GrafCompounder 3.210

Working with the "GrafCompounder" Program

July 2018

www.grafcompounder.com

GrafCompounder

- **The "GrafCompounder" is a software program, which enables you to create recipes using any recipe database of: e.g. Rubber, TPE, TP and similar compounds.**
  - **Database must contain formulas with ingredients, their proportions and measured properties of the compounds.**
- **This software helps you save time and effort in recipe development by:**
  - **Elimination of Reinvention**
  - **Allowing faster and more accurate decisions on starting formulas**
  - **Creation of better ideas about further compound development**
  - **Useage of historic data in compound development**

- **Designed to support the plant chemist**

GrafCompounder

- The GrafCompounder uses a Multiple Linear Iteration Method [MLI] to calculate a recipe according to target or specification.
- The GrafCompounder enables to analyze a happenstance database.
- It is displaying the ratio of contribution of each compound recipe on the final formulation. This helps to identify faulty compound data.
  - If your confirmation experiment does not match the prediction inside confidence intervall, it is possible to track back all data used for the calculated compound.

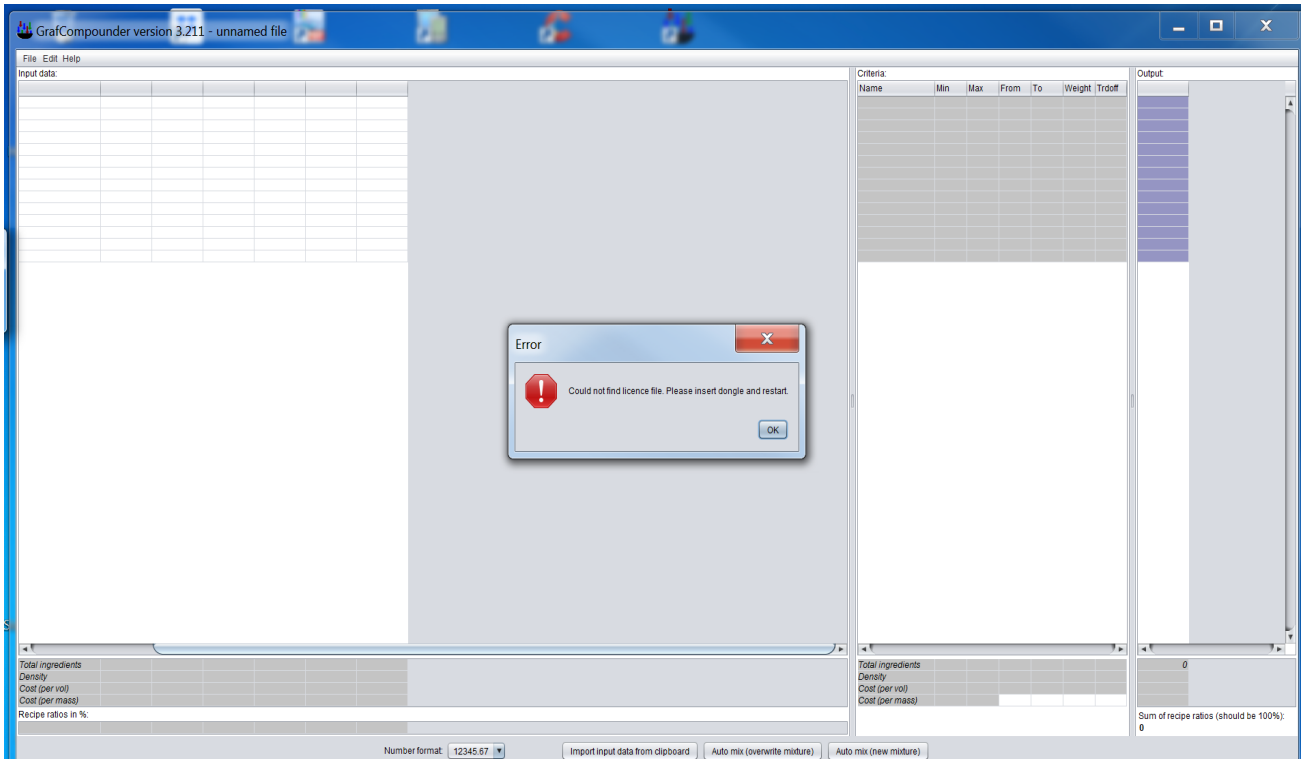
GrafCompounder

- **This tutorial familiarizes you with the advantage, potential and the best way to use the “GrafCompounder 3.211”**
  - **It shows all program features.**
  - **Explains this “easy to use” program**
  - **Guides you step wise through the program features**

GrafCompounder

- **Import of Data from other sources**
  - **Any Table Calculation Program**
    - **Excel®**
    - **Open Office Calc**
    - **.....**

Start Grafcompounder



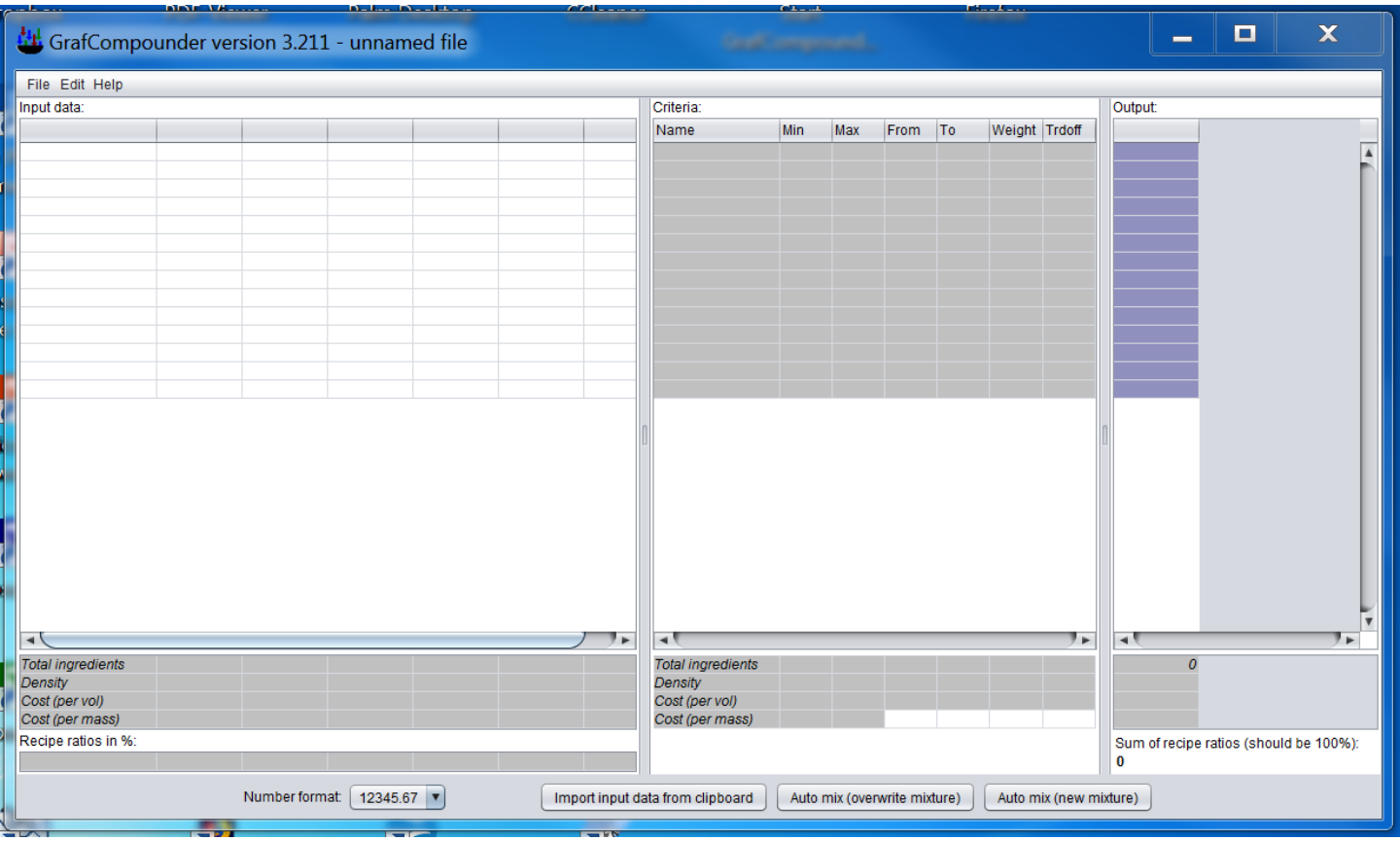
Insert the license Dongle into a USB port on your PC/Laptop computer

Once the dongle is in place, open the GrafCompounder program.

If you try to do this in the reverse order an error message will be displayed.

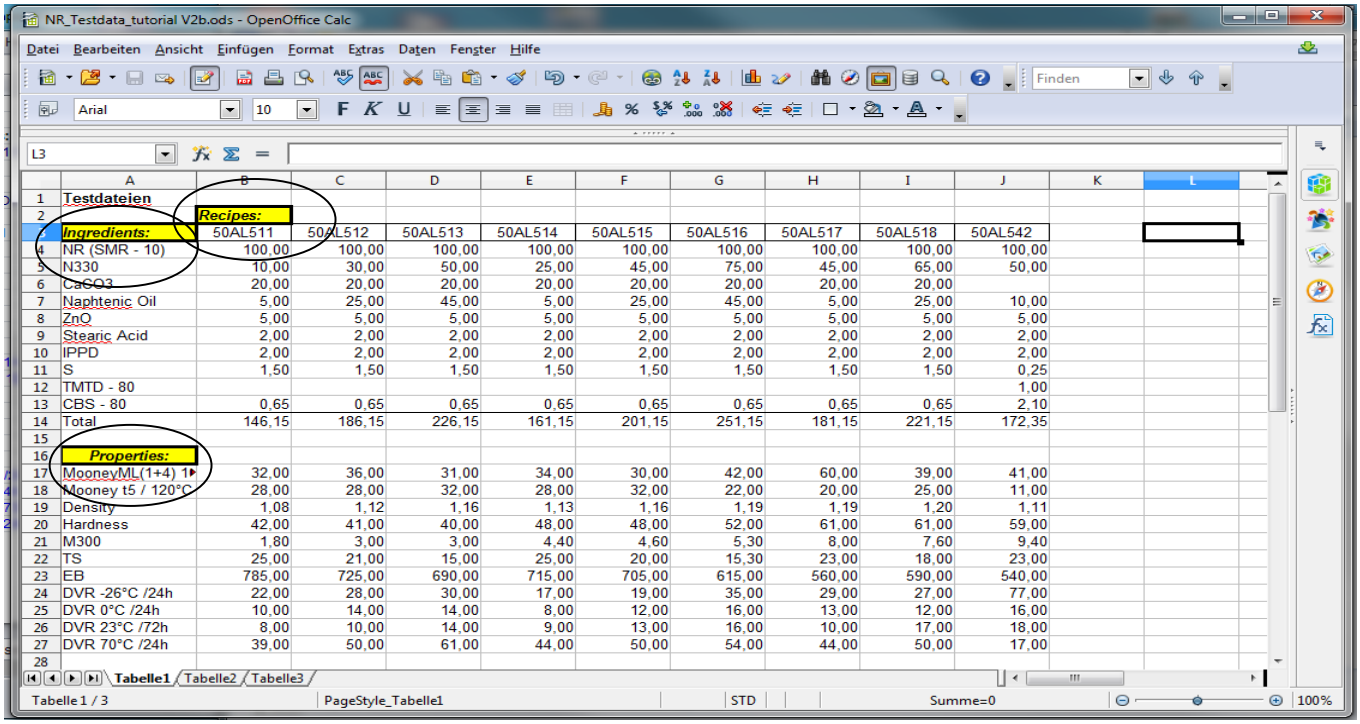
Click ok and the Program is closing

Data Transfer



- **After insertion of the dongle and start of the GrafCompounder program the screen should appear as shown**

Data format



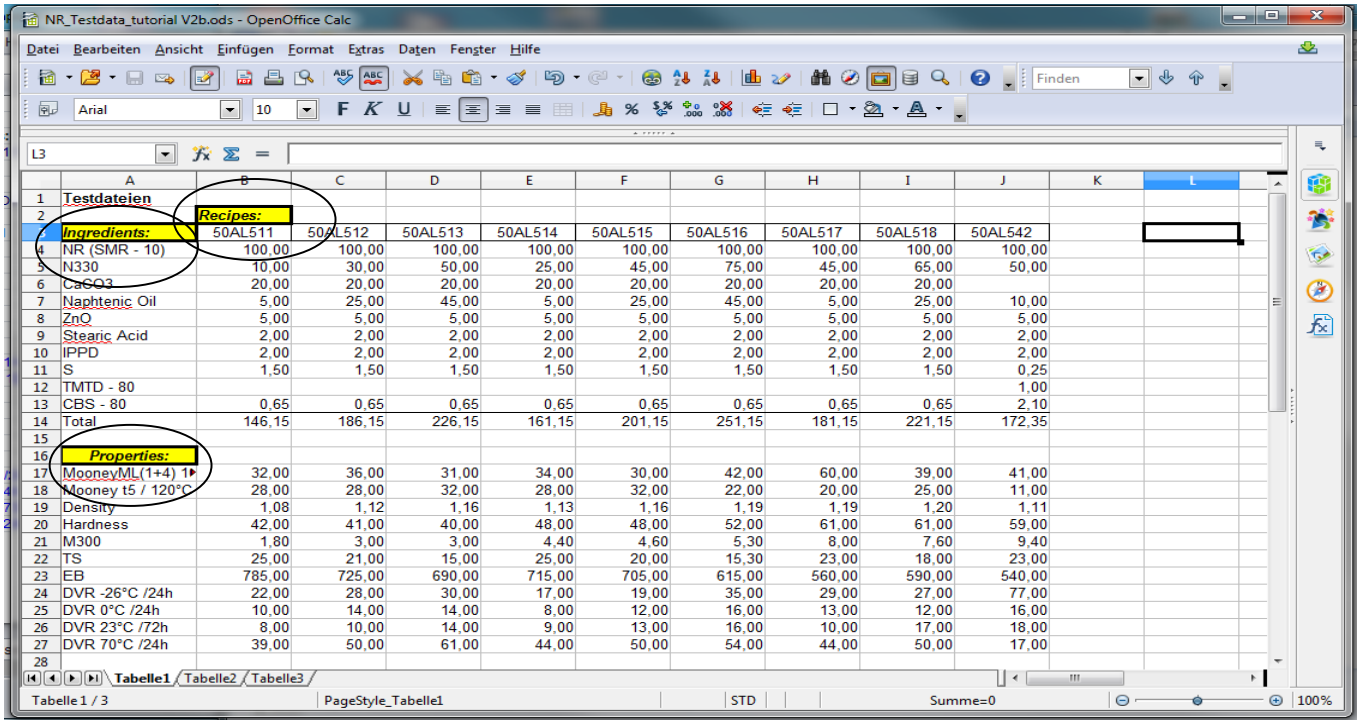
	A	B	C	D	E	F	G	H	I	J	K	L
1	Testdateien											
2		Recipes:										
3	Ingredients:	50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50AL517	50AL518	50AL542		
4	NR (SMR - 10)	100,00	100,00	100,00	100,00	100,00	100,00	100,00	100,00	100,00		
5	N330	10,00	30,00	50,00	25,00	45,00	75,00	45,00	65,00	50,00		
6	CaCO3	20,00	20,00	20,00	20,00	20,00	20,00	20,00	20,00			
7	Naphtenic Oil	5,00	25,00	45,00	5,00	25,00	45,00	5,00	25,00	10,00		
8	ZnO	5,00	5,00	5,00	5,00	5,00	5,00	5,00	5,00	5,00		
9	Stearic Acid	2,00	2,00	2,00	2,00	2,00	2,00	2,00	2,00	2,00		
10	IPPD	2,00	2,00	2,00	2,00	2,00	2,00	2,00	2,00	2,00		
11	S	1,50	1,50	1,50	1,50	1,50	1,50	1,50	1,50	0,25		
12	TMTD - 80									1,00		
13	CBS - 80	0,65	0,65	0,65	0,65	0,65	0,65	0,65	0,65	2,10		
14	Total	146,15	186,15	226,15	161,15	201,15	251,15	181,15	221,15	172,35		
15												
16	Properties:											
17	MooneyML(1+4) 1	32,00	36,00	31,00	34,00	30,00	42,00	60,00	39,00	41,00		
18	Mooney t5 / 120°C	28,00	28,00	32,00	28,00	32,00	22,00	20,00	25,00	11,00		
19	Density	1,08	1,12	1,16	1,13	1,16	1,19	1,19	1,20	1,11		
20	Hardness	42,00	41,00	40,00	48,00	48,00	52,00	61,00	61,00	59,00		
21	M300	1,80	3,00	3,00	4,40	4,60	5,30	8,00	7,60	9,40		
22	TS	25,00	21,00	15,00	25,00	20,00	15,30	23,00	18,00	23,00		
23	EB	785,00	725,00	690,00	715,00	705,00	615,00	560,00	590,00	540,00		
24	DVR -26°C /24h	22,00	28,00	30,00	17,00	19,00	35,00	29,00	27,00	77,00		
25	DVR 0°C /24h	10,00	14,00	14,00	8,00	12,00	16,00	13,00	12,00	16,00		
26	DVR 23°C /72h	8,00	10,00	14,00	9,00	13,00	16,00	10,00	17,00	18,00		
27	DVR 70°C /24h	39,00	50,00	61,00	44,00	50,00	54,00	44,00	50,00	17,00		
28												

Tabelle1 / Tabelle2 / Tabelle3

Tabelle 1 / 3 | PageStyle_Tabelle1 | STD | Summe=0 | 100%

- **The spreadsheet should contain formulas (minimum 3) with their properties.**
- **The first column cell named “Ingredients:” with the list of ingredients underneath,**
- **A cell “Properties:” with the list of properties.**
  - **There is no limitation: Whatever can be turned into a number can be listed.**
- **The next columns first cell named “Recipes:”**
  - **Please insert the required cell names exactly as shown. The above example shows how to format any data table.**
  - **The program will not work without this cells highlighted in yellow**

Data format and transfer



NR_Testdata_tutorial V2b.ods - OpenOffice Calc

Datei Bearbeiten Ansicht Einfügen Format Extras Daten Fenster Hilfe

	A	B	C	D	E	F	G	H	I	J	K	L
1	Testdateien											
2		Recipes:										
3	Ingredients:	50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50AL517	50AL518	50AL542		
4	NR (SMR - 10)	100,00	100,00	100,00	100,00	100,00	100,00	100,00	100,00	100,00		
5	N330	10,00	30,00	50,00	25,00	45,00	75,00	45,00	65,00	50,00		
6	CaCO3	20,00	20,00	20,00	20,00	20,00	20,00	20,00	20,00			
7	Naphtenic Oil	5,00	25,00	45,00	5,00	25,00	45,00	5,00	25,00	10,00		
8	ZnO	5,00	5,00	5,00	5,00	5,00	5,00	5,00	5,00	5,00		
9	Stearic Acid	2,00	2,00	2,00	2,00	2,00	2,00	2,00	2,00	2,00		
10	IPPD	2,00	2,00	2,00	2,00	2,00	2,00	2,00	2,00	2,00		
11	S	1,50	1,50	1,50	1,50	1,50	1,50	1,50	1,50	0,25		
12	TMTD - 80									1,00		
13	CBS - 80	0,65	0,65	0,65	0,65	0,65	0,65	0,65	0,65	2,10		
14	Total	146,15	186,15	226,15	161,15	201,15	251,15	181,15	221,15	172,35		
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19	Density	1,08	1,12	1,16	1,13	1,16	1,19	1,19	1,20	1,11		
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22	TS	25,00	21,00	15,00	25,00	20,00	15,30	23,00	18,00	23,00		
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24	DVR -26°C /24h	22,00	28,00	30,00	17,00	19,00	35,00	29,00	27,00	77,00		
25	DVR 0°C /24h	10,00	14,00	14,00	8,00	12,00	16,00	13,00	12,00	16,00		
26	DVR 23°C /72h	8,00	10,00	14,00	9,00	13,00	16,00	10,00	17,00	18,00		
27	DVR 70°C /24h	39,00	50,00	61,00	44,00	50,00	54,00	44,00	50,00	17,00		
28												

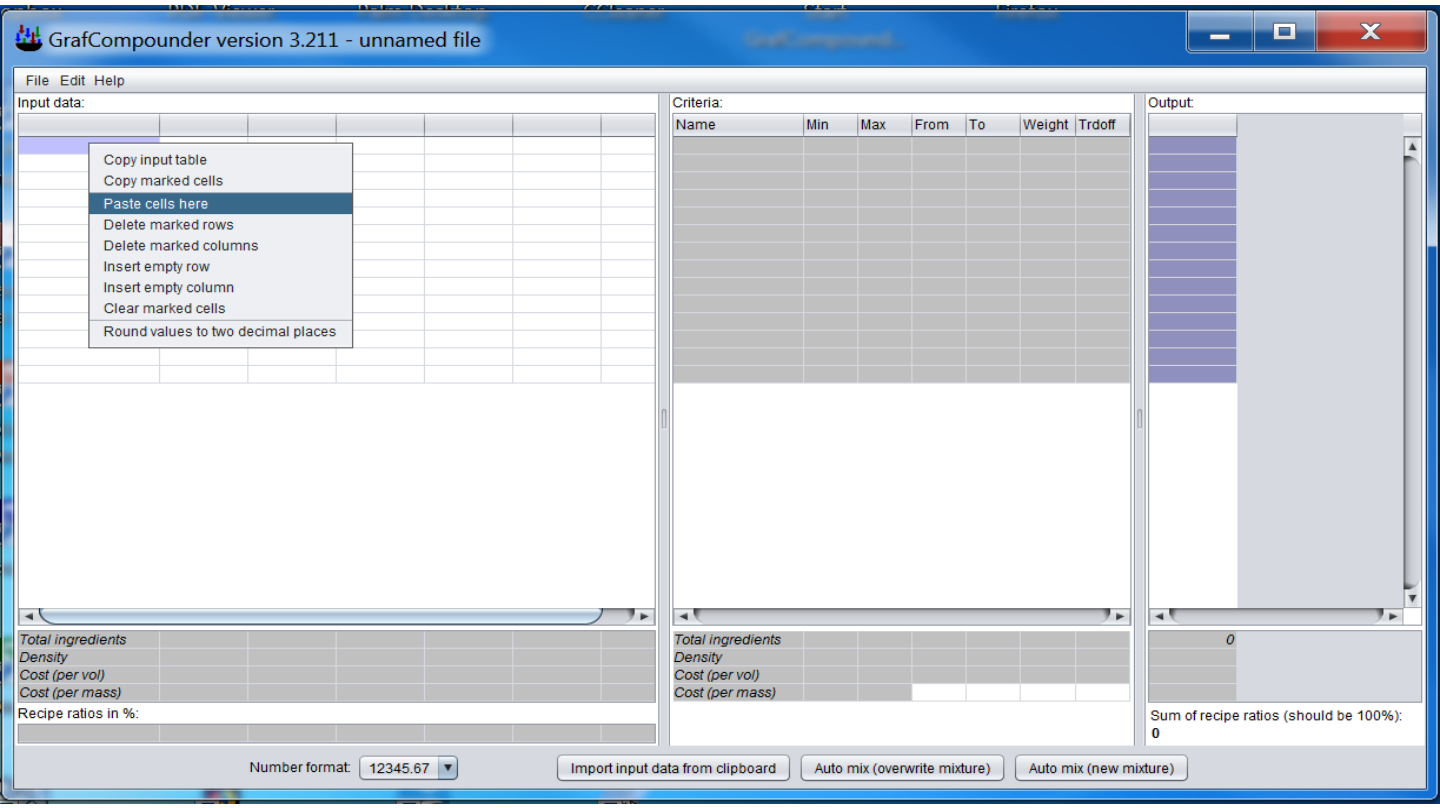
Tabelle1 Tabelle2 Tabelle3

Tabelle 1 / 3 | PageStyle_Tabelle1 | STD | Summe=0 | 100%

With copy / paste

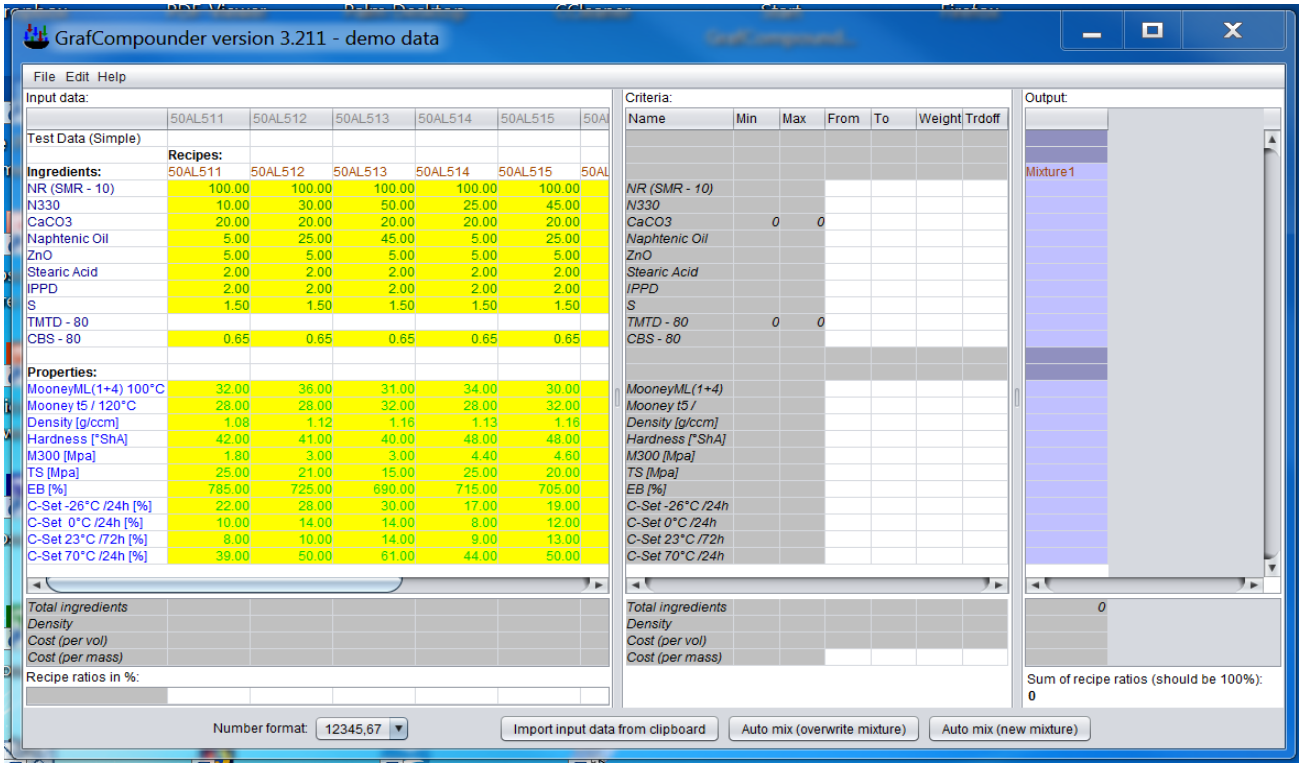
this table can be inserted in GrafCompounder

Data Insertion



- **Transfer the data into the GrafCompounder program. There are three options to assign the data:**
  - **Paste the information from the table calculation sheet: Click first cell, then right click. Select “Paste cell here” from Pull Down Menue**

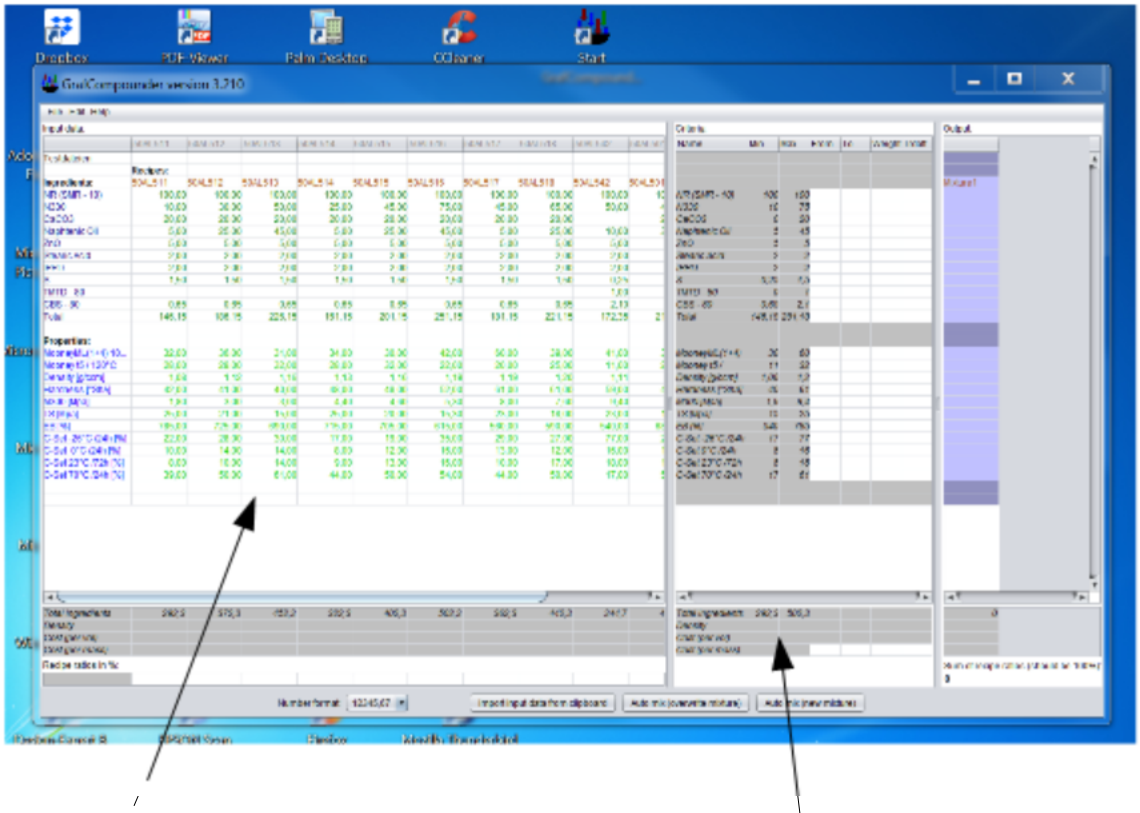
Data Insertion



Program screen would look like shown.

- **The yellow cells indicate, that the number format is different from the pre set format.GC program will not work.**
  - **Min & Max rows in “Criteria” window are empty**
- **Choose the number format in the example select “komma” instead of point**

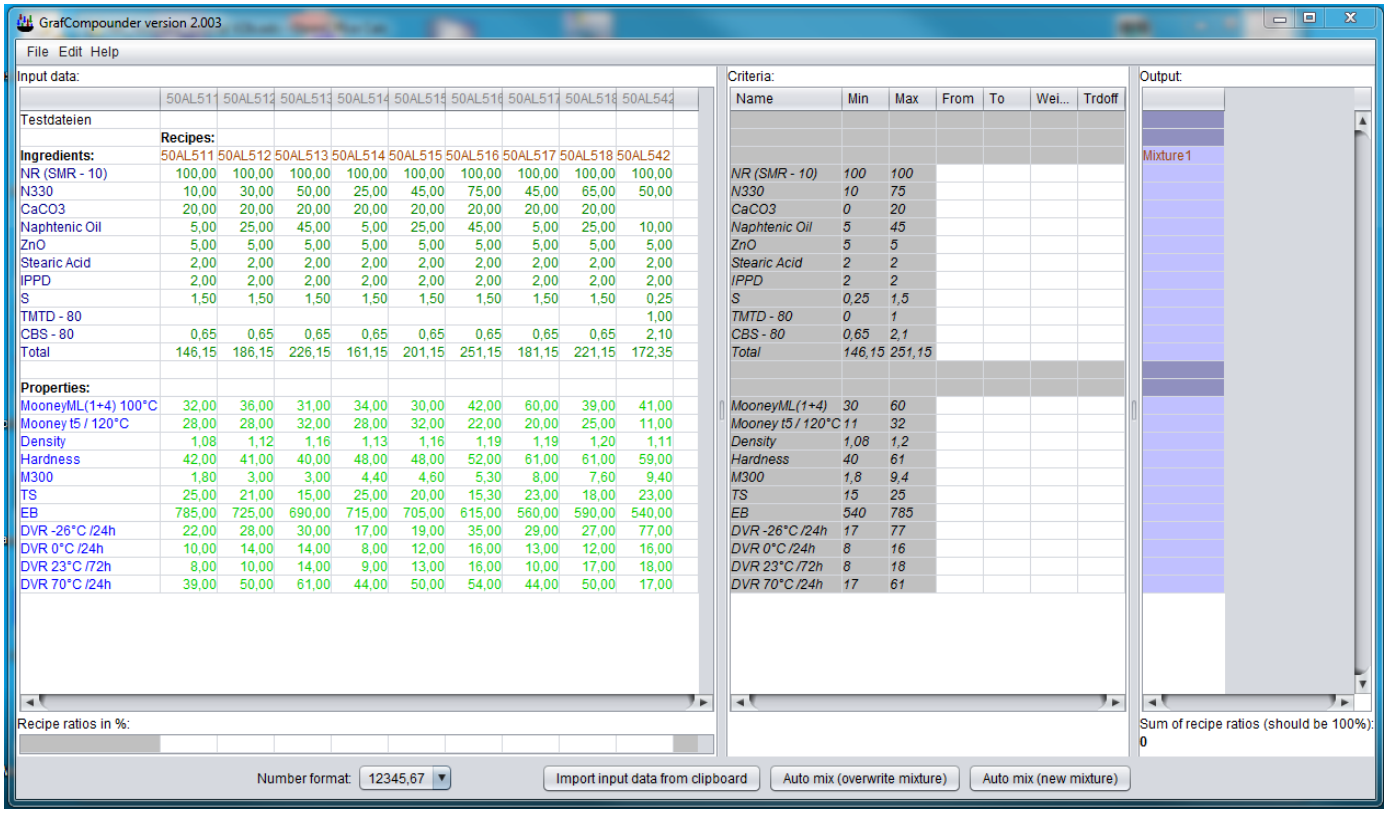
Data Insertion



- **Program screen would now look like shown above.**
  - **Ingredients and Property named in blue**
  - **Recipe numbers are in red**
  - **Property numbers are in green**

- **In the area next to “Input data”**
  - **“Criteria” window**
    - **1. Column: Ingredients & Property names**
    - **2. Column: Minimum values**
    - **3. Column: Maximum Values**

Data Transfer



Testdateien									
	Recipes:								
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CaCO3	20,00	20,00	20,00	20,00	20,00	20,00	20,00	20,00	
Naphtenic Oil	5,00	25,00	45,00	5,00	25,00	45,00	5,00	25,00	10,00
ZnO	5,00	5,00	5,00	5,00	5,00	5,00	5,00	5,00	5,00
Stearic Acid	2,00	2,00	2,00	2,00	2,00	2,00	2,00	2,00	2,00
IPPD	2,00	2,00	2,00	2,00	2,00	2,00	2,00	2,00	2,00
S	1,50	1,50	1,50	1,50	1,50	1,50	1,50	1,50	0,25
TMTD - 80									1,00
CBS - 80	0,65	0,65	0,65	0,65	0,65	0,65	0,65	0,65	2,10
Total	146,15	186,15	226,15	161,15	201,15	251,15	181,15	221,15	172,35
Properties:									
MooneyML(1+4) 100°C	32,00	36,00	31,00	34,00	30,00	42,00	60,00	39,00	41,00
Mooney t5 / 120°C	28,00	28,00	32,00	28,00	32,00	22,00	20,00	25,00	11,00
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TS	25,00	21,00	15,00	25,00	20,00	15,30	23,00	18,00	23,00
EB	785,00	725,00	690,00	715,00	705,00	615,00	560,00	590,00	540,00
DVR -26°C /24h	22,00	28,00	30,00	17,00	19,00	35,00	29,00	27,00	77,00
DVR 0°C /24h	10,00	14,00	14,00	8,00	12,00	16,00	13,00	12,00	16,00
DVR 23°C /72h	8,00	10,00	14,00	9,00	13,00	16,00	10,00	17,00	18,00
DVR 70°C /24h	39,00	50,00	61,00	44,00	50,00	54,00	44,00	50,00	17,00

Name	Min	Max	From	To	Wei...	Trdoff
NR (SMR - 10)	100	100				
N330	10	75				
CaCO3	0	20				
Naphtenic Oil	5	45				
ZnO	5	5				
Stearic Acid	2	2				
IPPD	2	2				
S	0,25	1,5				
TMTD - 80	0	1				
CBS - 80	0,65	2,1				
Total	146,15	251,15				
MooneyML(1+4)	30	60				
Mooney t5 / 120°C	11	32				
Density	1,08	1,2				
Hardness	40	61				
M300	1,8	9,4				
TS	15	25				
EB	540	785				
DVR -26°C /24h	17	77				
DVR 0°C /24h	8	16				
DVR 23°C /72h	8	18				
DVR 70°C /24h	17	61				

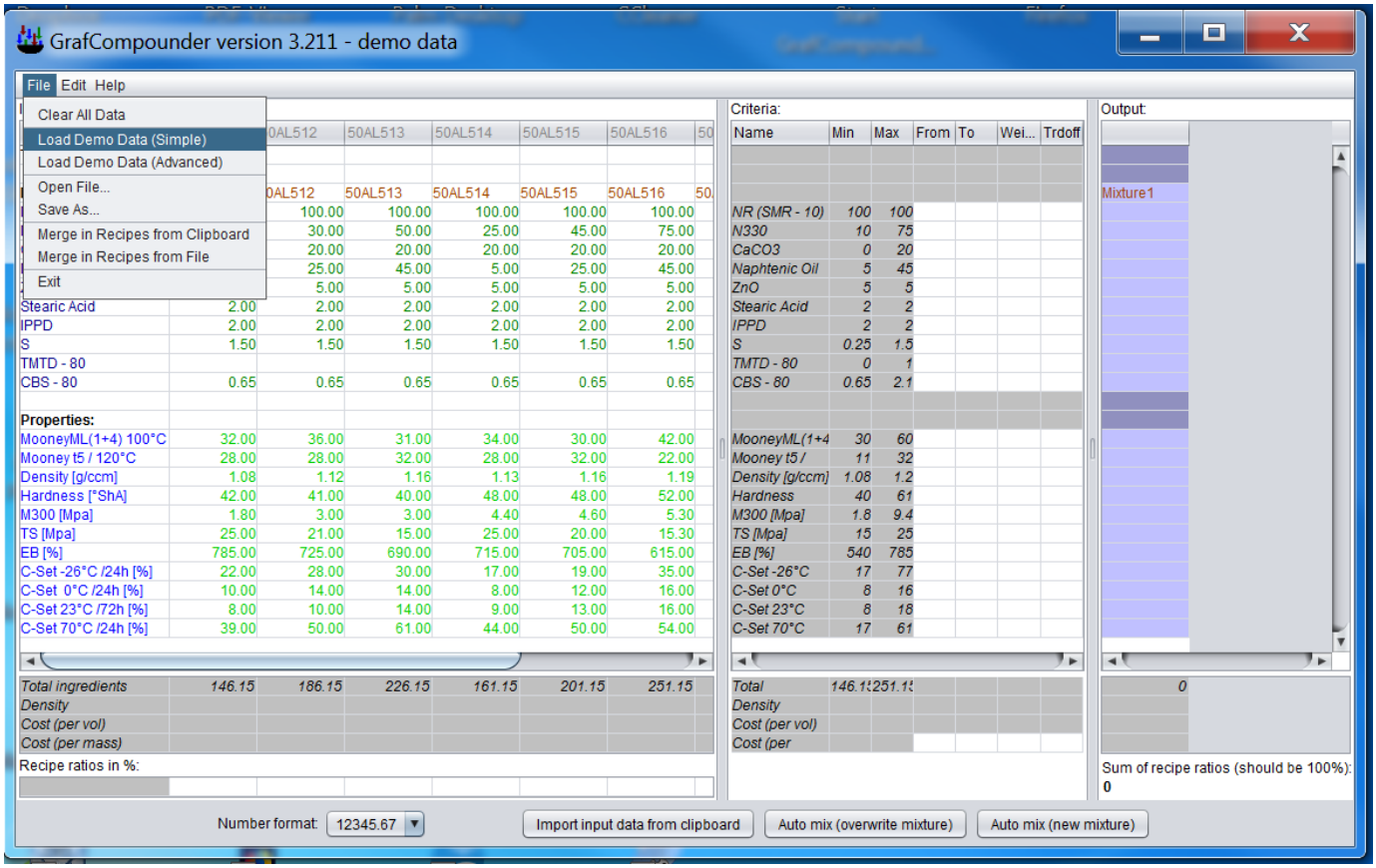
Output:

Mixture1

- **Once the "Number format" is adjusted to accommodate the comma:**
  - **The recipes now appear red and the properties show as green**
  - **The Min and Max columns show the highest and lowest numbers of the related row.**

Now you are ready for calculation, if you choose this option and want to move on

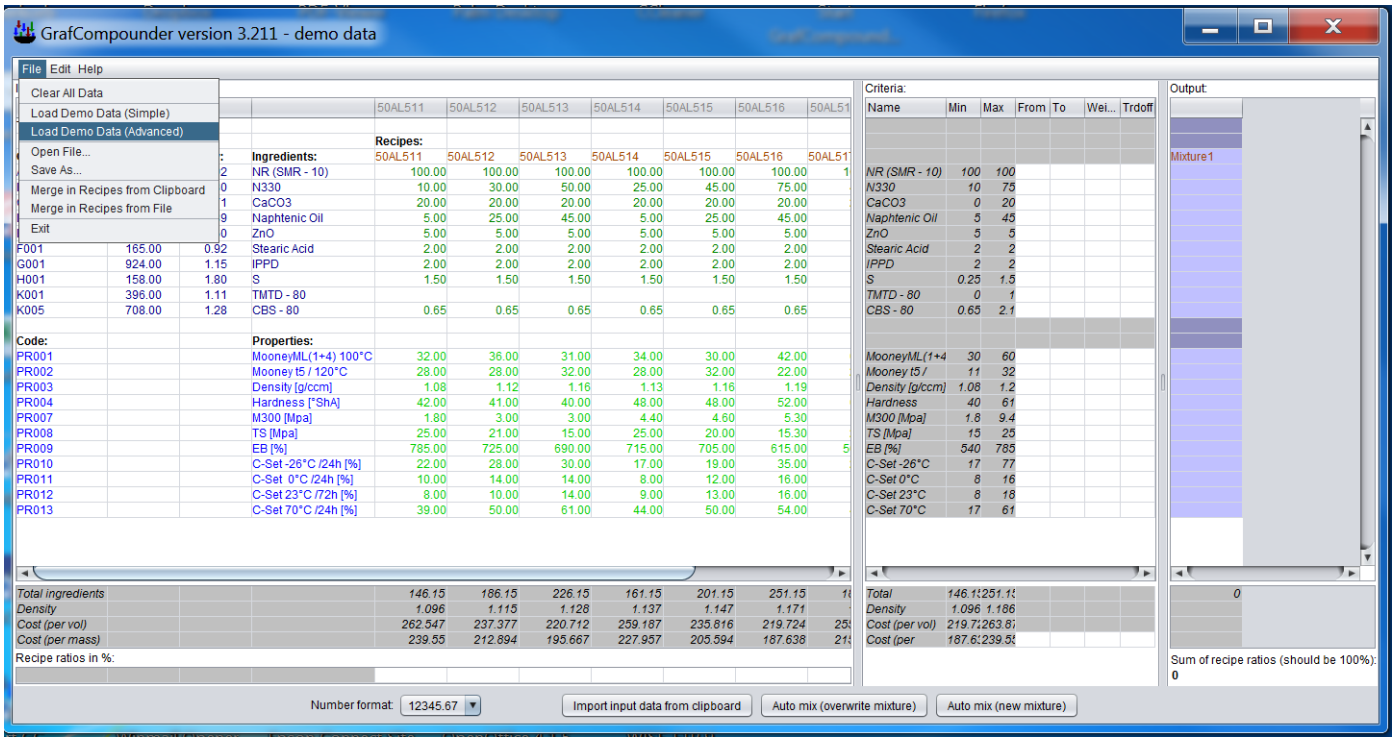
Open File



- **Other options for adding data:**

- **As a second option you can open the GrafCompounder program**
  - **Click “File”**
  - **and "LoadDemo Data (simple)“ in the pull down menu.**

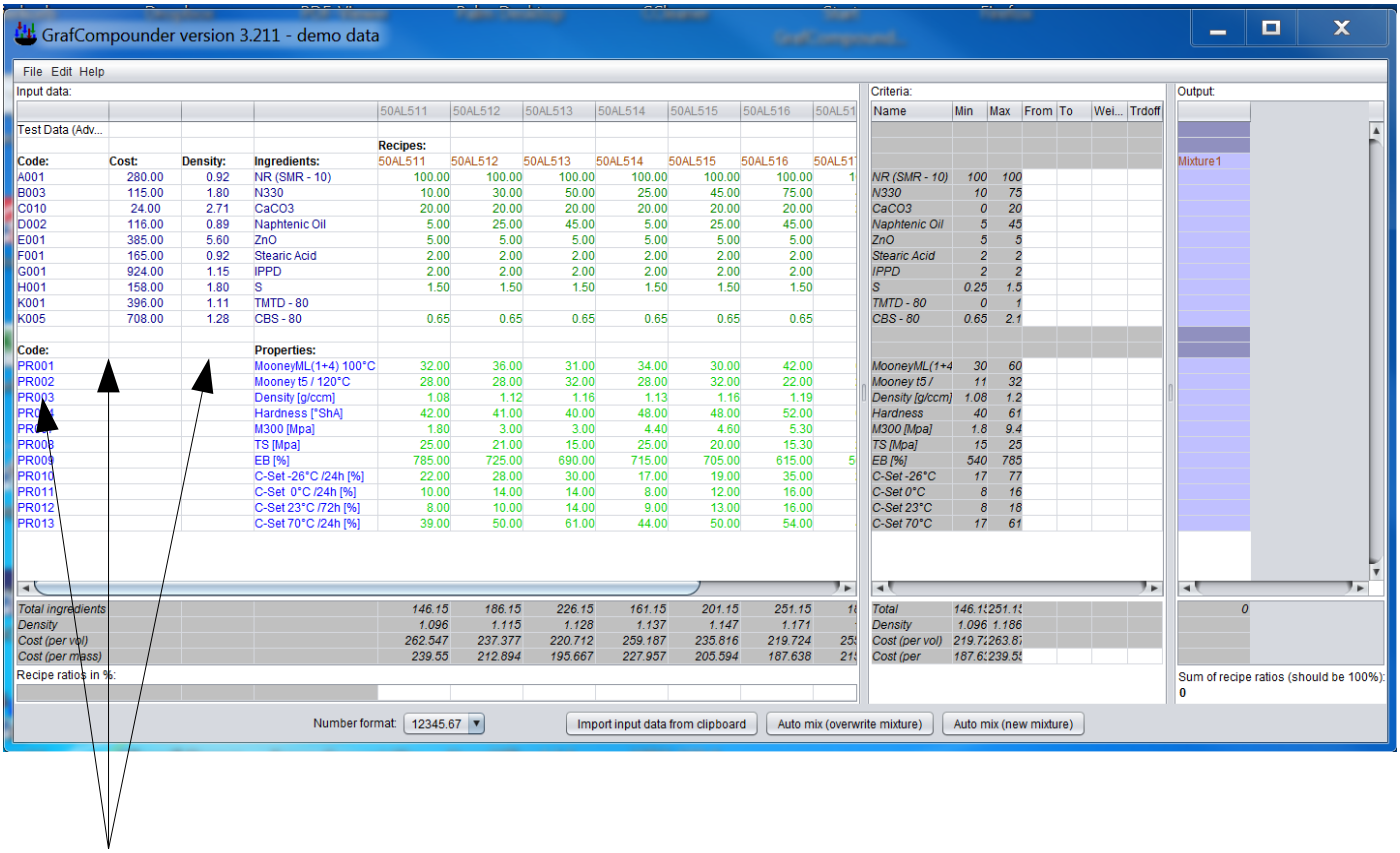
Open File



- **Other options for adding data:**

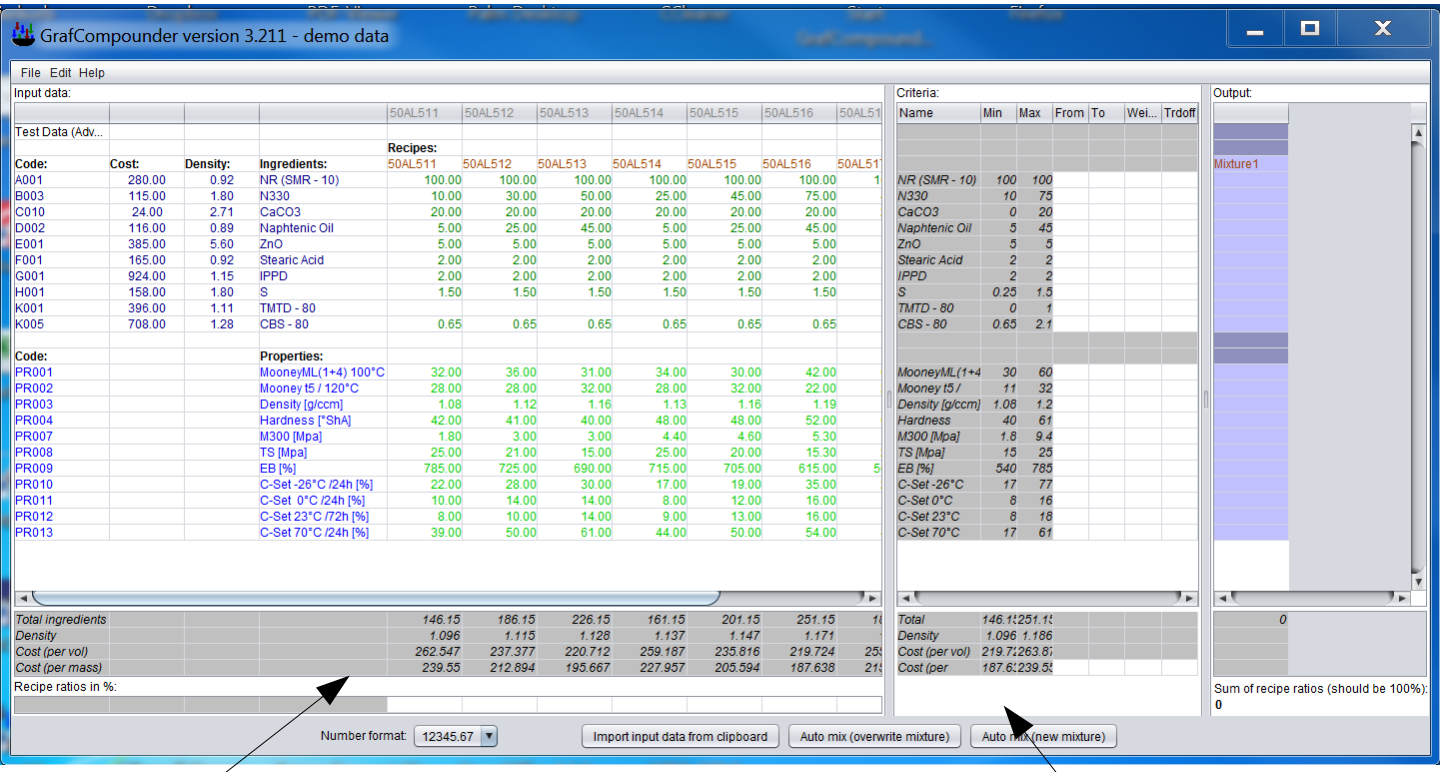
- **As a second option you can open the GrafCompounder program**
  - **Click “File”**
  - **and "LoadDemo Data (advanced)“ in the pull down menu.**

Open File



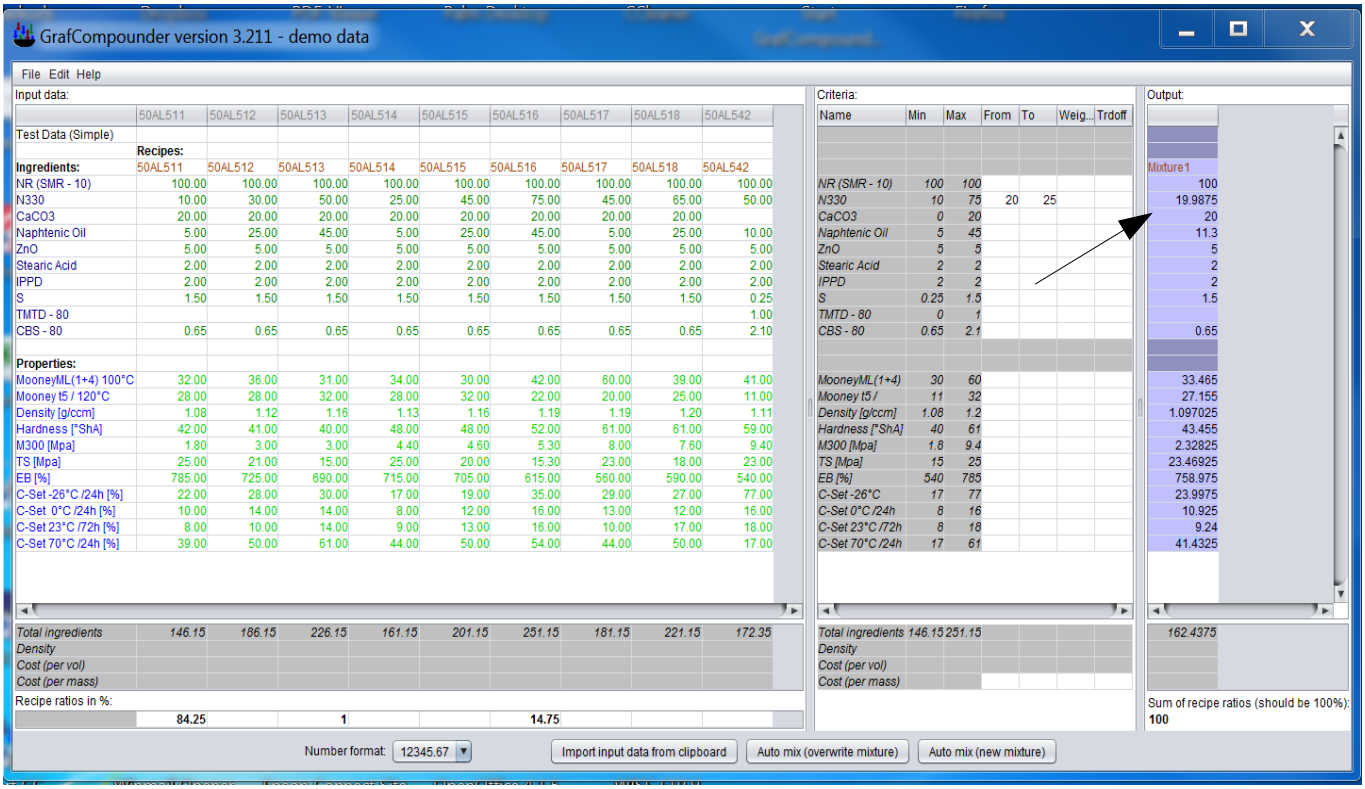
- **"LoadDemo Data (advanced)“**
- **This Data File has additional columns**
  - **Density:**
  - **Cost:**
  - **Code:**

Open File



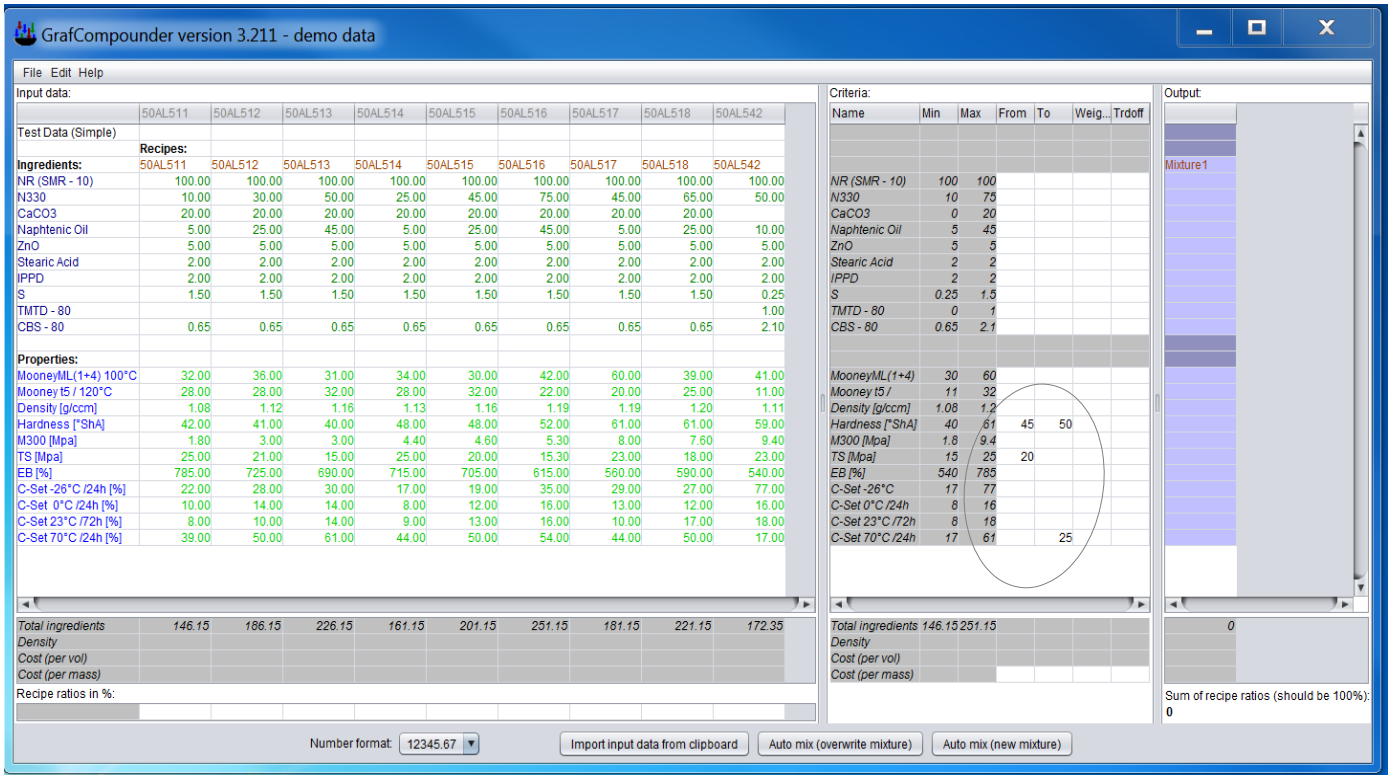
- "LoadDemo Data (advanced)“
  - The columns are necessary to calculate
    - Compound density
    - Cost per Volume
    - Cost per mass
  - The criteria Window shows the spread of data regarding denisty, cost per volume and cost per mass

Data analysis
(Demo Data Simple)



- To start, enter values in the “From” “To” columns
- Example: Ingredients
  - A minimum amount - “From” 20 phr
  - A target amount - “From” 20 phr “To” 25 phr
  - A maximum amount - “To” 25 phr
- The calculated compound has N330 19.98 phr
  - *As soon as the lower limit reached, program stops further calculation – as a general rule*
  - *(Comment: it would make sense only for larger datasets)*

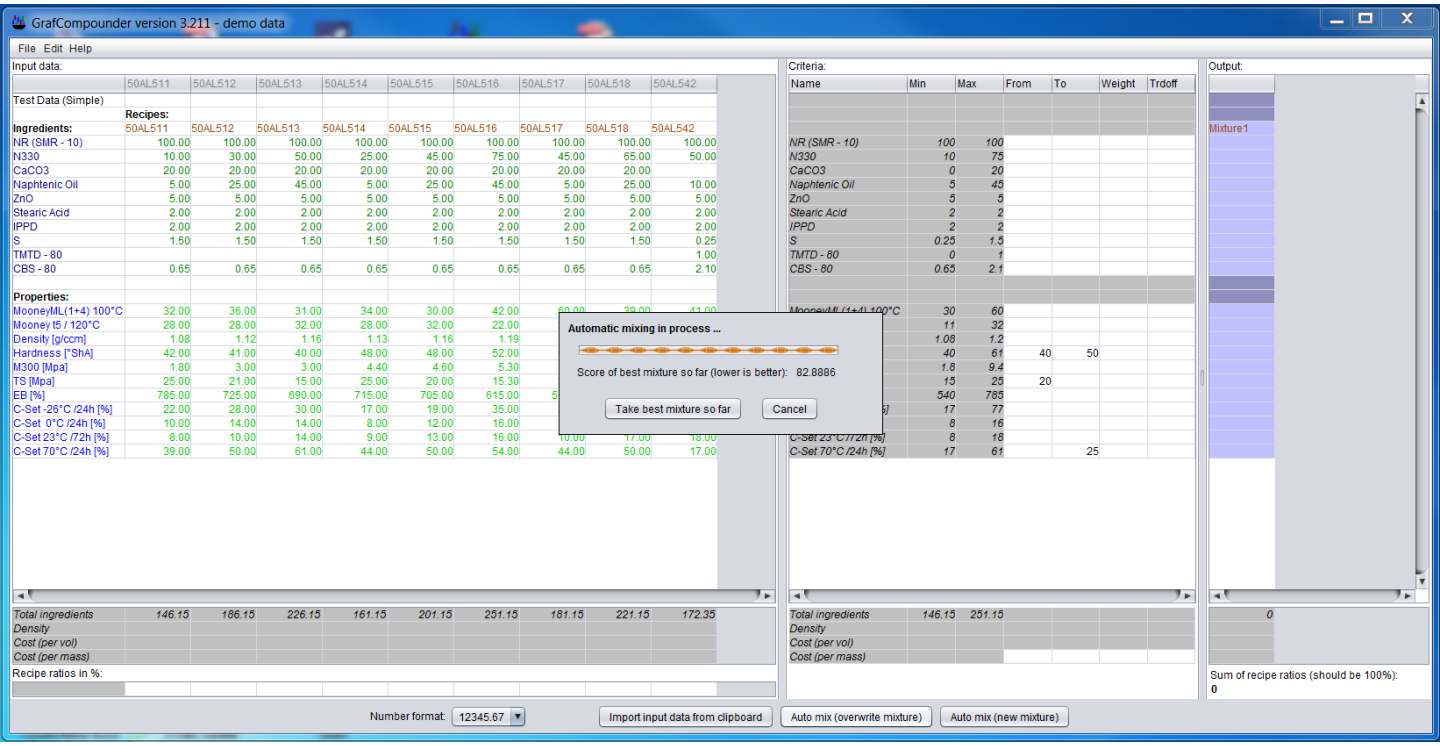
Data analysis
(Demo Data Simple)



- **To start more realistic:**
  Enter values in the “From” “To” columns in the criteria indow / Property section
- **The example shows the following criteria:**
  - **Target Hardness “From” 45 ShA “To” 50 ShA**
  - **Maximum C-Set (70°C/24h) - “To” 25 %**
  - **Minimum Tensile - “From” 20 MPa**

Data analysis

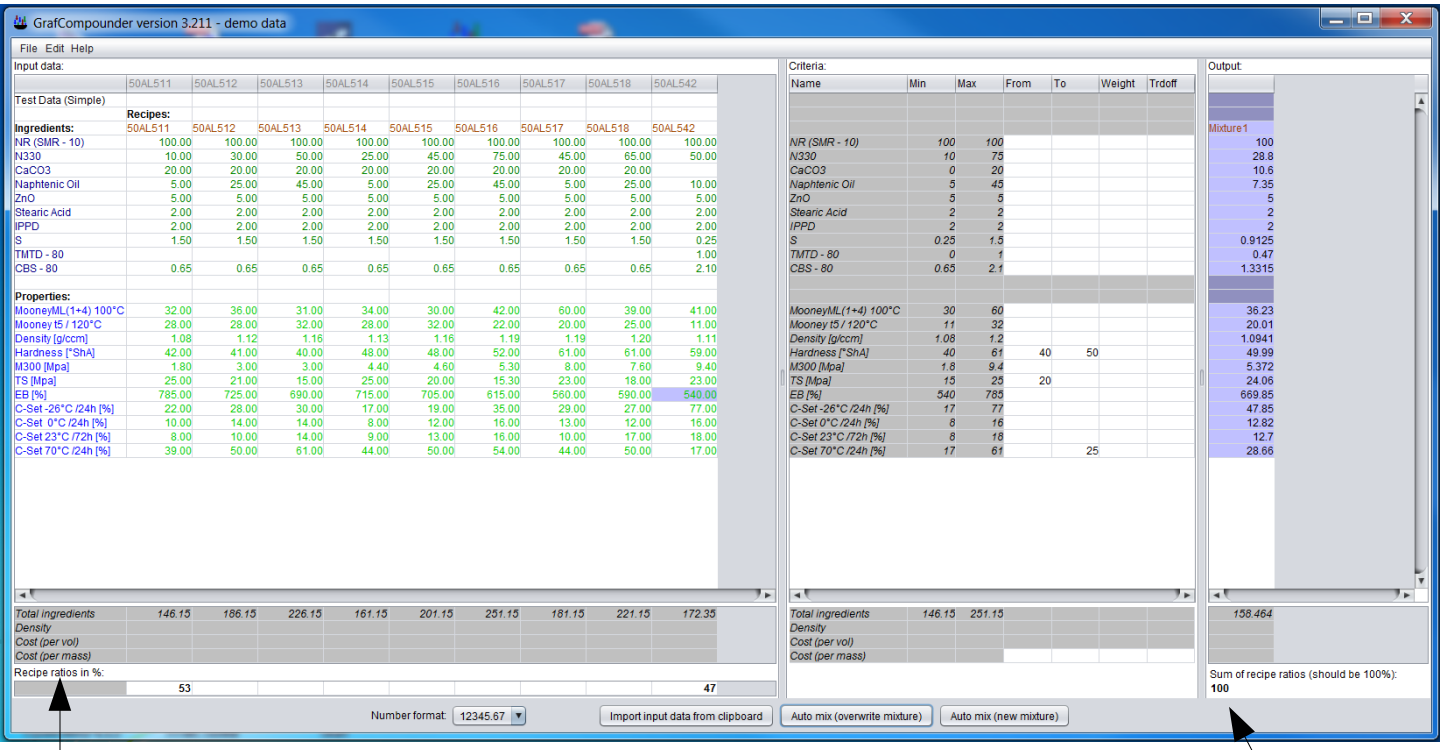
(Demo Data Simple)



- **Click on “auto mix (overwrite mixture)”**
  - **This tells the program to mix and to place the result in the highlighted column in the output window.**
- **The mixture is calculated,**
  - **But with a score of 82: No 100% match of the target is achieved**
  - **If all criteria are met the “Score of best mixture so far (lower is better)” will equal 0**
  - **Otherwise the score will be a number greater than 0.**

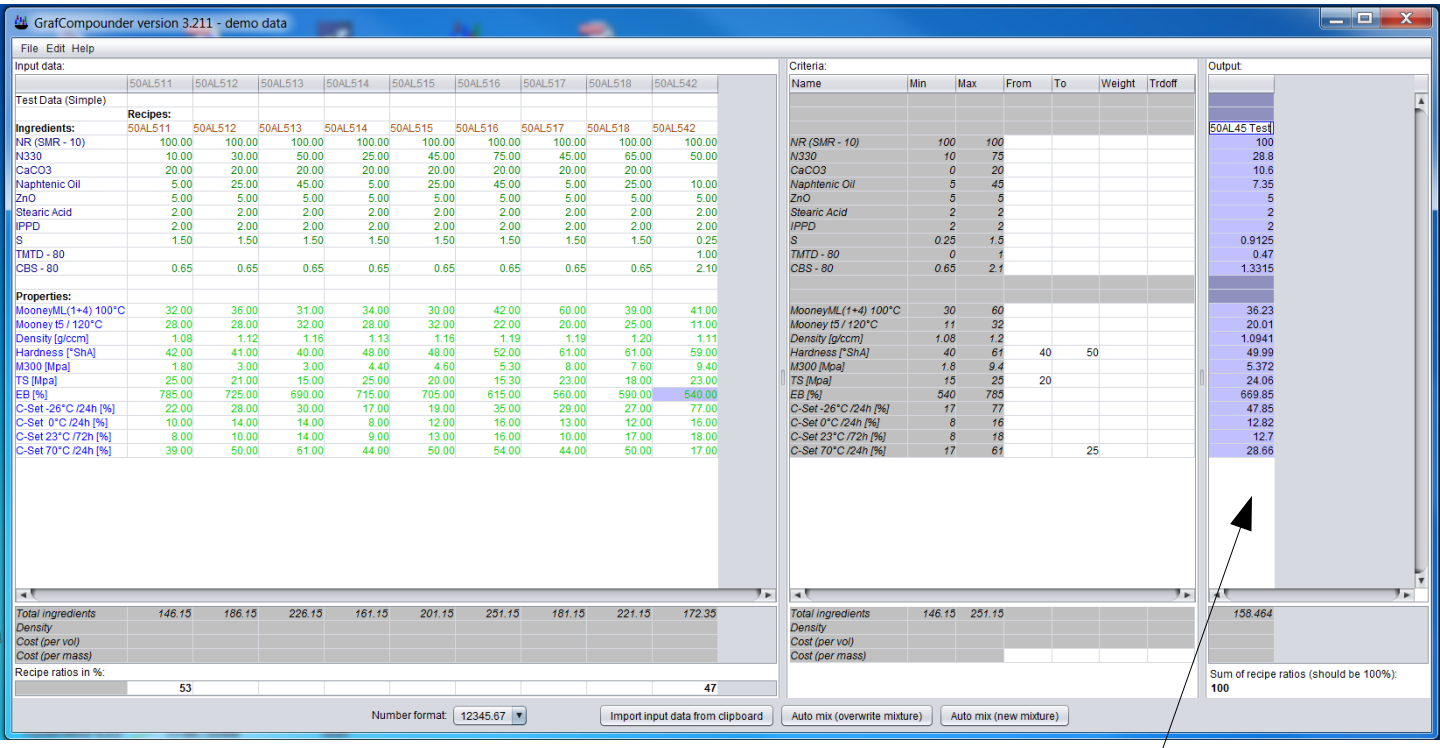
Data analysis

(Demo Data Simple)



- **Click on "take this mixture"**
  - **Because we chose "Auto mix (overwrite mixture)", the application has placed it in the highlighted column and automatically assigned the name "Mixture1" to it.**
- **This mixture is a combination of several compounds. The ratios the formula is made of can be seen from the line at the bottom of the page: "Recipe ratios in %"**
- **The line sum should always equal 100%**

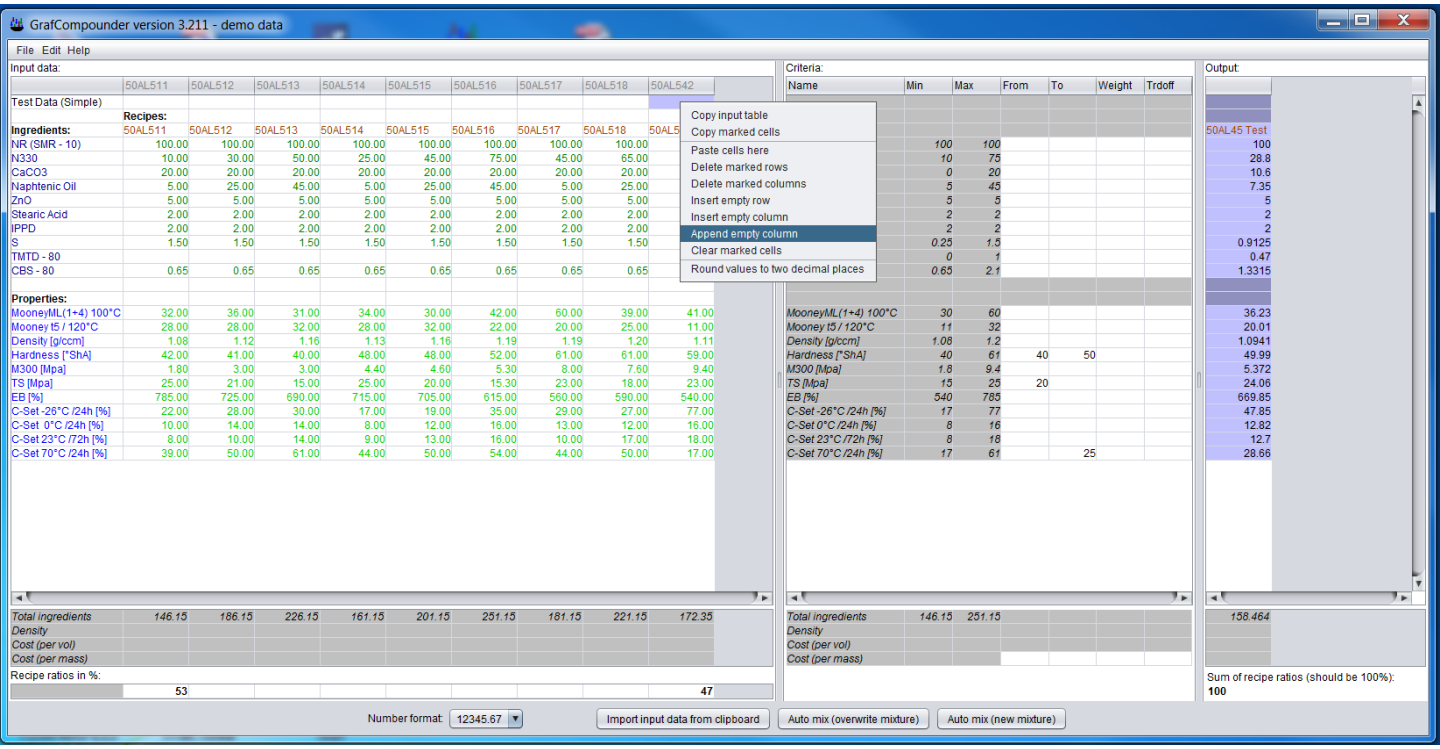
Naming the mixture



- **You can double-click the cell “Mixture 1“ to rename it**
  - **In the example above, the cell is being renamed to "50 AL45Test"**
- **In the example taget for C-Set is not met. All other values in target.**
- **You can take this mixture and do confirmation experiment.**

Compound Analysis

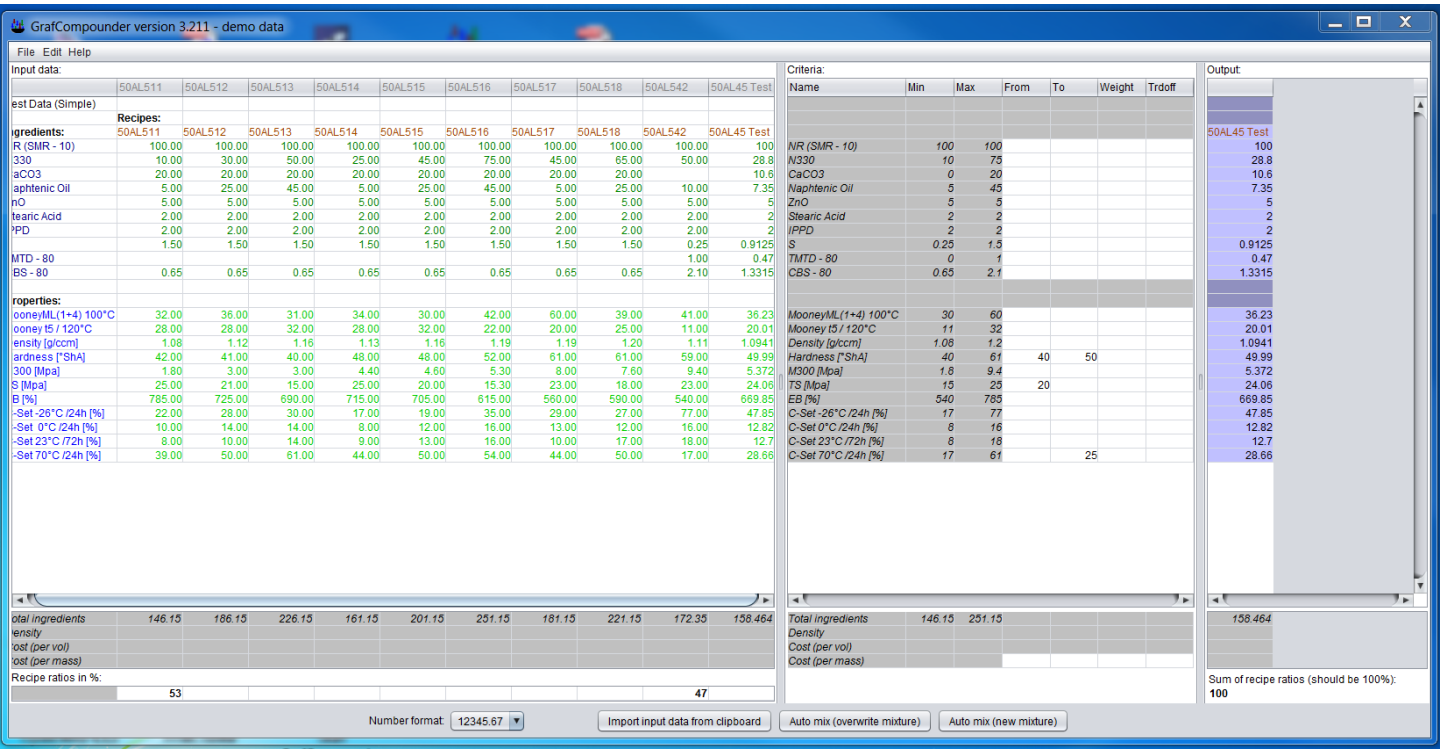
Review Calculation



- **Before the confirmation experiment you can work on the compound.**
  - **Click first cell in Data Tabel**
  - **Make a right click**
  - **Pull Down Menue select “Append empty column”**
    - **Comment:**
      If you click on theh fist cell in another column than the last you get
      “Insert empty column”

Compound Analysis

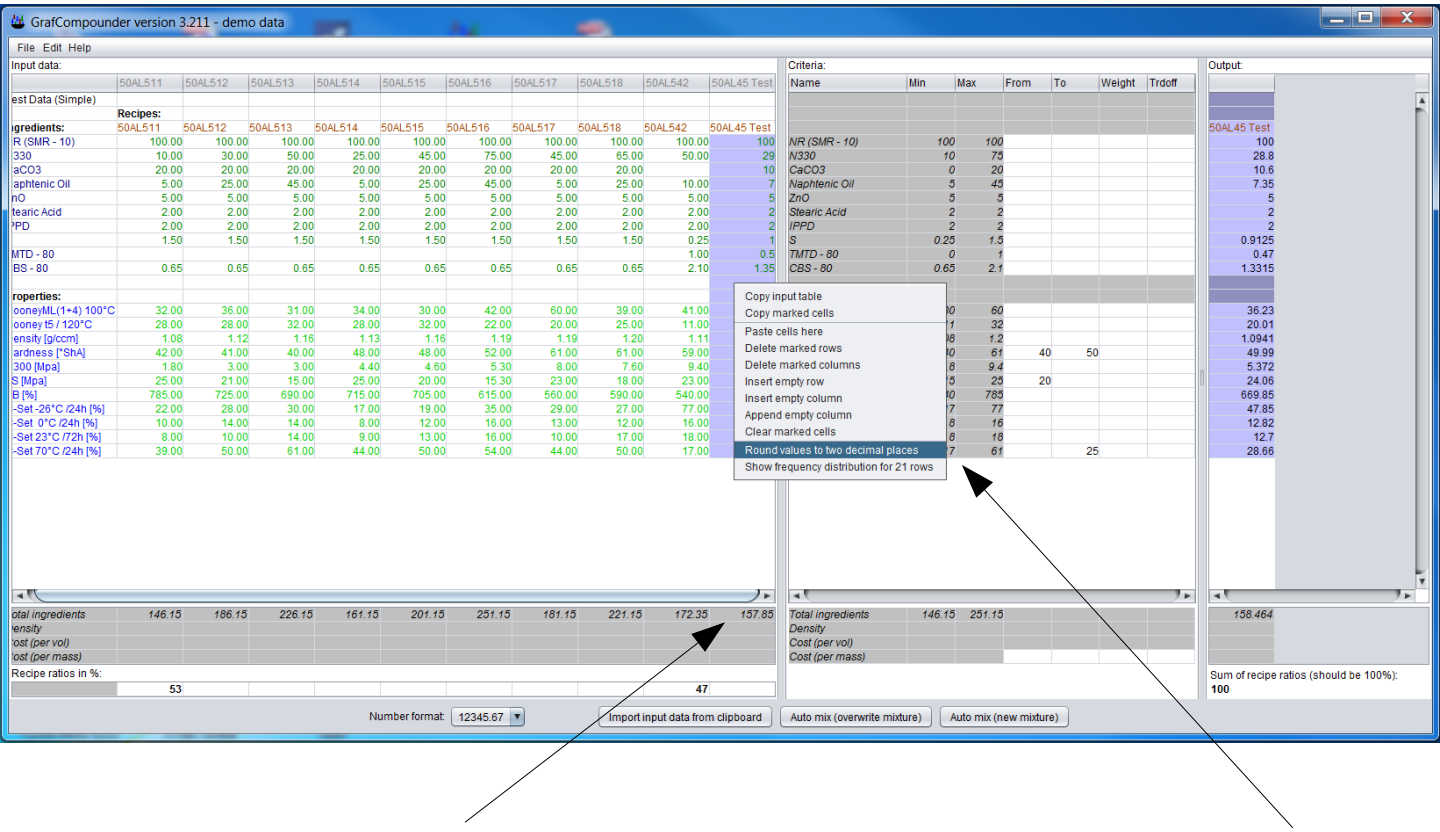
Review Calculation



- **Continue with right click into output column**
  - **Select “Copy mixture to clippboard”**
  - **Click first cell in appended empty data column**
  - **Make right click, select: “Paste cells here”**
- **Test compound is now tranferred in the data table with it name**
  - **Review and straight out odd numbers**

Compound Analysis

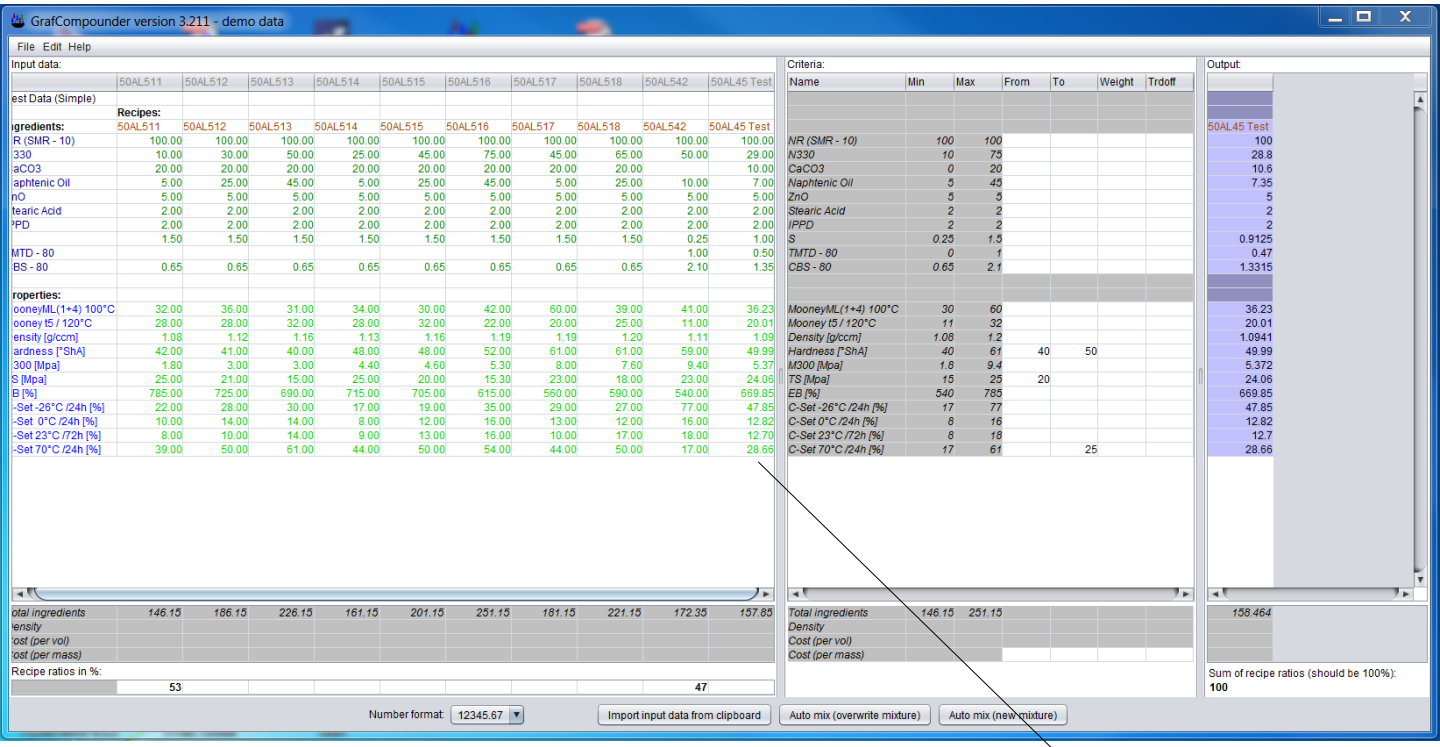
Review Calculation



- **After elimination of all odd numbers**
- ***Total ingredients is automatically recalculated***
  - **Highlight Compound data**
  - **Make right click and choose "Round values to two decimal places"**
    - **You can do same with property values**

Compound Analysis

Review Calculation



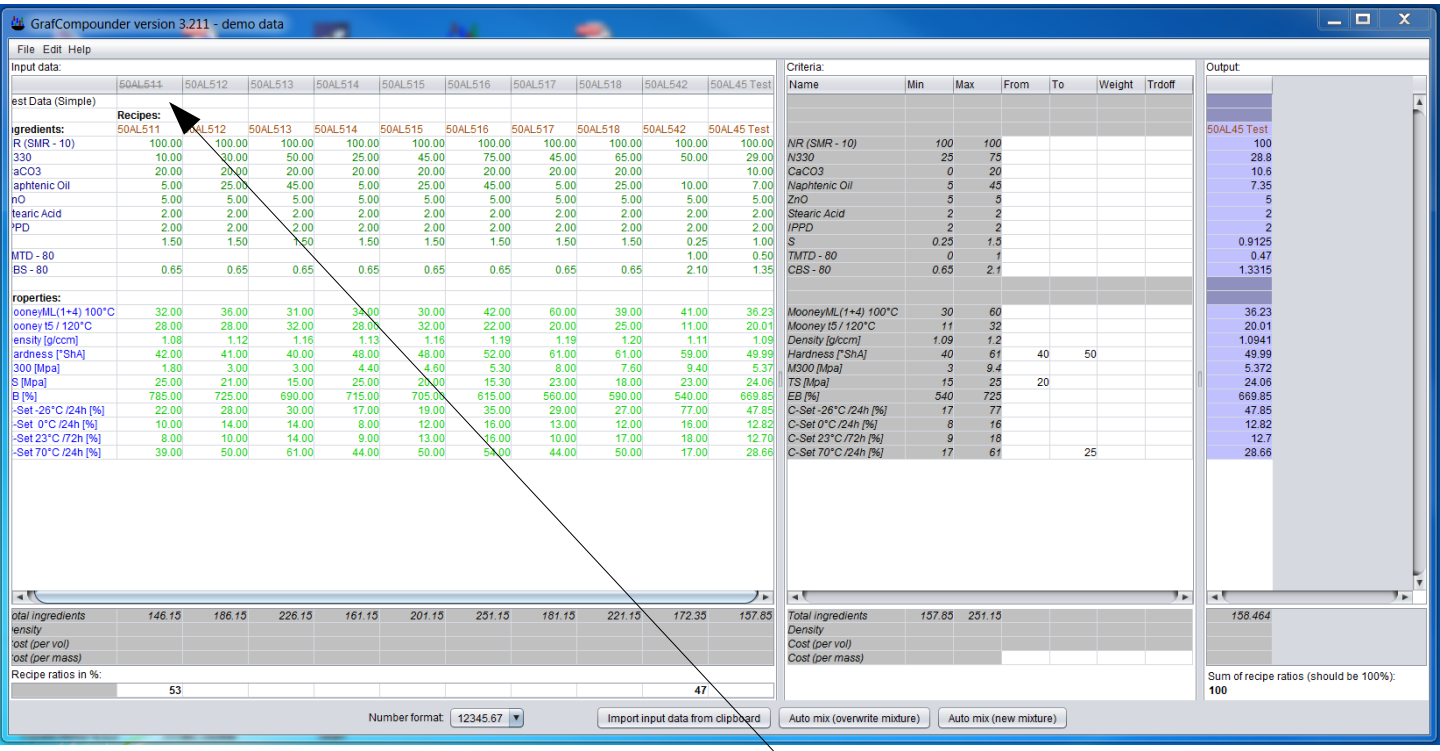
- **After compound review go to confirmation experiment with the reviewed formula**
  - **Replace property data with new measured data**
  - **Result should be in 95% confidence intervall**
- **Review the formula by analyzing it with the formulas it was compounded from.**
  - **If result is sufficient close, leave compound in the dataset as new**

    'formula&property data colum' for further calculation
    - ***You may rename the compound with double click in name cell***

Compound Analysis

Review Calculation

Example 1

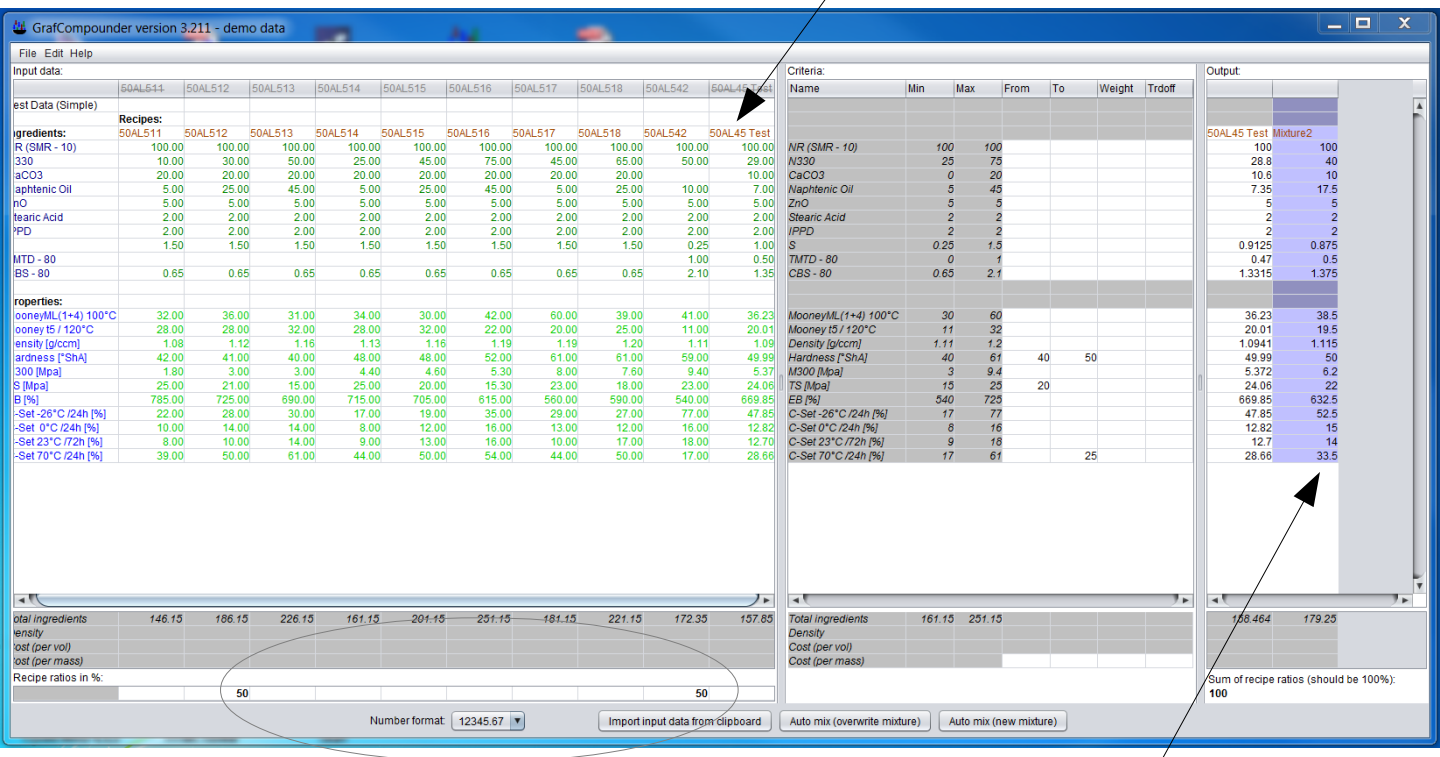


- **Result of confirmation experiment was not sufficient:**
  - **Assumption: First compound column has faulty data**
  - **Disable formula with right click on name**
  - **Name in cell turns ~~50AL511~~**
  - **Compound will be excluded from calculation**
    - ***You can reverse by right click again***

Compound Analysis

Review Calculation

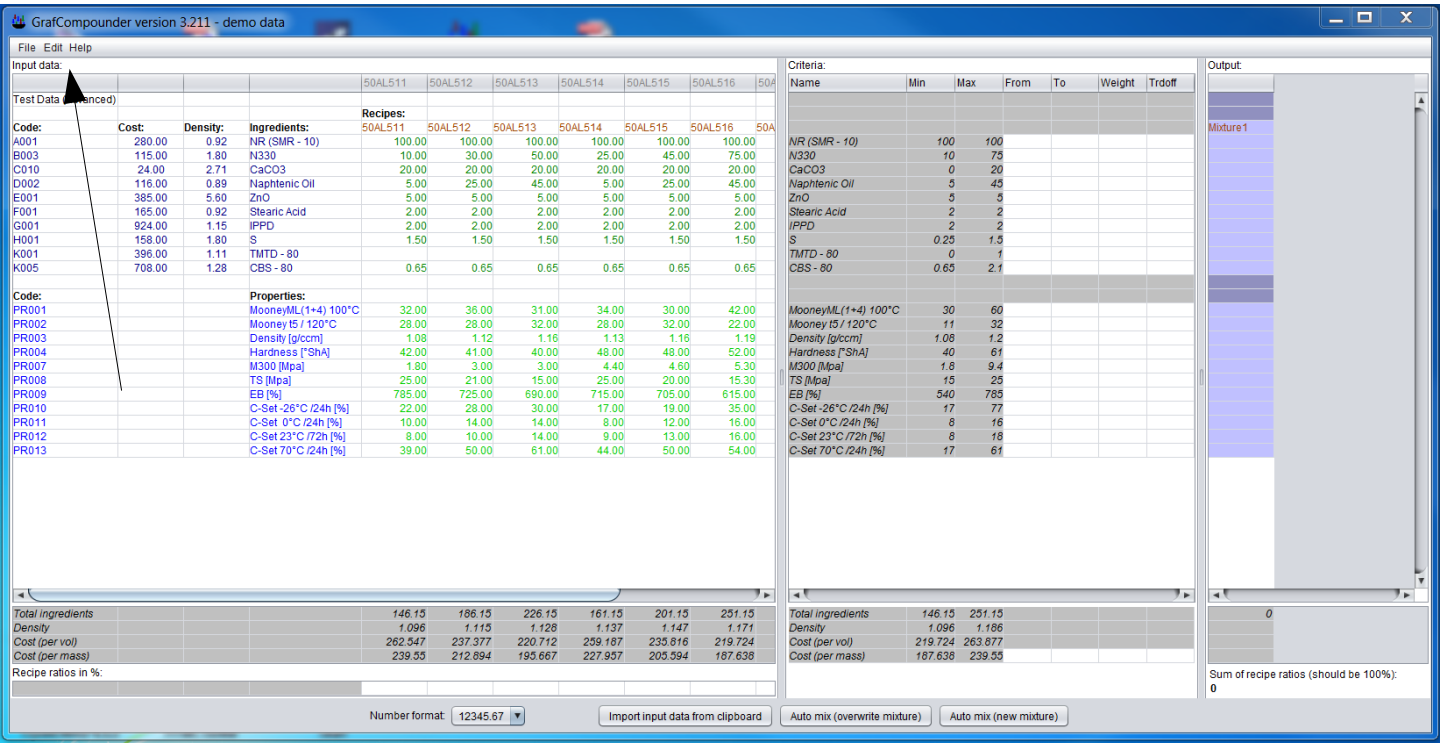
Example 1



- **Recalculate using *"Automix(new mixture)***
  - ***Allows to compare result of first with second run (50AL512 excluded)***
  - ***Warning: Do not forget to exclude Test compound as well (if not cnfirmed yet and physicals corrected with measrued ones)***
- **Compare results of fist with second run**
  - **If more acceptable replace test compound with mixture 2**
    - **In the example C-Set is farer off, which give higher score (*192 instead of 82*)**

Data analysis

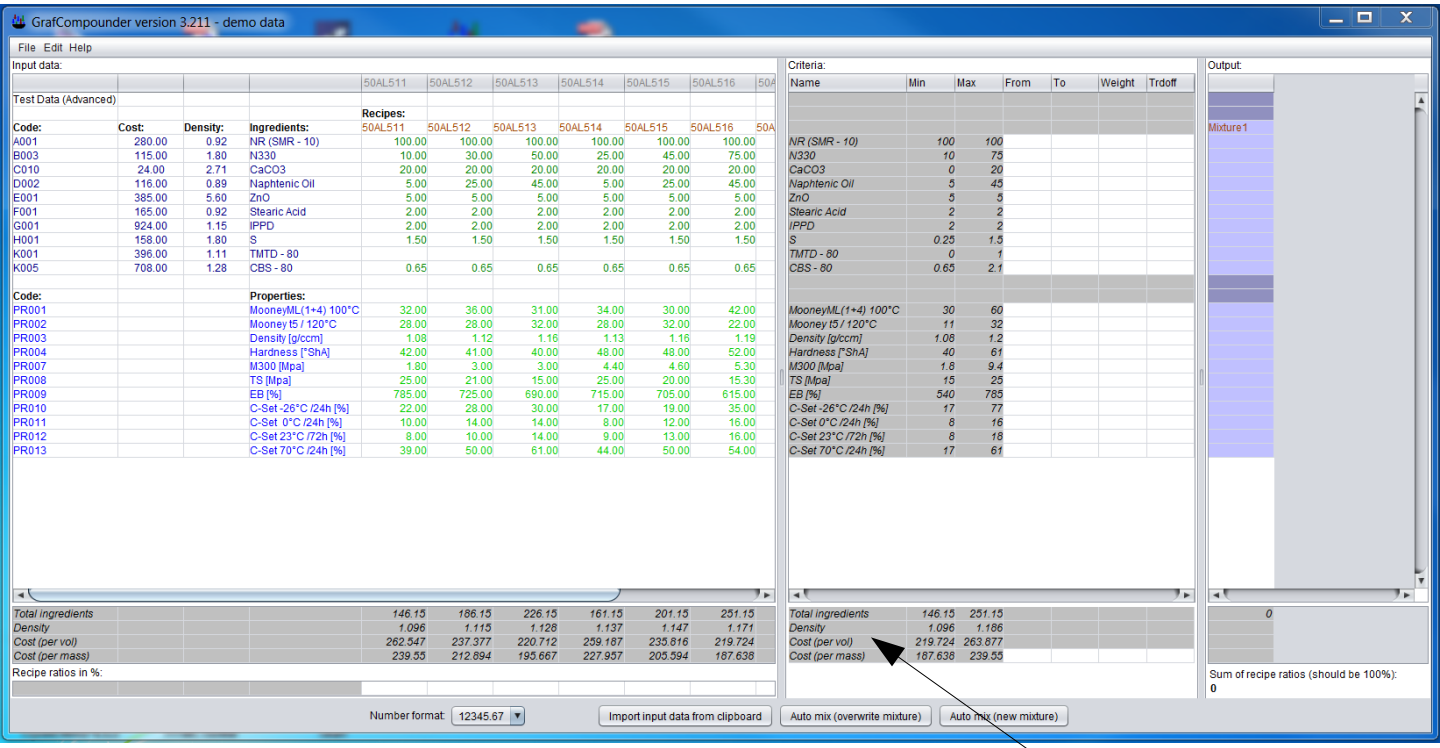
(Demo Data Advanced)



- **Load Demo Data Advanced**
  - **Click “File” and then “Clear all Data”**
  - **Click “File”, select “Load Demo data (advanced)” from Pull down Menue**
- **Screen appears with**
  - **Column – Code:**
    Ingredients are coded
    Physical properties with code as well
- **Code is needed for the “Merger” of different set of data files.**

Data analysis

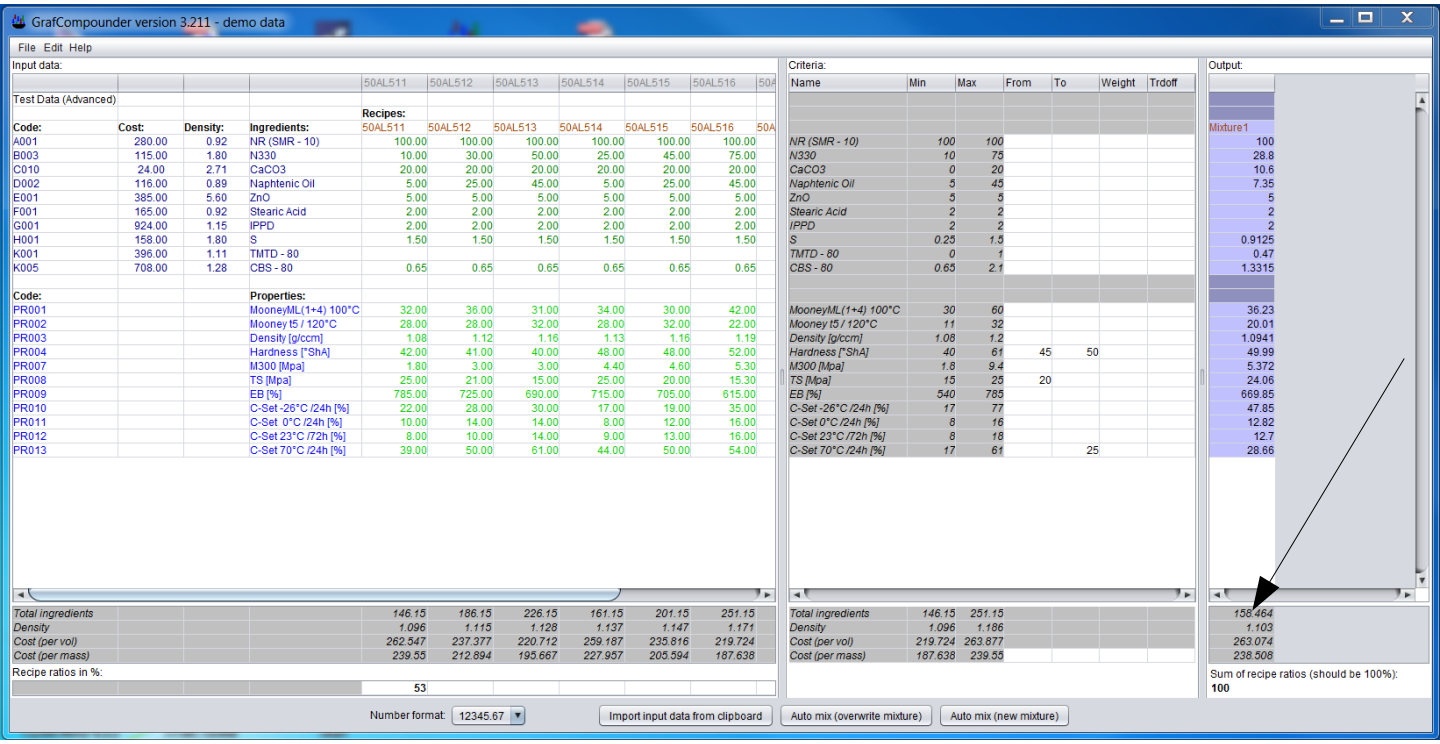
(Demo Data Advanced)



- **Load Demo Data Advanced**
  - **From File Pull down Menue**
- **Cost Column**
  - **It is neede to calculate volume & weight cost**
- **Denisty Column**
  - **Denisty value follows the ingredients ratio in percent (in terms of phr it is not linear and there fore need to be calulated separately**

Data analysis

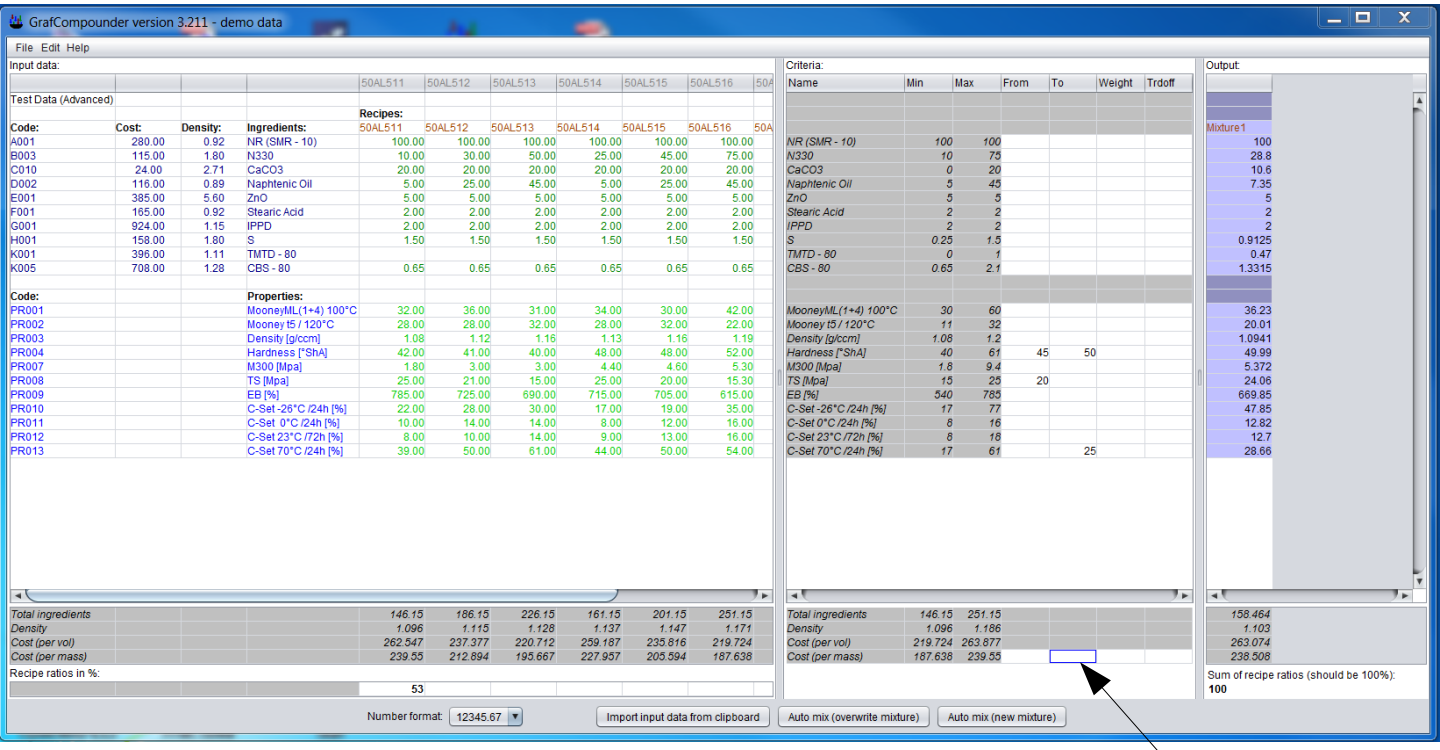
(Demo Data Advanced)



- **With same target values as in the previous example**
  - **Hardness “From” 45 ShA “To” 50 ShA**
  - **C-Set (70°C/24h) - “To” 25 %**
  - **Tensile - “From” 20 Mpa**
- **Create a new mixture with “Auto Mix (overwrite mixture)”**
  - **Result comes with**
    - ***Volume Cost***
    - ***Weight Cost***

Data analysis

(Demo Data Advanced)

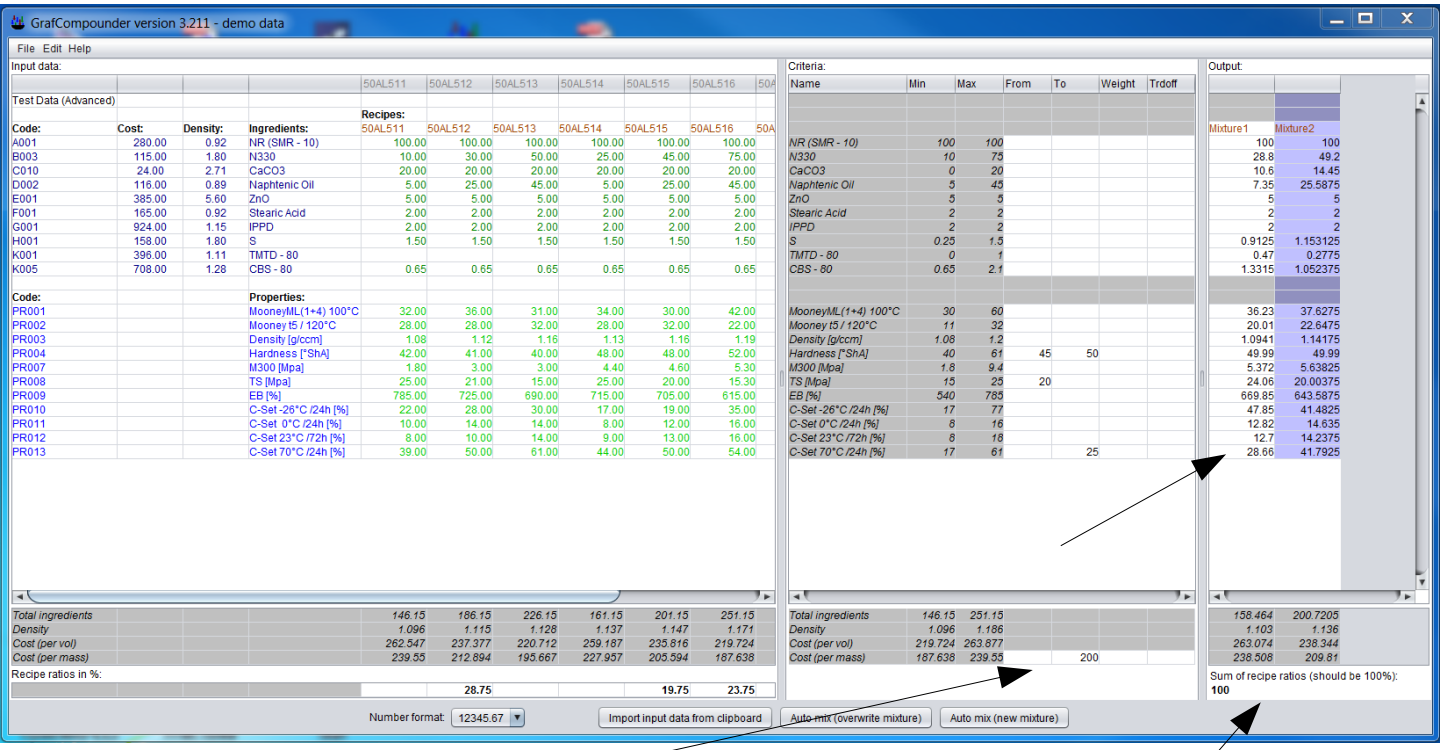


Cost targets

- ***It is possible to put a "cost (per mass)" target in.***
  - ***But not density: because formula is not created yet***
  - ***And volume cost target is not possible due to same reason.***

Data analysis

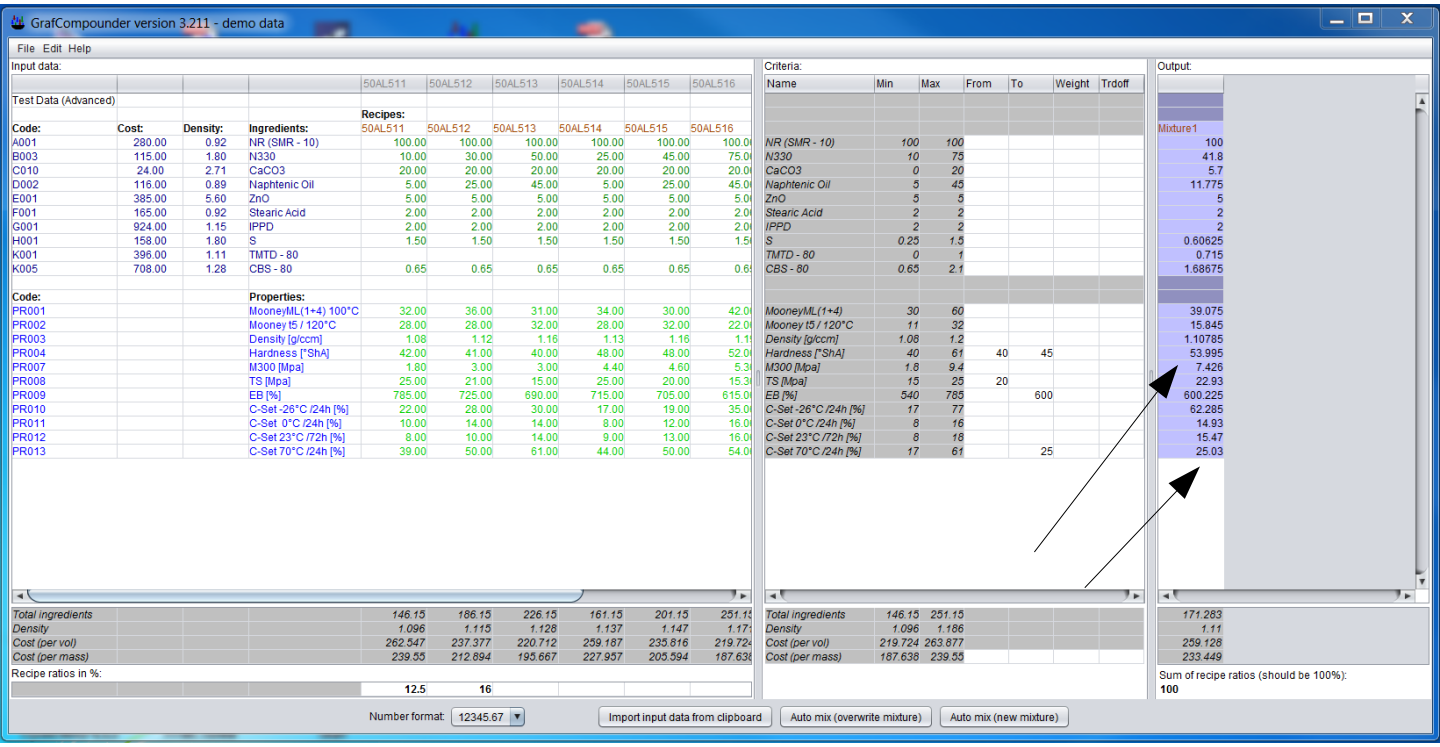
(Demo Data Advanced)



- ***Cost targets***
  - ***In the example we put in 200 as a "cost (per mass)" target in.***
    - ***It can be any unit***
      - ***In the example EU / 100 kg***
    - ***Processing with "Auto mix (new mixture)"***
      we are able to compoare influence of cost taget on results
- ***Cost per mass ist very close to target, consequently filler content is higher, but C-Set farer off.***
  Score with 650 compared to 82 for Mixture 1

Creating Formulas

Using “Weight” and “Trdoff”

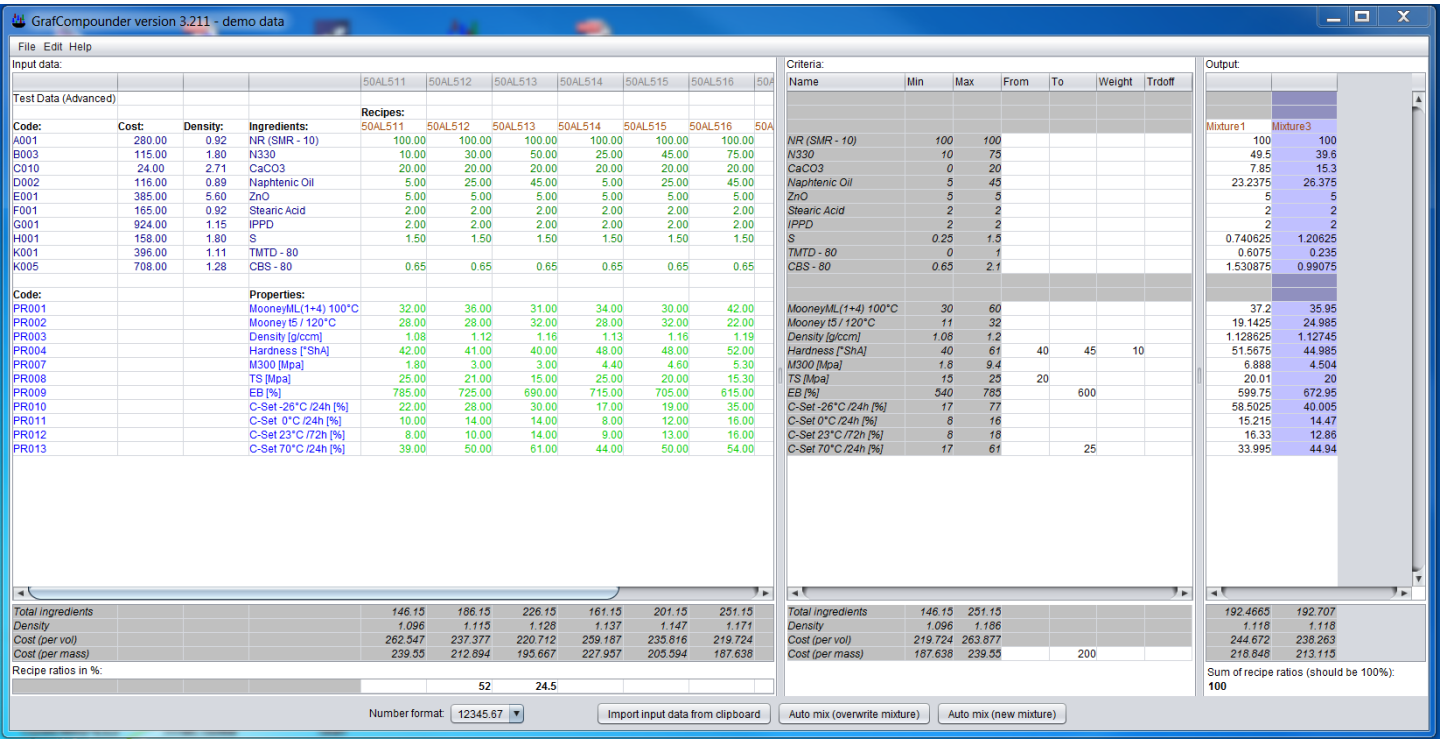


- **To show the use of “weight” and “Trd off” it is helpful to create a conflicting target:**
  - **Hardness: 40 – 45°ShA !**
  - **Tensile > 20 Mpa**
  - **Elongation < 600 %**
  - **C-set < 25%**

- **With Auto mix (Over write mixture) we calculate a new formula**
  - **Score is around 430**
    Due to mismatch of Hardness: 54°ShA

Creating Formulas

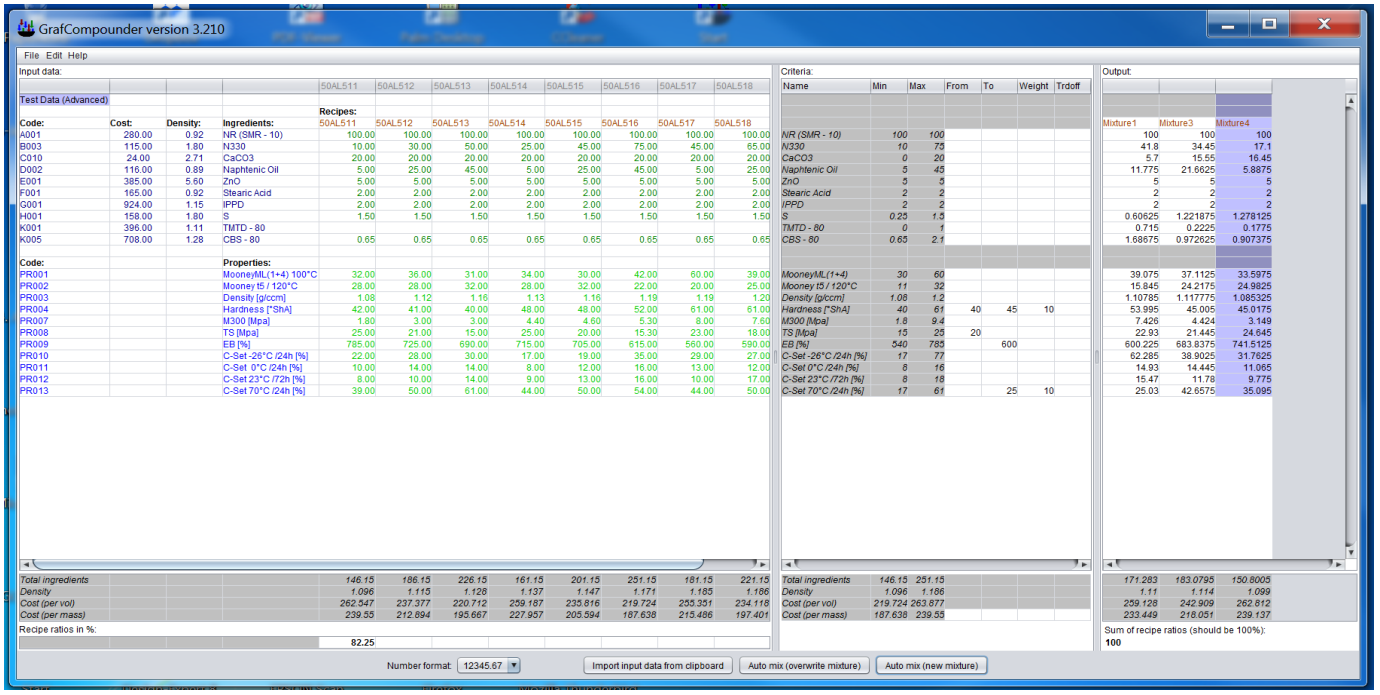
Using “Weight” and “Trdoff”



- **In our example we noticed that Hardness is out of target**
  - **But Hardness is the first property in any specification**
  - **To get result into hardness specification we put a “weight” of 10 in the criteria column (*Any other number > 0 will do*)**
  - **Choose “Auto mix (new mixture)” to follow changes**
- **Hardenss is now 45°ShA – in target**
- **C-Set is farer off target with 42 %**
- **Elongation is off with 683 %**
  - **Score point with 744 higher as well**

Creating Formulas

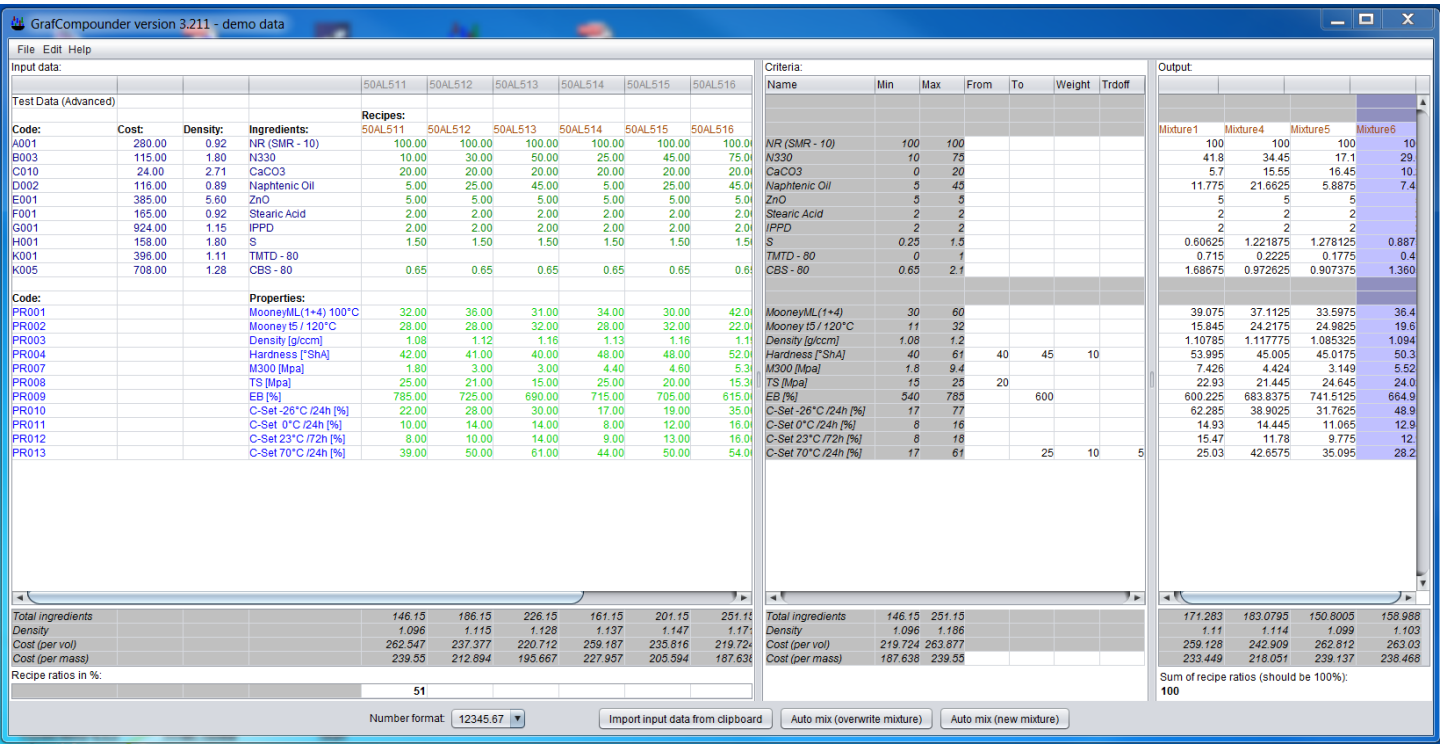
Using “Weight” and “Trdoff”



- **While Hardness is close to upper limit:**
  - **We do not want C-Set that high.**
- **How to find the best compromise?**
  - **We leave the “ weight” on Hardness**
  - **Put an additional “weight” on C-Cet (example 10)**
  -
- **Result:**
  C-Set now from 42% down to 35%
  while hardness is in specification
  (notice that elongaton has increased further)
  - **Consequently we have higher score 2878**

Creating Formulas

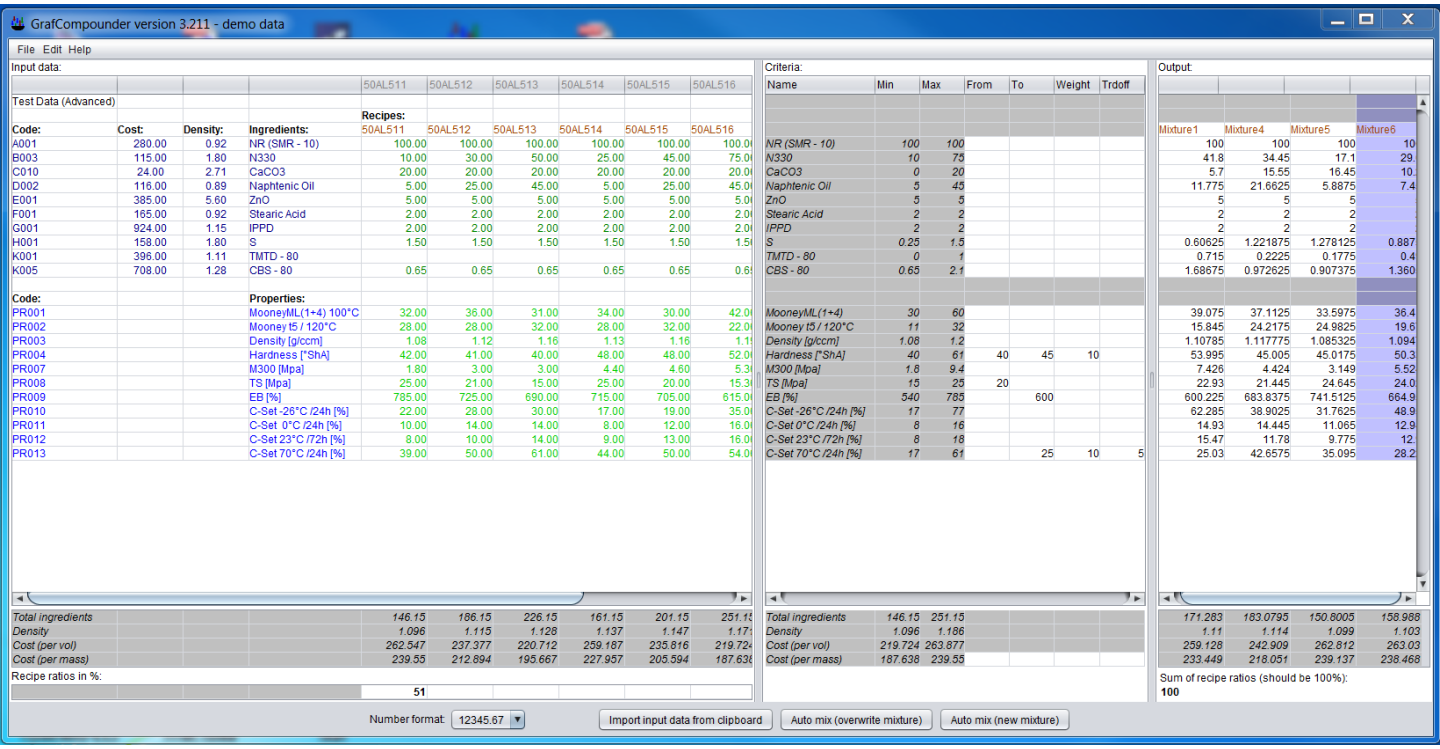
Using “Weight” and “Trdoff”



- **Result:**
  C-Set now from 42% down to 35%
  while hardness is in specification
  (notice that elongaton has increased further)
- **We want still better compression set with the chance to get hardness only a few points out of upper limit.**
  - **We want a preference on C-Set putting a “trdoff” of 5, while leaving both “weights”**
- **Result:**
  - **C-Set with 28% closer to upper limit and acceptable**
  - **Hardness has increased to 50°ShA**
  - **Elongation now at 665% lower than before**
- **Tentatively this results acceptable and will take in confirmation experiment.**

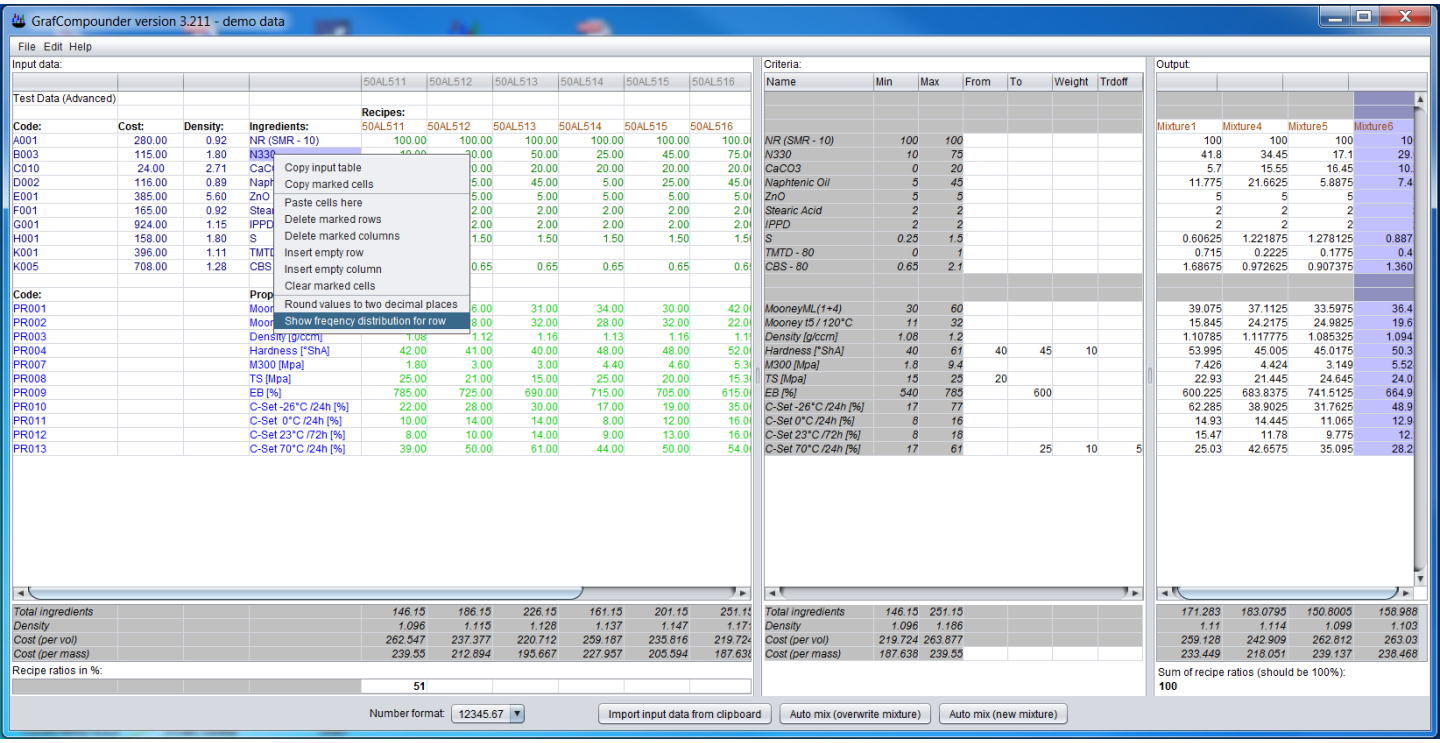
Creating Formulas

Using “Weight” and “Trdoff”



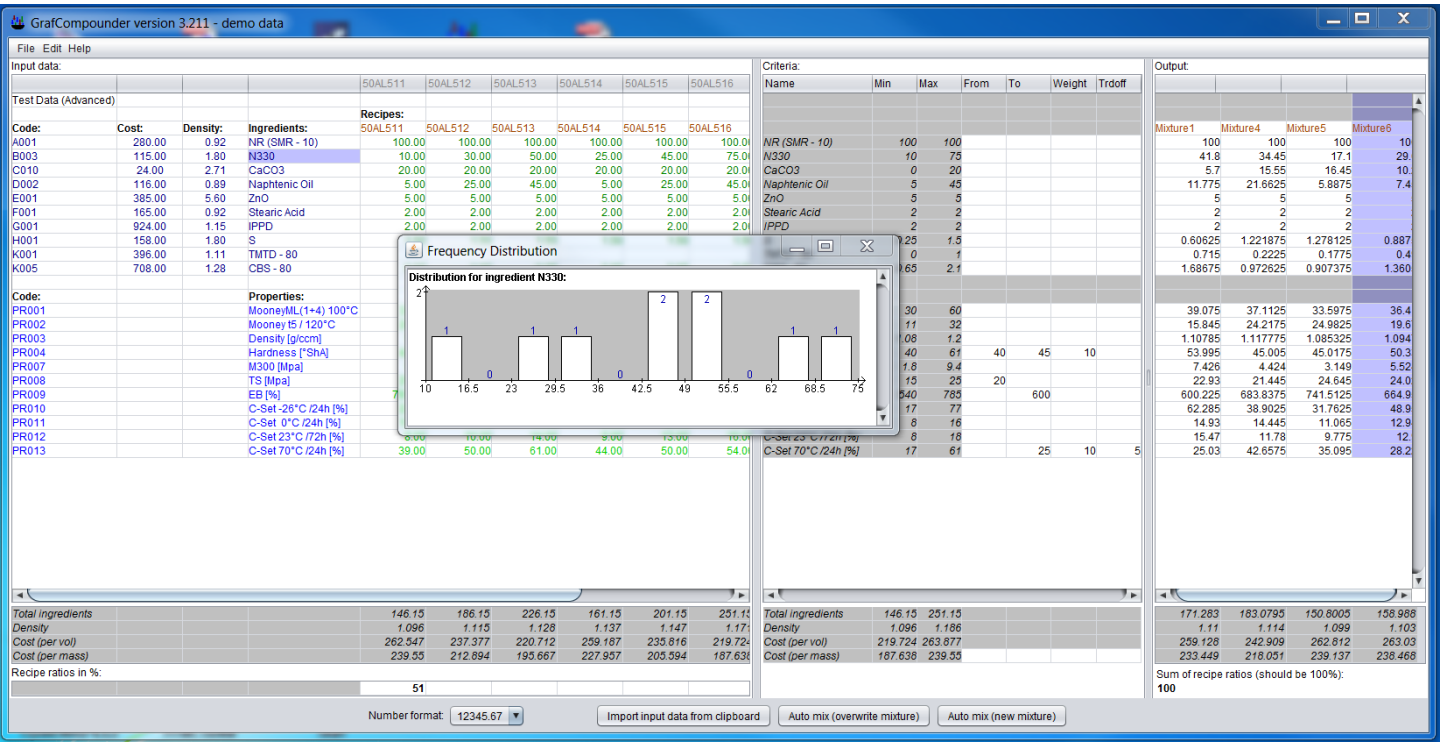
- **As demonstrated**
  - **“weight” helps to give a preference to properties, we have the freedom to select**
  - **In case of confliciting targets “trdoff” shifts the preference towards one of the weighted properties.**
  -
- **The search for the best compromise in case of conflicting properties in specification can be done with the “trdoff” command.**

Database Tools



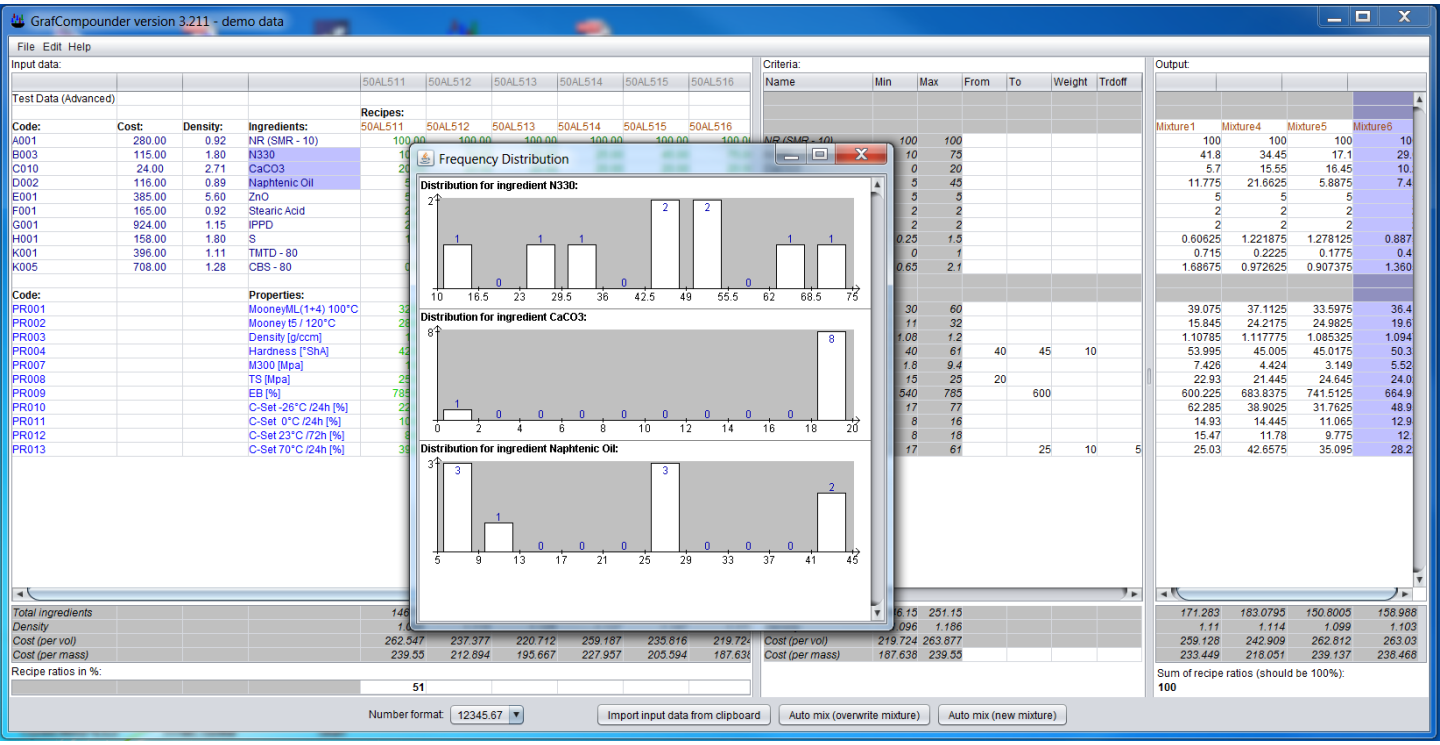
- Criteria window shows the Min / Max values for any ingredient and property
- In case you want more information about the distribution of any ingredient or property
  - Click mouse pointer in Cell: Example N 330
  - Right click to get into pull down menue select “fruequency distributio for row”

Database Tools



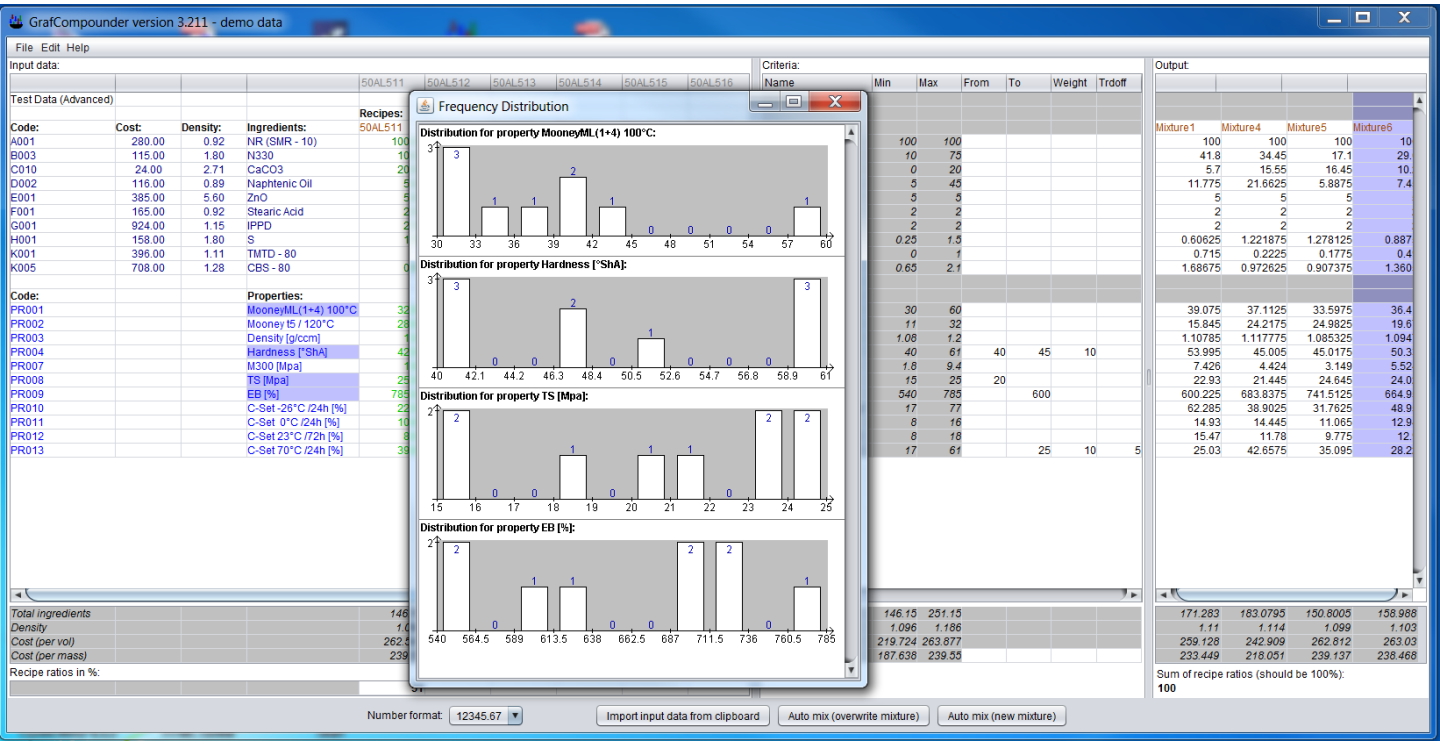
- “fruequency distributio for row”
  - Example N330 fruequency distribution is shown.
  - For ingredients with larger phr value the bar diagram is made of 10 steps starting with lowest value to max value

Database Tools



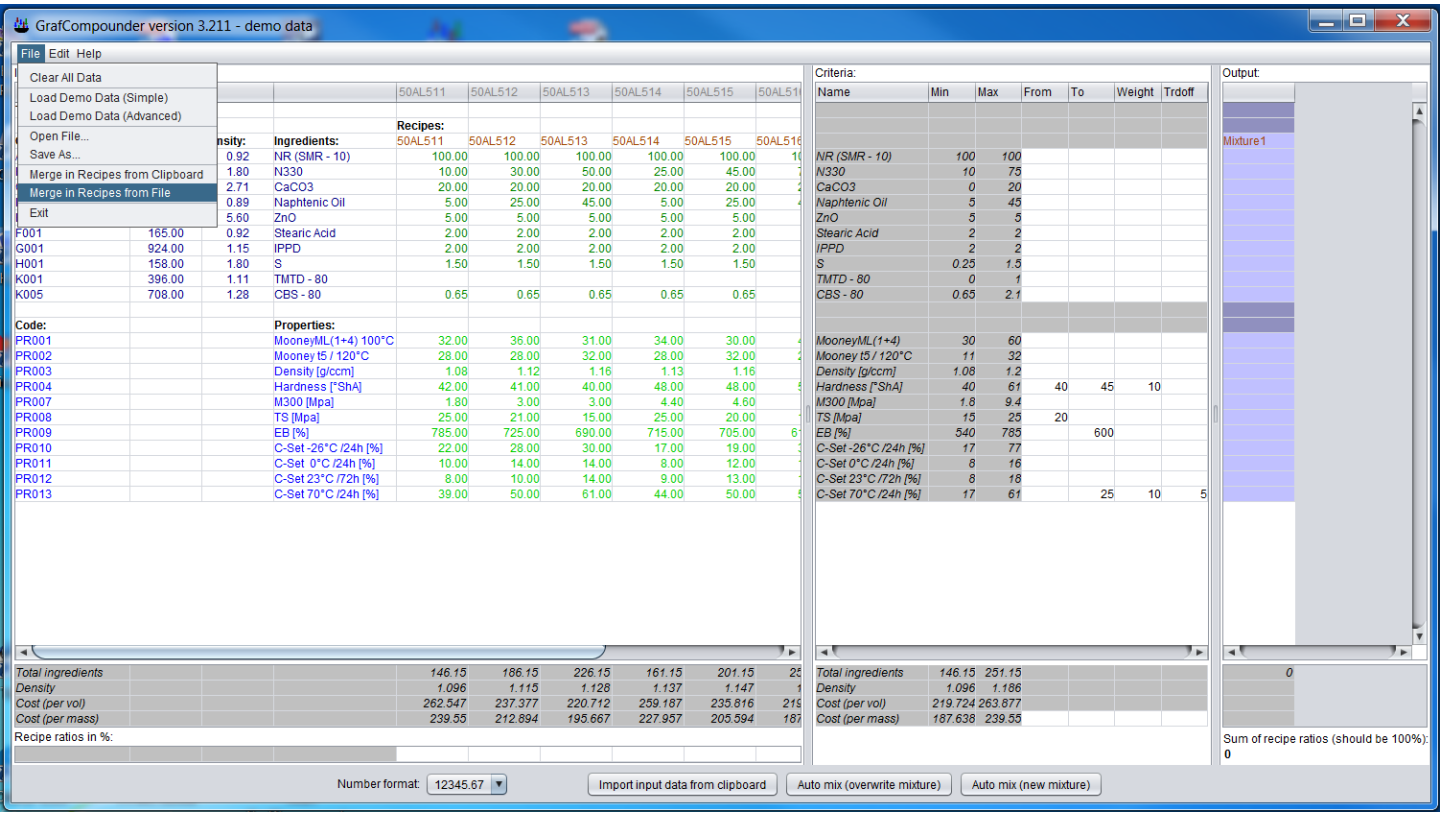
- **“fruequency distribution for x rows”**
  - **Example fruequency distribution for more than on ingredient:**
  - **Highlight all ingredients you want to see: Example: N330, CaCO3 and Naphtenic Oil**
  - **Pull Down menue with right click**
  - **Select “fruequency distribuion for 3 rows”**

Database Tools



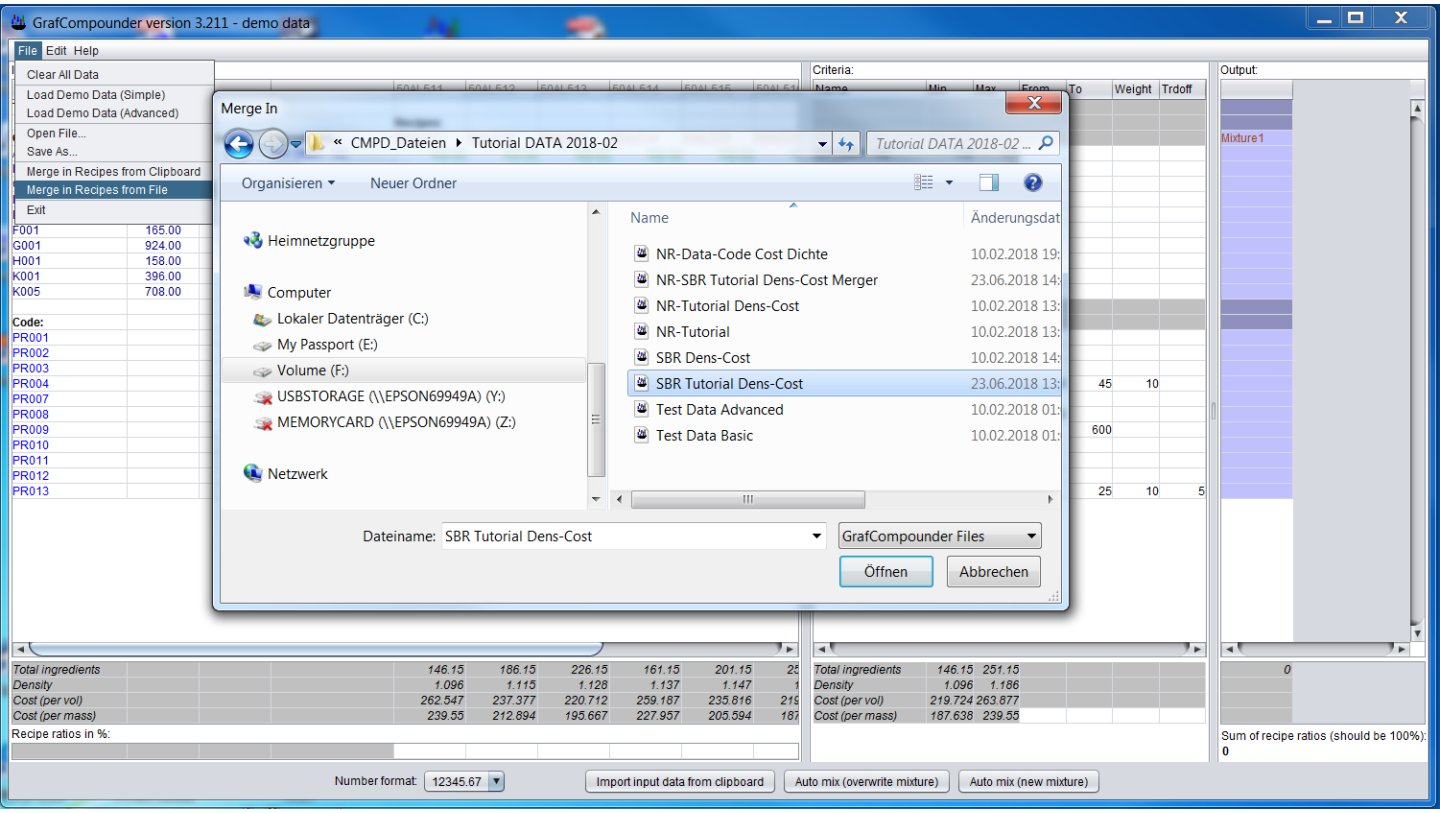
- "fruequency distribution for x rows"
  - Example fruequency distribution for more than on Property:
  - Highlight all properties you want to see: Example: Mooney, Hardness, TS-Tensile, EB-Elongation
  - Pull Down menue with right click
  - Select "fruequency distribuion for 4 rows"
- As in our previous example distributions are uneven *(what is expected with a small sample database)*

Database
Merger of Data Tables



- **Because of insufficient Data base you want to expand and add more data**
  - **Click File**
    Right click pull down menue:
    - **Option 1: Merge in Recipes from Clipboard**
    - **If you have copied Data from any other Table Data sheet**
    - **Option 2: Merge in Recipes from File**
      If you have stored a File in GC format
- **We take Option 2**

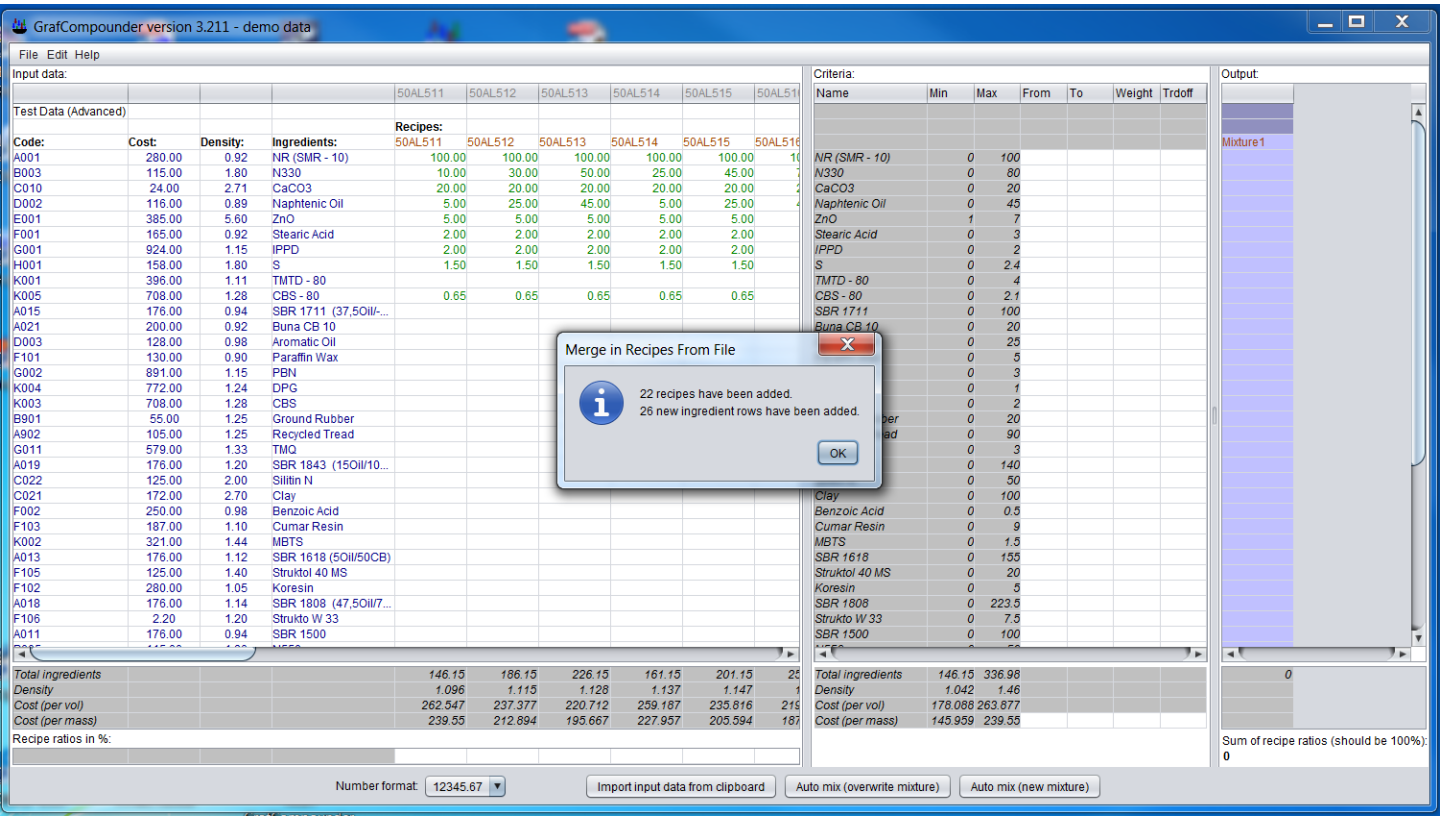
Database
Merger of Data Tables



- **Because of insufficient Data base you want to expand and add more data**
- **We take Option 2**
  - **Load Demo Data Advanced which is a set of NR Formulas**
  - **Click File**
  - **Select from Pull Down Menue: Merge in Recipes from File**
    - **Example: *SBR Tutorial Dens-Cost***
    - **Click Open**

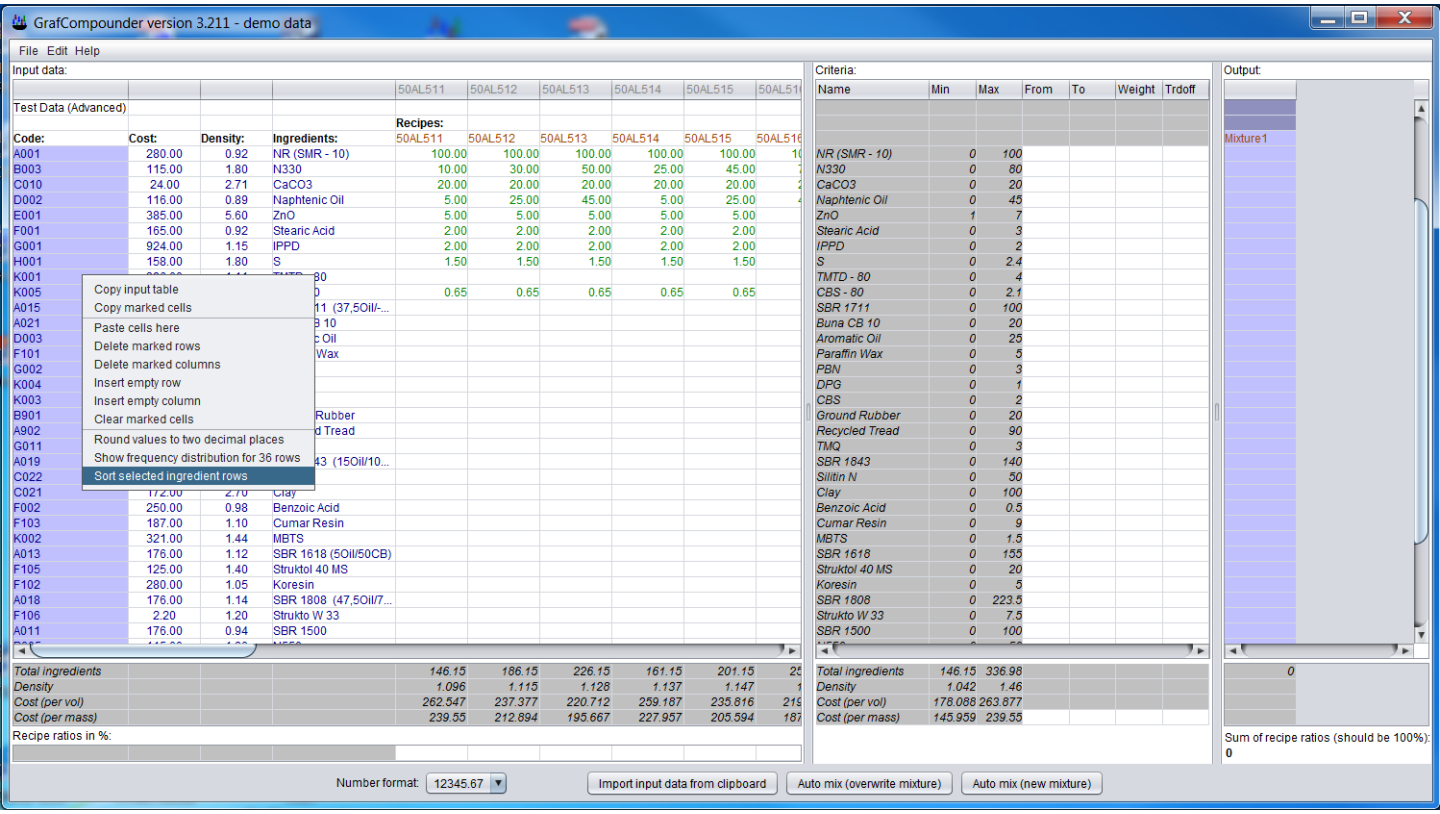
Database

Merger of Data Tables



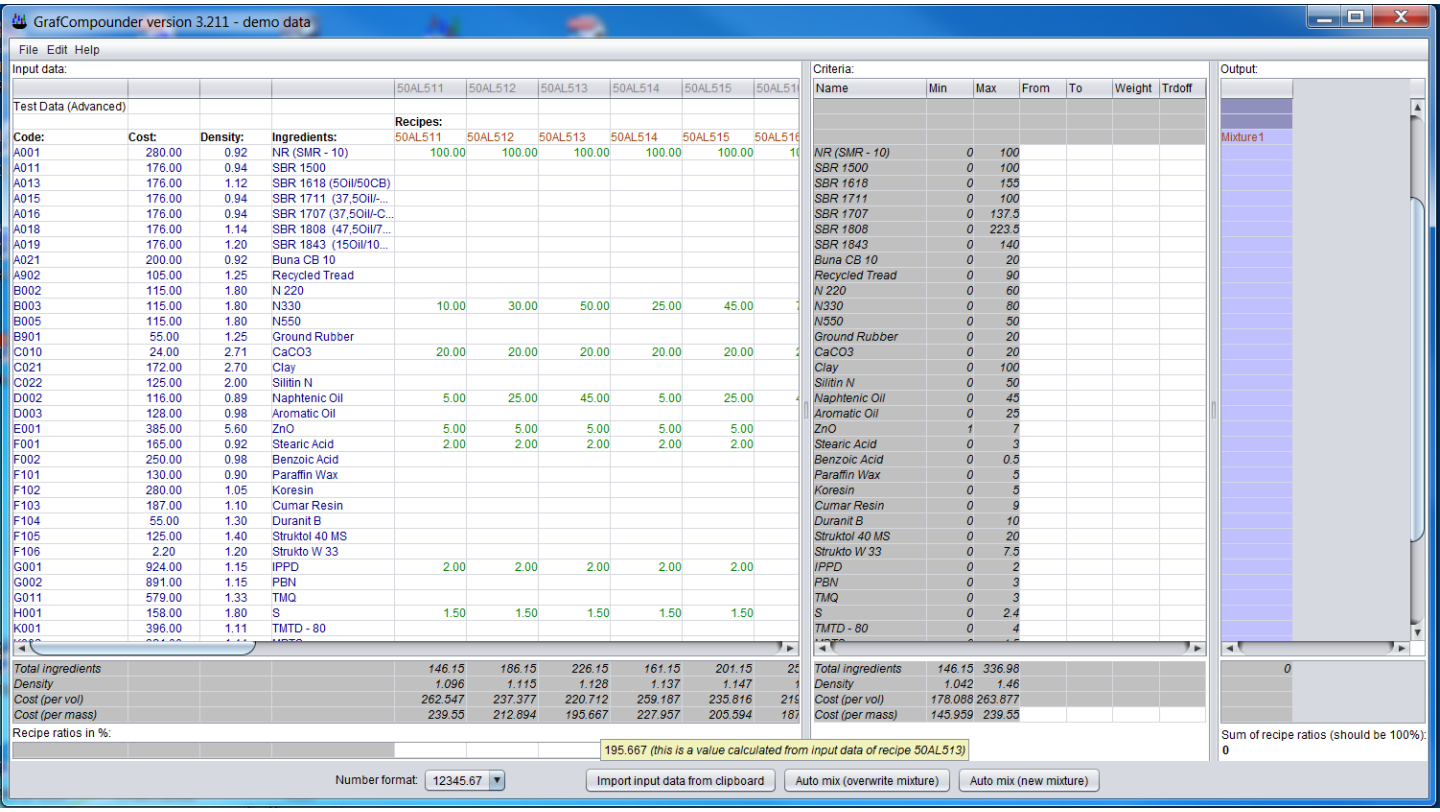
- **Because of insufficient Data base you want to expand and add more data**
- **With Option 2**
  - **Screen Appears with information window**
    - **xx Recipes have been added**
      (*in the example 22 recipes)*
    - **xx New ingredients have been added**
      (*in the example 26 new ingredient rows have been added)*
    - **xx new properties have been added**

Database
Merger of Data Tables



- Expanding the Data base with “Merger”
- Option 2
  - After the merger of files organization of data is necessary to have a table in the standard way
    - Polymer
    - Carbon Black
    - Whiting .....beside all other ingredients
    - Properties as well
- Click on all Ingredient Code: cells
- Right Click, Select “Sort by selected ingredient rows”

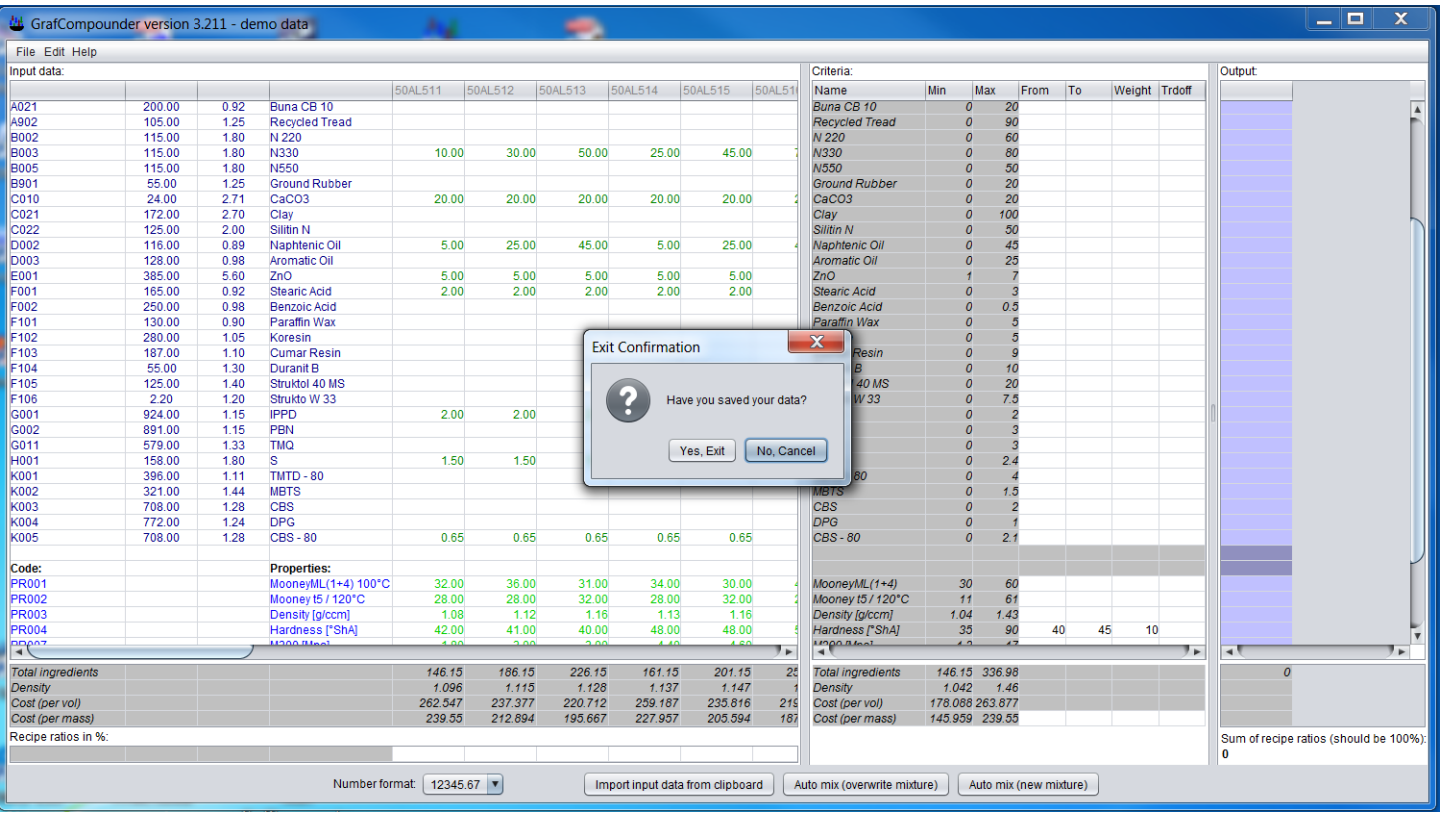
Database
Merger of Data Tables



- **Expanding the Data base with "Merger"**
  - **With Option 2:**
    - **After "Sort by selected ingredient rows" Ingredients in the table are organized in the standard way.**
      - ***Reminder: Sort properties separately.***
    - **Proceed with analysis and simulation**
- **Consideration:**
  - **Merge data sets with soluble polymers only**
    - **Insolubility cause second order effects None linearity) due to morphology influence of physicals**
  - **Data sets need same number format (dot, comma) for merger**

GrafCompounder

Data Storage



- **Store your results before closing the program**
  - **Click on x in upper right corner**
  - **Window appears: have you saved your data**

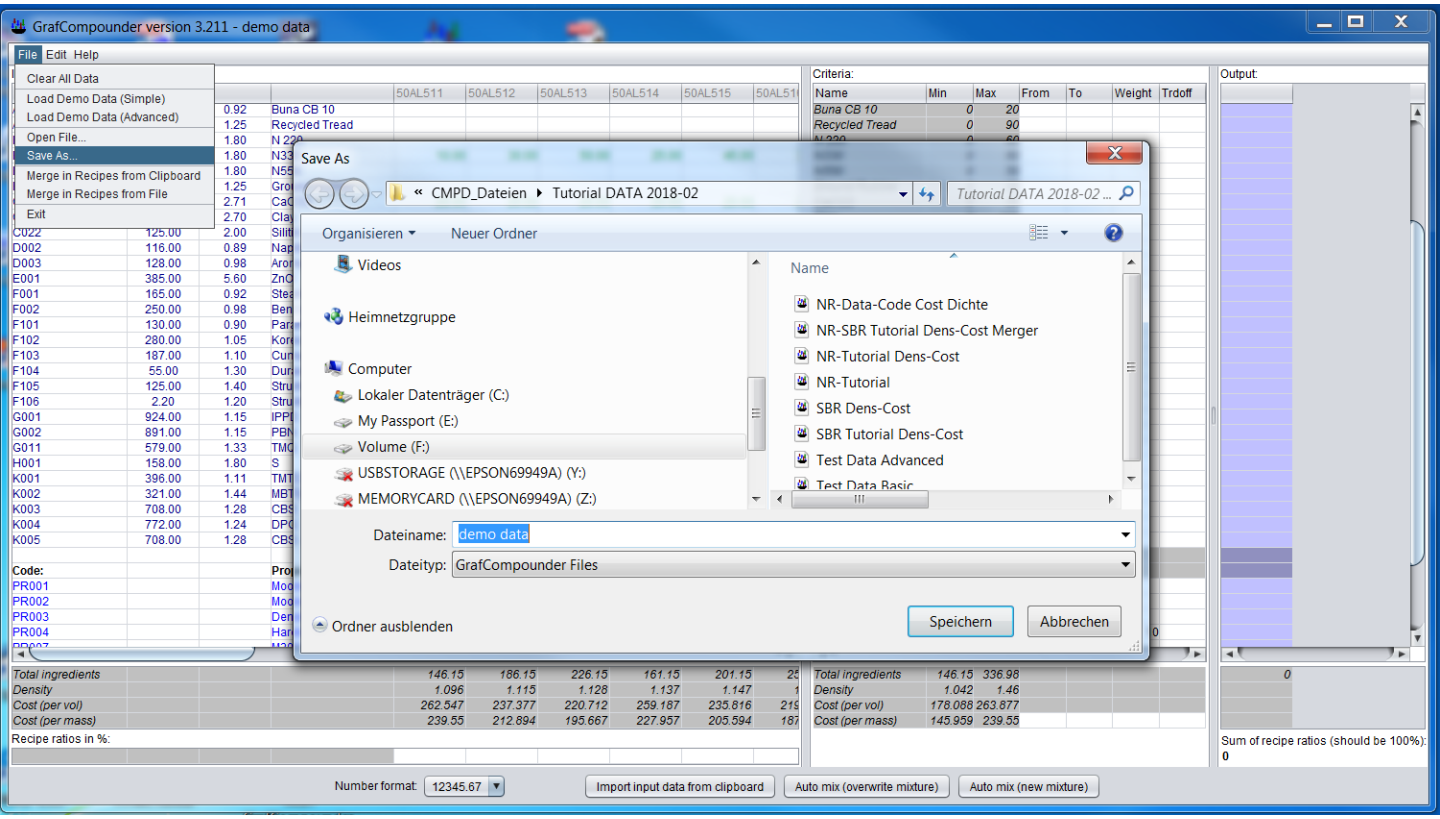
- There are two options:

1) Copy the data table and paste it into your table calculation spread sheet

2.) Store as ...gc (GrafCompounder) Format

GrafCompounder

Data Storage



- With 2nd option:
  - Select “No, Cancel”
  - Click “File”
  - Select: Folder
  - Name the File
  - Select “Store”

Note that this format can be opened by the GrafCompounder only

Summary

- With the GrafCompounder you have a newly created tool, which allows you to analyse a compound database using:
  - Limits,
  - “Weight” and
  - “Trade off”

  It is a formula simulation tool.
- “Weight” and “Trade off” allow to fine tune the simulation in case of conflicting targets
- Diagnose Tools show the spread / distribution of ingredients / physicals in the database
  - Min and Max Values are shown as well
- It is possible to merge different data sets from different sources
  - It is recommended to merge data with soluble polymers only

Summary

- With the GrafCompounder you can see the influence of each formula on the result.
  - Helps to track back to failure in the data base
- Cost of compound (Mass / Volume) are calculated.
  - Cost per mass can be used as a criteria in addition to physicals
- Quick analysis of the compounds, which are the result of different criteria and formulation inputs, enables you to make fast and accurate decisions, saving you time and money

Summary

- GrafCompounder recommendation
  - **Never ever go without a confirmation experiment**
    - Analyze the difference between measured and calculated data
      - If deviation out of confidence intervall
        - Look after faulty data in the database
        - Precision in Laboratory
        - Investigate other sources for failure
  - **Use the calculated Formula as a start in a “Statistic Experimental Design” (DoE)**
    - Use DoE for process optimization in Scale up
  - **Visit www.grafcompounder.com FAQ page**

Summary

- The formulas produced due to the selection criteria correspond to the general rules of compounding.
- These formulas will show property scores larger than the 95% confidence interval compared to those seen in the confirmation experiment as long as measurement errors in similar range.