RootProf

TUTORIAL 2

Unsupervised quantitative analysis

Contents

Chapter 1

The data set

Unidimensional patterns from X-ray diffraction measurements on polycrystalline mixtures form our dataset. Experimental samples have been produced by crystallization processes aiming at obtaining co-crystals formed by an active pharmaceutical ingredient (API) and a co-former. In our case polymorph III of carbamazepine constitutes the API, saccharine the co-former. The experimentally determined weight fractions of carbamazepine (CBZ III), saccharine (SAC) and co-crystal (CBZ-SAC) are reported in Table 1. The corresponding files are included as demo files. They are formed by two columns, the first containing the 2θ values, the second the corresponding values of diffracted intensity.

Table 1: Weight fractions of prepared mixtures. Samples 6-8 (shadowed) are composed by pure phases.

Sample n.	CBZ III	SAC	CBZ-SAC	File name
0	0	0.565	0.435	Rocco_S3_mac.txt
1	0.500	0.500	0	Rocco_S5_mac.txt
2	0.500	0	0.500	Rocco_S7_Como.txt
3	0.347	0.334	0.319	Rocco_S11_mac.txt
4	0.263	0.482	0.255	Rocco_S21_mac.txt
5	0.238	0.364	0.399	Rocco_S22_mac.txt
6	1	0	0	Rocco_CBZ_III_nomac.txt
7	0	1	0	Rocco_SAC_pura_nomac.txt
8	0	0	1	Rocco_CBZSAC_90511_n.txt

Chapter 2

Quantitative analysis by MultiFit

Motivation

Assessing the weight fraction of pure phases in mixtures by using least-squares fitting of related profiles.

The command file

The list of commands is the following.

```
whichanalysis 3
figpaper 1
dataType 2
range 10 50
preprocess 0 2 100
file   Rocco_S3_mac.txt
file   Rocco_S5_mac.txt
file   Rocco_S7_Como.txt
file   Rocco_S11_mac.txt
file   Rocco_S21_mac.txt
file   Rocco_S22_mac.txt
file   Rocco_CBZ_III_nomac.txt
purephase
file   Rocco_SAC_pura_nomac.txt
purephase
file   Rocco_CBZSAC_90511_n.txt
purephase
```

They have been included in the demo file named *fileInputQuantitative*. See the user guide for an explanation of each command.

Running RootProf

Start ROOT by clicking on his icon, or by typing "root" on a terminal window. Then write the root command:

Root> .x RootProf.C("fileInputQuantitative")

or

Root> .> outputQuantitative

Root> .x RootProf.C("fileInputQuantitative")

Root> .>

After some seconds, graphic windows will start appearing on your screen, while text output will appear on the terminal window, or redirected in the file named *outputQuantitative*. When the run ends, the root prompt will appear again on the ROOT terminal, and you will be able to edit each single graphic window and read the output file by your text editor.

The graphic output

Many graphic windows will appear on your terminal during the MultiSpecra run, each showing the result of the fitting of a given input spectrum (black full line) with a calculated spectrum composed by the weighted sum of the pure phase profiles (dashed red line). An example is given in Fig.1. The pure phase profiles have to be included among the input profiles, identified by the command *purephase*.
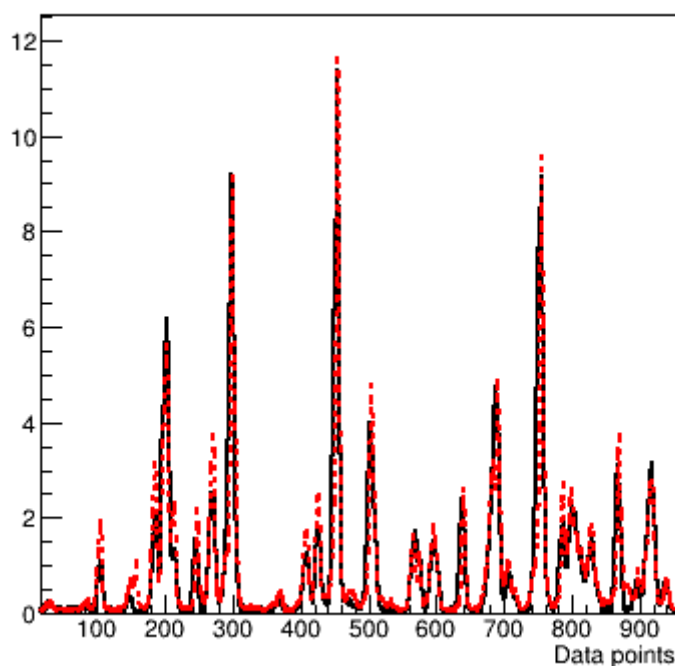

Fig.1 MultiFit on Sample 0

The weights of the calculated spectrum are the fitted parameters, and, properly rescaled, represent the weight fraction of the pure phases in each mixture spectrum. The overall set of weights is shown in Fig.2, as a function of the input spectrum Their sum is also shown (blue line): it is expected to be 1 if the considered pure phases are the only constituent of the mixture. Sum values below 1 (as it occurs for samples 0-5) indicate that other phases are present in the mixture, or it include amorphous content.
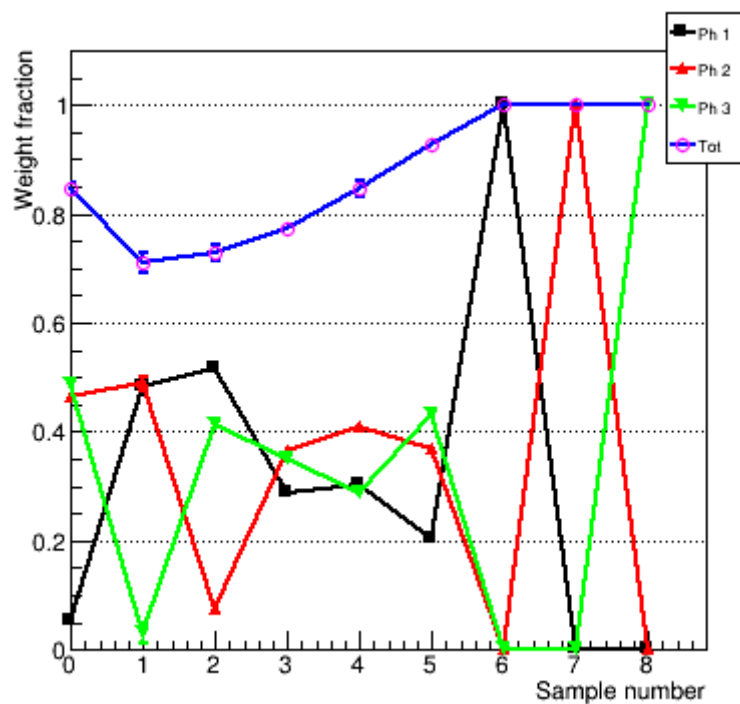
Fig.2 Quantitative Fit graph

The fitted weights of one pure phase are shown correlated to those of another pure phase in Figs. 3 pure phases 1-2) and Fig.4 (pure phases 1-3). The resulting scatter plot look similar to the score plots obtained in the PCA analysis of the same dataset (see tutorial on qualitative analysis), indicating that the fitted weight fraction follow the classification obtained in the principal components space.
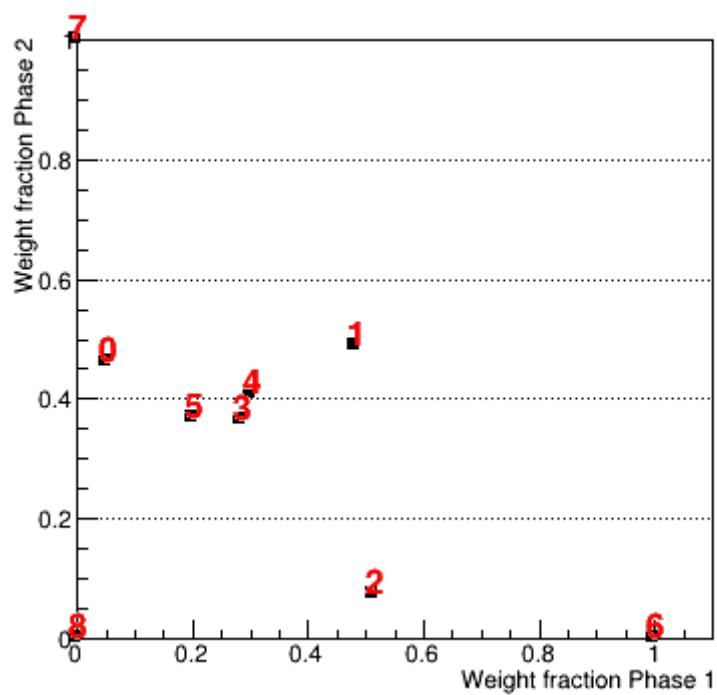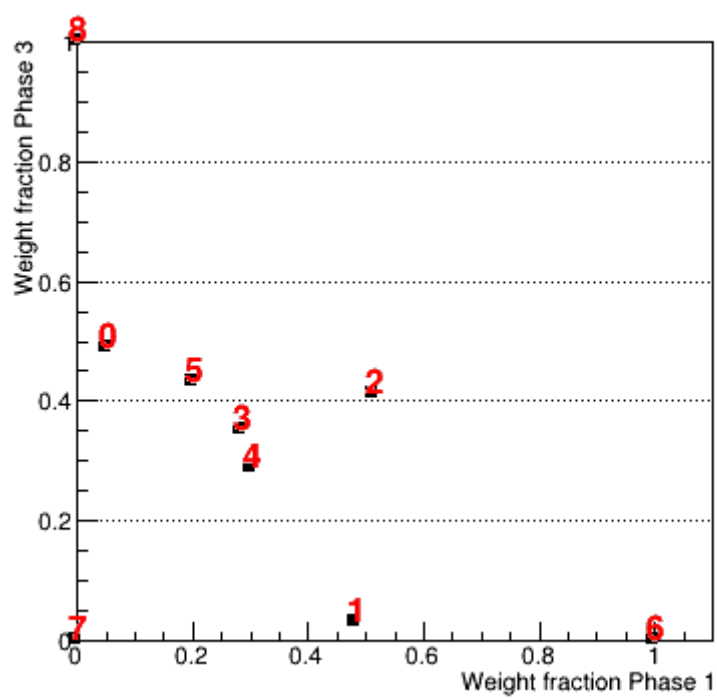
Fig.3 Quantitative Fit plot 1-2
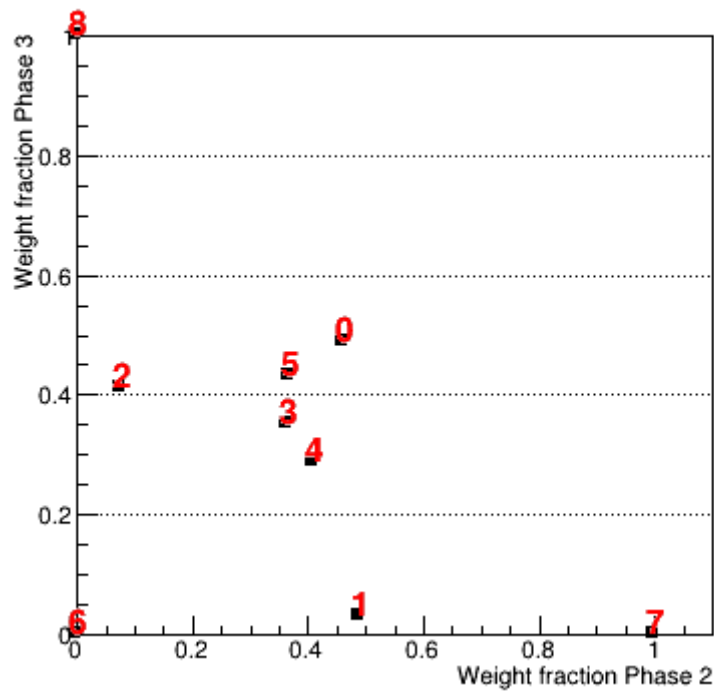

Fig.4 Quantitative Fit plot 1-3

Fig.5 Quantitative Fit plot 2-3

The output file

The content of the output file named *outputQuantitative* is reported below, with comments added.

```
 Input from file: fileInputQuantitative
-------------------------------
  whichanalysis 3

  figpaper 1

  dataType 2

  range 10 50

  preprocess 0 2 100

  file   Rocco_S3_mac.txt

  file   Rocco_S5_mac.txt

  file   Rocco_S7_Como.txt

  file   Rocco_S11_mac.txt

  file   Rocco_S21_mac.txt

  file   Rocco_S22_mac.txt

  file   Rocco_CBZ_III_nomac.txt
```

```
  purephase

  file  Rocco_SAC_pura_nomac.txt

  purephase

  file  Rocco_CBZSAC_90511_n.txt

  purephase
```

The above section shows the commands read from the command file. It should be checked to ensure that they are interpreted correctly.

```
Reading input files:
 ----------------------
Sample 0 -> file Rocco_S3_mac.txt
        Found 1999  points
Sample 1 -> file Rocco_S5_mac.txt
        Found 1999  points
Sample 2 -> file Rocco_S7_Como.txt
        Found 1999  points
Sample 3 -> file Rocco_S11_mac.txt
        Found 1999  points
Sample 4 -> file Rocco_S21_mac.txt
        Found 1999  points
Sample 5 -> file Rocco_S22_mac.txt
        Found 1999  points
Sample 6 -> file Rocco_CBZ_III_nomac.txt
        Found 1999  points
Sample 7 -> file Rocco_SAC_pura_nomac.txt
        Found 1999  points
Sample 8 -> file Rocco_CBZSAC_90511_n.txt
        Found 1999  points
```

The above section reports the number of data points read within each input file.

```
Starting Quantitative analysis
```

```
FIT RESULTS:
 ------------------------
 Spectrum 0: Rocco_S3_mac.txt
 Chi-Square=4.23e+02, Reduced Chi-Square=2.12e-01, NDF=1995
 Weight fraction Phase 1  0.043 +- 0.006
 Weight fraction Phase 2  0.390 +- 0.005
 Weight fraction Phase 3  0.411 +- 0.008
 Total weight fraction 0.844 +- 0.011
 Rescaled weight fraction Phase 1  0.051 +- 0.007
 Rescaled weight fraction Phase 2  0.462 +- 0.006
 Rescaled weight fraction Phase 3  0.487 +- 0.007
 ------------------------
 Spectrum 1: Rocco_S5_mac.txt
 Chi-Square=1.28e+03, Reduced Chi-Square=6.42e-01, NDF=1995
 Weight fraction Phase 1  0.342 +- 0.011
 Weight fraction Phase 2  0.347 +- 0.008
 Weight fraction Phase 3  0.022 +- 0.014
 Total weight fraction 0.710 +- 0.019
```

```
Rescaled weight fraction Phase 1  0.481 +- 0.013
Rescaled weight fraction Phase 2  0.488 +- 0.013
Rescaled weight fraction Phase 3  0.031 +- 0.019
------------------------
Spectrum 2: Rocco_S7_Como.txt
Chi-Square=6.49e+02, Reduced Chi-Square=3.25e-01, NDF=1995
Weight fraction Phase 1  0.374 +- 0.008
Weight fraction Phase 2  0.054 +- 0.006
Weight fraction Phase 3  0.300 +- 0.010
Total weight fraction 0.729 +- 0.014
Rescaled weight fraction Phase 1  0.513 +- 0.010
Rescaled weight fraction Phase 2  0.075 +- 0.008
Rescaled weight fraction Phase 3  0.412 +- 0.010
------------------------
Spectrum 3: Rocco_S11_mac.txt
Chi-Square=3.94e+02, Reduced Chi-Square=1.98e-01, NDF=1995
Weight fraction Phase 1  0.220 +- 0.006
Weight fraction Phase 2  0.281 +- 0.005
Weight fraction Phase 3  0.270 +- 0.008
Total weight fraction 0.771 +- 0.011
Rescaled weight fraction Phase 1  0.286 +- 0.007
Rescaled weight fraction Phase 2  0.364 +- 0.006
Rescaled weight fraction Phase 3  0.350 +- 0.007
------------------------
Spectrum 4: Rocco_S21_mac.txt
Chi-Square=6.86e+02, Reduced Chi-Square=3.44e-01, NDF=1995
Weight fraction Phase 1  0.257 +- 0.008
Weight fraction Phase 2  0.347 +- 0.006
Weight fraction Phase 3  0.243 +- 0.010
Total weight fraction 0.846 +- 0.014
Rescaled weight fraction Phase 1  0.303 +- 0.008
Rescaled weight fraction Phase 2  0.410 +- 0.008
Rescaled weight fraction Phase 3  0.287 +- 0.009
------------------------
Spectrum 5: Rocco_S22_mac.txt
Chi-Square=3.83e+02, Reduced Chi-Square=1.92e-01, NDF=1995
Weight fraction Phase 1  0.187 +- 0.006
Weight fraction Phase 2  0.340 +- 0.005
Weight fraction Phase 3  0.398 +- 0.007
Total weight fraction 0.925 +- 0.011
Rescaled weight fraction Phase 1  0.202 +- 0.006
Rescaled weight fraction Phase 2  0.368 +- 0.005
Rescaled weight fraction Phase 3  0.430 +- 0.006
------------------------
Spectrum 6: Rocco_CBZ_III_nomac.txt
Chi-Square=1.26e-06, Reduced Chi-Square=6.32e-10, NDF=1995
Weight fraction Phase 1  1.000 +- 0.000
Weight fraction Phase 2  0.000 +- 0.000
Weight fraction Phase 3  0.000 +- 0.000
Total weight fraction 1.000 +- 0.000
Rescaled weight fraction Phase 1  1.000 +- 0.000
Rescaled weight fraction Phase 2  0.000 +- 0.000
Rescaled weight fraction Phase 3  0.000 +- 0.000
------------------------
Spectrum 7: Rocco_SAC_pura_nomac.txt
Chi-Square=1.68e-06, Reduced Chi-Square=8.44e-10, NDF=1995
Weight fraction Phase 1  0.000 +- 0.000
Weight fraction Phase 2  1.000 +- 0.000
Weight fraction Phase 3  0.000 +- 0.000
Total weight fraction 1.000 +- 0.000
```

```
Rescaled weight fraction Phase 1  0.000 +- 0.000
Rescaled weight fraction Phase 2  1.000 +- 0.000
Rescaled weight fraction Phase 3  0.000 +- 0.000
------------------------
Spectrum 8: Rocco_CBZSAC_90511_n.txt
Chi-Square=1.18e-06, Reduced Chi-Square=5.92e-10, NDF=1995
Weight fraction Phase 1  0.000 +- 0.000
Weight fraction Phase 2  0.000 +- 0.000
Weight fraction Phase 3  1.000 +- 0.000
Total weight fraction 1.000 +- 0.000
Rescaled weight fraction Phase 1  0.000 +- 0.000
Rescaled weight fraction Phase 2  0.000 +- 0.000
Rescaled weight fraction Phase 3  1.000 +- 0.000
```

The above section reports the results of the fitting procedure applied to each input spectrum separately. Fit results include goodness-of-fit estimates (Chi Square and Reduced Chi Square), number of degrees of freedom (NDF), and the best fit estimates of the pure phases weight fractions. Finally, the rescaled weights are reported.

Chapter 3

Assessing quantitative analysis results

Motivation

Comparing the weight fractions of pure phases in mixtures estimated by RootProf with those measured experimentally.

The command file

The list of commands is the following.

```
whichanalysis 3
figpaper 1
dataType 2
range 10 50
preprocess 0 2 100
file  Rocco_S3_mac.txt
referw 0 0.565 0.435
file  Rocco_S5_mac.txt
referw 0.5 0.5 0
file  Rocco_S7_Como.txt
referw 0.5 0 0.5
file  Rocco_S11_mac.txt
referw 0.347 0.334 0.319
file  Rocco_S21_mac.txt
referw 0.263 0.482 0.255
file  Rocco_S22_mac.txt
referw 0.238 0.364 0.399
file  Rocco_CBZ_III_nomac.txt
referw 1 0 0
purephase
file  Rocco_SAC_pura_nomac.txt
referw 0 1 0
purephase
file  Rocco_CBZSAC_90511_n.txt
purephase
referw 0 0 1
```

The commands have been included in the demo file named *fileInputQuantitativeTrue*. See the user guide for an explanation of their meaning.

Running RootProf

Start ROOT by clicking on his icon, or by typing "root" on a terminal window. Then write the root command:

Root> .x RootProf.C("fileInputQuantitativeTrue")

or

Root> .> outputQuantitativeTrue

.x RootProf.C("fileInputQuantitativeTrue")

.>

After some seconds, graphic windows will start appearing on your screen, while text output will appear on the terminal window, or redirected in the file named *outputQuantitativeTrue*. When the run ends, the root prompt will appear again on the ROOT terminal, and you are able to edit each single graphic window and read the output file by your text editor.

The graphical output

The graphic window in Fig.1 shows the overall phase abundances known in advance (reference abundances). They can be obtained experimentally, or determined by other methods, and have been put in the input file through the command *referw*. This plot should be compared with that of Quantitative Fig graph window (Fig.1, Chapter 1), where the phase abundances estimated by RootProf are reported with the same layout.
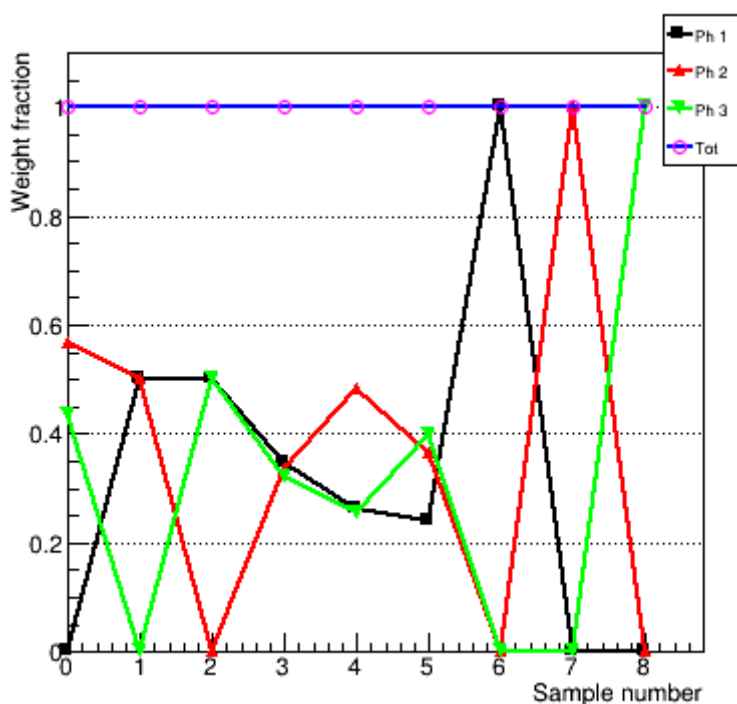
Fig.1 Quantitative Fit graph (reference weight fractions)

Figs. 2-4 show the calibration plots of each pure phase:, i.e. the scatter plots of the reference versus estimated weight fractions. The best fit line is shown in red, a dashed black line along the diagonal is drawn for reference, and error bars on data points, representing the uncertainty of the estimated weight fraction value are also included (in most of the cases they are hidden by the data point symbol). These plots can be used to assess the quality of the RootProf estimates, considering the spread of the points around the diagonal or the best fit line.
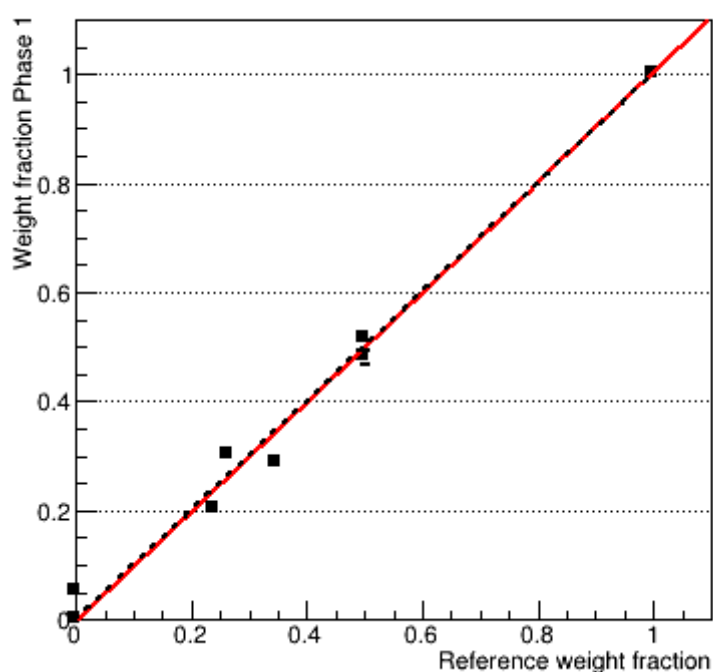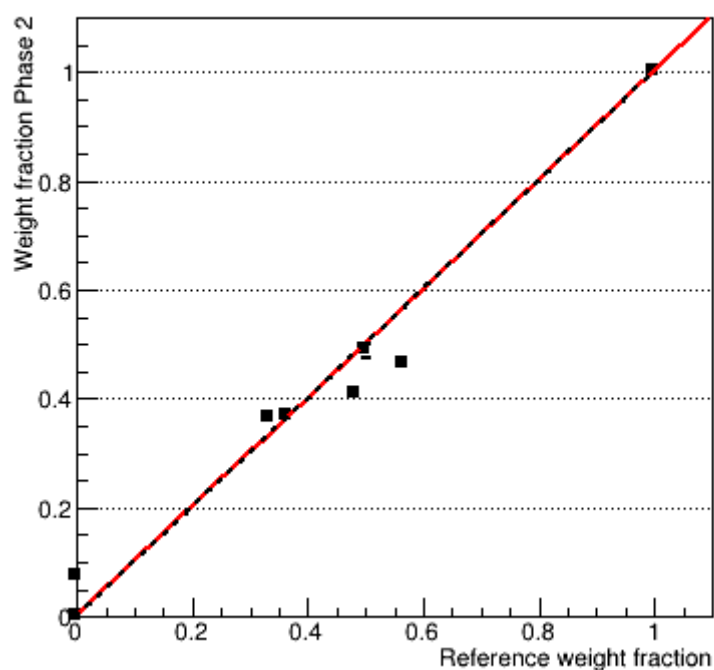

Fig.2 Calibration plot Phase 1
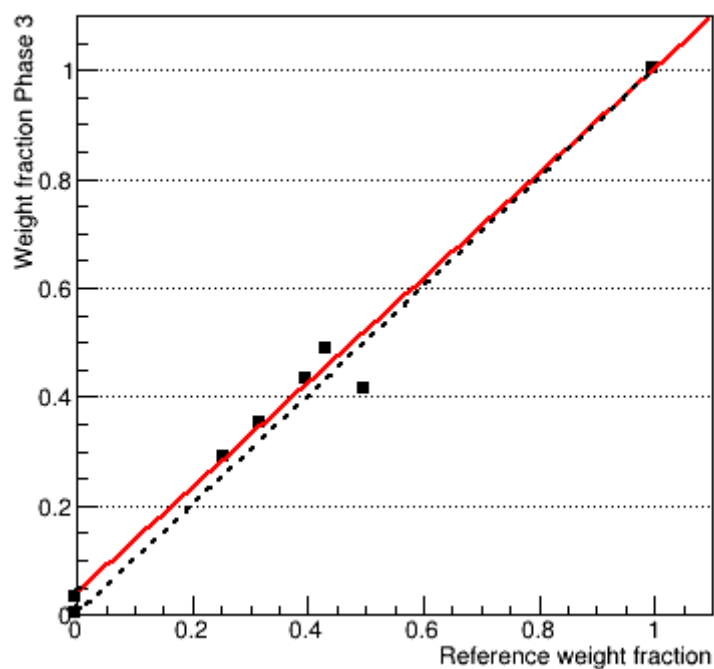
Fig.3 Calibration plot Phase 2

Fig.4 Calibration plot Phase 3

Figs. 5-8 show the difference between the true abundances and those calculated by RootProf, as a function of these latter. An hint about the estimation error can be inferred for the each pure phase, considering the spread of the points around the dashed line at y=0.
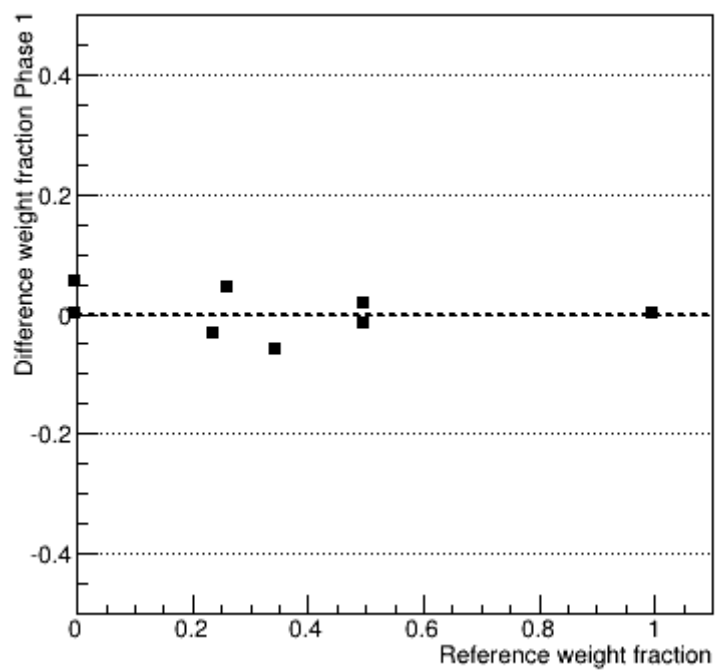
Fig.5 Difference plot Phase 1
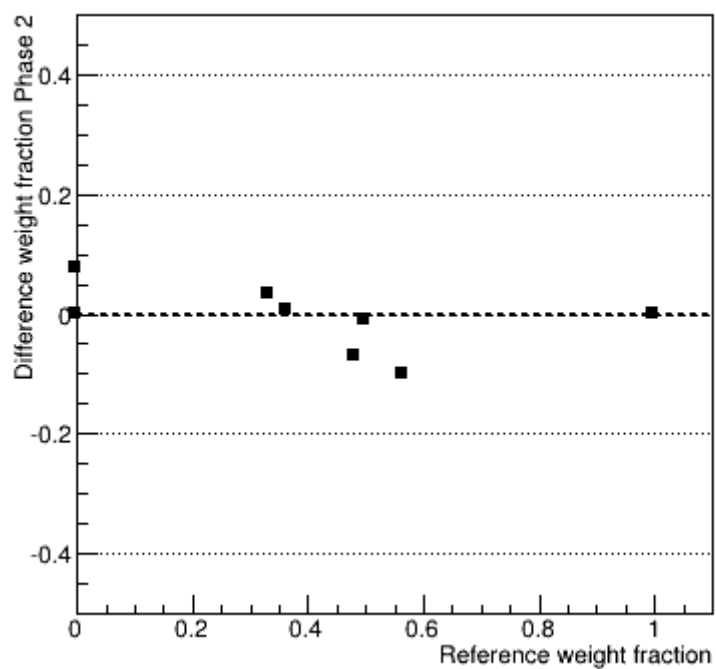
Fig.6 Difference plot Phase 2
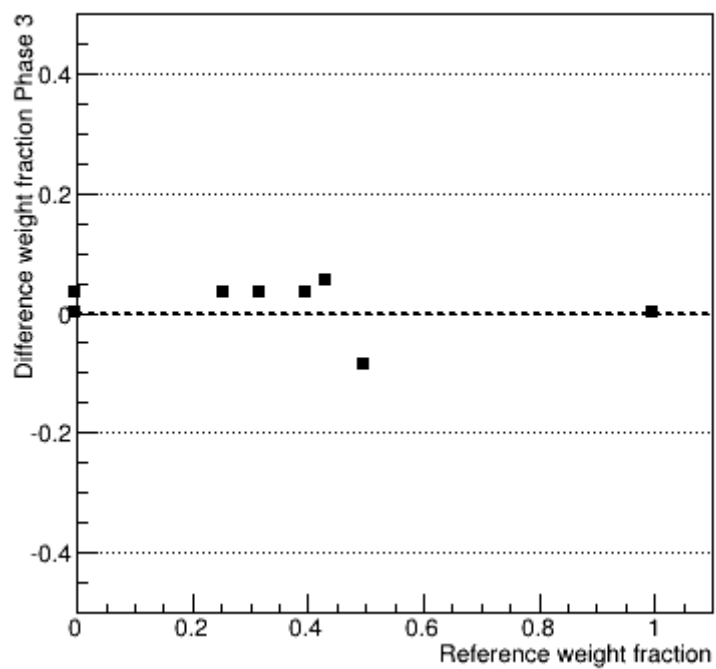
Fig.7 Difference plot Phase 3

The output file

The content of the output file named *outputQuantitativeTrue* is reported below, with comments added.

```
Input from file: fileInputQuantitativeTrue
--------------------------------
 whichanalysis 3

 figpaper 1

 dataType 2

 range 10 50

 preprocess 0 2 100

 file   Rocco_S3_mac.txt

 referw 0 0.565 0.435

 file   Rocco_S5_mac.txt

 referw 0.5 0.5 0

 file   Rocco_S7_Como.txt
```

```
referw 0.5 0 0.5

file  Rocco_S11_mac.txt

referw 0.347 0.334 0.319

file  Rocco_S21_mac.txt

referw 0.263 0.482 0.255

file  Rocco_S22_mac.txt

referw 0.238 0.364 0.399

file  Rocco_CBZ_III_nomac.txt

referw 1 0 0

purephase

file  Rocco_SAC_pura_nomac.txt

referw 0 1 0

purephase

file  Rocco_CBZSAC_90511_n.txt

purephase

referw 0 0 1
```

The above section shows the commands read from the command file. It should be checked to ensure that they are interpreted correctly.

```
Reading input files:
 ----------------------
Sample 0 -> file Rocco_S3_mac.txt
        Found 1999  points
Sample 1 -> file Rocco_S5_mac.txt
        Found 1999  points
Sample 2 -> file Rocco_S7_Como.txt
        Found 1999  points
Sample 3 -> file Rocco_S11_mac.txt
        Found 1999  points
Sample 4 -> file Rocco_S21_mac.txt
        Found 1999  points
Sample 5 -> file Rocco_S22_mac.txt
        Found 1999  points
Sample 6 -> file Rocco_CBZ_III_nomac.txt
        Found 1999  points
Sample 7 -> file Rocco_SAC_pura_nomac.txt
        Found 1999  points
Sample 8 -> file Rocco_CBZSAC_90511_n.txt
        Found 1999  points
```

The above section reports the number of data points read within each input file.

```
Starting Quantitative analysis

FIT RESULTS:
------------------------
Spectrum 0: Rocco_S3_mac.txt
Chi-Square=4.23e+02, Reduced Chi-Square=2.12e-01, NDF=1995
Weight fraction Phase 1  0.043 +- 0.006
Weight fraction Phase 2  0.390 +- 0.005
Weight fraction Phase 3  0.411 +- 0.008
Total weight fraction 0.844 +- 0.011
Rescaled weight fraction Phase 1  0.051 +- 0.007
Rescaled weight fraction Phase 2  0.462 +- 0.006
Rescaled weight fraction Phase 3  0.487 +- 0.007
------------------------
Spectrum 1: Rocco_S5_mac.txt
Chi-Square=1.28e+03, Reduced Chi-Square=6.42e-01, NDF=1995
Weight fraction Phase 1  0.342 +- 0.011
Weight fraction Phase 2  0.347 +- 0.008
Weight fraction Phase 3  0.022 +- 0.014
Total weight fraction 0.710 +- 0.019
Rescaled weight fraction Phase 1  0.481 +- 0.013
Rescaled weight fraction Phase 2  0.488 +- 0.013
Rescaled weight fraction Phase 3  0.031 +- 0.019
------------------------
Spectrum 2: Rocco_S7_Como.txt
Chi-Square=6.49e+02, Reduced Chi-Square=3.25e-01, NDF=1995
Weight fraction Phase 1  0.374 +- 0.008
Weight fraction Phase 2  0.054 +- 0.006
Weight fraction Phase 3  0.300 +- 0.010
Total weight fraction 0.729 +- 0.014
Rescaled weight fraction Phase 1  0.513 +- 0.010
Rescaled weight fraction Phase 2  0.075 +- 0.008
Rescaled weight fraction Phase 3  0.412 +- 0.010
------------------------
Spectrum 3: Rocco_S11_mac.txt
Chi-Square=3.94e+02, Reduced Chi-Square=1.98e-01, NDF=1995
Weight fraction Phase 1  0.220 +- 0.006
Weight fraction Phase 2  0.281 +- 0.005
Weight fraction Phase 3  0.270 +- 0.008
Total weight fraction 0.771 +- 0.011
Rescaled weight fraction Phase 1  0.286 +- 0.007
Rescaled weight fraction Phase 2  0.364 +- 0.006
Rescaled weight fraction Phase 3  0.350 +- 0.007
------------------------
Spectrum 4: Rocco_S21_mac.txt
Chi-Square=6.86e+02, Reduced Chi-Square=3.44e-01, NDF=1995
Weight fraction Phase 1  0.257 +- 0.008
Weight fraction Phase 2  0.347 +- 0.006
Weight fraction Phase 3  0.243 +- 0.010
Total weight fraction 0.846 +- 0.014
Rescaled weight fraction Phase 1  0.303 +- 0.008
Rescaled weight fraction Phase 2  0.410 +- 0.008
Rescaled weight fraction Phase 3  0.287 +- 0.009
------------------------
Spectrum 5: Rocco_S22_mac.txt
Chi-Square=3.83e+02, Reduced Chi-Square=1.92e-01, NDF=1995
Weight fraction Phase 1  0.187 +- 0.006
Weight fraction Phase 2  0.340 +- 0.005
Weight fraction Phase 3  0.398 +- 0.007
Total weight fraction 0.925 +- 0.011
```

```
 Rescaled weight fraction Phase 1  0.202 +- 0.006
 Rescaled weight fraction Phase 2  0.368 +- 0.005
 Rescaled weight fraction Phase 3  0.430 +- 0.006
 ------------------------
 Spectrum 6: Rocco_CBZ_III_nomac.txt
 Chi-Square=1.26e-06, Reduced Chi-Square=6.32e-10, NDF=1995
 Weight fraction Phase 1  1.000 +- 0.000
 Weight fraction Phase 2  0.000 +- 0.000
 Weight fraction Phase 3  0.000 +- 0.000
 Total weight fraction 1.000 +- 0.000
 Rescaled weight fraction Phase 1  1.000 +- 0.000
 Rescaled weight fraction Phase 2  0.000 +- 0.000
 Rescaled weight fraction Phase 3  0.000 +- 0.000
 ------------------------
 Spectrum 7: Rocco_SAC_pura_nomac.txt
 Chi-Square=1.68e-06, Reduced Chi-Square=8.44e-10, NDF=1995
 Weight fraction Phase 1  0.000 +- 0.000
 Weight fraction Phase 2  1.000 +- 0.000
 Weight fraction Phase 3  0.000 +- 0.000
 Total weight fraction 1.000 +- 0.000
 Rescaled weight fraction Phase 1  0.000 +- 0.000
 Rescaled weight fraction Phase 2  1.000 +- 0.000
 Rescaled weight fraction Phase 3  0.000 +- 0.000
 ------------------------
 Spectrum 8: Rocco_CBZSAC_90511_n.txt
 Chi-Square=1.18e-06, Reduced Chi-Square=5.92e-10, NDF=1995
 Weight fraction Phase 1  0.000 +- 0.000
 Weight fraction Phase 2  0.000 +- 0.000
 Weight fraction Phase 3  1.000 +- 0.000
 Total weight fraction 1.000 +- 0.000
 Rescaled weight fraction Phase 1  0.000 +- 0.000
 Rescaled weight fraction Phase 2  0.000 +- 0.000
 Rescaled weight fraction Phase 3  1.000 +- 0.000
```

The above section reports the results of the fitting procedure applied to each input spectrum separately. Fit results include goodness-of-fit estimates (Chi Square and Reduced Chi Square), number of degrees of freedom (NDF), and the best fit estimates of the pure phases weight fractions. Finally, the rescaled weights are reported.

```
    ------------------------------------
 Phase 1: RMSE=0.033 RMSE'=0.035 R2=0.989 R2(NPP)=0.947 AKLD=0.029
      Calibration fit: Chi-Square=2.11e+02 intercept=-0.006+-0.004
slope=1.006+-0.004
      Limits estimates: LOD=1.32  LOQ=4.00
 NPP: Calibration fit: Chi-Square=1.56e+02 intercept=0.028+-0.006
slope=0.860+-0.020
 NPP: Limits estimates: LOD=2.33  LOQ=7.06
    ------------------------------------
 Phase 2: RMSE=0.050 RMSE'=0.053 R2=0.977 R2(NPP)=0.955 AKLD=0.039
      Calibration fit: Chi-Square=4.76e+02 intercept=0.002+-0.004
slope=0.998+-0.004
      Limits estimates: LOD=1.39  LOQ=4.22
 NPP: Calibration fit: Chi-Square=9.14e+01 intercept=0.106+-0.007
slope=0.682+-0.017
 NPP: Limits estimates: LOD=3.27  LOQ=9.92
    ------------------------------------
 Phase 3: RMSE=0.040 RMSE'=0.047 R2=0.984 R2(NPP)=0.919 AKLD=0.039
      Calibration fit: Chi-Square=1.49e+02 intercept=0.039+-0.005
slope=0.961+-0.005
```

```
      Limits estimates: LOD=1.73  LOQ=5.25
 NPP: Calibration fit: Chi-Square=1.37e+02 intercept=0.079+-0.013
slope=0.851+-0.033
 NPP: Limits estimates: LOD=4.95  LOQ=15.00
  -----------------------------------
 Average total weight fraction: 0.804 +- 0.006
 Overall agreement: FOM=0.123 AKLD: 0.108
```

The section above includes the comparison between the phase abundances estimated by RootProf with the true ones. The following quantities are reported to express the agreement between estimated and reference weight fractions: the Root Mean Square Error (RMSE), the same quantity calculated by including only samples for which the reference weight fraction of the given pure phase is not zero (RMSE'), the Squared Pearson's correlation coefficient (R2), and the same quantity calculated without considering pure phases [R2(NPP)]. Optimal RMSE and RMSE' values should be close to 0, optimal R2 values should be close to 1. The Chi-Square, intercept and slope of the best fit line determined by the calibrations plots are also reported. The slope parameter is used to obtain estimates of the Limit of Quantification (LOQ) and Limit of Detection (LOD). The same calculations are repeated by excluding pure phases from the fit of the calibration plots (NPP). A measure of the overall agreement between estimated and true weight fractions is given through the parameter FOM, which is the sum of the RMSE calculated over all the three pure phases, and the absolute value of the Kullback-Leibner distance (AKLD), calculated as a sum over the three pure phases. Note that AKLD has finite values only if reference weight fraction are different from zero.

Chapter 4

Quantitative analysis by unfolding

Motivation

Assessing the weight fraction of pure phases in mixtures by using the unfolding algorithm.

The command file

The list of commands is the following.

```
whichanalysis 3
unfold 1
figpaper 1
dataType 2
angle 10 50
preprocess 0 2 100
file   Rocco_S3_mac.txt
referw 0 0.565 0.435
file   Rocco_S5_mac.txt
referw 0.5 0.5 0
file   Rocco_S7_Como.txt
referw 0.5 0 0.5
file   Rocco_S11_mac.txt
referw 0.347 0.334 0.319
file   Rocco_S21_mac.txt
referw 0.263 0.482 0.255
file   Rocco_S22_mac.txt
referw 0.238 0.364 0.399
file   Rocco_CBZ_III_nomac.txt
referw 1 0 0
purephase
file   Rocco_SAC_pura_nomac.txt
referw 0 1 0
purephase
file   Rocco_CBZSAC_90511_n.txt
purephase
referw 0 0 1
```

They have been included in the demo file named *fileInputQuantitativeUnfolding*. See the user guide for an explanation of each command.

Running RootProf

Start ROOT by clicking on his icon, or by typing "root" on a terminal window. Then write the root command:

Root> .x RootProf.C("fileInputQuantitativeUnfolding")

Or

Root> .> outputQuantitativeUnfolding

.x RootProf.C("fileInputQuantitativeUnfolding")

.>

After some seconds, graphic windows will start appearing on your screen, while text output will appear on the terminal window, or redirected in the file named *outputQuantitativeUnfolding*. When the run ends, the root prompt will appear again on the ROOT terminal, and you will be able to edit each single graphic window and read the output file by your text editor. It should be noted that a quantitative run with Unfolding is much faster than that with MultiFit approach.

The graphic output

The graphic windows produced are the same as those produced by the MultiFir approach through the fileInputQuantitativeTrue command file (see Chapters 1 and 2). They are here reported only to appreciate the differences from those shown in Chapters 1 and 2.
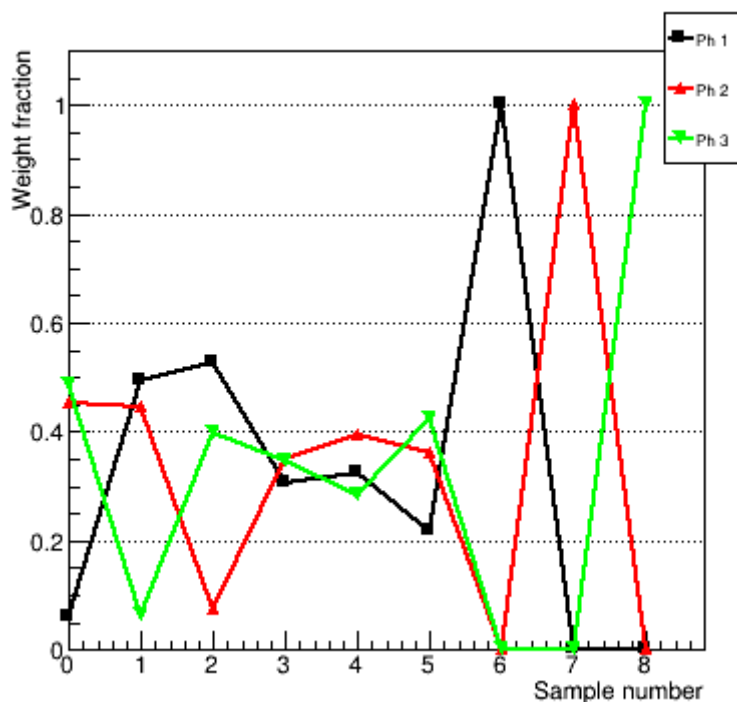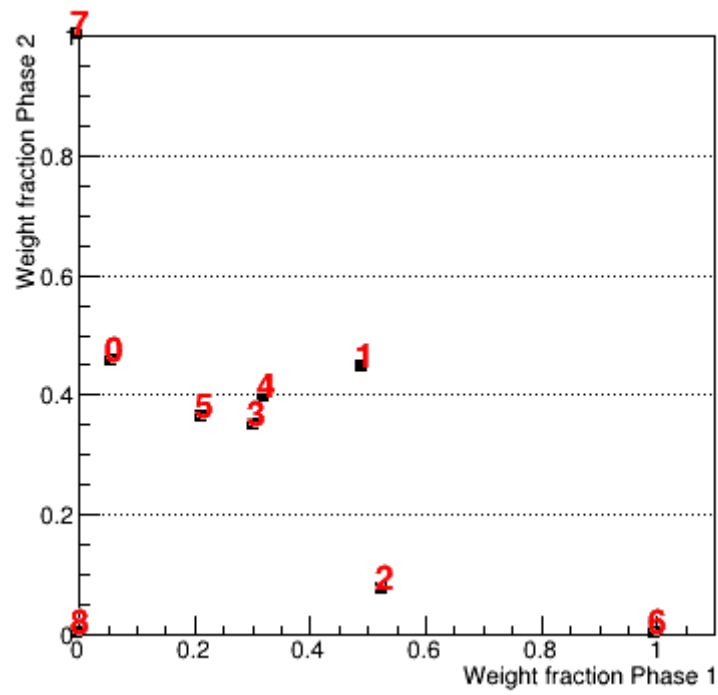

Fig.1 Quantitative Fit graph
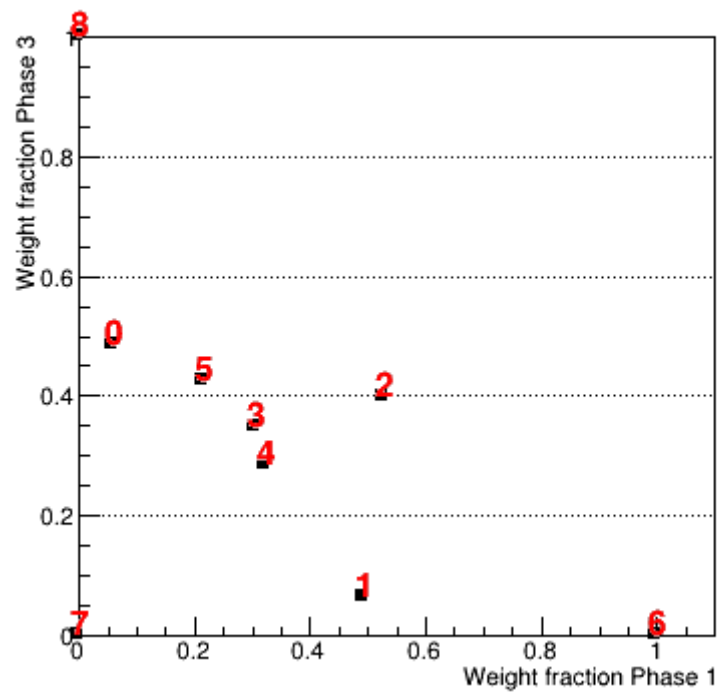
Fig.2 Quantitative Fit plot 1-2
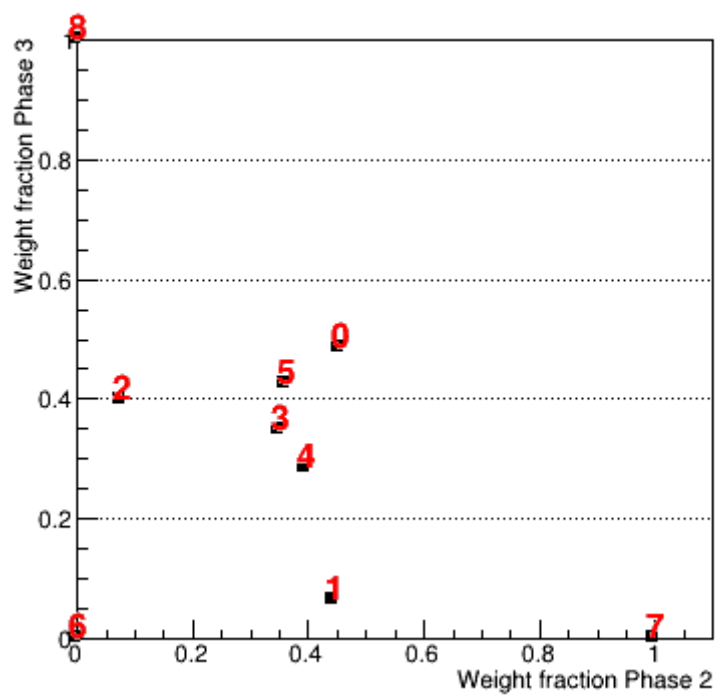

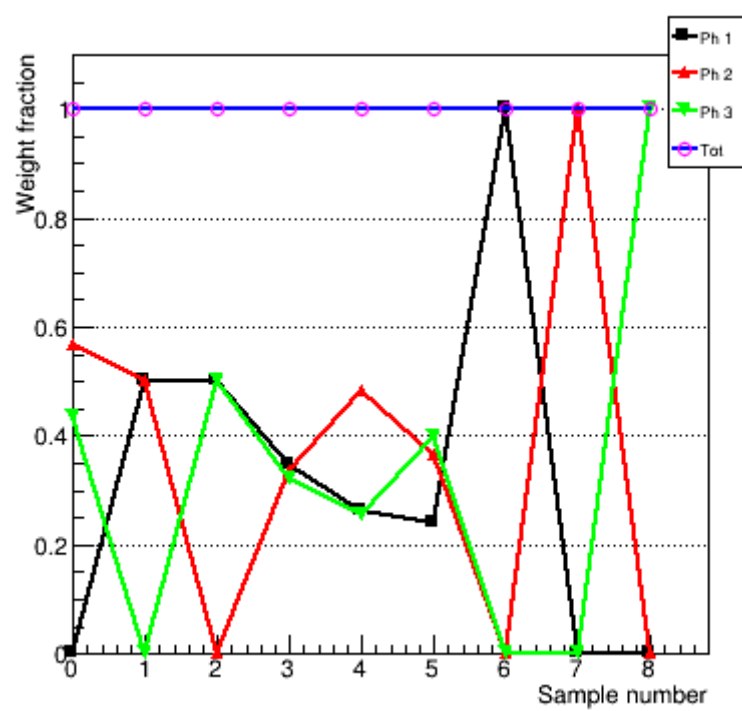Fig.3 Quantitative Fit plot 1-3

Fig.4 Quantitative Fit plot 2-3

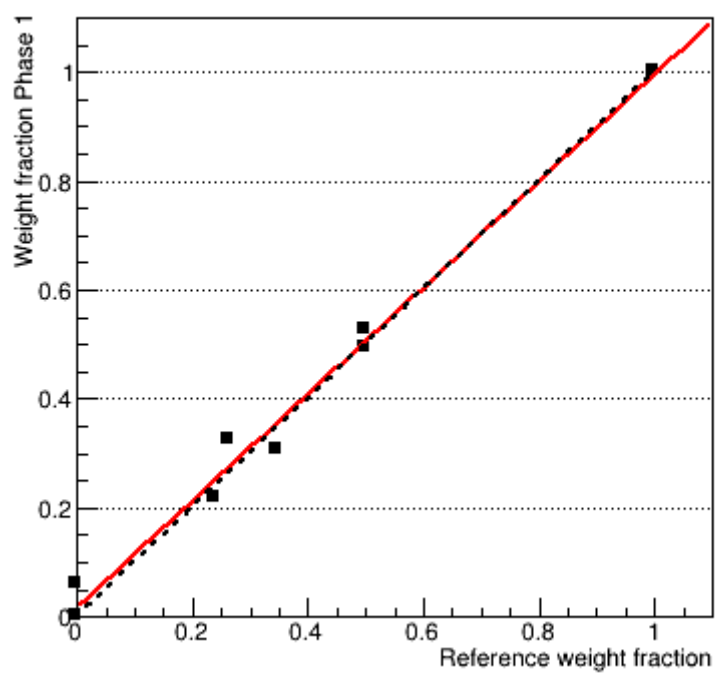Fig.5 Quantitative Fit graph (reference weight fractions)

Fig.6 Calibration plot Phase 1
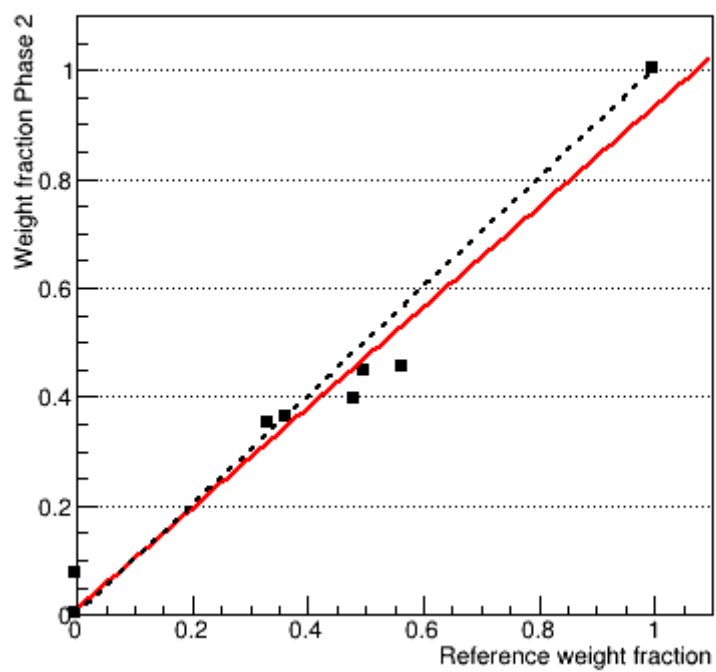
Fig.7 Calibration plot Phase 2
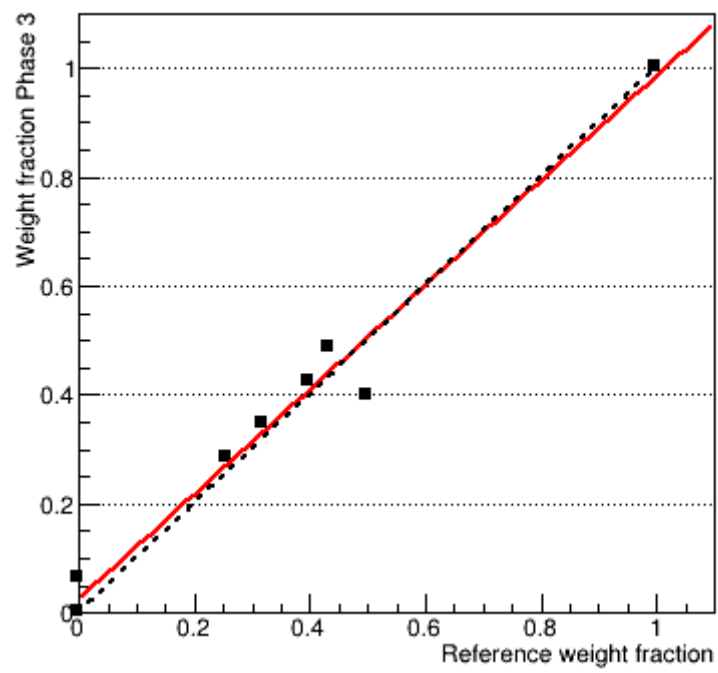
Fig.8 Calibration plot Phase 2
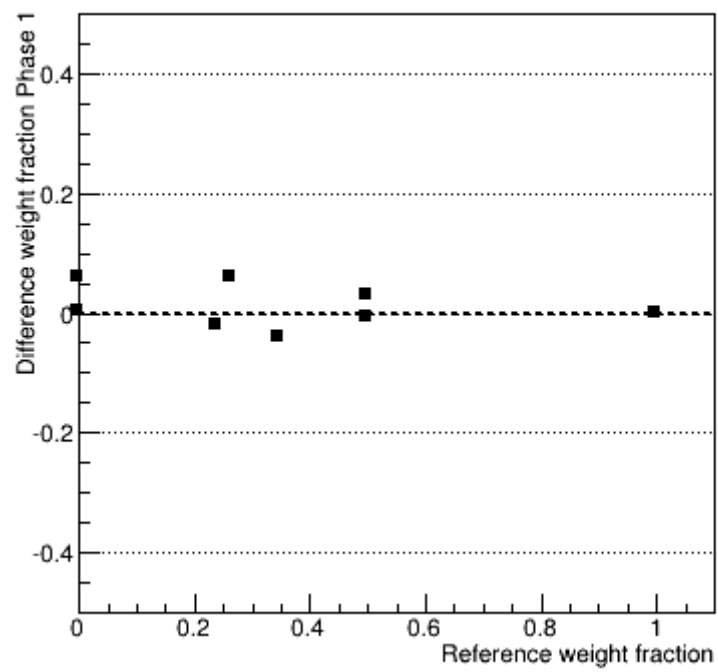
Fig.9 Difference plot Phase 1
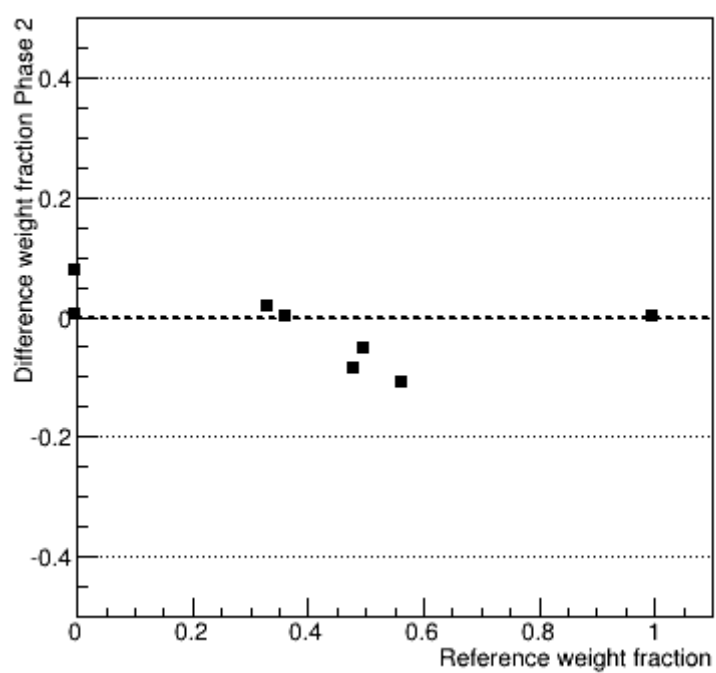
Fig.10 Difference plot Phase 2
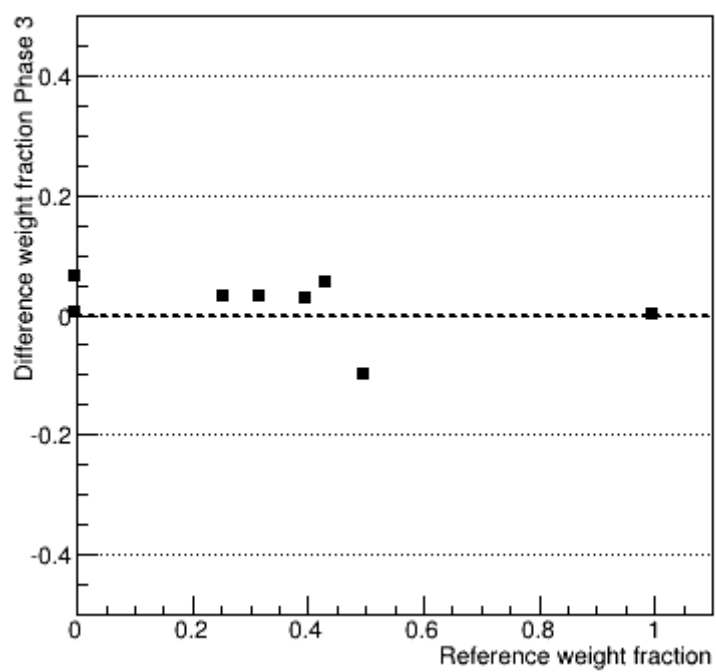
Fig.11 Difference plot Phase 3

The output file

The content of the output file named *outputQuantitativeUnfolding* is reported below, with comments added.

```
Input from file: fileInputQuantitativeUnfolding
-----------------------------
 whichanalysis 3

 unfold 1

 figpaper 1

 dataType 2

 range 10 50

 preprocess 0 2 100

 file  Rocco_S3_mac.txt

 referw 0 0.565 0.435

 file  Rocco_S5_mac.txt

 referw 0.5 0.5 0

 file  Rocco_S7_Como.txt

 referw 0.5 0 0.5

 file  Rocco_S11_mac.txt

 referw 0.347 0.334 0.319

 file  Rocco_S21_mac.txt

 referw 0.263 0.482 0.255

 file  Rocco_S22_mac.txt

 referw 0.238 0.364 0.399

 file  Rocco_CBZ_III_nomac.txt

 referw 1 0 0

 purephase

 file  Rocco_SAC_pura_nomac.txt

 referw 0 1 0

 purephase

 file  Rocco_CBZSAC_90511_n.txt

 purephase
```

```
  referw 0 0 1
```

The above section shows the commands read from the command file. It should be checked to ensure that they are interpreted correctly.

```
Reading input files:
 ----------------------
Sample 0 -> file Rocco_S3_mac.txt
         Found 1999  points
Sample 1 -> file Rocco_S5_mac.txt
         Found 1999  points
Sample 2 -> file Rocco_S7_Como.txt
         Found 1999  points
Sample 3 -> file Rocco_S11_mac.txt
         Found 1999  points
Sample 4 -> file Rocco_S21_mac.txt
         Found 1999  points
Sample 5 -> file Rocco_S22_mac.txt
         Found 1999  points
Sample 6 -> file Rocco_CBZ_III_nomac.txt
         Found 1999  points
Sample 7 -> file Rocco_SAC_pura_nomac.txt
         Found 1999  points
Sample 8 -> file Rocco_CBZSAC_90511_n.txt
         Found 1999  points
```

The above section reports the number of data points read within each input file.

```
Starting Quantitative analysis
```

```
UNFOLDING RESULTS:
 ------------------------
 Spectrum 0: Rocco_S3_mac.txt
 Weight fraction Phase 1  6181.286 + 0.000
 Weight fraction Phase 2  46952.293 + 0.000
 Weight fraction Phase 3  50353.484 + 0.000
 Rescaled weight fraction Phase 1  0.060 + 0.000
 Rescaled weight fraction Phase 2  0.454 + 0.000
 Rescaled weight fraction Phase 3  0.487 + 0.000
 ------------------------
 Spectrum 1: Rocco_S5_mac.txt
 Weight fraction Phase 1  47144.859 + 0.000
 Weight fraction Phase 2  42580.141 + 0.000
 Weight fraction Phase 3  6082.123 + 0.000
 Rescaled weight fraction Phase 1  0.492 + 0.000
 Rescaled weight fraction Phase 2  0.444 + 0.000
 Rescaled weight fraction Phase 3  0.063 + 0.000
 ------------------------
 Spectrum 2: Rocco_S7_Como.txt
 Weight fraction Phase 1  50416.996 + 0.000
 Weight fraction Phase 2  7133.152 + 0.000
 Weight fraction Phase 3  38147.168 + 0.000
 Rescaled weight fraction Phase 1  0.527 + 0.000
 Rescaled weight fraction Phase 2  0.075 + 0.000
 Rescaled weight fraction Phase 3  0.399 + 0.000
 ------------------------
 Spectrum 3: Rocco_S11_mac.txt
 Weight fraction Phase 1  29783.451 + 0.000
```

```
Weight fraction Phase 2  34026.340 + 0.000
Weight fraction Phase 3  33867.691 + 0.000
Rescaled weight fraction Phase 1  0.305 + 0.000
Rescaled weight fraction Phase 2  0.348 + 0.000
Rescaled weight fraction Phase 3  0.347 + 0.000
------------------------
Spectrum 4: Rocco_S21_mac.txt
Weight fraction Phase 1  34247.609 + 0.000
Weight fraction Phase 2  41771.691 + 0.000
Weight fraction Phase 3  30160.977 + 0.000
Rescaled weight fraction Phase 1  0.323 + 0.000
Rescaled weight fraction Phase 2  0.393 + 0.000
Rescaled weight fraction Phase 3  0.284 + 0.000
------------------------
Spectrum 5: Rocco_S22_mac.txt
Weight fraction Phase 1  24237.797 + 0.000
Weight fraction Phase 2  40614.102 + 0.000
Weight fraction Phase 3  47613.461 + 0.000
Rescaled weight fraction Phase 1  0.216 + 0.000
Rescaled weight fraction Phase 2  0.361 + 0.000
Rescaled weight fraction Phase 3  0.423 + 0.000
------------------------
Spectrum 6: Rocco_CBZ_III_nomac.txt
Weight fraction Phase 1  131060.422 + 0.000
Weight fraction Phase 2  36.072 + 0.000
Weight fraction Phase 3  76.670 + 0.000
Rescaled weight fraction Phase 1  0.999 + 0.000
Rescaled weight fraction Phase 2  0.000 + 0.000
Rescaled weight fraction Phase 3  0.001 + 0.000
------------------------
Spectrum 7: Rocco_SAC_pura_nomac.txt
Weight fraction Phase 1  106.049 + 0.000
Weight fraction Phase 2  119602.828 + 0.000
Weight fraction Phase 3  42.662 + 0.000
Rescaled weight fraction Phase 1  0.001 + 0.000
Rescaled weight fraction Phase 2  0.999 + 0.000
Rescaled weight fraction Phase 3  0.000 + 0.000
------------------------
Spectrum 8: Rocco_CBZSAC_90511_n.txt
Weight fraction Phase 1  41.899 + 0.000
Weight fraction Phase 2  8.069 + 0.000
Weight fraction Phase 3  120413.766 + 0.000
Rescaled weight fraction Phase 1  0.000 + 0.000
Rescaled weight fraction Phase 2  0.000 + 0.000
Rescaled weight fraction Phase 3  1.000 + 0.000
```

The above section reports the results of the fitting procedure applied to each input spectrum separately. The rescaled weights are reported.

```
  ------------------------------------
 Phase 1: RMSE=0.034 RMSE'=0.033 R2=0.989 R2(NPP)=0.950 AKLD=0.026
     Calibration fit: Chi-Square=9.13e-03 intercept=0.015+0.017
slope=0.977+0.039
     Limits estimates: LOD=5.84  LOQ=17.71
 NPP: Calibration fit: Chi-Square=7.54e-03 intercept=0.043+0.036
slope=0.901+0.103
 NPP: Limits estimates: LOD=13.32  LOQ=40.38
  ------------------------------------
 Phase 2: RMSE=0.057 RMSE'=0.063 R2=0.973 R2(NPP)=0.969 AKLD=0.050
```

```
        Calibration fit: Chi-Square=2.04e-02 intercept=0.010+0.027
slope=0.921+0.058
        Limits estimates: LOD=9.85  LOQ=29.85
 NPP: Calibration fit: Chi-Square=2.98e-03 intercept=0.092+0.025
slope=0.678+0.060
 NPP: Limits estimates: LOD=12.23  LOQ=37.06
   ----------------------------------
 Phase 3: RMSE=0.046 RMSE'=0.050 R2=0.978 R2(NPP)=0.901 AKLD=0.040
        Calibration fit: Chi-Square=1.68e-02 intercept=0.024+0.024
slope=0.959+0.054
        Limits estimates: LOD=8.21  LOQ=24.89
 NPP: Calibration fit: Chi-Square=1.10e-02 intercept=0.081+0.047
slope=0.795+0.132
 NPP: Limits estimates: LOD=19.55  LOQ=59.25
   ----------------------------------
 Overall agreement: FOM=0.137 AKLD: 0.116
```

The above section includes the comparison between the phase abundances estimated by RootProf and the reference ones. The quantities reported are the same as those described in Chapter 2. Here it is interesting to note the very small differences with respect to the values obtained by MultiFit (Chapter 2). The overall AKLD is worse than that obtained by MultiFit (0.108).

Chapter 5

Combined quantitative analysis: MultiFit + Unfolding

Motivation

Combine quantitative estimates obtained by the MultiFit approach with those obtained by the Unfolding algorithm.

The command file

The input command file is *fileInputQuantitativeComb*, reported here below:

```
whichanalysis 3
unfold 2
figpaper 1
dataType 2
range 10 50
preprocess 0 2 100
file  Rocco_S3_mac.txt
referw 0 0.565 0.435
file  Rocco_S5_mac.txt
referw 0.5 0.5 0
file  Rocco_S7_Como.txt
referw 0.5 0 0.5
file  Rocco_S11_mac.txt
referw 0.347 0.334 0.319
file  Rocco_S21_mac.txt
referw 0.263 0.482 0.255
file  Rocco_S22_mac.txt
referw 0.238 0.364 0.399
file  Rocco_CBZ_III_nomac.txt
referw 1 0 0
purephase
file  Rocco_SAC_pura_nomac.txt
referw 0 1 0
purephase
file  Rocco_CBZSAC_90511_n.txt
purephase
referw 0 0 1
```

They have been included in the demo file named *fileInputQuantitativeComb*. See the user guide for an explanation of each command. The combined approach MultiFit+Unfolding is triggered by using the command *unfold* 2.

Running RootProf

Start ROOT by clicking on his icon, or by typing "root" on a terminal window. Then write the root command:

Root> .x RootProf.C("fileInputQuantitativeComb")

or

Root> .> outputQuantitativeComb

.x RootProf.C("fileInputQuantitativeComb")

.>

After some seconds, graphic windows will start appearing on your screen, while text output will appear on the text window, or redirected in the file named *outputQuantitativeComb*. When the run ends, the root prompt will appear again on the ROOT terminal, and you are able to edit each single graphic window and read the output file by your text editor.

The graphic output

The graphic output is the same as that described in Chapters 1 and 2.

The output file

The output file, named *outputQuantitativeComb,* is reported in the following:

```
 Input from file: fileInputQuantitativeComb
-----------------------------
  whichanalysis 3

  unfold 2

  figpaper 1

  dataType 2

  range 10 50

  preprocess 0 2 100

  file  Rocco_S3_mac.txt

  referw 0 0.565 0.435

  file  Rocco_S5_mac.txt

  referw 0.5 0.5 0

  file  Rocco_S7_Como.txt

  referw 0.5 0 0.5

  file  Rocco_S11_mac.txt

  referw 0.347 0.334 0.319
```

```
file  Rocco_S21_mac.txt

referw 0.263 0.482 0.255

file  Rocco_S22_mac.txt

referw 0.238 0.364 0.399

file  Rocco_CBZ_III_nomac.txt

referw 1 0 0

purephase

file  Rocco_SAC_pura_nomac.txt

referw 0 1 0

purephase

file  Rocco_CBZSAC_90511_n.txt

purephase

referw 0 0 1
```

The above section shows the commands read from the command file. It should be checked to ensure that they are interpreted correctly.

```
Reading input files:
 ---------------------
Sample 0 -> file Rocco_S3_mac.txt
        Found 1999  points
Sample 1 -> file Rocco_S5_mac.txt
        Found 1999  points
Sample 2 -> file Rocco_S7_Como.txt
        Found 1999  points
Sample 3 -> file Rocco_S11_mac.txt
        Found 1999  points
Sample 4 -> file Rocco_S21_mac.txt
        Found 1999  points
Sample 5 -> file Rocco_S22_mac.txt
        Found 1999  points
Sample 6 -> file Rocco CBZ III_nomac.txt
        Found 1999  points
Sample 7 -> file Rocco_SAC_pura_nomac.txt
        Found 1999  points
Sample 8 -> file Rocco_CBZSAC_90511_n.txt
        Found 1999  points
```

The above section reports the number of data points read within each input file.

```
Starting Quantitative analysis

 FIT RESULTS:
 ------------------------
 Spectrum 0: Rocco_S3_mac.txt
```

```
Chi-Square=4.23e+02, Reduced Chi-Square=2.12e-01, NDF=1995
Weight fraction Phase 1  0.043 +- 0.006
Weight fraction Phase 2  0.390 +- 0.005
Weight fraction Phase 3  0.411 +- 0.008
Total weight fraction 0.844 +- 0.011
Rescaled weight fraction Phase 1  0.051 +- 0.007
Rescaled weight fraction Phase 2  0.462 +- 0.006
Rescaled weight fraction Phase 3  0.487 +- 0.007
------------------------
Spectrum 1: Rocco_S5_mac.txt
Chi-Square=1.28e+03, Reduced Chi-Square=6.42e-01, NDF=1995
Weight fraction Phase 1  0.342 +- 0.011
Weight fraction Phase 2  0.347 +- 0.008
Weight fraction Phase 3  0.022 +- 0.014
Total weight fraction 0.710 +- 0.019
Rescaled weight fraction Phase 1  0.481 +- 0.013
Rescaled weight fraction Phase 2  0.488 +- 0.013
Rescaled weight fraction Phase 3  0.031 +- 0.019
------------------------
Spectrum 2: Rocco_S7_Como.txt
Chi-Square=6.49e+02, Reduced Chi-Square=3.25e-01, NDF=1995
Weight fraction Phase 1  0.374 +- 0.008
Weight fraction Phase 2  0.054 +- 0.006
Weight fraction Phase 3  0.300 +- 0.010
Total weight fraction 0.729 +- 0.014
Rescaled weight fraction Phase 1  0.513 +- 0.010
Rescaled weight fraction Phase 2  0.075 +- 0.008
Rescaled weight fraction Phase 3  0.412 +- 0.010
------------------------
Spectrum 3: Rocco_S11_mac.txt
Chi-Square=3.94e+02, Reduced Chi-Square=1.98e-01, NDF=1995
Weight fraction Phase 1  0.220 +- 0.006
Weight fraction Phase 2  0.281 +- 0.005
Weight fraction Phase 3  0.270 +- 0.008
Total weight fraction 0.771 +- 0.011
Rescaled weight fraction Phase 1  0.286 +- 0.007
Rescaled weight fraction Phase 2  0.364 +- 0.006
Rescaled weight fraction Phase 3  0.350 +- 0.007
------------------------
Spectrum 4: Rocco_S21_mac.txt
Chi-Square=6.86e+02, Reduced Chi-Square=3.44e-01, NDF=1995
Weight fraction Phase 1  0.257 +- 0.008
Weight fraction Phase 2  0.347 +- 0.006
Weight fraction Phase 3  0.243 +- 0.010
Total weight fraction 0.846 +- 0.014
Rescaled weight fraction Phase 1  0.303 +- 0.008
Rescaled weight fraction Phase 2  0.410 +- 0.008
Rescaled weight fraction Phase 3  0.287 +- 0.009
------------------------
Spectrum 5: Rocco_S22_mac.txt
Chi-Square=3.83e+02, Reduced Chi-Square=1.92e-01, NDF=1995
Weight fraction Phase 1  0.187 +- 0.006
Weight fraction Phase 2  0.340 +- 0.005
Weight fraction Phase 3  0.398 +- 0.007
Total weight fraction 0.925 +- 0.011
Rescaled weight fraction Phase 1  0.202 +- 0.006
Rescaled weight fraction Phase 2  0.368 +- 0.005
Rescaled weight fraction Phase 3  0.430 +- 0.006
------------------------
Spectrum 6: Rocco_CBZ_III_nomac.txt
```

```
Chi-Square=1.26e-06, Reduced Chi-Square=6.32e-10, NDF=1995
Weight fraction Phase 1  1.000 +- 0.000
Weight fraction Phase 2  0.000 +- 0.000
Weight fraction Phase 3  0.000 +- 0.000
Total weight fraction 1.000 +- 0.000
Rescaled weight fraction Phase 1  1.000 +- 0.000
Rescaled weight fraction Phase 2  0.000 +- 0.000
Rescaled weight fraction Phase 3  0.000 +- 0.000
-----------------------
Spectrum 7: Rocco_SAC_pura_nomac.txt
Chi-Square=1.68e-06, Reduced Chi-Square=8.44e-10, NDF=1995
Weight fraction Phase 1  0.000 +- 0.000
Weight fraction Phase 2  1.000 +- 0.000
Weight fraction Phase 3  0.000 +- 0.000
Total weight fraction 1.000 +- 0.000
Rescaled weight fraction Phase 1  0.000 +- 0.000
Rescaled weight fraction Phase 2  1.000 +- 0.000
Rescaled weight fraction Phase 3  0.000 +- 0.000
-----------------------
Spectrum 8: Rocco_CBZSAC_90511_n.txt
Chi-Square=1.18e-06, Reduced Chi-Square=5.92e-10, NDF=1995
Weight fraction Phase 1  0.000 +- 0.000
Weight fraction Phase 2  0.000 +- 0.000
Weight fraction Phase 3  1.000 +- 0.000
Total weight fraction 1.000 +- 0.000
Rescaled weight fraction Phase 1  0.000 +- 0.000
Rescaled weight fraction Phase 2  0.000 +- 0.000
Rescaled weight fraction Phase 3  1.000 +- 0.000
```

The above section reports the results of the MultiFit fitting procedure.

```
UNFOLDING RESULTS:
-----------------------
Spectrum 0: Rocco_S3_mac.txt
Weight fraction Phase 1  6181.286 +- 0.000
Weight fraction Phase 2  46952.293 +- 0.000
Weight fraction Phase 3  50353.484 +- 0.000
Rescaled weight fraction Phase 1  0.060 +- 0.000
Rescaled weight fraction Phase 2  0.454 +- 0.000
Rescaled weight fraction Phase 3  0.487 +- 0.000
-----------------------
Spectrum 1: Rocco_S5_mac.txt
Weight fraction Phase 1  47144.859 +- 0.000
Weight fraction Phase 2  42580.141 +- 0.000
Weight fraction Phase 3  6082.123 +- 0.000
Rescaled weight fraction Phase 1  0.492 +- 0.000
Rescaled weight fraction Phase 2  0.444 +- 0.000
Rescaled weight fraction Phase 3  0.063 +- 0.000
-----------------------
Spectrum 2: Rocco_S7_Como.txt
Weight fraction Phase 1  50416.996 +- 0.000
Weight fraction Phase 2  7133.152 +- 0.000
Weight fraction Phase 3  38147.168 +- 0.000
Rescaled weight fraction Phase 1  0.527 +- 0.000
Rescaled weight fraction Phase 2  0.075 +- 0.000
Rescaled weight fraction Phase 3  0.399 +- 0.000
-----------------------
Spectrum 3: Rocco_S11_mac.txt
Weight fraction Phase 1  29783.451 +- 0.000
```

```
 Weight fraction Phase 2  34026.340 +- 0.000
 Weight fraction Phase 3  33867.691 +- 0.000
 Rescaled weight fraction Phase 1  0.305 +- 0.000
 Rescaled weight fraction Phase 2  0.348 +- 0.000
 Rescaled weight fraction Phase 3  0.347 +- 0.000
 -----------------------
 Spectrum 4: Rocco_S21_mac.txt
 Weight fraction Phase 1  34247.609 +- 0.000
 Weight fraction Phase 2  41771.691 +- 0.000
 Weight fraction Phase 3  30160.977 +- 0.000
 Rescaled weight fraction Phase 1  0.323 +- 0.000
 Rescaled weight fraction Phase 2  0.393 +- 0.000
 Rescaled weight fraction Phase 3  0.284 +- 0.000
 -----------------------
 Spectrum 5: Rocco_S22_mac.txt
 Weight fraction Phase 1  24237.797 +- 0.000
 Weight fraction Phase 2  40614.102 +- 0.000
 Weight fraction Phase 3  47613.461 +- 0.000
 Rescaled weight fraction Phase 1  0.216 +- 0.000
 Rescaled weight fraction Phase 2  0.361 +- 0.000
 Rescaled weight fraction Phase 3  0.423 +- 0.000
 -----------------------
 Spectrum 6: Rocco_CBZ_III_nomac.txt
 Weight fraction Phase 1  131060.422 +- 0.000
 Weight fraction Phase 2  36.072 +- 0.000
 Weight fraction Phase 3  76.670 +- 0.000
 Rescaled weight fraction Phase 1  0.999 +- 0.000
 Rescaled weight fraction Phase 2  0.000 +- 0.000
 Rescaled weight fraction Phase 3  0.001 +- 0.000
 -----------------------
 Spectrum 7: Rocco_SAC_pura_nomac.txt
 Weight fraction Phase 1  106.049 +- 0.000
 Weight fraction Phase 2  119602.828 +- 0.000
 Weight fraction Phase 3  42.662 +- 0.000
 Rescaled weight fraction Phase 1  0.001 +- 0.000
 Rescaled weight fraction Phase 2  0.999 +- 0.000
 Rescaled weight fraction Phase 3  0.000 +- 0.000
 -----------------------
 Spectrum 8: Rocco_CBZSAC_90511_n.txt
 Weight fraction Phase 1  41.899 +- 0.000
 Weight fraction Phase 2  8.069 +- 0.000
 Weight fraction Phase 3  120413.766 +- 0.000
 Rescaled weight fraction Phase 1  0.000 +- 0.000
 Rescaled weight fraction Phase 2  0.000 +- 0.000
 Rescaled weight fraction Phase 3  1.000 +- 0.000
```

The above section reports the results of the Unfolding fitting procedure.

```
Combining MultiFit with Unfolding estimates
  ----------------------------------
 Phase 1: RMSE=0.033 RMSE'=0.033 R2=0.989 R2(NPP)=0.949 AKLD=0.028
     Calibration fit: Chi-Square=9.14e-03 intercept=0.010+-0.017
slope=0.978+-0.039
     Limits estimates: LOD=5.84  LOQ=17.71
 NPP: Calibration fit: Chi-Square=7.69e-03 intercept=0.036+-0.037
slope=0.899+-0.104
 NPP: Limits estimates: LOD=13.49  LOQ=40.89
  ----------------------------------
 Phase 2: RMSE=0.053 RMSE'=0.057 R2=0.976 R2(NPP)=0.964 AKLD=0.044
```

```
     Calibration fit: Chi-Square=1.87e-02 intercept=0.013+-0.026
slope=0.927+-0.055
     Limits estimates: LOD=9.37  LOQ=28.40
 NPP: Calibration fit: Chi-Square=3.78e-03 intercept=0.092+-0.028
slope=0.698+-0.068
 NPP: Limits estimates: LOD=13.38  LOQ=40.54
  ----------------------------------
 Phase 3: RMSE=0.043 RMSE'=0.049 R2=0.981 R2(NPP)=0.911 AKLD=0.040
     Calibration fit: Chi-Square=1.46e-02 intercept=0.021+-0.022
slope=0.968+-0.050
     Limits estimates: LOD=7.60  LOQ=23.04
 NPP: Calibration fit: Chi-Square=1.08e-02 intercept=0.067+-0.047
slope=0.837+-0.131
 NPP: Limits estimates: LOD=18.40  LOQ=55.76
  ----------------------------------
 Overall agreement: FOM=0.128 AKLD: 0.112
```

The above section includes the comparison between the phase abundances estimated by RootProf+Unfolding and the reference ones. The quantities reported are the same as those described in Chapter 2. Here it is interesting to note the very small differences with respect to the values obtained by MultiFit (Chapter 2), and by Unfolding (paragraph above) separately. The overall AKLD is intermediate between those obtained by MultiFit (0.108) and by Unfolding (0.116).