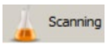
# DiscoveryMat Software User Manual

This software has been developed and optimised within HE-Arc as part of various funded research project under an academic free license 3.0. It was created to collect data (corrosion potentials of metallic materials when in contact with a solution), to interpret them in order to propose a plausible composition and to share data between several partners. The English language was chosen for better sharing.

The software has three tools displayed in the settings window on the left of the homepage (Fig. 1):

1. **Data collection** (button  ),
2. **Data processing** (button  ),
3. **Data sharing** (button  ).

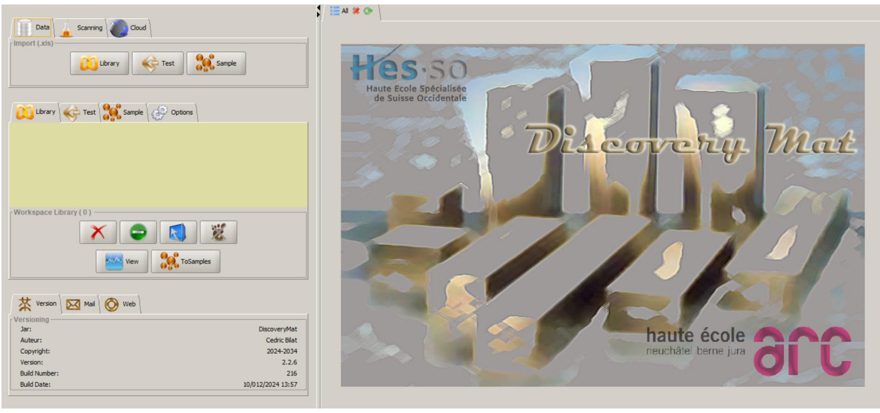
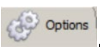
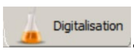



Fig. 1: "Discovery Mat" software homepage with the settings window on the left and the graphic area on the right.

The Data sharing tool has not yet been implemented. In the following, we detail the use of the first two tools that are operational.

## 1. Data collection (Scanning tool)

The file *Measurement_Protocol* (*Protocol for data collection and processing with the "Discovery Mat" software)* details the measurement of potentials and the main functions of the developed tool.

With the Scanning tool, it is possible to automatically collect data by driving an interfaced multimeter. This tool works either with the Metrix M3282 multimeter or with the Yoctopuce voltmeter (see the file *Equipment for measuring potentials*). The choice of a measurement tool is made by clicking on , then on . The measurement system options appear (Fig. 2).

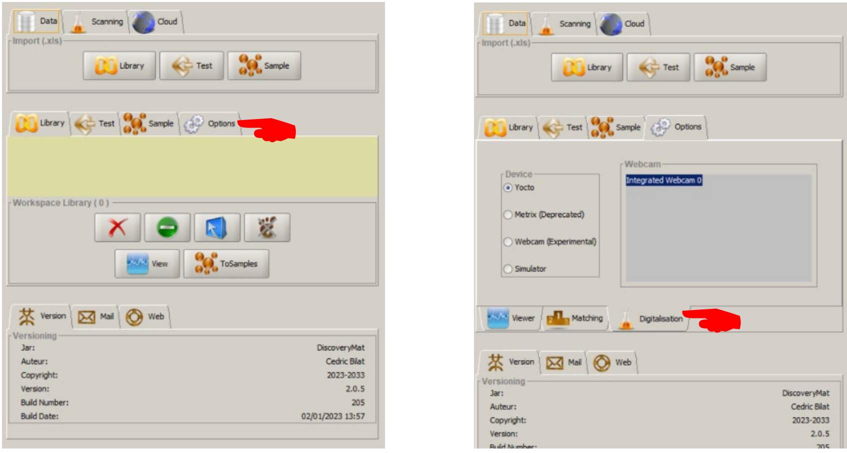
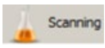
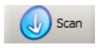


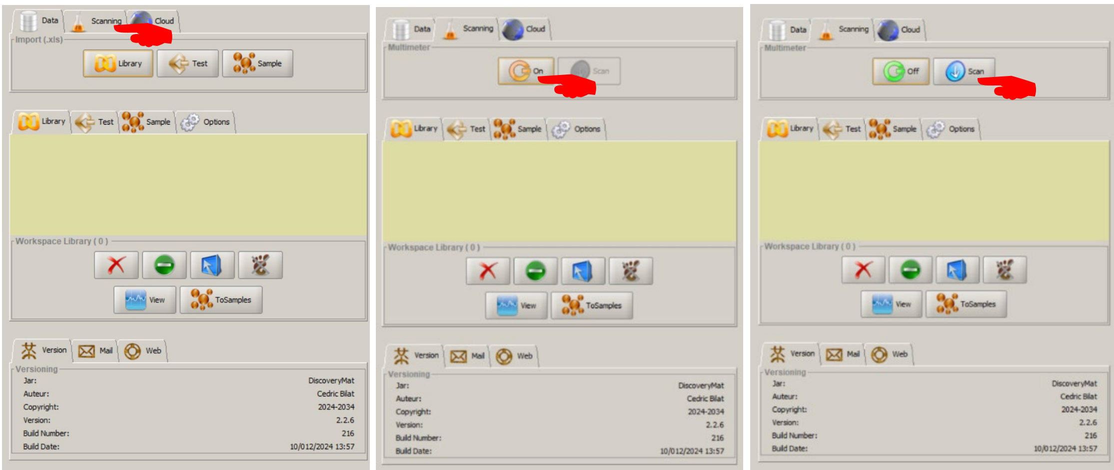
Fig. 2: Choice of measurement system.

Once the various connections for data collection have been made, the measurement control is started by clicking the 

button in the settings window (Fig. 3a), then press the 

(Fig. 3b). If the connection between the laptop and the multimeter is not effective, the error message "Multimeter on failure" appears. Otherwise the setup window will appear as in Fig. 3c and the Scanner tool is ready for measurement. To do this, simply click on the 

button.



a/ b/ c/

Fig. 3: Data collection control operations.

The measured potentials depend in particular on the surface preparation of the materials tested. As the polishing is not always the same, these potentials are not identical from one measurement to another. The Scanning tool measures potentials over a period of 5 to 15 minutes (the window below shows a continuous display of the measurements taken every second - Fig. 4). At least three plots (2 of 5min. (i.e. 300 measurement points) and 1 of 15min. (i.e. 900 measurement points)) are necessary to check the reproducibility of the results but only the 15min. plot counts for the analysis of the materials.

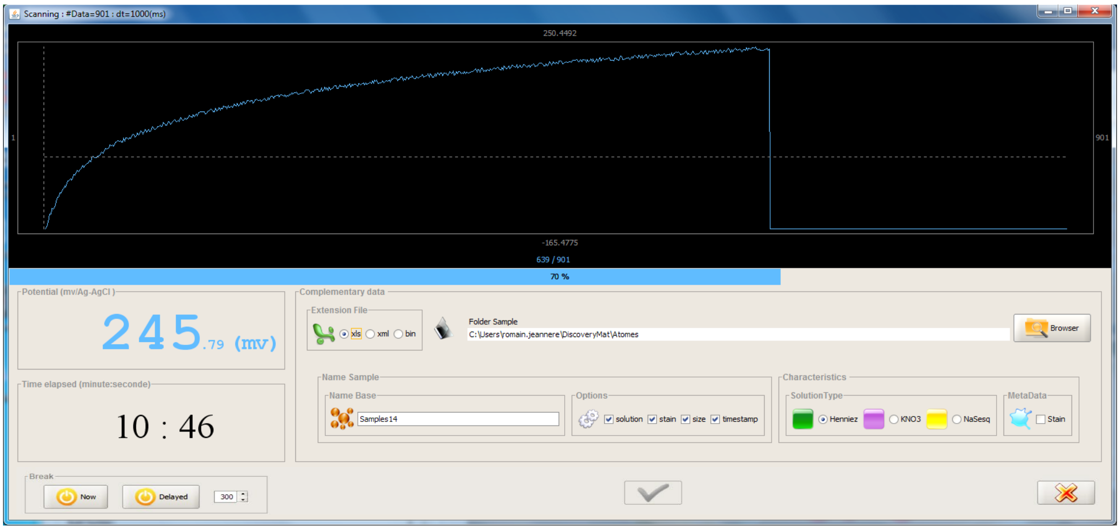
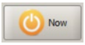
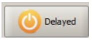
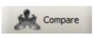



Fig. 4: Visualisation of the monitoring of the measured potentials.

The Scanning tool has been designed in such a way that the measurement stops automatically after 15 minutes. Also for measurements over 5 min. one has to stop the plot manually with the  button or on  button, once one has inserted the number 300 in the box on the right. The elapsed time is given under the potential value but also with the displacement of the blue cursor.

A certain amount of information about the plot must be recorded by the operator during the duration of the plot:

- Final data format (xls (Excel format), xml (text format) or bin (binary format)),
- Plot name (whether or not associated with the name of the solution tested, the number of points in the plot, the time and date of the plot and the possible presence of a stain - information selected in the Options box),
- Recording folder (on the laptop hard disk),
- Solution tested (each solution is colour coded: green for Henniez or Evian mineral water, purple for KNO3 1%(w/v) and yellow for sodium sesquicarbonate (NaSesq) 0.44NaHC+0.21Na2Cg/100mL),
- Presence or not of a stain left by the solution (information difficult to give at this level of the experiment).

After this, the first two 5-minute plots appear in the Sample workspace (blue area) of the settings window. The reproducibility of these can be checked by selecting them with the  button and clicking on the  button (Fig. 5). If the plots overlap, the plots are considered to be reproducible.

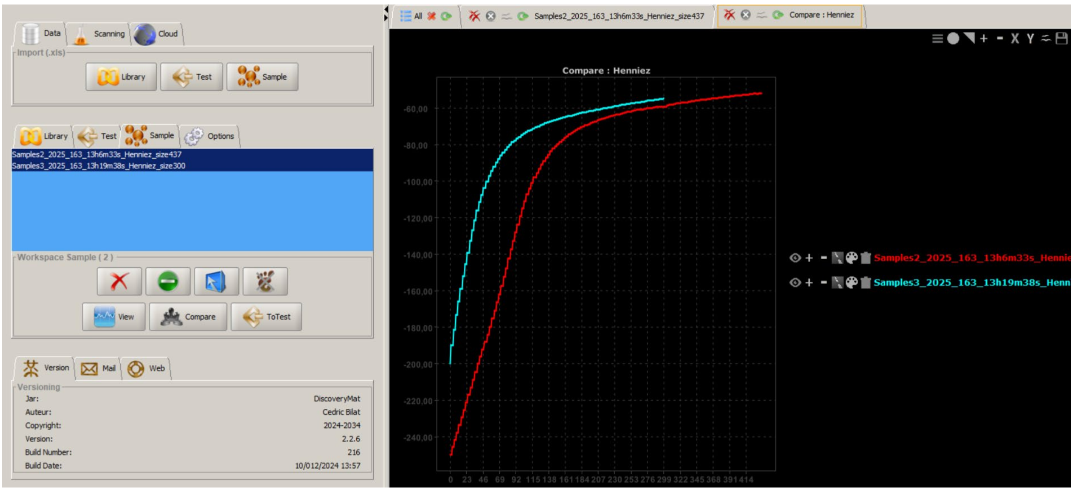
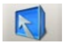



Fig. 5: Comparison of two plots to check their reproducibility.

The file Protocol for *data collection and processing with Discovery Mat software* indicates what to do if reproducibility problems are encountered.

The operator can permanently delete one or more plots from the workspace and the hard disk of the laptop at any time with the  button, or simply remove them from the workspace while keeping them on the hard drive with the  button. He can also select all the plots in the workspace with the  button or deselect them with the  button. It is also possible to view one or more plots with the  button.

At the end of this step, the operator has at least 9 plots for an unknown material under test (3 for each solution).

## 2. Data processing (Data tool)

The file *Protocol for data collection and processing with the "Discovery Mat" software* details the steps involved in processing the results and the main functions of the tool developed in this context.

The operator starts with data in the Sample workspace.

### 2.1. Identification of an unknown material tested from its plots obtained automatically with the "Discovery Mat" software

In the case of data obtained with the "Discovery Mat" software, the 3 plots of 900 points (corresponding to 15min.) obtained for each solution are selected in the Sample workspace with the Ctrl key on the laptop keyboard (Fig. 6).

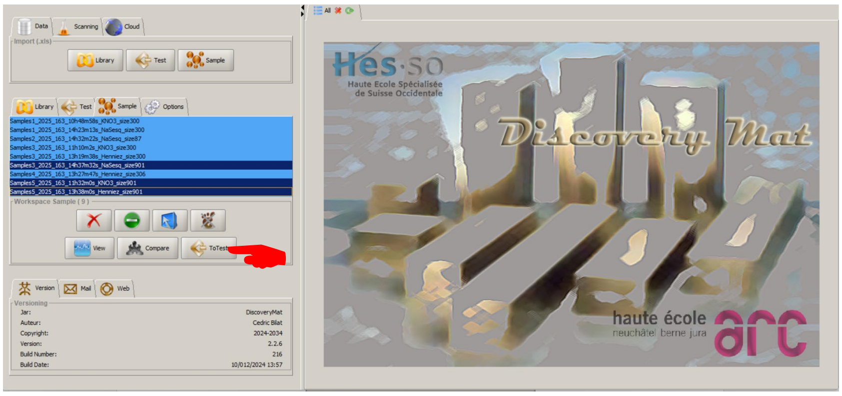



Fig. 6: Selection in the workspace Sample of the 3 plots over 15min. of the unknown material tested.

By clicking on the ToTest button, the window shown in Fig. 7 appears. Here again, the operator must note a certain amount of information related to the compilation of the three plots for the same material in the three solutions considered: data format, recording file, name of the material, whether or not the date and time of the compilation are associated with the test. In addition, certain characteristics of the plots in each of the solutions must be mentioned (existence or not of a horizontal shift between the plots made in the same solution (2 plots 5 min and 1 plot 15 min), fluctuations in potential and a stain left by the solution on the metal surface). The window also shows the rough appearance of the three plots with their respective colours. When all the information is entered, click on th button.

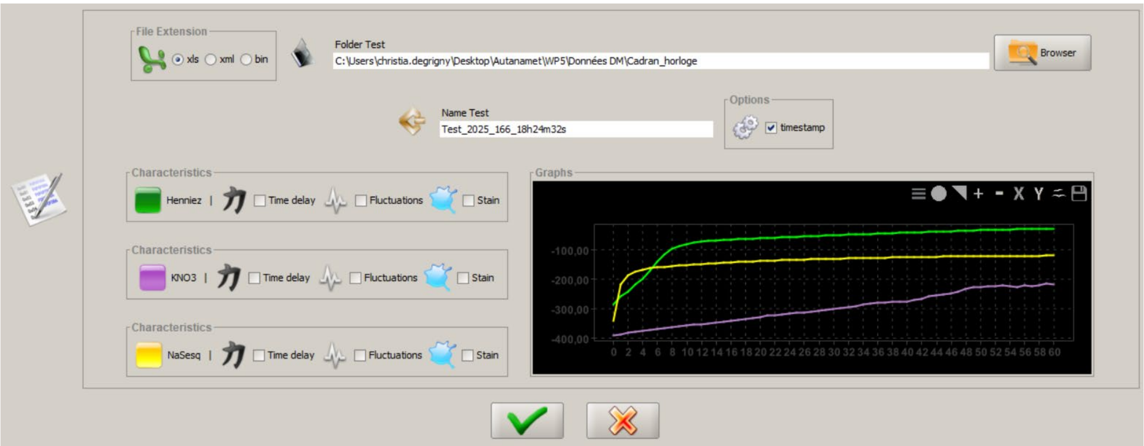



Fig. 7: Recording of the compilation of the three plots of the unknown material tested, their characteristics and a rough visualisation of all the plots.

The following window (Fig. 8) appears with the name of the Test material in the Test workspace in the settings window and its plots in the three solutions considered on the right-hand side, with the box indicating the characteristics of the plots at the bottom right.

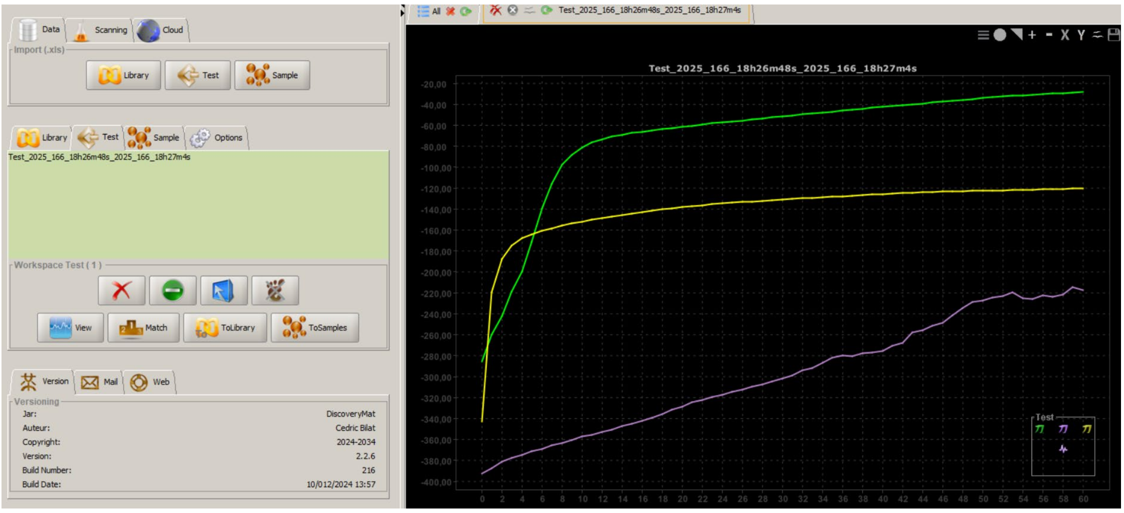
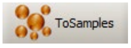


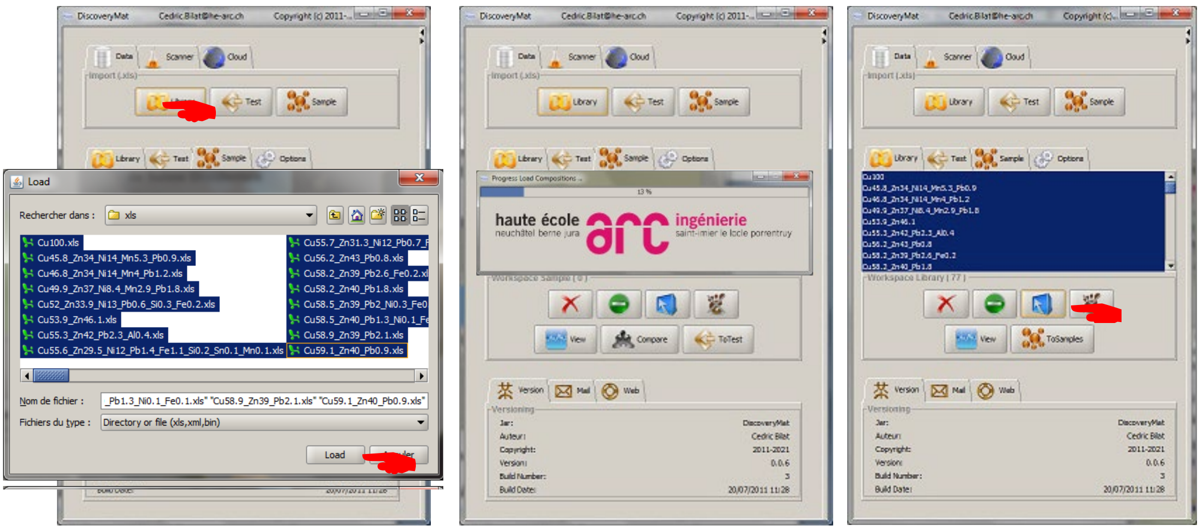

Fig. 8: Visualisation of the three plots of unknown material tested and their characteristics.

This last operation smoothes out the initial plots since the 900 measurement points are reduced to only 60 points (those corresponding to the 15s measurements). By clicking on the 

button, the three plots can be ununited as a Sample file, but the points between the 15s are also lost.

In order to analyse this test material via the Data tool of the Discovery Mat software, it is necessary to select a database located on the hard disk of the laptop and made up of materials of known composition whose electrochemical plots will be compared with those of the test material. By clicking on the 

button, the appropriate database is downloaded from the laptop by selecting the corresponding folder and highlighting the files to be considered (Fig. 9a). The download % window appears (Fig. 9b). The download is long if the number of materials in the database is large and the files are in xls format. It is faster with xlm and bin files. When the operation is complete, the database files appear in the Library workspace of the settings window. Select them all by clicking o  (Fig. 9c).




a/ b/ c/

Fig. 9: Control operations for downloading files from a database in the Library workspace.

The next step is to compare the plots of the Test material with those of the materials in the selected database. To do this, return to the Test workspace by clicking on Test button, check that the material to be tested is over-lit and click on Match button (Fig. 10).

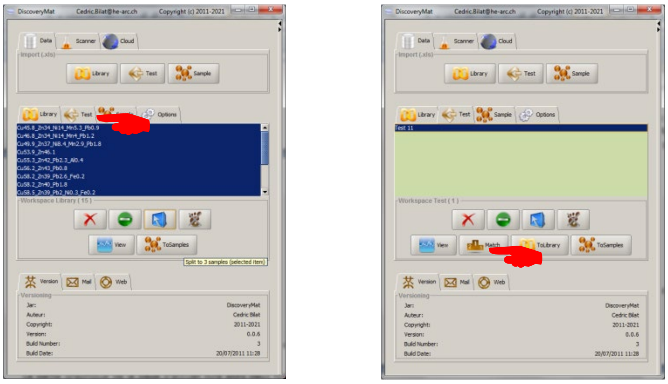
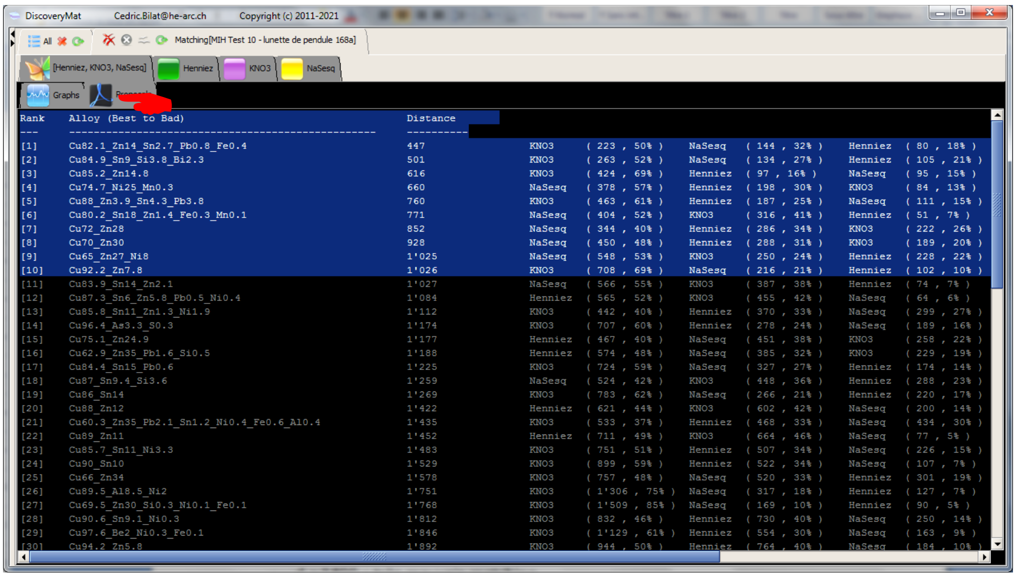


Fig. 10: Control operation of the comparison of the plots of the unknown material tested with those of the materials in the selected database.

The graphic part of the homepage then provides two types of information: by clicking on the Proposals button, a list of proposed compositions is obtained by calculating the distances between the plots of the materials in the selected database and those of the unknown test material (Fig. 11). The smaller the distances indicated, the more plausible the matching. Thus, proposal 1 in the list is the most plausible, the last the least.



| Rank | Alloy (Best to Bad) | Distance | | | | | | |
|---|---|---|---|---|---|---|---|---|
| [1] | Cu82.1_Zn14_Sn2.7_Pb0.8_Fe0.4 | 447 | KNO3 | ( 223 , 50% ) | NaSesq | ( 144 , 32% ) | Henniez | ( 80 , 18% ) |
| [2] | Cu84.9_Sn9_Si3.8_Bi2.3 | 501 | KNO3 | ( 263 , 52% ) | NaSesq | ( 134 , 27% ) | Henniez | ( 105 , 21% ) |
| [3] | Cu85.2_Zn14.8 | 616 | KNO3 | ( 424 , 69% ) | Henniez | ( 97 , 16% ) | NaSesq | ( 95 , 15% ) |
| [4] | Cu74.7_Ni25_Mn0.3 | 660 | NaSesq | ( 378 , 57% ) | Henniez | ( 198 , 30% ) | KNO3 | ( 84 , 13% ) |
| [5] | Cu88_Zn3.9_Sn4.3_Pb3.8 | 760 | KNO3 | ( 463 , 61% ) | Henniez | ( 187 , 25% ) | NaSesq | ( 111 , 15% ) |
| [6] | Cu80.2_Sn18_Zn1.4_Fe0.3_Mn0.1 | 771 | NaSesq | ( 404 , 52% ) | KNO3 | ( 316 , 41% ) | Henniez | ( 51 , 7% ) |
| [7] | Cu72_Zn28 | 852 | NaSesq | ( 344 , 40% ) | Henniez | ( 286 , 34% ) | KNO3 | ( 222 , 26% ) |
| [8] | Cu70_Zn30 | 928 | NaSesq | ( 450 , 48% ) | Henniez | ( 288 , 31% ) | KNO3 | ( 189 , 20% ) |
| [9] | Cu65_Zn27_Ni8 | 1'025 | NaSesq | ( 548 , 53% ) | KNO3 | ( 250 , 24% ) | Henniez | ( 228 , 22% ) |
| [10] | Cu92.2_Zn7.8 | 1'026 | KNO3 | ( 708 , 69% ) | NaSesq | ( 216 , 21% ) | Henniez | ( 102 , 10% ) |
| [11] | Cu83.9_Sn14_Zn2.1 | 1'027 | NaSesq | ( 566 , 55% ) | KNO3 | ( 387 , 38% ) | Henniez | ( 74 , 7% ) |
| [12] | Cu87.3_Sn6_Zn5.8_Pb0.5_Ni0.4 | 1'084 | Henniez | ( 565 , 52% ) | KNO3 | ( 455 , 42% ) | NaSesq | ( 64 , 6% ) |
| [13] | Cu85.8_Sn11_Zn1.3_Ni1.9 | 1'112 | KNO3 | ( 442 , 40% ) | Henniez | ( 370 , 33% ) | NaSesq | ( 299 , 27% ) |
| [14] | Cu96.4_As3.3_S0.3 | 1'174 | KNO3 | ( 707 , 60% ) | Henniez | ( 278 , 24% ) | NaSesq | ( 189 , 16% ) |
| [15] | Cu75.1_Zn24.9 | 1'177 | Henniez | ( 467 , 40% ) | NaSesq | ( 451 , 38% ) | KNO3 | ( 258 , 22% ) |
| [16] | Cu62.9_Zn35_Pb1.6_Si0.5 | 1'188 | Henniez | ( 574 , 48% ) | NaSesq | ( 385 , 32% ) | KNO3 | ( 229 , 19% ) |
| [17] | Cu84.4_Sn15_Pb0.6 | 1'225 | KNO3 | ( 724 , 59% ) | NaSesq | ( 327 , 27% ) | Henniez | ( 174 , 14% ) |
| [18] | Cu87_Sn9.4_Si3.6 | 1'259 | NaSesq | ( 524 , 42% ) | KNO3 | ( 448 , 36% ) | Henniez | ( 288 , 23% ) |
| [19] | Cu86_Sn14 | 1'269 | KNO3 | ( 783 , 62% ) | NaSesq | ( 266 , 21% ) | Henniez | ( 220 , 17% ) |
| [20] | Cu88_Zn12 | 1'422 | Henniez | ( 621 , 44% ) | KNO3 | ( 602 , 42% ) | NaSesq | ( 200 , 14% ) |
| [21] | Cu60.3_Zn35_Pb2.1_Sn1.2_Ni0.4_Fe0.6_Al0.4 | 1'435 | KNO3 | ( 533 , 37% ) | Henniez | ( 468 , 33% ) | NaSesq | ( 434 , 30% ) |
| [22] | Cu89_Zn11 | 1'452 | Henniez | ( 711 , 49% ) | KNO3 | ( 664 , 46% ) | NaSesq | ( 77 , 5% ) |
| [23] | Cu85.7_Sn11_Ni3.3 | 1'483 | KNO3 | ( 751 , 51% ) | Henniez | ( 507 , 34% ) | NaSesq | ( 226 , 15% ) |
| [24] | Cu90_Sn10 | 1'529 | KNO3 | ( 899 , 59% ) | Henniez | ( 522 , 34% ) | NaSesq | ( 107 , 7% ) |
| [25] | Cu66_Zn34 | 1'578 | KNO3 | ( 757 , 48% ) | NaSesq | ( 520 , 33% ) | Henniez | ( 301 , 19% ) |
| [26] | Cu89.5_Al8.5_Ni2 | 1'751 | KNO3 | ( 1'306 , 75% ) | NaSesq | ( 317 , 18% ) | Henniez | ( 127 , 7% ) |
| [27] | Cu69.5_Zn30_Si0.3_Ni0.1_Fe0.1 | 1'768 | KNO3 | ( 1'509 , 85% ) | NaSesq | ( 169 , 10% ) | Henniez | ( 90 , 5% ) |
| [28] | Cu90.6_Sn9.1_Ni0.3 | 1'812 | KNO3 | ( 832 , 46% ) | Henniez | ( 730 , 40% ) | NaSesq | ( 250 , 14% ) |
| [29] | Cu97.6_Be2_Ni0.3_Fe0.1 | 1'846 | KNO3 | ( 1'129 , 61% ) | Henniez | ( 554 , 30% ) | NaSesq | ( 163 , 9% ) |
| [30] | Cu94.2_Zn5.8 | 1'892 | KNO3 | ( 944 , 50% ) | Henniez | ( 764 , 40% ) | NaSesq | ( 184 , 10% ) |

Fig. 11: List of proposed compositions of the unknown material tested proposed by the "DiscoveryMat" software.

The practical use of the Data tool of the Discovery Mat software shows that in the majority of cases the plots of the tested unknown materials do not find exact equivalents with those of the materials in the selected databases for the three solutions. This led us to define the following ranges of greater or lesser correspondence:

- d between 250-450: good matching ;
- - d between 450-700: fairly good matching;

christian.degrigny@he-arch.ch –

- - d between 700-900: poor matching;
- - d between 900-1100: fairly poor matching;
- - d between 1100-1400: poor matching;
- - d >1400: very poor matching.

These new matches are evolving as the database grows.

The second type of information allows this initial mathematical assessment of the plots to be refined. It consists of clicking on the Graphs button, visually compare the appearance of the plots of the Test material with those of each of the materials in the selected database (Fig. 12).

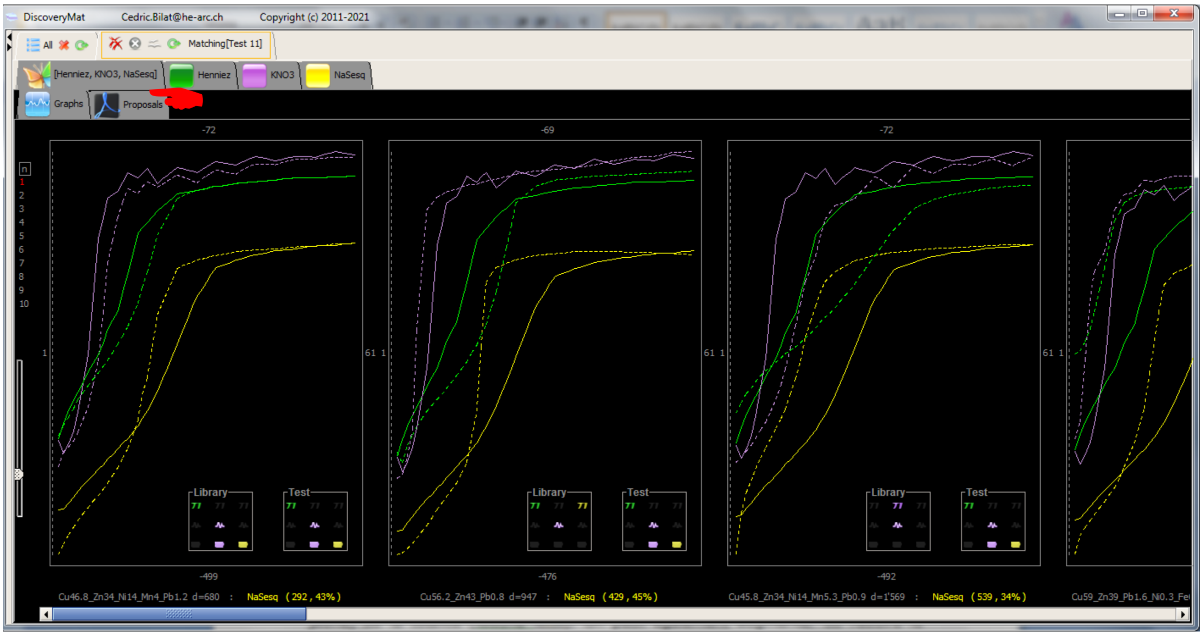



Fig. 12: Visual comparison of the plots of the unknown material tested with those of each of the materials in the selected database.

Several options exist to view a selection of plots (e.g. in a specific solution by clicking on the green, purple or yellow button) or all of them (button ). We can also increase or reduce the number of graph lines, decrease their size or zoom them by using the numbers and the slider on the left of the graph.

In addition to the plots, the bottom right-hand corner of each graph contains boxes giving the characteristics mentioned above (horizontal shift between the plots, fluctuations in potentials and presence or absence of a spot) for both the unknown material tested and the material considered in the selected database. Two very similar materials should, a priori, have the same characteristics.

At the end of this analysis and the preliminary condition report carried out on the unknown material tested, the operator is in a position to make composition proposals.

### 2.2. Database enrichment

If the comparison of the electrochemical plots of an unknown material tested with those of materials from the database selected via the Data tool of the "Discovery Mat" software shows that the distance calculated is significant (poor to very poor matching), it is advisable to analyse the unknown material tested with another elemental analysis tool (X-ray fluorescence spectrometer, energy dispersive spectrometer) in order to insert this material into the database and thus enrich it. To do this, click on the 

button, from the Test workspace of the settings window (Fig. 13).

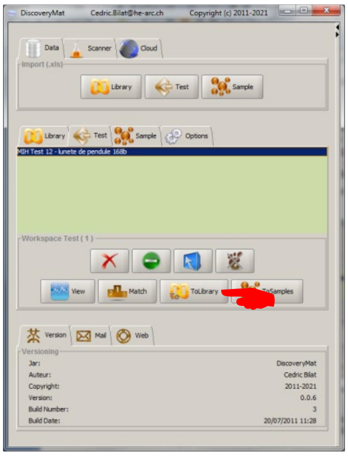



Fig. 13: Inserting plots of an unknown and identified material into a laptop database.

The following window appears (Fig. 14). Once again the operator must specify the format of the data to be saved, the selected folder (existing database) and the name of the corresponding file. Then click on the  button.

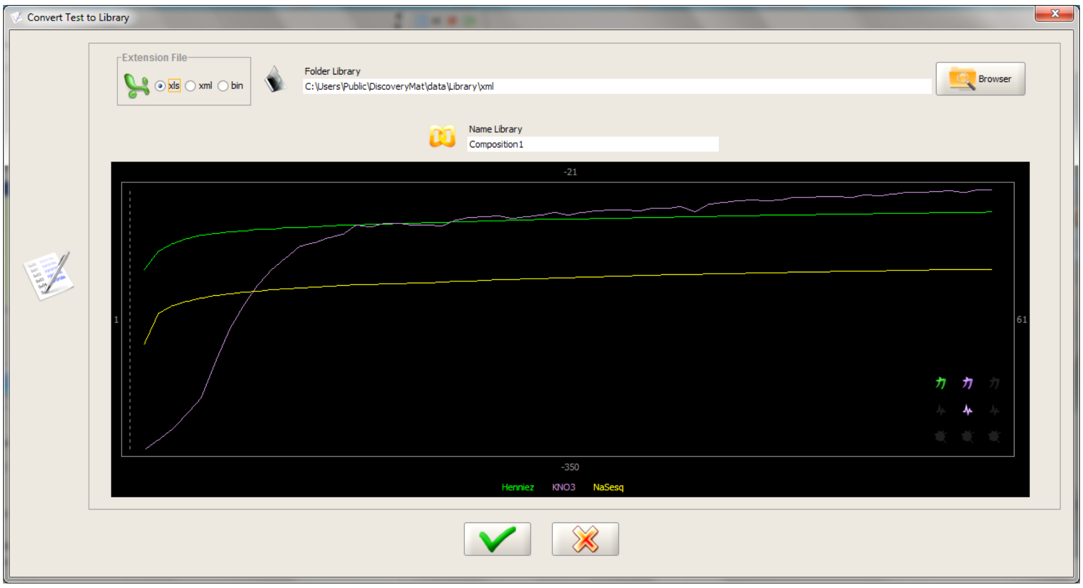



Fig. 14: Recording of the three plots of the unknown material tested and identified and their characteristics in an existing database.

christian.degrigny@he-arch.ch –

The following window appears if the given file name does not comply with the rules imposed below (Fig. 15).

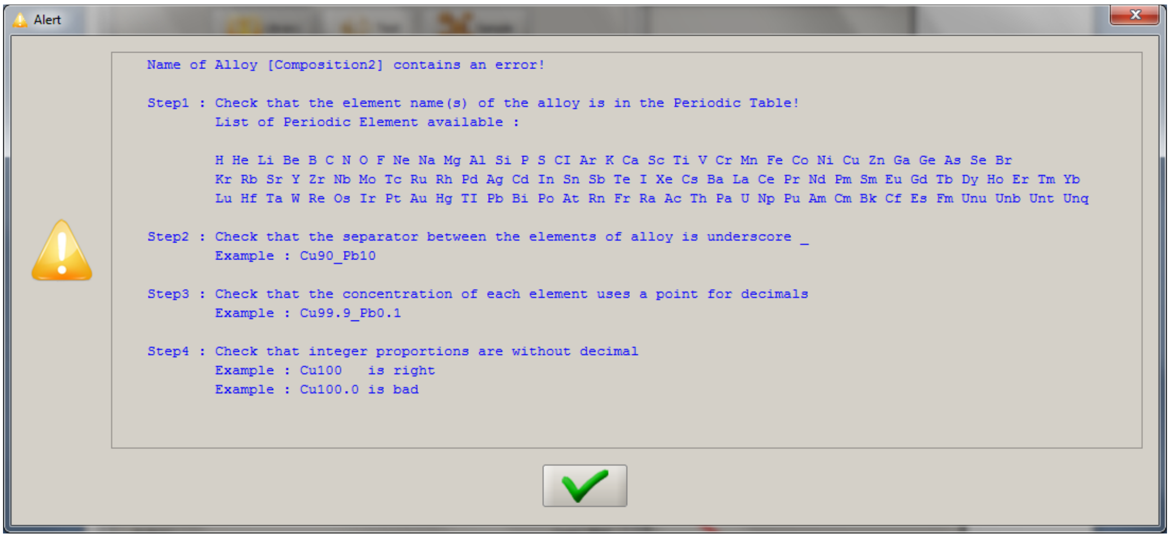


Fig. 15 : Guidelines for naming material files in the laptop databases.