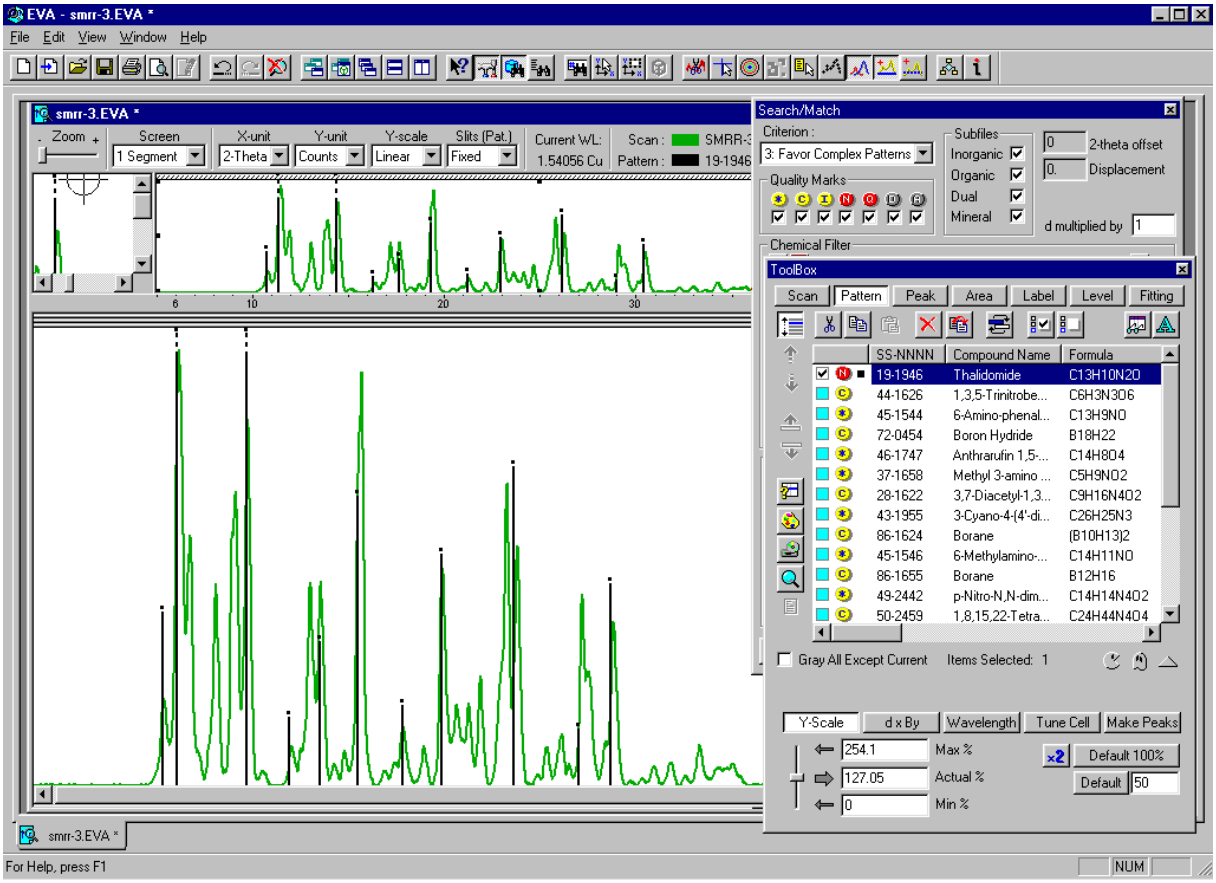

Figure 3: Organic from a pharmaceutical engineer

Sample 4 - Inorganic industrial processing plant sample

Normal procedure (background subtraction and search on the whole profile) was applied to these data. The identified phases are:

- Litharge PbO ICDD 05-0561
- Monoclinic lead oxide sulphate PbSO4,4PbO ICDD 23-0333
- Triclinic lead oxide sulphate PbSO4,3PbO,H2O ICDD 88-0552
- Massicot PbO ICDD 38-1477

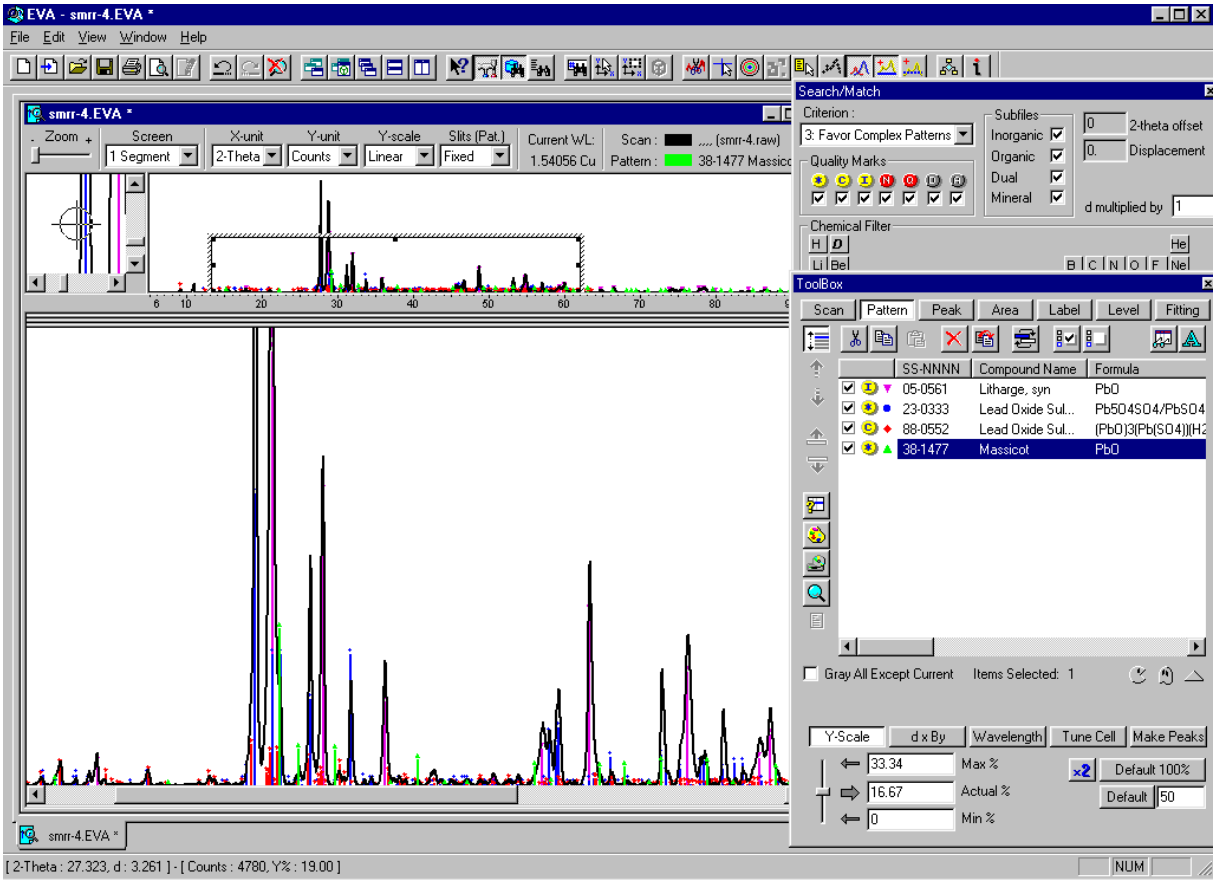

Figure 4: Inorganic industrial processing plant sample