Chemoface

TUTRIAL & CASE STUDIES

Installing

Chemoface was developed on the MATLAB environment.
It is a stand-alone application and does not require a MATLAB license installation to run.

Installation on Microsoft Windows(32 or 64 bits): http://www.ufla.br/chemoface/
Downloadand install MCR.⬚Download and install Chemoface

Running

Access the modules from Chemoface home screen (Figure 1).

A screen resolution lower than 1024x768 is not recommended.
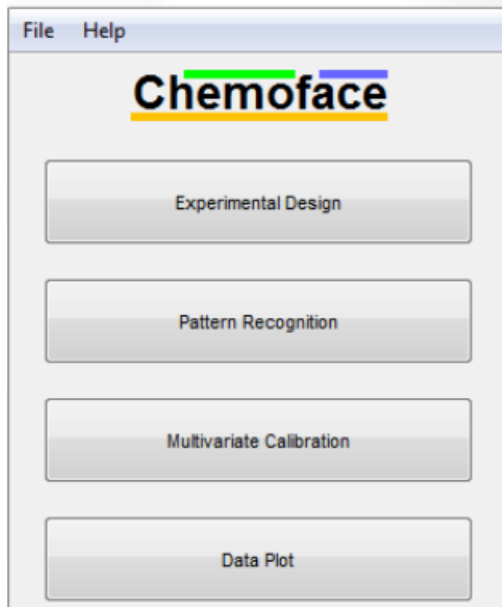
Chemoface uses dot (.) as decimal mark.

Figure 1.Chemoface home screen

Designing the experiment

- Select the design type (1).
- Select the number of factors (2).
- Select the number of replications for the response (dependent variable) (3).
- If appropriate, add central point (4) and select the number of replications (5).
- If Fractional Factorial is used, select the size of the fraction (6).
- If Mixture Design is used, select the Simplex type (7).

- Set the label of the response and the labels and levelsfor the factors (8).

- Note:If Full, Fractional, Central Composite or Plackett-Burman is used, provide only values for -1 and +1; additional levels (e.g. axial and central points) are automatically calculated.

- If Mixture Design is used, provide values ranging from 0 to 1; constraintscan be used, providing values>0 and/or <1.

- If Plackett-Burman is used, dummy factors are just left empty. Press Design button (9).

- Note:It is possible to alternate between coded and uncoded factor levels using menu Edit> Alternate coded-uncoed variables.

- The model will be fitted according to the provided levels (coded or uncoded).

<u>Inserting the responses</u>
Insert the responses (dependent variable) typing it on the table (10) or paste from a spread sheet using menu File> Paste responses.
Analyzing the design(not applicable toMixture Design)
Select the error type (11) and the confidencelevel (12).
Press Effectsbutton (13) to obtain the effects table (Figure 3A).
Press Pareto's Chartbutton (14) to obtain a Pareto's graph for the effects (Figure 3B).

File   Edit   Tools

Design Settings

Design Type: Central Composite **1**

N. of Factors: 3 **2**

N. of Replications: 1 **3**

4 ☑ Central Points: 3 **5**

Fraction Size: -1 **6**

Simplex Type: Lattice - 6 points **7**

	Labels	(-1)	(+1)
Y	Yeld(%)	---	---
X1	Temp.(°C)	35	50
X2	Time(h)	1	2
X3	Stir.(RPM)	100	200
X4			
X5			
X6			
X7			
X8			

8

Provide only –1 and +1 levels. Axial points are automatically calculated.

9 Design

Experimental Design

	Temp.(°C)	Time(h)	Stir.(RPM)	Yeld(%) 1
1	35	1	100	45
2	35	1	200	53
3	35	2	100	54
4	35	2	200	54
5	50	1	100	48
6	50	1	200	52
7	50	2	100	55
8	50	2	200	57
9	29.8866	1.5000	150	50
10	55.1134	1.5000	150	57
11	42.5000	0.6591	150	46
12	42.5000	2.3409	150	58
13	42.5000	1.5000	65.9104	50
14	42.5000	1.5000	234.0896	56
15	42.5000	1.5000	150	56
16	42.5000	1.5000	150	55
17	42.5000	1.5000	150	57

10

Design Analysis

Error based on: Pure Error **11**

Confidence level (%): ◄ **12** ► 95

Factor Effects

13 Effects   Pareto's Chart **14**

Surface

Model: Quadratic **15**

16 Coefficients

21 Surface   Type: 3D sur... **19**

X: Temp.(... **20**

22 Meas. x Pred.   Y: Time(h)

☑ Plot experimental responses **17**

☐ Ignore non-significant coefficients **18**

	Effect	Error	t	p	significant
Temp.(°C)(X1)	2.6027	0.5412	4.8092	0.0406	yes
Time(h)(X2)	6.1773	0.5412	11.4142	0.0076	yes
Stir.(RPM)(X3)	3.5280	0.5412	6.5189	0.0227	yes
X1*X2	0.5000	0.7071	0.7071	0.5528	no
X1*X3	-0.5000	0.7071	-0.7071	0.5528	no
X2*X3	-2.5000	0.7071	-3.5355	0.0715	no

A
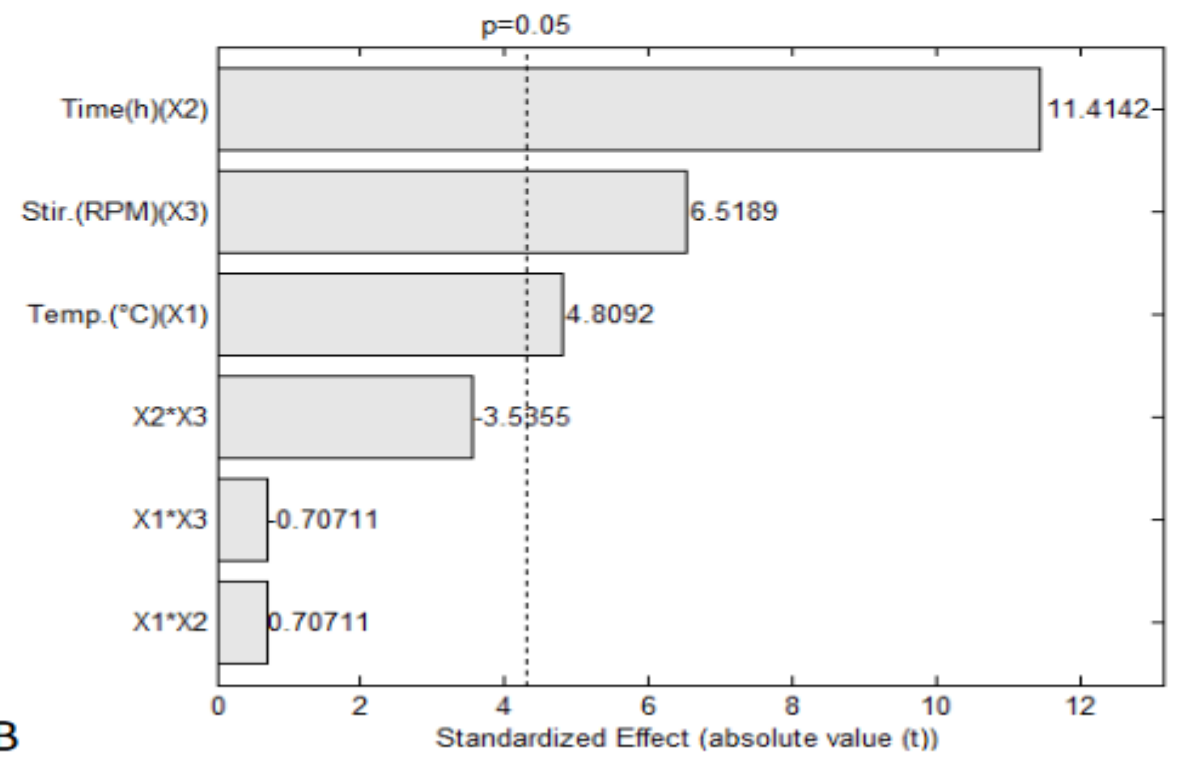
B

Figure 3. Table and graph for the effects

Building model and response surfaces(not applicable to *Fractional and Plackett-Burman* designs)

- Select the model type (15).
- Press Coefficients button(16) to obtain a table with the model coefficients (Figure 4A).
- Choose if experimental responses should be plotted (17) and if only significant coefficients (18) should be used for model fit.
- Select the graph type (19).
- For design with more than two factors, select the factors to be plotted (20) and set the level of the no plotted factor(s)(Figure 4B).
- Press Surface Plot button (21) to obtain the graph and the statistics for the model (Figure 4C-D).
- Press Meas. x Pred. button (22) to obtain the graph for measured x predicted values (Figure 4E)

b0(X=1)	-32.1661	14.6761	-2.1917	0.1597	no
Temp.(°C)(X1)	1.6404	0.4938	3.3219	0.0799	no
Time(h)(X2)	28.8569	5.7984	4.9767	0.0381	yes
Stir.(RPM)(X3)	0.2763	0.0580	4.7653	0.0413	yes
X1*X2	0.0667	0.0943	0.7071	0.5528	no
X1*X3	-6.6667e-04	9.4281e-04	-0.7071	0.5528	no
X2*X3	-0.0500	0.0141	-3.5355	0.0715	no
X1²	-0.0173	0.0053	-3.2594	0.0826	no
X2²	-6.0043	1.1913	-5.0400	0.0372	yes
X3²	-4.5901e-04	1.1913e-04	-3.8529	0.0612	no

A

B

Set value for Stir.(RPM):

150

OK   Cancel
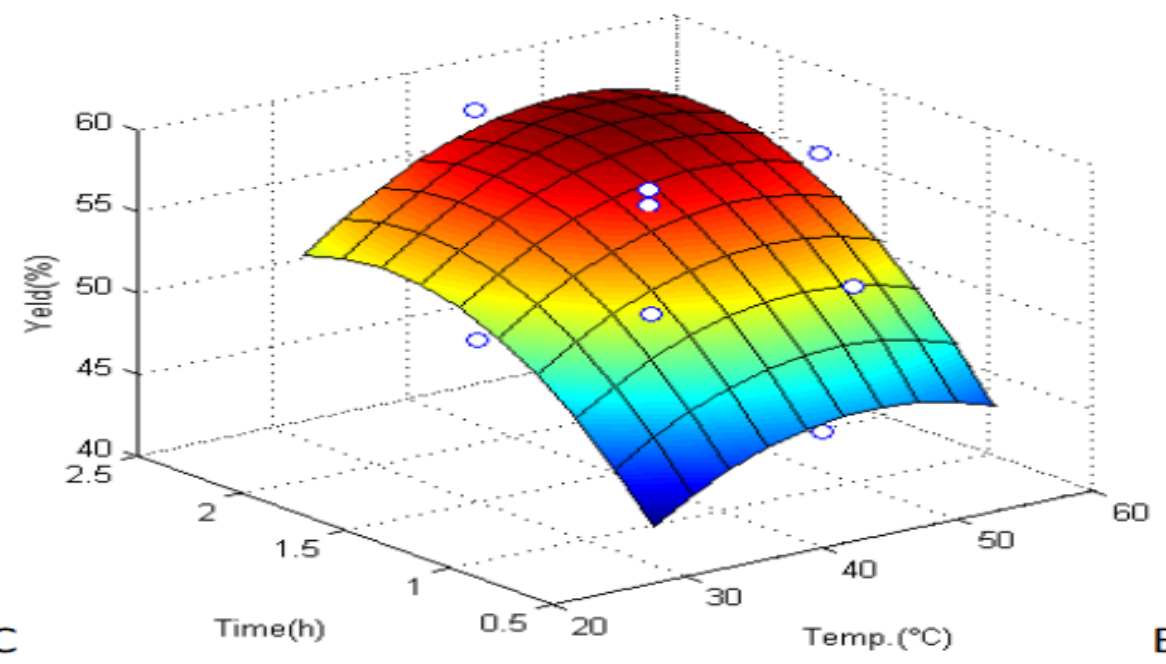
C
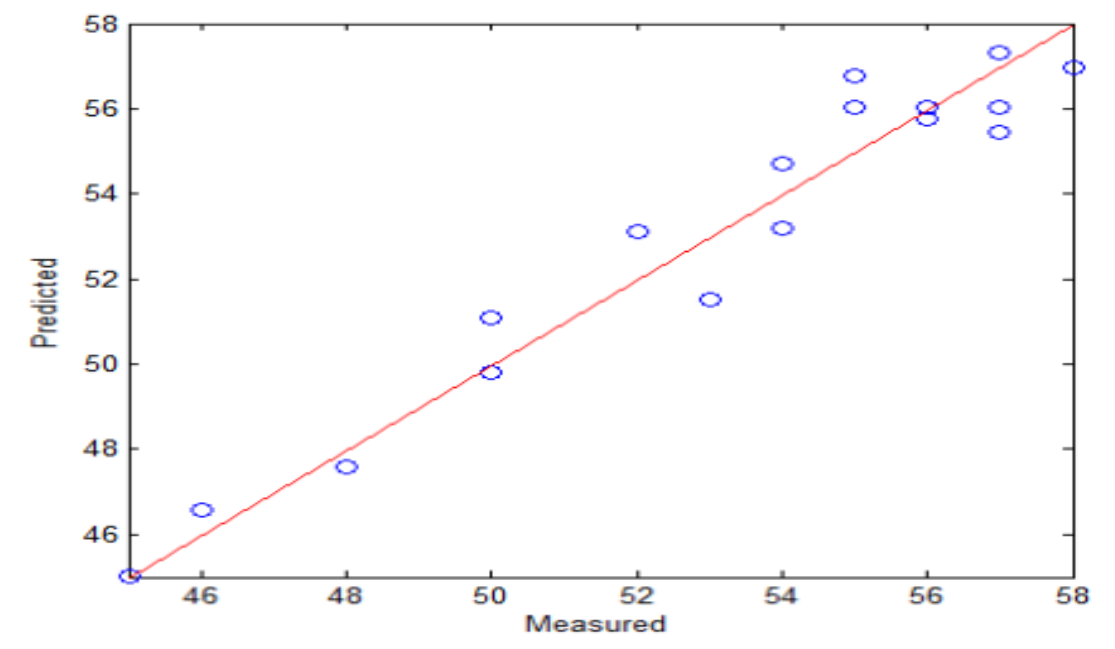
E

Figure 4.Tables and graph for the model

Additional features

- All obtained tables can be copied using menu Edit> Copy...
- A designed experiment can be saved using menu
- File> Save data.
- Later, this file can be opened using menu File> Open data.
- Experimental assays for a Mixture design can be plotted using menu Tools> Experimental points.
- Desirability functions can be used to combine multiple responses using menu Tools> Desirability Function(Figure 5).
- Insert each response set pasting it from a spreadsheet using menu File> Paste responses. Allocate replications abreast (In example, there are two replications, (1)).

Desirability fucntion

- Set optimization direction (2), the response name (3), the limit ranges (4), and the desirability power (5).

- Press Add>>button(6) to compute the desirability values for this response (7)

- and the global desirability (8).

- To compute a new response set, proceed similarly starting by menu File> Paste responses. When all response sets were added, copy the global desirability using Copy Global Desirability button (9).

- The copied desirability can be inserted as responses in the design table (Experimental Design module) using File> Paste responses
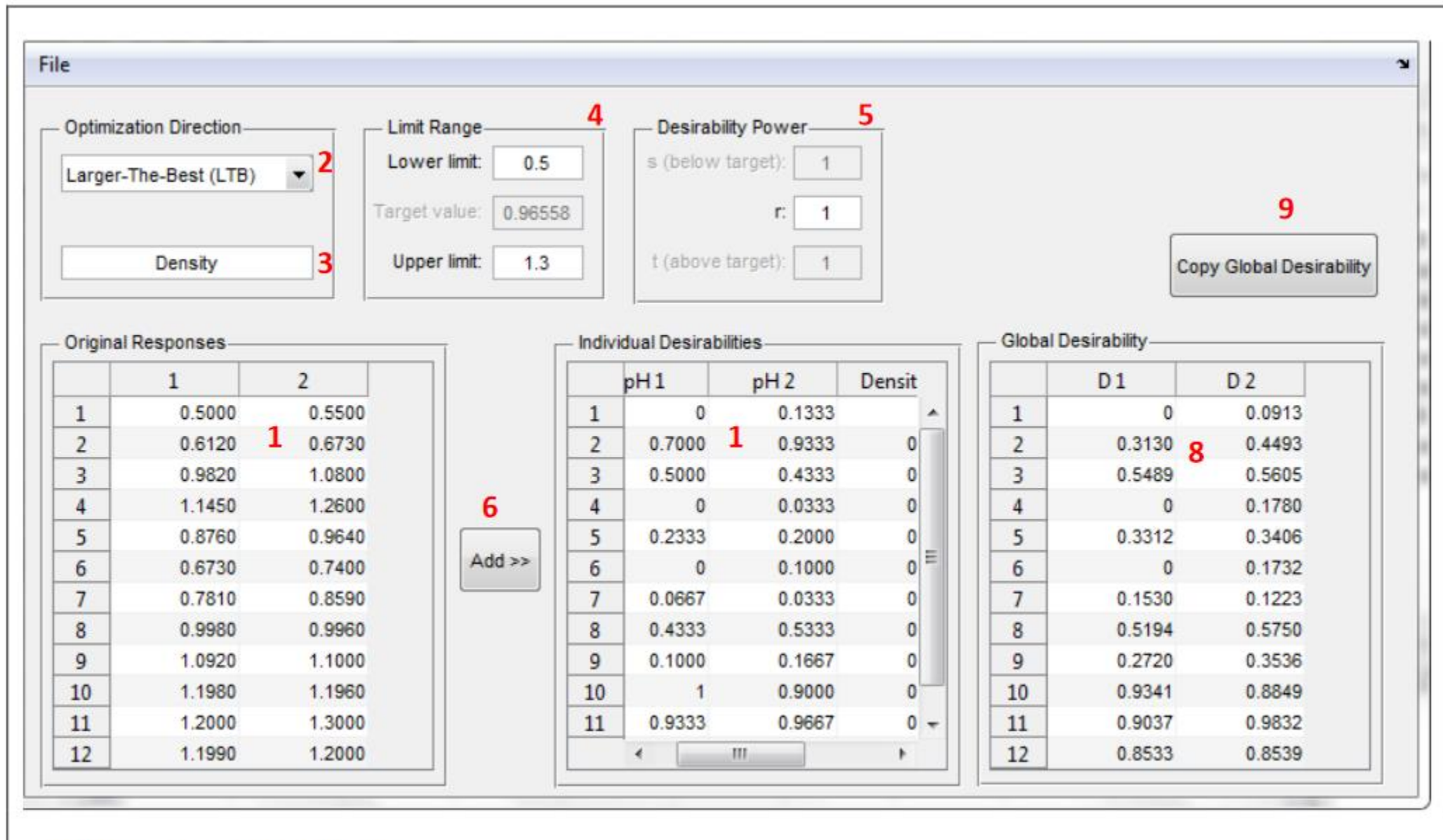
Figure 5. Desirability function

Pattern Recognition

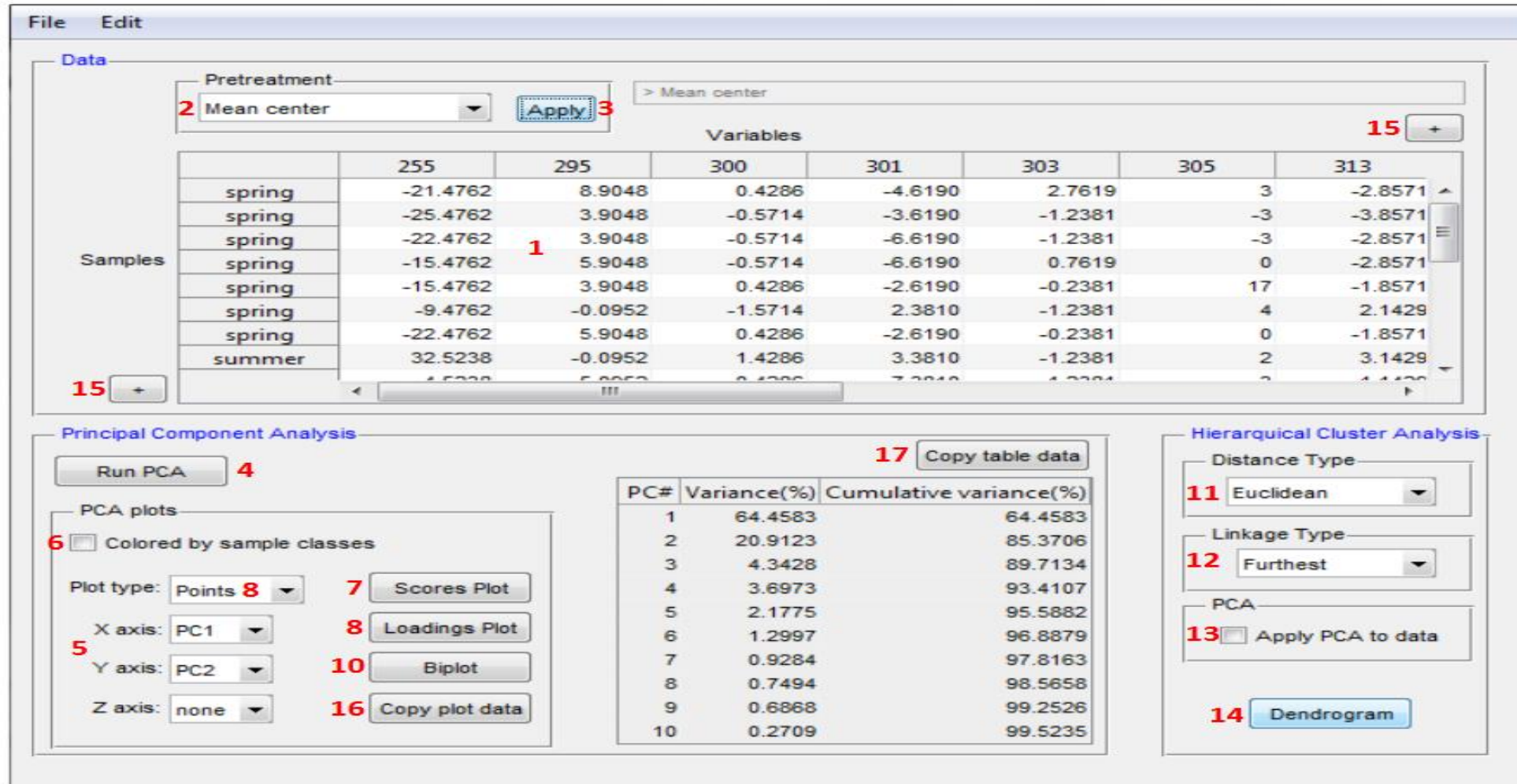**Figure 6.** Pattern recognition by PCA and HCA

Inserting data set

- Type data on the table (1) or paste it from a spreadsheet (or from Data Organization module)usingmenu File> Paste data. Only numeric data should be inserted. Use sample in rows and variables in columns.

- If appropriate, insert sample labels using menu Edit> Sample labels or classes. If there are sample classes, it can be inserted similarly (Figure 7A).

- If appropriated, insert variable labels using menu Edit> Variable labels. If dataset is from continuous variables, use > Continuous variables (Figure 7C) and insert the range. If dataset is from discrete variables, use > Generic variables(Figure 7B).
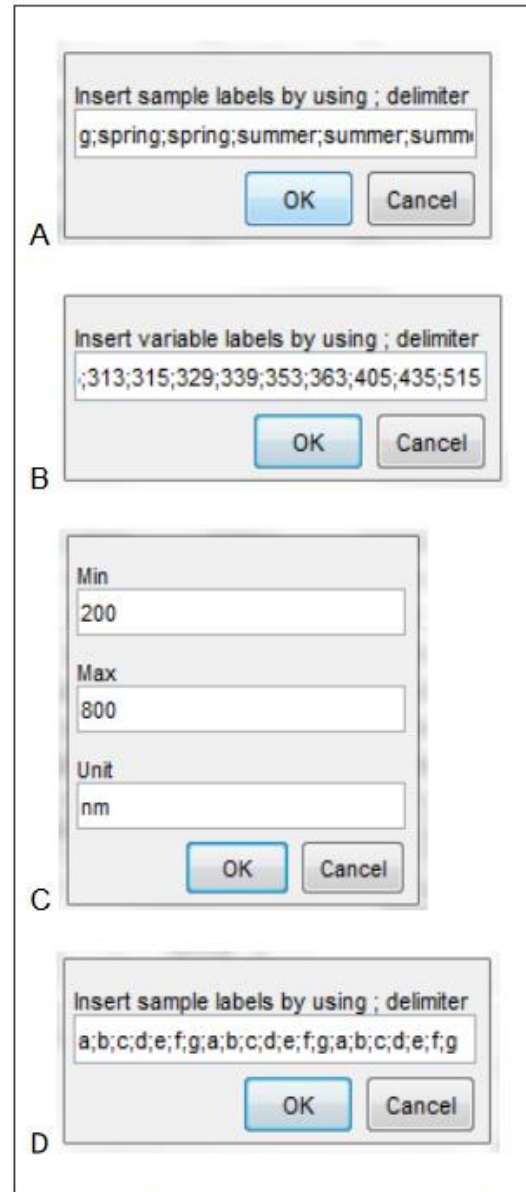
- Note: if labels are not provided, these are numbered.!!!

Figure 7. Inserting sample and variable labels

Data pretreatment

- Select the pretreatment method (2).

- Press Applybutton (3).

- Note:Multiple pretreatment methods can be applied just by selecting the mand pressing Apply. To return to the original data after a pretreatment, select "No preprocess" and press Apply

Performing PCA

- Press Run PCA button (4).

- Select PC to be plotted on X and Y axis (5). If a 2D plot is used, select PC to be plotted on X and Yaxis and set Z axis in "none". However, for a 3D plot (Figure 8D), select the PC to be plotted on all 3 axis: X, Y and Z.

- Note: If sample classes are provided, they may be colored on the scores plot: select "Colored by sample classes"(6).

- Optionally sample labels also can be inserted: just provide the labels when solicited (Figure 7D).

- For scores graph, press Scores plot button (7)(Figure 8A).

- For loadings graph (Figure 8B), select the plot type: points or vectors (8).

- Press Loadings plot button (9)

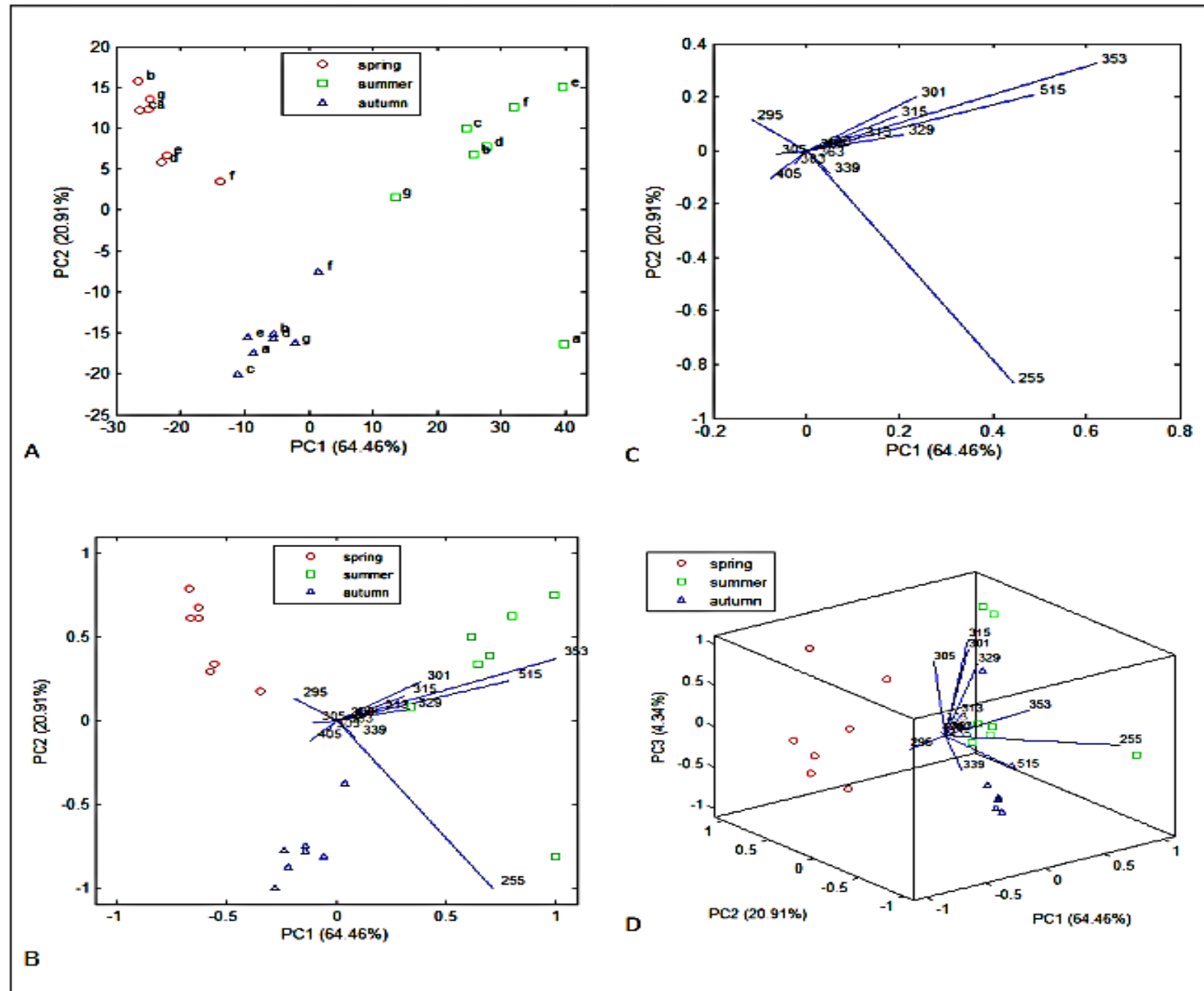- **For a scores and loadings graph (Figure 8C), press Biplot button (10)**

Figure 8. PCA plots

Performing HCA

- Select the distance type (11).
- Select the linkage type (12).
- Note:Optionally PCA can be preciously applied to HCA:
- select Apply PCA to data (13) and select the number of PC to be used when solicited.
- Press Dendrogram button (14) to run HCA and obtain the dendrogram (Figure 9B).
- Insert the threshold to color the similar groups (Figure 9A). ,
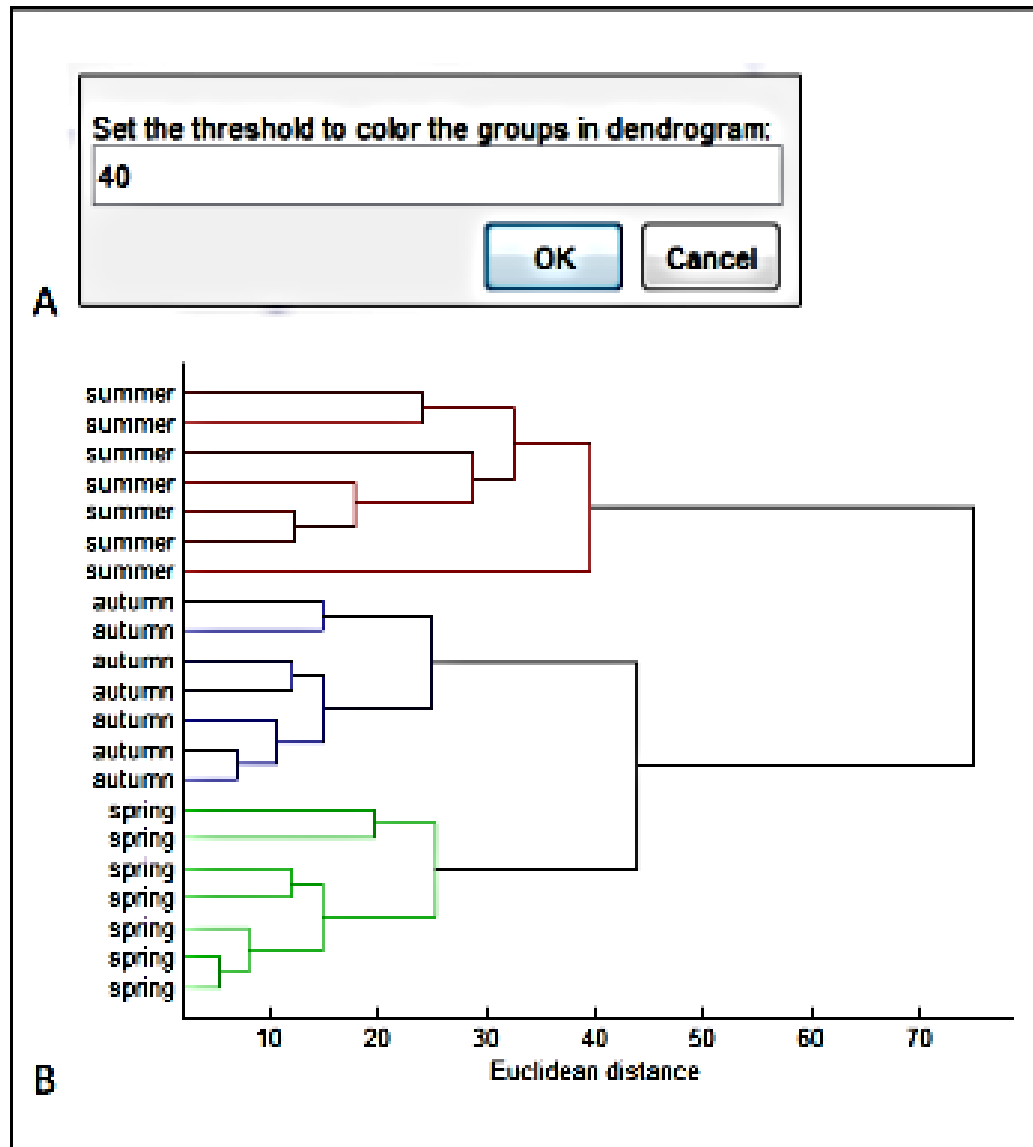- If it is not applicable, press Cancel.

Figure 9. HCA plot

Figure handling

- Saving figure with high resolution
- Access menu File> Export set up at the figure window.
- At the setup window (Figure 18A), access Rendering (1).
- Set the color to be saved, e.g., RGB color, gray scale, etc (2).
- Set the resolution to be saved, e.g., 600 dpi (3).
- Press Export button (4).
- Set the file name (5) (Figure 18B)
- Select the file type, e.g., .tif (6).⬚Press Savebutton(7)
- Note: If .fig (MATLAB figure) is selected in file type, the file can be opened only by using menu File > Open Figure in the Chemoface home screen or by Matlab software. Figures(.fig) can be edited (e.g., font size, font color) only on the Matlab software.
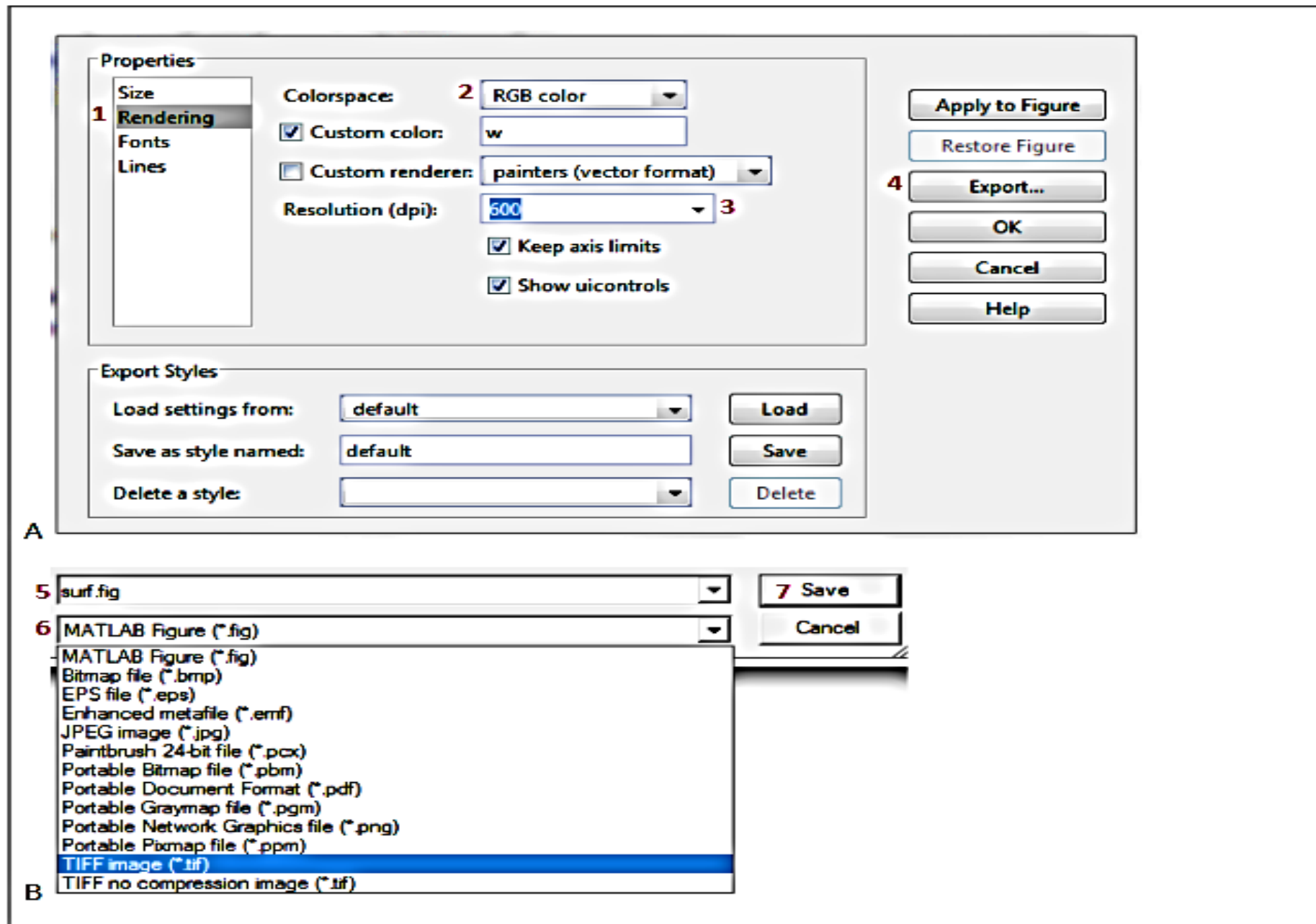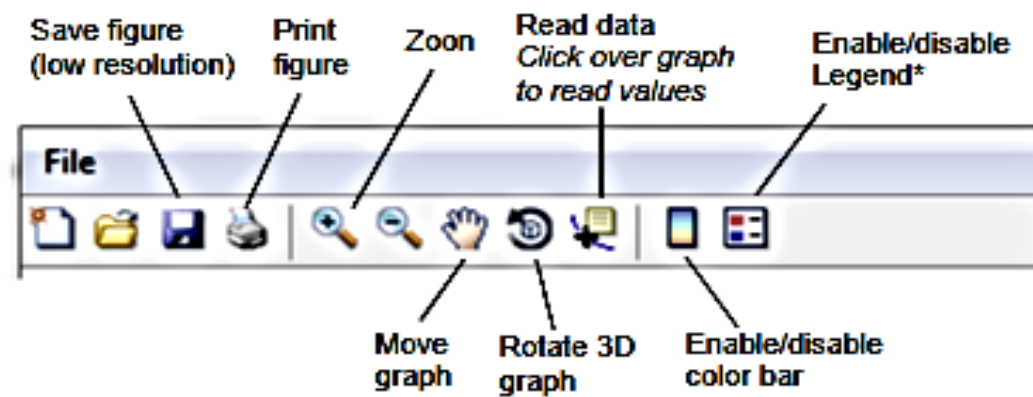
Figure 18. Exporting figure

Tools on the figure window

Save figure (low resolution)
Print figure
Zoon
Read data *Click over graph to read values*
Enable/disable Legend*

File

Move graph
Rotate 3D graph
Enable/disable color bar

To move legend, click with left mouse button and drag.