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# **GrafCompounder 3.210**

**Working with the  
“GrafCompounder”  
Program**

**July 2018**

[www.grafcompounder.com](http://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:

- λ Elimination of Reinvention
- λ Allowing faster and more accurate decisions on starting formulas
- λ Creation of better ideas about further compound development
- λ 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”

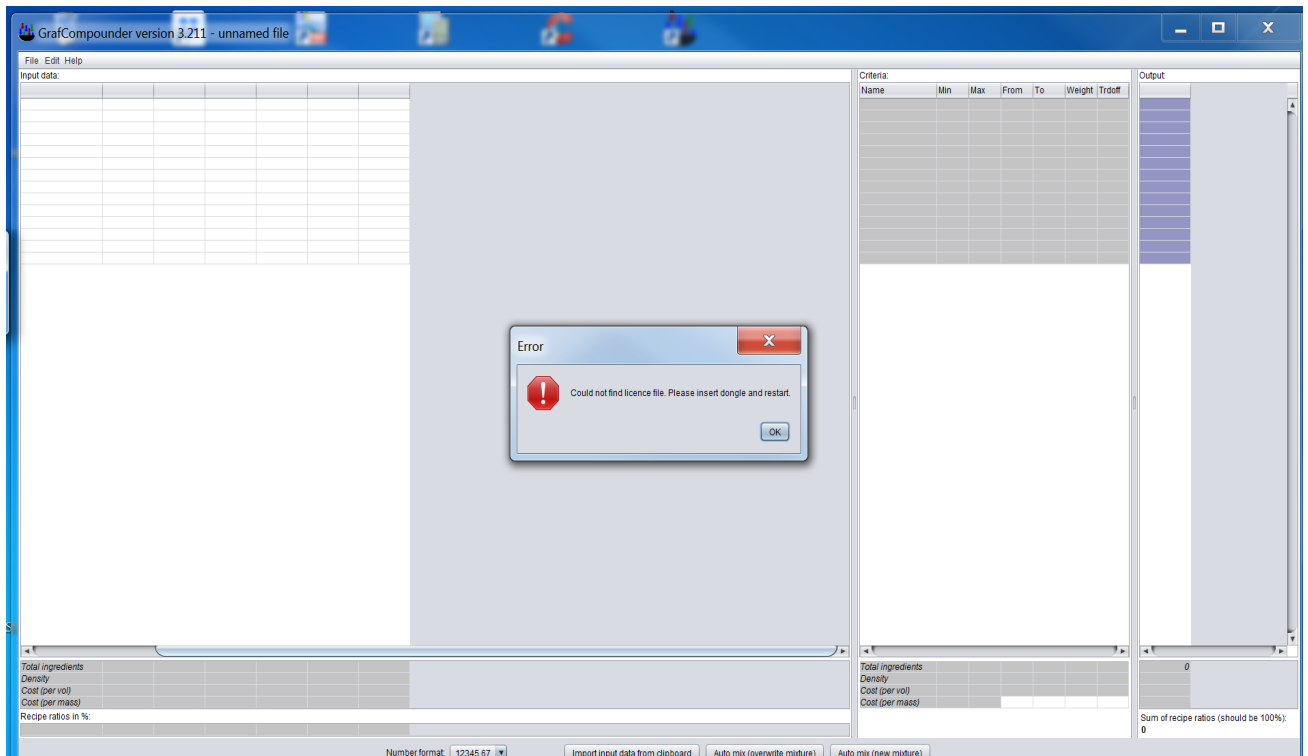
- **It shows all program features.**
- **Explains this “easy to use” program**
- **Guides you step wise through the program features**

# GrafCompounder

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

# Start Grafcompounder



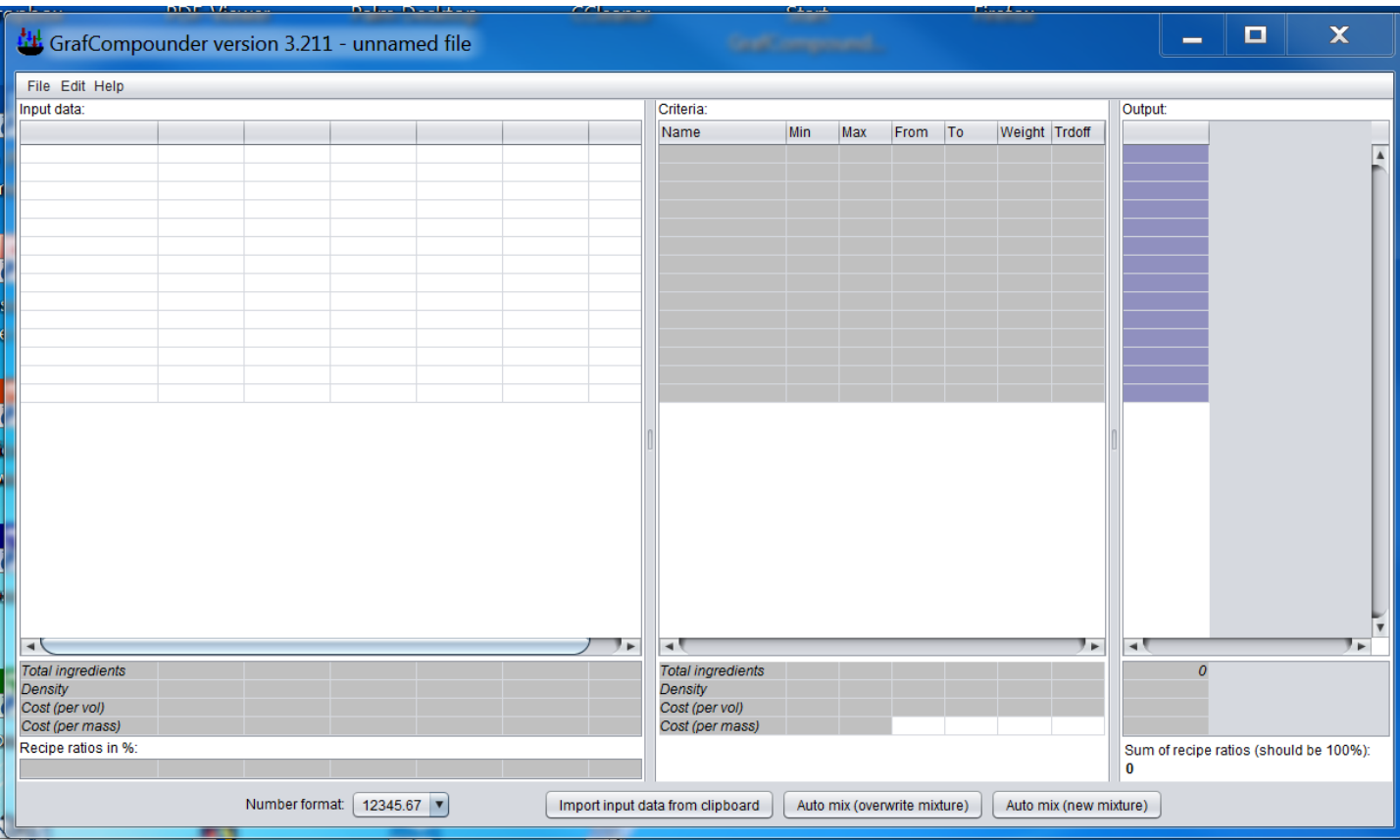
**Insert the license Dongle into a USB port on your PC/Laptop computer**

**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

The screenshot shows a spreadsheet with the following data:

	50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50AL517	50AL518	50AL542
Ingredients:									
NR (SMR - 10)	100,00	100,00	100,00	100,00	100,00	100,00	100,00	100,00	100,00
N330	10,00	30,00	50,00	25,00	45,00	75,00	45,00	65,00	50,00
CaCO <sub>3</sub>	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) 1*	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
Density	1,08	1,12	1,16	1,13	1,16	1,19	1,19	1,20	1,11
Hardness	42,00	41,00	40,00	48,00	48,00	52,00	61,00	61,00	59,00
M300	1,80	3,00	3,00	4,40	4,60	5,30	8,00	7,60	9,40
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

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

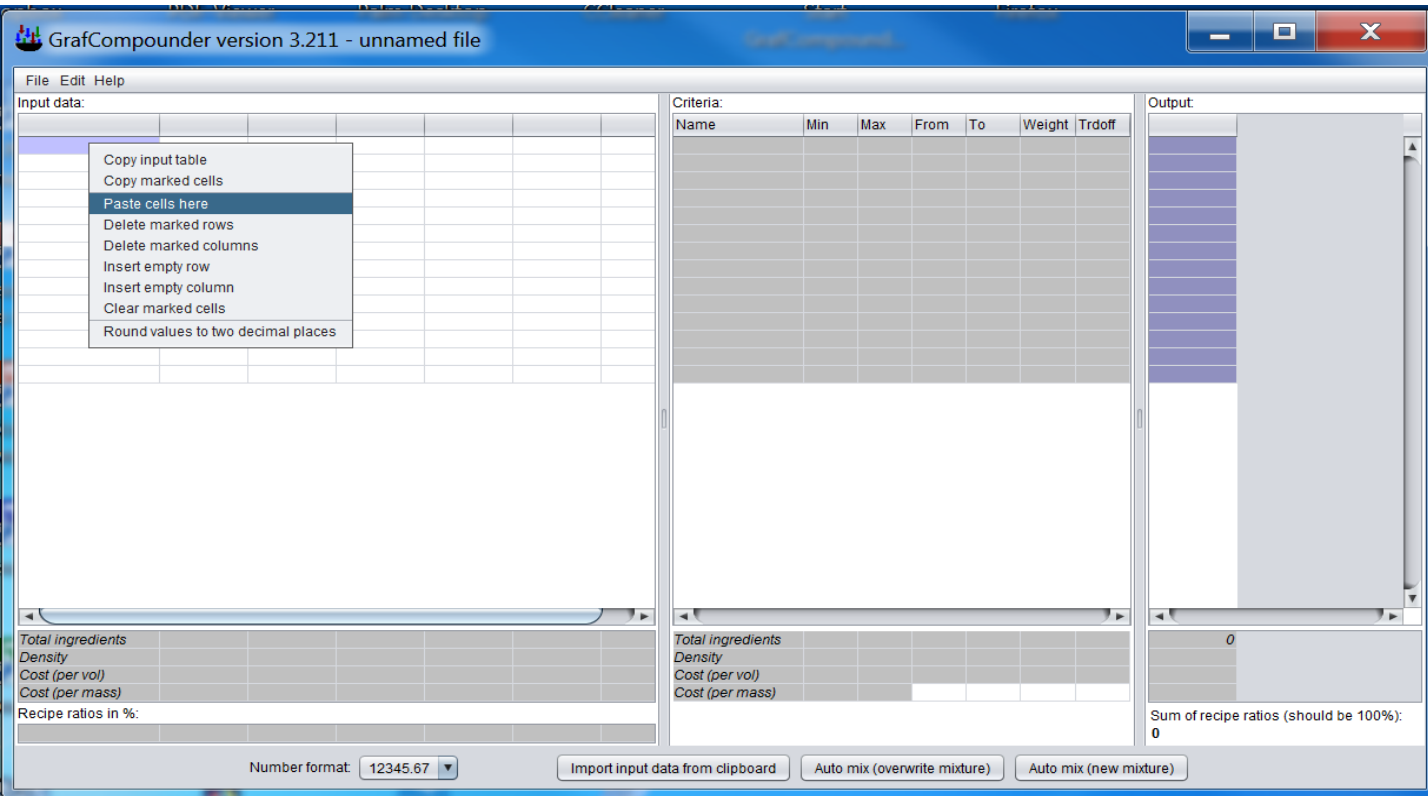
The screenshot shows a spreadsheet with the following data:

1	A	B	C	D	E	F	G	H	I	J	K	L
2	Testdaten	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												

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 Menu

# Data Insertion

The screenshot shows the GrafCompounder version 3.211 - demo data interface. The main window is divided into several sections:

- Input data:** A table with columns for recipes (50AL511 to 50AL515) and rows for ingredients and properties. Yellow cells indicate that the number format is different from the pre-set format.
- Criteria:** A table with columns for Name, Min, Max, From, To, Weight, and Trdoff. The Min and Max rows are empty.
- Output:** A list of ingredients and properties, including "Mixture 1".
- Bottom Panel:** Includes a "Number format" dropdown set to "12345,67", and buttons for "Import input data from clipboard", "Auto mix (overwrite mixture)", and "Auto mix (new mixture)".

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

The screenshot displays the GnuCompass 3.710 software interface. The main window is titled "GnuCompass version 3.710" and shows a table with columns for ingredients and properties. The table is organized into sections: "Input data", "Criteria", and "Output". The "Input data" section contains a table with columns for ingredients and properties, and rows for various items like "Wheatflour", "Rice", "Soya", etc. The "Criteria" section contains a table with columns for ingredients and properties, and rows for various items like "Wheatflour", "Rice", "Soya", etc. The "Output" section contains a table with columns for ingredients and properties, and rows for various items like "Wheatflour", "Rice", "Soya", etc. Arrows point to the "Criteria" window and the "Input data" table.

Ingredients	Wheatflour	Rice	Soya	...	...	...	...	...	...
Wheatflour	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
Rice	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00
Soya	10.00	10.00	10.00	10.00	10.00	10.00	10.00	10.00	10.00
...	...	...	...	...	...	...	...	...	...

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

The screenshot shows the GrafCompounder version 2.003 software interface. The main window is titled "GrafCompounder version 2.003" and has a menu bar with "File", "Edit", and "Help".

The interface is divided into several sections:

- Input data:** A table with columns for ingredients and rows for various materials. The table is color-coded: ingredients are in red, and properties are in green.
- Criteria:** A table with columns for Name, Min, Max, From, To, Wei..., and Trdoff. It lists various materials and their minimum and maximum values.
- Output:** A list of materials, including "Mixture 1".
- Properties:** A table with columns for properties and rows for various materials. The table is color-coded: properties are in green, and ingredients are in red.

At the bottom of the window, there is a "Recipe ratios in %" section and a "Number format" dropdown menu set to "12345,67". There are also buttons for "Import input data from clipboard", "Auto mix (overwrite mixture)", and "Auto mix (new mixture)".

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

GrafCompunder version 3.211 - demo data

File Edit Help

- Clear All Data
- Load Demo Data (Simple)
- Load Demo Data (Advanced)
- Open File...
- Save As...
- Merge in Recipes from Clipboard
- Merge in Recipes from File
- Exit

	50AL512	50AL513	50AL514	50AL515	50AL516	50AL517
100.00	100.00	100.00	100.00	100.00	100.00	100.00
30.00	50.00	25.00	45.00	75.00		
20.00	20.00	20.00	20.00	20.00		
25.00	45.00	5.00	25.00	45.00		
	5.00	5.00	5.00	5.00	5.00	
Stearic Acid	2.00	2.00	2.00	2.00	2.00	2.00
IPPD	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
TMTD - 80						
CBS - 80	0.65	0.65	0.65	0.65	0.65	0.65
<b>Properties:</b>						
MooneyML(1+4) 100°C	32.00	36.00	31.00	34.00	30.00	42.00
Mooney t5 / 120°C	28.00	28.00	32.00	28.00	32.00	22.00
Density [g/ccm]	1.08	1.12	1.16	1.13	1.16	1.19
Hardness [°ShA]	42.00	41.00	40.00	48.00	48.00	52.00
M300 [Mpa]	1.80	3.00	3.00	4.40	4.60	5.30
TS [Mpa]	25.00	21.00	15.00	25.00	20.00	15.30
EB [%]	785.00	725.00	690.00	715.00	705.00	615.00
C-Set -26°C /24h [%]	22.00	28.00	30.00	17.00	19.00	35.00
C-Set 0°C /24h [%]	10.00	14.00	14.00	8.00	12.00	16.00
C-Set 23°C /72h [%]	8.00	10.00	14.00	9.00	13.00	16.00
C-Set 70°C /24h [%]	39.00	50.00	61.00	44.00	50.00	54.00
Total Ingredients	146.15	186.15	226.15	161.15	201.15	251.15
Density						
Cost (per vol)						
Cost (per mass)						
Recipe ratios in %:						

Criteria:

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				
MooneyML(1+4)	30	60				
Mooney t5 /	11	32				
Density [g/ccm]	1.08	1.2				
Hardness	40	61				
M300 [Mpa]	1.8	9.4				
TS [Mpa]	15	25				
EB [%]	540	785				
C-Set -26°C	17	77				
C-Set 0°C	8	16				
C-Set 23°C	8	18				
C-Set 70°C	17	61				

Output:

Mixture 1

0

Sum of recipe ratios (should be 100%):  
0

Number format: 12345.67

Import input data from clipboard    Auto mix (overwrite mixture)    Auto mix (new mixture)

## Other options for adding data:

As a second option you can open the GrafCompunder program

- Click "File"
- and "LoadDemo Data (simple)" in the pull down menu.

# Open File

Criteria:

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				
MooneyML(1+4)	30	60				
Mooney t5 /	11	32				
Density [g/ccm]	1.08	1.2				
Hardness [ShA]	40	61				
M300 [Mpa]	1.8	9.4				
TS [Mpa]	15	25				
EB [%]	540	785				
C-Set -26°C	17	77				
C-Set 0°C	8	16				
C-Set 23°C	8	18				
C-Set 70°C	17	61				

Output

Name	Min	Max	From	To	Wei...	Trdoff
Mixture1						

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

GrafCompounder version 3.211 - demo data

File Edit Help

Input data:

Test Data (Adv...)				50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50AL517	
<b>Code:</b>	<b>Cost:</b>	<b>Density:</b>	<b>Ingredients:</b>	<b>Recipes:</b>							
A001	280.00	0.92	NR (SMR - 10)	100.00	100.00	100.00	100.00	100.00	100.00	100.00	
B003	115.00	1.80	N330	10.00	30.00	50.00	25.00	45.00	75.00		
C010	24.00	2.71	CaCO3	20.00	20.00	20.00	20.00	20.00	20.00		
D002	116.00	0.89	Naphtenic Oil	5.00	25.00	45.00	5.00	25.00	45.00		
E001	385.00	5.60	ZnO	5.00	5.00	5.00	5.00	5.00	5.00		
F001	165.00	0.92	Stearic Acid	2.00	2.00	2.00	2.00	2.00	2.00		
G001	924.00	1.15	IPPD	2.00	2.00	2.00	2.00	2.00	2.00		
H001	158.00	1.80	S	1.50	1.50	1.50	1.50	1.50	1.50		
K001	396.00	1.11	TMTD - 80								
K005	708.00	1.28	CBS - 80	0.65	0.65	0.65	0.65	0.65	0.65		
<b>Code:</b>			<b>Properties:</b>								
PR001			MooneyML(1+4) 100°C	32.00	36.00	31.00	34.00	30.00	42.00		
PR002			Mooney t5 / 120°C	28.00	28.00	32.00	28.00	32.00	22.00		
PR003			Density [g/ccm]	1.08	1.12	1.16	1.13	1.16	1.19		
PR004			Hardness [°SHA]	42.00	41.00	40.00	48.00	48.00	52.00		
PR005			M300 [Mpa]	1.80	3.00	3.00	4.40	4.60	5.30		
PR008			TS [Mpa]	25.00	21.00	15.00	25.00	20.00	15.30		
PR009			EB [%]	785.00	725.00	690.00	715.00	705.00	615.00		
PR010			C-Set -26°C /24h [%]	22.00	28.00	30.00	17.00	19.00	35.00		
PR011			C-Set 0°C /24h [%]	10.00	14.00	14.00	8.00	12.00	16.00		
PR012			C-Set 23°C /72h [%]	8.00	10.00	14.00	9.00	13.00	16.00		
PR013			C-Set 70°C /24h [%]	39.00	50.00	61.00	44.00	50.00	54.00		
<b>Total ingredients</b>				146.15	166.15	226.15	161.15	201.15	251.15		
<b>Density</b>				1.096	1.115	1.128	1.137	1.147	1.171		
<b>Cost (per vol)</b>				262.547	237.377	220.712	259.187	235.816	219.724		
<b>Cost (per mass)</b>				239.55	212.894	195.667	227.957	205.594	187.638		
<b>Recipe ratios in %:</b>											

Criteria:

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				
MooneyML(1+4)	30	60				
Mooney t5 /	11	32				
Density [g/ccm]	1.08	1.2				
Hardness	40	61				
M300 [Mpa]	1.8	9.4				
TS [Mpa]	15	25				
EB [%]	540	785				
C-Set -26°C	17	77				
C-Set 0°C	8	16				
C-Set 23°C	8	18				
C-Set 70°C	17	61				

Output:

Mixture1

Sum of recipe ratios (should be 100%): 0

Number format: 12345.67

Import input data from clipboard Auto mix (overwrite mixture) Auto mix (new mixture)

"LoadDemo Data (advanced)"

This Data File has additional columns

- Density:
- Cost:
- Code:



# Open File

GrafCompoander version 3.211 - demo data

File Edit Help

Input data:

			50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50AL517	
Code:	Cost:	Density:	Recipes:							
A001	280.00	0.92	100.00	100.00	100.00	100.00	100.00	100.00	100.00	
B003	115.00	1.80	10.00	30.00	50.00	25.00	45.00	75.00		
C010	24.00	2.71	20.00	20.00	20.00	20.00	20.00	20.00		
D002	116.00	0.89	5.00	25.00	45.00	5.00	25.00	45.00		
E001	385.00	5.60	5.00	5.00	5.00	5.00	5.00	5.00		
F001	165.00	0.92	2.00	2.00	2.00	2.00	2.00	2.00		
G001	924.00	1.15	2.00	2.00	2.00	2.00	2.00	2.00		
H001	158.00	1.80	1.50	1.50	1.50	1.50	1.50	1.50		
K001	396.00	1.11								
K005	708.00	1.28	0.65	0.65	0.65	0.65	0.65	0.65		

Code: PR001 PR002 PR003 PR004 PR007 PR008 PR009 PR010 PR011 PR012 PR013

Properties:

	50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50AL517
MooneyML(1+4) 100°C	32.00	36.00	31.00	34.00	30.00	42.00	
Mooney t5 / 120°C	28.00	28.00	32.00	28.00	32.00	22.00	
Density [g/ccm]	1.08	1.12	1.16	1.13	1.16	1.19	
Hardness [°ShA]	42.00	41.00	40.00	48.00	48.00	52.00	
M300 [Mpa]	1.80	3.00	3.00	4.40	4.60	5.30	
TS [Mpa]	25.00	21.00	15.00	25.00	20.00	15.30	
EB [%]	785.00	725.00	690.00	715.00	705.00	615.00	5
C-Set -26°C /24h [%]	22.00	28.00	30.00	17.00	19.00	35.00	
C-Set 0°C /24h [%]	10.00	14.00	14.00	8.00	12.00	16.00	
C-Set 23°C /72h [%]	8.00	10.00	14.00	9.00	13.00	16.00	
C-Set 70°C /24h [%]	39.00	50.00	61.00	44.00	50.00	54.00	

Criteria:

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				
MooneyML(1+4)	30	60				
Mooney t5 /	11	32				
Density [g/ccm]	1.08	1.2				
Hardness	40	61				
M300 [Mpa]	1.8	9.4				
TS [Mpa]	15	25				
EB [%]	540	785				
C-Set -26°C	17	77				
C-Set 0°C	8	16				
C-Set 23°C	8	18				
C-Set 70°C	17	61				

Output:

Mixture1

0

Sum of recipe ratios (should be 100%): 0

Total ingredients: 146.15 186.15 226.15 161.15 201.15 251.15 11

Density: 1.096 1.115 1.128 1.137 1.147 1.171

Cost (per vol): 262.547 237.377 220.712 259.187 235.816 219.724 25

Cost (per mass): 239.55 212.894 195.667 227.957 205.594 187.638 21

Recipe ratios in %:

Number format: 12345.67

Import input data from clipboard

Auto mix (overwrite mixture)

Auto mix (new mixture)

"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 density, cost per volume and cost per mass

# Data analysis

## (Demo Data Simple)

GrafCompounder version 3.211 - demo data

File Edit Help

Input data:

	50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50AL517	50AL518	50AL542
<b>Test Data (Simple)</b>									
<b>Ingredients:</b>									
NR (SMR - 10)	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
N330	10.00	30.00	50.00	25.00	45.00	75.00	45.00	65.00	50.00
CaCO3	20.00	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
<b>Properties:</b>									
MooneyML(1+4) 100°C	32.00	36.00	31.00	34.00	30.00	42.00	60.00	39.00	41.00
Mooney 15 / 120°C	28.00	28.00	32.00	28.00	32.00	22.00	20.00	25.00	11.00
Density [g/ccm]	1.08	1.12	1.16	1.13	1.16	1.19	1.19	1.20	1.11
Hardness [°ShA]	42.00	41.00	40.00	48.00	48.00	52.00	61.00	61.00	59.00
M300 [Mpa]	1.80	3.00	3.00	4.40	4.60	5.30	8.00	7.60	9.40
TS [Mpa]	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
C-Set -26°C /24h [%]	22.00	28.00	30.00	17.00	19.00	35.00	29.00	27.00	77.00
C-Set 0°C /24h [%]	10.00	14.00	14.00	8.00	12.00	16.00	13.00	12.00	16.00
C-Set 23°C /72h [%]	8.00	10.00	14.00	9.00	13.00	16.00	10.00	17.00	18.00
C-Set 70°C /24h [%]	39.00	50.00	61.00	44.00	50.00	54.00	44.00	50.00	17.00
<b>Criteria:</b>									
Name	Min	Max	From	To	Weig.	Trdoff			
NR (SMR - 10)	100	100							
N330	10	75	20	25					
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							
<b>Output:</b>									
<b>Mixture 1</b>									
NR (SMR - 10)	100					100			
N330	19.9875					19.9875			
CaCO3	20					20			
Naphtenic Oil	11.3					11.3			
ZnO	5					5			
Stearic Acid	2					2			
IPPD	2					2			
S	1.5					1.5			
TMTD - 80									
CBS - 80	0.65					0.65			
<b>MooneyML(1+4)</b>									
MooneyML(1+4)	30	60				33.465			
Mooney 15 /	11	32				27.155			
Density [g/ccm]	1.08	1.2				1.097025			
Hardness [°ShA]	40	61				43.455			
M300 [Mpa]	1.8	9.4				2.32825			
TS [Mpa]	15	25				23.46925			
EB [%]	540	785				758.975			
C-Set -26°C	17	77				23.9975			
C-Set 0°C /24h	8	16				10.925			
C-Set 23°C /72h	8	18				9.24			
C-Set 70°C /24h	17	61				41.4325			
<b>Total Ingredients</b>									
Total Ingredients	146.15	251.15				162.4375			
Density									
Cost (per vol)									
Cost (per mass)									
<b>Recipe ratios in %:</b>									
	84.25	1				14.75			

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)

GrafCompunder version 3.211 - demo data

File Edit Help

Input data:

	50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50AL517	50AL518	50AL542
<b>Test Data (Simple)</b>									
<b>Ingredients:</b>									
NR (SMR - 10)	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
N330	10.00	30.00	50.00	25.00	45.00	75.00	45.00	65.00	50.00
CaCO3	20.00	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
<b>Properties:</b>									
MooneyML(1+4) 100°C	32.00	36.00	31.00	34.00	30.00	42.00	60.00	39.00	41.00
Mooney I5 / 120°C	28.00	28.00	32.00	28.00	32.00	22.00	20.00	25.00	11.00
Density [g/ccm]	1.08	1.12	1.16	1.13	1.16	1.19	1.19	1.20	1.11
Hardness [°ShA]	42.00	41.00	40.00	48.00	48.00	52.00	61.00	61.00	59.00
M300 [Mpa]	1.80	3.00	3.00	4.40	4.60	5.30	8.00	7.60	9.40
TS [Mpa]	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
C-Set -26°C /24h [%]	22.00	28.00	30.00	17.00	19.00	35.00	29.00	27.00	77.00
C-Set 0°C /24h [%]	10.00	14.00	14.00	8.00	12.00	16.00	13.00	12.00	16.00
C-Set 23°C /72h [%]	8.00	10.00	14.00	9.00	13.00	16.00	10.00	17.00	18.00
C-Set 70°C /24h [%]	39.00	50.00	61.00	44.00	50.00	54.00	44.00	50.00	17.00
<b>Criteria:</b>									
Name	Min	Max	From	To	Weig...	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							
<b>Output:</b>									
Mixture1									
Total ingredients 146.15 251.15									
Density									
Cost (per vol)									
Cost (per mass)									
Sum of recipe ratios (should be 100%): 0									

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)

The screenshot shows the GrafCompounder version 3.2111 - demo data interface. It features a main data table with columns for various recipes (50AL511 to 50AL542) and rows for ingredients and properties. A 'Criteria' table is visible on the right, listing parameters like NR (SMR - 10), N330, CaCO3, etc., with their respective Min, Max, From, To, Weight, and Trdff values. An 'Automatic mixing in process' dialog box is overlaid on the data table, displaying a progress bar and a 'Score of best mixture so far (lower is better): 82.8886'. The dialog has 'Take best mixture so far' and 'Cancel' buttons. The 'Output' window on the far right shows 'Mixture1' with a 'Sum of recipe ratios (should be 100%): 0'.

### 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)

The screenshot shows the GrafCompounder version 3.2111 - demo data interface. It is divided into several sections:

- Input data:** A table with columns for recipes (50AL511 to 50AL542) and rows for ingredients and properties.
- Criteria:** A table with columns for Name, Min, Max, From, To, Weight, and Trdoff. It lists various material properties like NR (SMR - 10), N330, CaCO3, etc.
- Output:** A list of results for 'Mixture1', including values for Total ingredients (158.464), Density, Cost (per vol), and Cost (per mass). A note at the bottom states 'Sum of recipe ratios (should be 100%): 100'.
- Recipe ratios in %:** A row at the bottom of the input data table showing ratios for each recipe, with a total of 53 for recipe 50AL511 and 47 for recipe 50AL542.

### 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

The screenshot shows the GrafCompoinder software interface with three main data tables:

Test Data (Simple)	50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50AL517	50AL518	50AL542
<b>Ingredients:</b>									
NR (SMR - 10)	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
N330	10.00	30.00	50.00	25.00	45.00	75.00	45.00	65.00	50.00
CaCO3	20.00	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
<b>Properties:</b>									
MooneyML(1+4) 100°C	32.00	36.00	31.00	34.00	30.00	42.00	60.00	39.00	41.00
Mooney 15 / 120°C	28.00	28.00	32.00	28.00	32.00	22.00	20.00	25.00	11.00
Density [g/ccm]	1.08	1.12	1.16	1.13	1.16	1.19	1.19	1.20	1.11
Hardness ["ShA]	42.00	41.00	40.00	48.00	48.00	52.00	61.00	61.00	59.00
M300 [Mpa]	1.80	3.00	3.00	4.40	4.60	5.30	8.00	7.60	9.40
TS [Mpa]	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
C-Set -26°C /24h [%]	22.00	28.00	30.00	17.00	19.00	35.00	29.00	27.00	77.00
C-Set 0°C /24h [%]	10.00	14.00	14.00	8.00	12.00	16.00	13.00	12.00	16.00
C-Set 23°C /72h [%]	8.00	10.00	14.00	9.00	13.00	16.00	10.00	17.00	18.00
C-Set 70°C /24h [%]	39.00	50.00	61.00	44.00	50.00	54.00	44.00	50.00	17.00
<b>Total ingredients</b>	146.15	186.15	226.15	161.15	201.15	251.15	181.15	221.15	172.35
Density									
Cost (per vol)									
Cost (per mass)									
Recipe ratios in %:	53								47

Criteria:	Name	Min	Max	From	To	Weight	Tdroff
	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			
	MooneyML(1+4) 100°C		30	60			
	Mooney 15 / 120°C		11	32			
	Density [g/ccm]		1.08	1.2			
	Hardness ["ShA]		40	61	40	50	
	M300 [Mpa]		1.8	9.4			
	TS [Mpa]		15	25	20		
	EB [%]		540	785			
	C-Set -26°C /24h [%]		17	77			
	C-Set 0°C /24h [%]		8	16			
	C-Set 23°C /72h [%]		8	18			
	C-Set 70°C /24h [%]		17	61	25		

Output	50AL45 Test1
	100
	28.8
	10.6
	7.35
	5
	2
	2
	0.9125
	0.47
	1.3315
	36.23
	20.01
	1.0941
	49.99
	5.372
	24.05
	669.85
	47.85
	12.82
	12.7
	28.66
	158.464
	Sum of recipe ratios (should be 100%):
	100

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 target for C-Set is not met. All other values in target.

You can take this mixture and do confirmation experiment.

# Compound Analysis

## Review Calculation

GrafCompounder version 3.211 - demo data

File Edit Help

Input data

Test Data (Simple)	50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50AL517	50AL518	50AL519	50AL520
<b>Ingredients:</b>										
NR (SMR - 10)	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
N330	10.00	30.00	50.00	25.00	45.00	75.00	45.00	65.00		
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		
ZnO	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		
IPPD	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		
TMTD - 80										
CBS - 80	0.65	0.65	0.65	0.65	0.65	0.65	0.65	0.65		
<b>Properties:</b>										
MooneyML(1+4) 100°C	32.00	36.00	31.00	34.00	30.00	42.00	60.00	39.00	41.00	
Mooney 15 / 120°C	28.00	28.00	32.00	28.00	32.00	22.00	20.00	25.00	11.00	
Density [g/ccm]	1.08	1.12	1.16	1.13	1.16	1.19	1.19	1.20	1.11	
Hardness [°ShA]	42.00	41.00	40.00	48.00	48.00	52.00	61.00	61.00	59.00	
M300 [Mpa]	1.80	3.00	3.00	4.40	4.60	5.30	8.00	7.60	9.40	
TS [Mpa]	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	
C-Set -26°C /24h [%]	22.00	28.00	30.00	17.00	19.00	35.00	29.00	27.00	77.00	
C-Set 0°C /24h [%]	10.00	14.00	14.00	8.00	12.00	19.00	13.00	12.00	16.00	
C-Set 23°C /72h [%]	8.00	10.00	14.00	9.00	13.00	19.00	10.00	17.00	18.00	
C-Set 70°C /24h [%]	39.00	50.00	61.00	44.00	50.00	54.00	44.00	50.00	17.00	
<b>Criteria:</b>										
Name	Min	Max	From	To	Weight	Trdoff				
		100	100							
		10	75							
		0	20							
		5	45							
		5	5							
		2	2							
		2	2							
		0.25	1.5							
		0	1							
		0.65	2.1							
<b>Output</b>										
50AL45 Test										
										100
										28.8
										10.6
										7.35
										5
										2
										2
										0.9125
										0.47
										1.3315
										36.23
										20.01
										1.0941
										49.99
										5.372
										24.06
										669.85
										47.85
										12.82
										12.7
										28.86
<b>Total ingredients</b>	146.15	186.15	226.15	161.15	201.15	251.15	181.15	221.15	172.35	
<b>Density</b>										158.464
<b>Cost (per vol)</b>										
<b>Cost (per mass)</b>										
<b>Recipe ratios in %:</b>										
	53									47

Before the confirmation experiment you can work on the compound.

- Click first cell in Data Table
- Make a right click
- Pull Down Menu select “Append empty column”
  - Comment:  
If you click on the first cell in another column than the last you get “Insert empty column”

# Compound Analysis

## Review Calculation

The screenshot displays the GrafCompounder software interface. The main window is titled "GrafCompounder version 3.211 - demo data". It features a menu bar (File, Edit, Help) and a toolbar. The interface is divided into several sections:

- Input data:** A large table with columns for various compounds (50AL511 to 50AL542) and rows for different properties (e.g., R (SMR - 10), aCO3, Naphtenic Oil, nO, Stearic Acid, YPD, MTD - 80, BS - 80, MooneyML, Density, Hardness, TS, EB, C-Set).
- Criteria:** A table listing criteria with columns for Name, Min, Max, From, To, Weight, and Trdff.
- Output:** A table showing the results of the calculation, including values for the same properties as in the input data.
- Summary:** A section at the bottom showing "Total ingredients" (146.15), "Density" (251.15), and "Sum of recipe ratios (should be 100%): 100".

Continue with right click into output column

- Select "Copy mixture to clipboard"
- 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

GrafCompounder version 3.2111 - demo data

File Edit Help

Input data:

	50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50AL517	50AL518	50AL542	50AL45 Test
Ingredients:										
R (SMR - 10)	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
S30	10.00	30.00	50.00	25.00	45.00	75.00	45.00	65.00	50.00	
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	
hO	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	
MTD - 80									1.00	
BS - 80	0.65	0.65	0.65	0.65	0.65	0.65	0.65	0.65	2.10	
Properties:										
coneYML(1+4) 100°C	32.00	36.00	31.00	34.00	30.00	42.00	60.00	39.00	41.00	
coneY15 / 120°C	28.00	28.00	32.00	28.00	32.00	22.00	20.00	25.00	11.00	
ensity [g/ccm]	1.08	1.12	1.16	1.13	1.16	1.19	1.19	1.20	1.11	
ardness [°Sh]	42.00	41.00	40.00	48.00	48.00	52.00	61.00	61.00	59.00	
300 [Mpa]	1.80	3.00	3.00	4.40	4.60	5.30	8.00	7.60	9.40	
S [Mpa]	25.00	21.00	15.00	25.00	20.00	15.30	23.00	18.00	23.00	
B [%]	785.00	725.00	690.00	715.00	705.00	615.00	560.00	590.00	540.00	
-Set -28°C /24h [%]	22.00	28.00	30.00	17.00	19.00	35.00	29.00	27.00	77.00	
-Set 0°C /24h [%]	10.00	14.00	14.00	8.00	12.00	16.00	13.00	12.00	16.00	
-Set 23°C /72h [%]	8.00	10.00	14.00	9.00	13.00	16.00	10.00	17.00	18.00	
-Set 70°C /24h [%]	39.00	50.00	61.00	44.00	50.00	54.00	44.00	50.00	17.00	
Total ingredients	146.15	186.15	226.15	161.15	201.15	251.15	181.15	221.15	172.35	157.85
Density										
Cost (per vol)										
Cost (per mass)										
Recipe ratios in %:	53								47	

Criteria:

Name	Min	Max	From	To	Weight	Trdff
NR (SMR - 10)	100	100				
NS30	10	75				
CaCO3	0	20				
Naphtenic Oil	5	45				
ZnO	5	5				
Stearic Acid	2	2				
IPPD	2	2				
S	0.25	1.5				
MTD - 80	0	1				
CBS - 80	0.65	2.1				

Output:

Name	Value
50AL45 Test	100
NR (SMR - 10)	100
NS30	28.8
CaCO3	10.6
Naphtenic Oil	7.35
ZnO	5
Stearic Acid	2
IPPD	2
S	0.9125
MTD - 80	0.47
CBS - 80	1.3315
Total ingredients	158.464
Density	
Cost (per vol)	
Cost (per mass)	
Sum of recipe ratios (should be 100%):	100

Context menu options:

- Copy input table
- Copy marked cells
- Paste cells here
- Delete marked rows
- Delete marked columns
- Insert empty row
- Insert empty column
- Append empty column
- Clear marked cells
- Round values to two decimal places
- Show frequency distribution for 21 rows

Number format: 12345.67

Import input data from clipboard

Auto mix (overwrite mixture)

Auto mix (new mixture)

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

GrafCompounder version 3.211 - demo data

Input data:	50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50AL517	50AL518	50AL542	50AL45 Test
est Data (Simple)										
Recipes:										
Ingredients:										
R (SMR - 10)	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
N330	10.00	30.00	50.00	25.00	45.00	75.00	45.00	65.00	50.00	29.00
CaCO3	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00	10.00
Naphthenic Oil	5.00	25.00	45.00	5.00	25.00	45.00	5.00	25.00	10.00	7.00
ZnO	5.00	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	2.00
IPPD	2.00	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	1.00
MTD - 80										0.50
BS - 80	0.65	0.65	0.65	0.65	0.65	0.65	0.65	0.65	2.10	1.35
Properties:										
MooneyML(1+4) 100°C	32.00	36.00	31.00	34.00	30.00	42.00	60.00	39.00	41.00	36.23
Mooney 15 / 120°C	28.00	28.00	32.00	28.00	32.00	22.00	20.00	25.00	11.00	20.01
Density [g/ccm]	1.08	1.12	1.16	1.13	1.16	1.19	1.19	1.20	1.11	1.09
Hardness [°ShA]	42.00	41.00	40.00	48.00	48.00	52.00	61.00	61.00	59.00	49.99
M300 [Mpa]	1.80	3.00	3.00	4.40	4.60	5.30	8.00	7.60	9.40	5.37
TS [Mpa]	25.00	21.00	15.00	25.00	20.00	15.30	23.00	18.00	23.00	24.06
EB [%]	785.00	725.00	690.00	715.00	705.00	615.00	560.00	590.00	540.00	669.85
C-Set -26°C /24h [%]	22.00	28.00	30.00	17.00	19.00	35.00	29.00	27.00	77.00	47.85
C-Set 0°C /24h [%]	10.00	14.00	14.00	8.00	12.00	16.00	13.00	12.00	16.00	12.82
C-Set 23°C /72h [%]	8.00	10.00	14.00	9.00	13.00	16.00	10.00	17.00	18.00	12.70
C-Set 70°C /24h [%]	39.00	50.00	61.00	44.00	50.00	54.00	44.00	50.00	17.00	28.66
Total ingredients	146.15	186.15	226.15	161.15	201.15	251.15	181.15	221.15	172.35	157.85
Density										
Cost (per vol)										
Cost (per mass)										
Recipe ratios in %:	53								47	

Criteria:

Name	Min	Max	From	To	Weight	Trdoff
NR (SMR - 10)		100	100			
N330		10	75			
CaCO3		0	20			
Naphthenic Oil		5	45			
ZnO		5	5			
Stearic Acid		2	2			
IPPD		2	2			
S		0.25	1.5			
MTD - 80		0	1			
CBS - 80		0.65	2.1			
MooneyML(1+4) 100°C	30	60				
Mooney 15 / 120°C	11	32				
Density [g/ccm]	1.08	1.2				
Hardness [°ShA]	40	61	40	50		
M300 [Mpa]	1.8	9.4				
TS [Mpa]	15	25	20			
EB [%]	540	785				
C-Set -26°C /24h [%]	17	77				
C-Set 0°C /24h [%]	8	16				
C-Set 23°C /72h [%]	8	18				
C-Set 70°C /24h [%]	17	61		25		

Output:

50AL45 Test	
NR (SMR - 10)	100
N330	28.8
CaCO3	10.6
Naphthenic Oil	7.35
ZnO	5
Stearic Acid	2
IPPD	2
S	0.9125
MTD - 80	0.47
CBS - 80	1.3315
MooneyML(1+4) 100°C	36.23
Mooney 15 / 120°C	20.01
Density [g/ccm]	1.0941
Hardness [°ShA]	49.99
M300 [Mpa]	5.372
TS [Mpa]	24.06
EB [%]	669.85
C-Set -26°C /24h [%]	47.85
C-Set 0°C /24h [%]	12.82
C-Set 23°C /72h [%]	12.7
C-Set 70°C /24h [%]	28.66
Total ingredients	158.464
Density	
Cost (per vol)	
Cost (per mass)	
Sum of recipe ratios (should be 100%):	100

After compound review go to confirmation experiment with the reviewed formula

- Replace property data with new measured data
- Result should be in 95% confidence interval

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

The screenshot shows the GrafCompunder software interface. The main window displays a recipe table with columns for various compounds (50AL511 to 50AL518) and rows for different ingredients and properties. The 'Ingredients' column for '50AL511' is highlighted in blue, and an arrow points to it from the text below. The 'Criteria' table on the right shows various properties like MooneyML, Density, and Hardness. The 'Output' table on the far right shows the calculated values for each property.

Ingredients	50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50AL517	50AL518	50AL542	50AL45 Test
R (SMR - 10)	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
330	10.00	30.00	50.00	25.00	45.00	75.00	45.00	65.00	50.00	29.00
acCO3	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00	10.00
aphentic Oil	5.00	25.00	45.00	5.00	25.00	45.00	5.00	25.00	10.00	7.00
nO	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
tearic Acid	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00
PD	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00
MTD - 80	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	0.25	1.00
BS - 80	0.65	0.65	0.65	0.65	0.65	0.65	0.65	0.65	2.10	1.35
roperties:										
MooneyML(1+4) 100°C	32.00	36.00	31.00	34.00	30.00	42.00	60.00	39.00	41.00	36.23
Mooney 15 / 120°C	28.00	28.00	32.00	28.00	32.00	22.00	20.00	25.00	11.00	20.01
ensity [g/ccm]	1.08	1.12	1.16	1.13	1.16	1.19	1.19	1.20	1.11	1.09
ardness [°ShA]	42.00	41.00	40.00	48.00	48.00	52.00	61.00	61.00	59.00	49.99
300 [Mpa]	1.60	3.00	3.00	4.40	4.90	5.30	8.00	7.80	9.40	5.37
S [Mpa]	25.00	21.00	15.00	25.00	20.00	15.30	23.00	18.00	23.00	24.06
B [%]	785.00	725.00	690.00	715.00	705.00	615.00	560.00	590.00	540.00	669.85
-Set -28°C /24h [%]	22.00	28.00	30.00	17.00	19.00	35.00	29.00	27.00	77.00	47.85
-Set 0°C /24h [%]	10.00	14.00	14.00	8.00	12.00	16.00	13.00	12.00	16.00	12.82
-Set 23°C /72h [%]	8.00	10.00	14.00	9.00	13.00	15.00	10.00	17.00	18.00	12.70
-Set 70°C /24h [%]	39.00	50.00	61.00	44.00	50.00	54.00	44.00	50.00	17.00	28.66

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

The screenshot displays the GrafCompounder software interface. The main window is titled "GrafCompounder version 3.2111 - demo data". It features a menu bar (File, Edit, Help) and a toolbar. The interface is divided into several sections:

- Input data:** A table with columns for recipes 50AL511 through 50AL518, 50AL542, and 50AL45 Test. The table contains numerical values for various ingredients and properties.
- Recipes:** A section listing the recipes being compared.
- Ingredients:** A list of ingredients including NR (SMR - 10), N330, CaCO3, Naphthenic Oil, ZnO, Stearic Acid, IPPD, S, TMTD - 80, and CBS - 80.
- Properties:** A list of material properties such as Mooney/ML(1+4) 100°C, Mooney T5 / 120°C, Density [g/ccm], Hardness [°ShA], M300 [Mpa], TS [Mpa], EB [%], C-Set -26°C /24h [%], C-Set 0°C /24h [%], C-Set 23°C /72h [%], and C-Set 70°C /24h [%].
- Criteria:** A table with columns for Name, Min, Max, From, To, Weight, and Trdoff.
- Output:** A table showing the results of the comparison, including values for Total ingredients, Density, Cost (per vol), and Cost (per mass).

Arrows in the image point to specific areas: one points to the "50AL45 Test" column in the input data table, and another points to the "Sum of recipe ratios (should be 100%): 100" text at the bottom right of the output section.

### 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 confirmed yet and physicals corrected with measured 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)

GrafCompounder version 3.211 - demo data

File Edit Help

Input data:

Test Data (Advanced)				50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50AL517	
Code:	Cost	Density:	Ingredients:	Recipes:	50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50AL517
A001	280.00	0.92	NR (SMR - 10)		100.00	100.00	100.00	100.00	100.00	100.00	
B003	115.00	1.80	N330		10.00	30.00	50.00	25.00	45.00	75.00	
C010	24.00	2.71	CaCO3		20.00	20.00	20.00	20.00	20.00	20.00	
D002	116.00	0.89	Naphtenic Oil		5.00	25.00	45.00	5.00	25.00	45.00	
E001	385.00	5.60	ZnO		5.00	5.00	5.00	5.00	5.00	5.00	
F001	165.00	0.92	Stearic Acid		2.00	2.00	2.00	2.00	2.00	2.00	
G001	924.00	1.15	IPPD		2.00	2.00	2.00	2.00	2.00	2.00	
H001	158.00	1.80	S		1.50	1.50	1.50	1.50	1.50	1.50	
K001	396.00	1.11	TMTD - 80								
K005	708.00	1.28	CBS - 80		0.65	0.65	0.65	0.65	0.65	0.65	

Code: PR001 PR002 PR003 PR004 PR007 PR008 PR009 PR010 PR011 PR012 PR013

Properties:

Code:	MooneyML(1+4) 100°C	Mooney T5 / 120°C	Density [g/cm]	Hardness [ShA]	M300 [Mpa]	TS [Mpa]	EB [%]	C-Set -26°C /24h [%]	C-Set 0°C /24h [%]	C-Set 23°C /72h [%]	C-Set 70°C /24h [%]
PR001	32.00	36.00	31.00	34.00	30.00	42.00					
PR002	28.00	28.00	32.00	28.00	32.00	22.00					
PR003	1.08	1.12	1.16	1.13	1.18	1.19					
PR004	42.00	41.00	40.00	48.00	48.00	52.00					
PR007	1.80	3.00	3.00	4.40	4.60	5.30					
PR008	25.00	21.00	15.00	25.00	20.00	15.30					
PR009	785.00	725.00	690.00	715.00	705.00	615.00					
PR010	22.00	28.00	30.00	17.00	19.00	35.00					
PR011	10.00	14.00	14.00	8.00	12.00	16.00					
PR012	8.00	10.00	14.00	9.00	13.00	16.00					
PR013	39.00	50.00	61.00	44.00	50.00	54.00					

Criteria:

Name	Min	Max	From	To	Weight	Trdff
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				

Output:

Mixture 1	Total ingredients	Density	Cost (per vol)	Cost (per mass)
	146.15	1.096	219.724	167.638
	186.15	1.115	237.377	212.694
	226.15	1.128	259.187	193.667
	161.15	1.137	235.816	227.937
	201.15	1.147	255.916	205.994
	251.15	1.171	219.724	187.638

Sum of recipe ratios (should be 100%): 0

Number format: 12345.67

Import input data from clipboard

Auto mix (overwrite mixture)

Auto mix (new mixture)

### Load Demo Data Advanced

- Click “File” and then “Clear all Data”
- Click “File”, select “Load Demo data (advanced)” from Pull down Menu

### 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)

The screenshot displays the GrafCompoander software interface with the following data:

Code:	Cost:	Density:	Ingredients:	Recipes:	50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50AL517
A001	280.00	0.92	NR (SMR - 10)	50AL511	100.00	100.00	100.00	100.00	100.00	100.00	100.00
B003	115.00	1.80	N330	50AL512	10.00	30.00	50.00	25.00	45.00	75.00	
C010	24.00	2.71	CaCO3	50AL513	20.00	20.00	20.00	20.00	20.00	20.00	
D002	116.00	0.89	Naphtenic Oil	50AL514	5.00	25.00	45.00	5.00	25.00	45.00	
E001	385.00	5.60	ZnO	50AL515	5.00	5.00	5.00	5.00	5.00	5.00	
F001	165.00	0.92	Stearic Acid	50AL516	2.00	2.00	2.00	2.00	2.00	2.00	
G001	924.00	1.15	IPPD	50AL517	2.00	2.00	2.00	2.00	2.00	2.00	
H001	158.00	1.80	S		1.50	1.50	1.50	1.50	1.50	1.50	
K001	396.00	1.11	TMTD - 80								
K005	708.00	1.28	CBS - 80		0.65	0.65	0.65	0.65	0.65	0.65	

Code:	Properties:	50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50AL517
PR001	MooneyML(1+4) 100°C	32.00	36.00	31.00	34.00	30.00	42.00	
PR002	Mooney I5 / 120°C	28.00	28.00	32.00	28.00	32.00	22.00	
PR003	Density [g/ccm]	1.08	1.12	1.16	1.13	1.16	1.19	
PR004	Hardness [ShA]	42.00	41.00	40.00	48.00	48.00	52.00	
PR007	M300 [Mpa]	1.80	3.00	3.00	4.40	4.60	5.30	
PR008	TS [Mpa]	25.00	21.00	15.00	25.00	20.00	15.30	
PR009	EB [%]	785.00	725.00	690.00	715.00	705.00	615.00	
PR010	C-Set -26°C /24h [%]	22.00	28.00	30.00	17.00	19.00	35.00	
PR011	C-Set 0°C /24h [%]	10.00	14.00	14.00	8.00	12.00	16.00	
PR012	C-Set 23°C /72h [%]	8.00	10.00	14.00	9.00	13.00	16.00	
PR013	C-Set 70°C /24h [%]	39.00	50.00	61.00	44.00	50.00	54.00	

Criteria:	Name	Min	Max	From	To	Weight	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			
	MooneyML(1+4) 100°C		30	60			
	Mooney I5 / 120°C		11	32			
	Density [g/ccm]		1.08	1.2			
	Hardness [ShA]		40	61			
	M300 [Mpa]		1.6	9.4			
	TS [Mpa]		15	25			
	EB [%]		540	785			
	C-Set -26°C /24h [%]		17	77			
	C-Set 0°C /24h [%]		8	16			
	C-Set 23°C /72h [%]		8	18			
	C-Set 70°C /24h [%]		17	61			

Total ingredients	146.15	166.15	226.15	161.15	201.15	251.15
Density	1.096	1.115	1.128	1.137	1.147	1.171
Cost (per vol)	262.547	237.377	220.712	259.187	235.816	219.724
Cost (per mass)	239.55	212.694	195.667	227.957	205.994	187.638

### 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)

The screenshot displays the GrafCompounder software interface with the following data:

Code:	Cost:	Density:	Ingredients:	50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50A
A001	280.00	0.92	NR (SMR - 10)	100.00	100.00	100.00	100.00	100.00	100.00	
B003	115.00	1.80	N330	10.00	30.00	50.00	25.00	45.00	75.00	
C010	24.00	2.71	CaCO3	20.00	20.00	20.00	20.00	20.00	20.00	
D002	116.00	0.89	Naphtenic Oil	5.00	25.00	45.00	5.00	25.00	45.00	
E001	385.00	5.60	ZnO	5.00	5.00	5.00	5.00	5.00	5.00	
F001	165.00	0.92	Stearic Acid	2.00	2.00	2.00	2.00	2.00	2.00	
G001	924.00	1.15	IPPD	2.00	2.00	2.00	2.00	2.00	2.00	
H001	158.00	1.80	S	1.50	1.50	1.50	1.50	1.50	1.50	
K001	396.00	1.11	TMTD - 80							
K005	708.00	1.28	CBS - 80	0.65	0.65	0.65	0.65	0.65	0.65	

Code:	Properties:	50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50A
PR001	MooneyML(1+4) 100°C	32.00	36.00	31.00	34.00	30.00	42.00	
PR002	Mooney t5 / 120°C	28.00	28.00	32.00	28.00	32.00	22.00	
PR003	Density [g/ccm]	1.08	1.12	1.16	1.13	1.16	1.19	
PR004	Hardness [°ShA]	42.00	41.00	40.00	48.00	48.00	52.00	
PR007	M300 [Mpa]	1.80	3.00	3.00	4.40	4.60	5.30	
PR008	TS [Mpa]	25.00	21.00	15.00	25.00	20.00	15.30	
PR009	EB [%]	795.00	725.00	690.00	715.00	705.00	615.00	
PR010	C-Set -26°C /24h [%]	22.00	28.00	30.00	17.00	19.00	35.00	
PR011	C-Set 0°C /24h [%]	10.00	14.00	14.00	8.00	12.00	16.00	
PR012	C-Set 23°C /72h [%]	8.00	10.00	14.00	9.00	13.00	16.00	
PR013	C-Set 70°C /24h [%]	39.00	50.00	61.00	44.00	50.00	54.00	

Criteria:	Name	Min	Max	From	To	Weight	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				

Criteria:	Name	Min	Max	From	To	Weight	Trdoff
	MooneyML(1+4) 100°C	30	60				
	Mooney t5 / 120°C	11	32				
	Density [g/ccm]	1.08	1.2				
	Hardness [°ShA]	40	61	45	50		
	M300 [Mpa]	1.8	9.4				
	TS [Mpa]	15	25	20			
	EB [%]	540	768				
	C-Set -26°C /24h [%]	17	77				
	C-Set 0°C /24h [%]	8	16				
	C-Set 23°C /72h [%]	8	16				
	C-Set 70°C /24h [%]	17	61		25		

Output:	Mixture1
	100
	28.8
	10.6
	7.35
	5
	2
	2
	0.9125
	0.47
	1.3315
	36.23
	20.01
	1.0941
	49.99
	5.372
	24.06
	669.85
	47.85
	12.82
	12.7
	28.86

Total ingredients	146.15	186.15	226.15	161.15	201.15	251.15
Density	1.096	1.115	1.128	1.137	1.147	1.171
Cost (per vol)	262.547	237.377	220.712	259.187	235.816	219.724
Cost (per mass)	239.55	212.894	195.667	227.957	205.594	187.638

Total ingredients	146.15	251.15
Density	1.096	1.186
Cost (per vol)	219.724	263.877
Cost (per mass)	187.638	239.55

Sum of recipe ratios (should be 100%): 100

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)

GrafCompunder version 3.2111 - demo data

File Edit Help

Input data:

			50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50A	
Test Data (Advanced)										
Code:	Cost:	Density:	Recipes:							50A
A001	280.00	0.92	NR (SMR - 10)	100.00	100.00	100.00	100.00	100.00	100.00	
B003	115.00	1.80	N330	10.00	30.00	50.00	25.00	45.00	75.00	
C010	24.00	2.71	CaCO3	20.00	20.00	20.00	20.00	20.00	20.00	
D002	116.00	0.89	Naphtenic Oil	5.00	25.00	45.00	5.00	25.00	45.00	
E001	385.00	5.60	ZnO	5.00	5.00	5.00	5.00	5.00	5.00	
F001	165.00	0.92	Stearic Acid	2.00	2.00	2.00	2.00	2.00	2.00	
G001	924.00	1.15	IPPD	2.00	2.00	2.00	2.00	2.00	2.00	
H001	158.00	1.80	S	1.50	1.50	1.50	1.50	1.50	1.50	
K001	396.00	1.11	TMTD - 80							
K005	708.00	1.28	CBS - 80	0.65	0.65	0.65	0.65	0.65	0.65	
Properties:										
PR001			MooneyML(1+4) 100°C	32.00	36.00	31.00	34.00	30.00	42.00	
PR002			Mooney I5 / 120°C	28.00	28.00	32.00	28.00	32.00	22.00	
PR003			Density [g/ccm]	1.08	1.12	1.16	1.13	1.16	1.19	
PR004			Hardness [°ShA]	42.00	41.00	40.00	48.00	48.00	52.00	
PR007			M300 [Mpa]	1.80	3.00	3.00	4.40	4.60	5.30	
PR008			TS [Mpa]	25.00	21.00	15.00	25.00	20.00	15.30	
PR009			EB [%]	785.00	725.00	690.00	715.00	705.00	615.00	
PR010			C-Set -26°C /24h [%]	22.00	28.00	30.00	17.00	19.00	35.00	
PR011			C-Set 0°C /24h [%]	10.00	14.00	14.00	8.00	12.00	16.00	
PR012			C-Set 23°C /72h [%]	8.00	10.00	14.00	9.00	13.00	16.00	
PR013			C-Set 70°C /24h [%]	39.00	50.00	61.00	44.00	50.00	54.00	

Criteria:

Name	Min	Max	From	To	Weight	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				
MooneyML(1+4) 100°C	30	60				
Mooney I5 / 120°C	11	32				
Density [g/ccm]	1.08	1.2				
Hardness [°ShA]	40	61	45	50		
M300 [Mpa]	1.8	9.4				
TS [Mpa]	15	25	20			
EB [%]	540	785				
C-Set -26°C /24h [%]	17	77				
C-Set 0°C /24h [%]	8	16				
C-Set 23°C /72h [%]	8	18				
C-Set 70°C /24h [%]	17	61		25		

Output:

Mixture 1	Value
NR (SMR - 10)	100
N330	28.8
CaCO3	10.6
Naphtenic Oil	7.35
ZnO	5
Stearic Acid	2
IPPD	2
S	0.9125
TMTD - 80	0.47
CBS - 80	1.3315
MooneyML(1+4) 100°C	36.23
Mooney I5 / 120°C	20.01
Density [g/ccm]	1.0941
Hardness [°ShA]	49.99
M300 [Mpa]	5.372
TS [Mpa]	24.06
EB [%]	669.85
C-Set -26°C /24h [%]	47.85
C-Set 0°C /24h [%]	12.82
C-Set 23°C /72h [%]	12.7
C-Set 70°C /24h [%]	28.66
Total ingredients	158.464
Density	1.103
Cost (per vol)	263.074
Cost (per mass)	238.508
Sum of recipe ratios (should be 100%):	100

Recipe ratios in %:

	53
Total ingredients	146.15
Density	1.096
Cost (per vol)	262.547
Cost (per mass)	239.55

Number format: 12345.67

Import input data from clipboard

Auto mix (overwrite mixture)

Auto mix (new mixture)

### 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)

GrafCompoander version 3.211 - demo data

Input data:		50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50A	
<b>Test Data (Advanced)</b>									
<b>Code:</b>	<b>Cost:</b>	<b>Density:</b>	<b>Ingredients:</b>	<b>Recipes:</b>					
A001	280.00	0.92	NR (SMR - 10)	100.00	100.00	100.00	100.00	100.00	100.00
B003	115.00	1.80	N330	10.00	30.00	50.00	25.00	45.00	75.00
C010	24.00	2.71	CaCO3	20.00	20.00	20.00	20.00	20.00	20.00
D002	116.00	0.89	Naphtenic Oil	5.00	25.00	45.00	5.00	25.00	45.00
E001	385.00	5.60	ZnO	5.00	5.00	5.00	5.00	5.00	5.00
F001	165.00	0.92	Stearic Acid	2.00	2.00	2.00	2.00	2.00	2.00
G001	924.00	1.15	IPPD	2.00	2.00	2.00	2.00	2.00	2.00
H001	158.00	1.80	S	1.50	1.50	1.50	1.50	1.50	1.50
K001	395.00	1.11	TMTD - 80						
K005	708.00	1.28	CBS - 80	0.65	0.65	0.65	0.65	0.65	0.65
<b>Properties:</b>									
PR001	MooneyML(1+4) 100°C	32.00	36.00	31.00	34.00	30.00	42.00		
PR002	Mooney I5 / 120°C	28.00	28.00	32.00	28.00	32.00	22.00		
PR003	Density [g/ccm]	1.08	1.12	1.16	1.13	1.16	1.19		
PR004	Hardness [°ShA]	42.00	41.00	40.00	48.00	48.00	52.00		
PR007	M300 [mpa]	1.80	3.00	3.00	4.40	4.60	5.30		
PR008	TS [mpa]	25.00	21.00	15.00	25.00	20.00	15.30		
PR009	EB [%]	785.00	725.00	690.00	715.00	705.00	615.00		
PR010	C-Set -26°C /24h [%]	22.00	28.00	30.00	17.00	19.00	35.00		
PR011	C-Set 0°C /24h [%]	10.00	14.00	14.00	8.00	12.00	16.00		
PR012	C-Set 23°C /72h [%]	8.00	10.00	14.00	9.00	13.00	16.00		
PR013	C-Set 70°C /24h [%]	39.00	50.00	61.00	44.00	50.00	54.00		
<b>Criteria:</b>									
<b>Name</b>	<b>Min</b>	<b>Max</b>	<b>From</b>	<b>To</b>	<b>Weight</b>	<b>Troff</b>	<b>Output</b>		
NR (SMR - 10)	100	100					Mixture1	Mixture2	
N330	10	75					100	100	
CaCO3	0	20					28.8	49.2	
Naphtenic Oil	5	45					10.6	14.45	
ZnO	5	5					7.35	25.5875	
Stearic Acid	2	2					5	5	
IPPD	2	2					2	2	
S	0.25	1.5					0.9125	1.153125	
TMTD - 80	0	1					0.47	0.2775	
CBS - 80	0.65	2.1					1.3315	1.052375	
MooneyML(1+4) 100°C	30	60					36.23	37.6275	
Mooney I5 / 120°C	11	32					20.01	22.6475	
Density [g/ccm]	1.08	1.2					1.0941	1.14175	
Hardness [°ShA]	40	61	45	50			49.99	49.99	
M300 [mpa]	1.8	9.4					5.372	5.63825	
TS [mpa]	15	25	20				24.06	20.00375	
EB [%]	540	785					669.85	643.5875	
C-Set -26°C /24h [%]	17	77					47.85	41.4825	
C-Set 0°C /24h [%]	8	16					12.82	14.635	
C-Set 23°C /72h [%]	8	18					12.7	14.2375	
C-Set 70°C /24h [%]	17	61	25				28.66	41.7925	
<b>Output</b>									
Total ingredients	146.15	186.15	226.15	161.15	201.15	251.15	158.464	200.7205	
Density	1.096	1.115	1.128	1.137	1.147	1.171	1.103	1.136	
Cost (per vol)	262.547	237.377	220.712	259.187	235.816	219.724	263.074	238.344	
Cost (per mass)	239.95	212.894	195.667	227.957	205.994	187.638	238.508	209.81	
<b>Recipe ratios in %:</b>									
			28.75		19.75	23.75	Sum of recipe ratios (should be 100%): 100		

### 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 compare influence of cost target on results

Cost per mass is 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”

The screenshot shows the GrafCompounder software interface with the following data:

Input data:		50AL511	50AL512	50AL513	50AL514	50AL515	50AL516
<b>Code:</b>	<b>Cost:</b>						
A001	280.00	0.92	NR (SMR - 10)	100.00	100.00	100.00	100.00
B003	115.00	1.80	N330	10.00	30.00	50.00	25.00
C010	24.00	2.71	CaCO3	20.00	20.00	20.00	20.00
D002	116.00	0.89	Naphthenic Oil	5.00	25.00	45.00	5.00
E001	385.00	5.60	ZnO	5.00	5.00	5.00	5.00
F001	165.00	0.92	Stearic Acid	2.00	2.00	2.00	2.00
G001	924.00	1.15	IPPD	2.00	2.00	2.00	2.00
H001	158.00	1.80	S	1.50	1.50	1.50	1.50
K001	396.00	1.11	TMTD - 80				
K005	708.00	1.28	CBS - 80	0.65	0.65	0.65	0.65

Criteria:		Min	Max	From	To	Weight	Trdoff
NR (SMR - 10)		100	100				
N330		10	75				
CaCO3		0	20				
Naphthenic 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				

Output:		Weight	Trdoff
Mixture1			
NR (SMR - 10)		100	
N330		41.8	
CaCO3		5.7	
Naphthenic Oil		11.775	
ZnO		5	
Stearic Acid		2	
IPPD		2	
S		0.60825	
TMTD - 80		0.715	
CBS - 80		1.68675	
MooneyML(1+4)		39.075	
Mooney15/120°C		15.845	
Density [g/cm3]		1.10785	
Hardness [°ShA]		53.995	
M300 [Mpa]		7.426	
TS [Mpa]		22.93	
EB [%]		600.225	
C-Set -26°C/24h [%]		62.285	
C-Set 0°C/24h [%]		14.93	
C-Set 23°C/72h [%]		15.47	
C-Set 70°C/24h [%]		25.03	

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”

GrafCompounder version 3.211 - demo data

File Edit Help

Input data:

Test Data (Advanced)				50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50A
Code:	Cost:	Density:	Ingredients:	50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50A
A001	280.00	0.92	NR (SMR - 10)	100.00	100.00	100.00	100.00	100.00	100.00	
B003	115.00	1.80	N330	10.00	30.00	50.00	25.00	45.00	75.00	
C010	24.00	2.71	CaCO3	20.00	20.00	20.00	20.00	20.00	20.00	
D002	116.00	0.89	Naphtenic Oil	5.00	25.00	45.00	5.00	25.00	45.00	
E001	385.00	5.60	ZnO	5.00	5.00	5.00	5.00	5.00	5.00	
F001	165.00	0.92	Stearic Acid	2.00	2.00	2.00	2.00	2.00	2.00	
G001	924.00	1.15	IPP	2.00	2.00	2.00	2.00	2.00	2.00	
H001	158.00	1.80	S	1.50	1.50	1.50	1.50	1.50	1.50	
K001	396.00	1.11	TMTD - 80							
K005	708.00	1.28	CBS - 80	0.65	0.65	0.65	0.65	0.65	0.65	

Recipes:

	50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50A
PR001	32.00	36.00	31.00	34.00	30.00	42.00	
PR002	28.00	28.00	32.00	28.00	32.00	22.00	
PR003	1.08	1.12	1.16	1.13	1.16	1.19	
PR004	42.00	41.00	40.00	48.00	48.00	52.00	
PR007	1.80	3.00	3.00	4.40	4.60	5.30	
PR008	25.00	21.00	15.00	25.00	20.00	15.30	
PR009	785.00	725.00	690.00	715.00	705.00	615.00	
PR010	22.00	28.00	30.00	17.00	19.00	35.00	
PR011	10.00	14.00	14.00	8.00	12.00	16.00	
PR012	8.00	10.00	14.00	9.00	13.00	16.00	
PR013	39.00	50.00	61.00	44.00	50.00	54.00	

Properties:

	50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50A
MooneyML(1+4) 100°C	32.00	36.00	31.00	34.00	30.00	42.00	
Mooney 15 / 120°C	28.00	28.00	32.00	28.00	32.00	22.00	
Density (g/cm)	1.08	1.12	1.16	1.13	1.16	1.19	
Hardness [ShA]	42.00	41.00	40.00	48.00	48.00	52.00	
M300 [Mpa]	1.80	3.00	3.00	4.40	4.60	5.30	
TS [Mpa]	25.00	21.00	15.00	25.00	20.00	15.30	
EB [%]	785.00	725.00	690.00	715.00	705.00	615.00	
C-Set -26°C /24h [%]	22.00	28.00	30.00	17.00	19.00	35.00	
C-Set 0°C /24h [%]	10.00	14.00	14.00	8.00	12.00	16.00	
C-Set 23°C /72h [%]	8.00	10.00	14.00	9.00	13.00	16.00	
C-Set 70°C /24h [%]	39.00	50.00	61.00	44.00	50.00	54.00	

Criteria:

Name	Min	Max	From	To	Weight	Trdoff
NR (SMR - 10)	100	100				
N330	10	75				
CaCO3	0	20				
Naphtenic Oil	5	45				
ZnO	5	5				
Stearic Acid	2	2				
IPP	2	2				
S	0.25	1.5				
TMTD - 80	0	1				
CBS - 80	0.65	2.1				
MooneyML(1+4) 100°C	30	60				
Mooney 15 / 120°C	11	32				
Density (g/cm)	1.08	1.2				
Hardness [ShA]	40	61	40	45	10	
M300 [Mpa]	1.8	9.4				
TS [Mpa]	15	25	20			
EB [%]	540	785		600		
C-Set -26°C /24h [%]	17	77				
C-Set 0°C /24h [%]	8	16				
C-Set 23°C /72h [%]	8	18				
C-Set 70°C /24h [%]	17	61		25		

Output:

	Mixture1	Mixture3
NR (SMR - 10)	100	100
N330	49.5	39.6
CaCO3	7.85	15.3
Naphtenic Oil	23.2375	26.375
ZnO	5	5
Stearic Acid	2	2
IPP	2	2
S	0.740625	1.20625
TMTD - 80	0.6075	0.235
CBS - 80	1.530875	0.99075
MooneyML(1+4) 100°C	37.2	35.95
Mooney 15 / 120°C	19.1425	24.985
Density (g/cm)	1.128625	1.12745
Hardness [ShA]	51.5675	44.985
M300 [Mpa]	6.888	4.504
TS [Mpa]	20.01	20
EB [%]	599.75	672.95
C-Set -26°C /24h [%]	58.5025	40.005
C-Set 0°C /24h [%]	15.215	14.47
C-Set 23°C /72h [%]	16.33	12.86
C-Set 70°C /24h [%]	33.995	44.94

Total ingredients

	146.15	186.15	226.15	161.15	201.15	251.15
Density	1.096	1.115	1.128	1.137	1.147	1.171
Cost (per vol)	262.547	237.372	220.712	259.187	235.616	219.724
Cost (per mass)	239.55	212.694	195.667	227.957	205.594	187.638

Recipe ratios in %:

	52	24.5
Number format:	12345.67	

Import input data from clipboard

Auto mix (overwrite mixture) Auto mix (new mixture)

Total ingredients

	146.15	251.15
Density	1.096	1.186
Cost (per vol)	219.724	263.877
Cost (per mass)	187.638	239.55

Sum of recipe ratios (should be 100%): 100

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
  - Hardness 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”

The screenshot shows the GrafCompounder version 3.210 interface. The main window is titled "Input data" and contains several tables. The "Test Data (Advanced)" table lists ingredients like NR (SMR - 10), N330, CaCO3, Naphthenic Oil, ZnO, Stearic Acid, JPPD, S, TMTD - 80, and CBS - 80 across various recipes (50AL511 to 50AL518). The "Criteria" table lists properties such as MooneyML(1+4), Mooney 15 / 120°C, Density [g/cm³], Hardness [ShA], M300 [Mpa], TS [Mpa], EB [%], C-Set -26°C/24h [%], C-Set 0°C/24h [%], C-Set 23°C/72h [%], and C-Set 70°C/24h [%]. The "Output" table shows results for Mixture1, Mixture3, and Mixture4. At the bottom, there are summary tables for "Total ingredients", "Density", "Cost (per vol)", and "Cost (per mass)".

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 elongation has increased further)

- Consequently we have higher score 2878

# Creating Formulas

## Using “Weight” and “Trdoff”

GrafCompounder version 3.211 - demo data

Input data:				Recipes:							Criteria:						Output:			
				50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	Name	Min	Max	From	To	Weight	Trdoff	Mixture1	Mixture4	Mixture5	Mixture6
<b>Code:</b>	<b>Cost:</b>	<b>Density:</b>	<b>Ingredients:</b>																	
A001	280.00	0.92	NR (SMR - 10)	100.00	100.00	100.00	100.00	100.00	100.00	NR (SMR - 10)	100	100					100	100	100	100
B003	115.00	1.80	N330	10.00	30.00	50.00	25.00	45.00	75.00	N330	10	75					41.8	34.45	17.1	29
C010	24.00	2.71	CaCO3	20.00	20.00	20.00	20.00	20.00	20.01	CaCO3	0	20					5.7	15.55	16.45	10
D002	116.00	0.89	Naphtenic Oil	5.00	25.00	45.00	5.00	25.00	45.01	Naphtenic Oil	5	45					11.775	21.625	5.8875	7.4
E001	385.00	5.60	ZnO	5.00	5.00	5.00	5.00	5.00	5.01	ZnO	5	5					5	5	5	5
F001	165.00	0.92	Stearic Acid	2.00	2.00	2.00	2.00	2.00	2.01	Stearic Acid	2	2					2	2	2	2
G001	924.00	1.15	IPPD	2.00	2.00	2.00	2.00	2.00	2.01	IPPD	2	2					2	2	2	2
H001	158.00	1.80	S	1.50	1.50	1.50	1.50	1.50	1.51	S	0.25	1.5					0.60625	1.221875	1.278125	0.887
K001	396.00	1.11	TMTD - 80							TMTD - 80	0	1					0.715	0.2225	0.1775	0.4
K005	708.00	1.28	CBS - 80	0.65	0.65	0.65	0.65	0.65	0.61	CBS - 80	0.65	2.1					1.68675	0.972625	0.907375	1.360
<b>Code:</b>	<b>Properties:</b>																			
PR001			MooneyML(1+4) 100°C	32.00	36.00	31.00	34.00	30.00	42.01	MooneyML(1+4)	30	60					39.075	37.1125	33.5975	36.4
PR002			Mooney I5 / 120°C	28.00	28.00	32.00	28.00	32.00	22.01	Mooney I5 / 120°C	11	32					15.845	24.2175	24.9825	19.6
PR003			Density [g/ccm]	1.08	1.12	1.16	1.13	1.16	1.11	Density [g/ccm]	1.08	1.2					1.10785	1.117775	1.085325	1.094
PR004			Hardness [°ShA]	42.00	41.00	40.00	48.00	48.00	52.01	Hardness [°ShA]	40	61	40	45	10		53.995	45.005	45.0175	50.3
PR007			M300 [Mpa]	1.80	3.00	3.00	4.40	4.60	5.31	M300 [Mpa]	1.8	9.4					7.426	4.424	3.149	5.52
PR008			TS [Mpa]	25.00	21.00	15.00	25.00	20.00	15.31	TS [Mpa]	15	25	20				22.93	21.445	24.645	24.0
PR009			EB [%]	785.00	725.00	690.00	715.00	705.00	615.01	EB [%]	540	785		600			600.225	683.8375	741.5125	664.9
PR010			C-Set -26°C /24h [%]	22.00	28.00	30.00	17.00	19.00	35.01	C-Set -26°C /24h [%]	17	77					62.285	38.9025	31.7625	48.9
PR011			C-Set 0°C /24h [%]	10.00	14.00	14.00	8.00	12.00	16.01	C-Set 0°C /24h [%]	8	16					14.93	14.445	11.065	12.9
PR012			C-Set 23°C /72h [%]	8.00	10.00	14.00	9.00	13.00	16.01	C-Set 23°C /72h [%]	8	18					15.47	11.78	9.775	12
PR013			C-Set 70°C /24h [%]	39.00	50.00	61.00	44.00	50.00	54.01	C-Set 70°C /24h [%]	17	61		25	10	5	25.03	42.6575	35.095	28.2
<b>Total ingredients</b>				146.15	166.15	226.15	161.15	201.15	251.15	<b>Total ingredients</b>	146.15	251.15					171.283	183.0795	150.8005	158.988
<b>Density</b>				1.096	1.115	1.128	1.137	1.147	1.171	<b>Density</b>	1.096	1.186					1.11	1.114	1.099	1.103
<b>Cost (per vol)</b>				262.547	237.377	220.712	259.187	235.816	219.724	<b>Cost (per vol)</b>	219.724	263.877					259.128	242.909	262.812	263.03
<b>Cost (per mass)</b>				239.35	212.894	195.667	227.957	205.594	187.631	<b>Cost (per mass)</b>	187.638	239.55					233.449	218.051	239.137	238.468
<b>Recipe ratios in %:</b>				51													Sum of recipe ratios (should be 100%): 100			

**Result:**  
**C-Set now from 42% down to 35%**  
**while hardness is in specification**  
**(notice that elongation 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”

GrafCompunder version 3.211 - demo data

File Edit Help

Input data:

				50AL511	50AL512	50AL513	50AL514	50AL515	50AL516
<b>Test Data (Advanced)</b>									
<b>Code:</b>	<b>Cost:</b>	<b>Density:</b>	<b>Ingredients:</b>	<b>50AL511</b>	<b>50AL512</b>	<b>50AL513</b>	<b>50AL514</b>	<b>50AL515</b>	<b>50AL516</b>
A001	280.00	0.92	NR (SMR - 10)	100.00	100.00	100.00	100.00	100.00	100.00
B003	115.00	1.80	N330	10.00	30.00	50.00	25.00	45.00	75.00
C010	24.00	2.71	CaCO3	20.00	20.00	20.00	20.00	20.00	20.00
D002	116.00	0.89	Naphthenic Oil	5.00	25.00	45.00	5.00	25.00	45.00
E001	385.00	5.60	ZnO	5.00	5.00	5.00	5.00	5.00	5.00
F001	165.00	0.92	Stearic Acid	2.00	2.00	2.00	2.00	2.00	2.00
G001	924.00	1.15	IPPD	2.00	2.00	2.00	2.00	2.00	2.00
H001	158.00	1.80	S	1.50	1.50	1.50	1.50	1.50	1.50
K001	396.00	1.11	TMTD - 80						
K005	708.00	1.28	CBS - 80	0.65	0.65	0.65	0.65	0.65	0.65
<b>Properties:</b>									
PR001			MooneyML(1+4) 100°C	32.00	36.00	31.00	34.00	30.00	42.00
PR002			Mooney I5 / 120°C	28.00	28.00	32.00	28.00	32.00	22.00
PR003			Density [g/ccm]	1.08	1.12	1.16	1.13	1.16	1.11
PR004			Hardness [ShA]	42.00	41.00	40.00	48.00	48.00	52.00
PR007			M300 [Mpa]	1.80	3.00	3.00	4.40	4.60	5.30
PR008			TS [Mpa]	25.00	21.00	15.00	25.00	20.00	15.30
PR009			EB [%]	785.00	725.00	690.00	715.00	705.00	615.00
PR010			C-Set -26°C /24h [%]	22.00	28.00	30.00	17.00	19.00	35.00
PR011			C-Set 0°C /24h [%]	10.00	14.00	14.00	8.00	12.00	16.00
PR012			C-Set 23°C /72h [%]	8.00	10.00	14.00	9.00	13.00	16.00
PR013			C-Set 70°C /24h [%]	39.00	50.00	61.00	44.00	50.00	54.00
<b>Total ingredients</b>				146.15	186.15	226.15	161.15	201.15	251.15
<b>Density</b>				1.096	1.115	1.128	1.137	1.147	1.171
<b>Cost (per vol)</b>				262.547	237.377	220.712	259.167	235.616	219.721
<b>Cost (per mass)</b>				239.55	212.694	193.667	227.957	205.594	167.631
<b>Recipe ratios in %:</b>				51					

Criteria:

Name	Min	Max	From	To	Weight	Trdoff
NR (SMR - 10)	100	100				
N330	10	75				
CaCO3	0	20				
Naphthenic 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				
MooneyML(1+4)	30	60				
Mooney I5 / 120°C	11	32				
Density [g/ccm]	1.08	1.2	40	45	10	
Hardness [ShA]	40	61				
M300 [Mpa]	1.8	9.4				
TS [Mpa]	15	25	20			
EB [%]	540	785		600		
C-Set -26°C /24h [%]	17	77				
C-Set 0°C /24h [%]	8	16				
C-Set 23°C /72h [%]	8	18				
C-Set 70°C /24h [%]	17	61	25	10	5	

Output:

Mixture1	Mixture4	Mixture5	Mixture6
100	100	100	100
41.8	34.45	17.1	29
5.7	15.55	16.45	10
11.775	21.6625	5.8875	7.4
5	5	5	5
2	2	2	2
2	2	2	2
0.60625	1.221875	1.278125	0.887
0.715	0.2225	0.1775	0.4
1.68675	0.972625	0.907375	1.360
39.075	37.1125	33.5975	36.4
15.845	24.2175	24.9825	19.6
1.10785	1.117775	1.085325	1.094
53.995	45.005	45.0175	50.3
7.426	4.424	3.149	5.52
22.93	21.445	24.645	24.0
600.225	683.8375	741.5125	664.9
62.285	38.9025	31.7625	48.9
14.93	14.445	11.065	12.9
15.47	11.78	9.775	12
25.03	42.6575	35.095	28.2

Sum of recipe ratios (should be 100%): 100

Number format: 12345.67

Import input data from clipboard

Auto mix (overwrite mixture)

Auto mix (new mixture)

### As demonstrated

- “weight” helps to give a preference to properties, we have the freedom to select
- In case of conflicting 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

The screenshot displays the GrafCompounder software interface. The main window is titled "GrafCompounder version 3.211 - demo data". It features a menu bar (File, Edit, Help) and a toolbar. The central area is divided into several panes:

- Input Data (Advanced):** A table with columns for ingredients (50AL511 to 50AL516) and properties (Code, Cost, Density, Ingredients, Recipes, Prop). A context menu is open over the "NR (SMR - 10)" cell, showing options like "Copy input table", "Copy marked cells", "Paste cells here", "Delete marked rows", "Delete marked columns", "Insert empty row", "Insert empty column", and "Clear marked cells".
- Criteria:** A table with columns for Name, Min, Max, From, To, Weight, and Trdoff. It lists various ingredients and properties with their respective ranges.
- Output:** A table showing the results of the calculation, including mixture ratios and total ingredients.

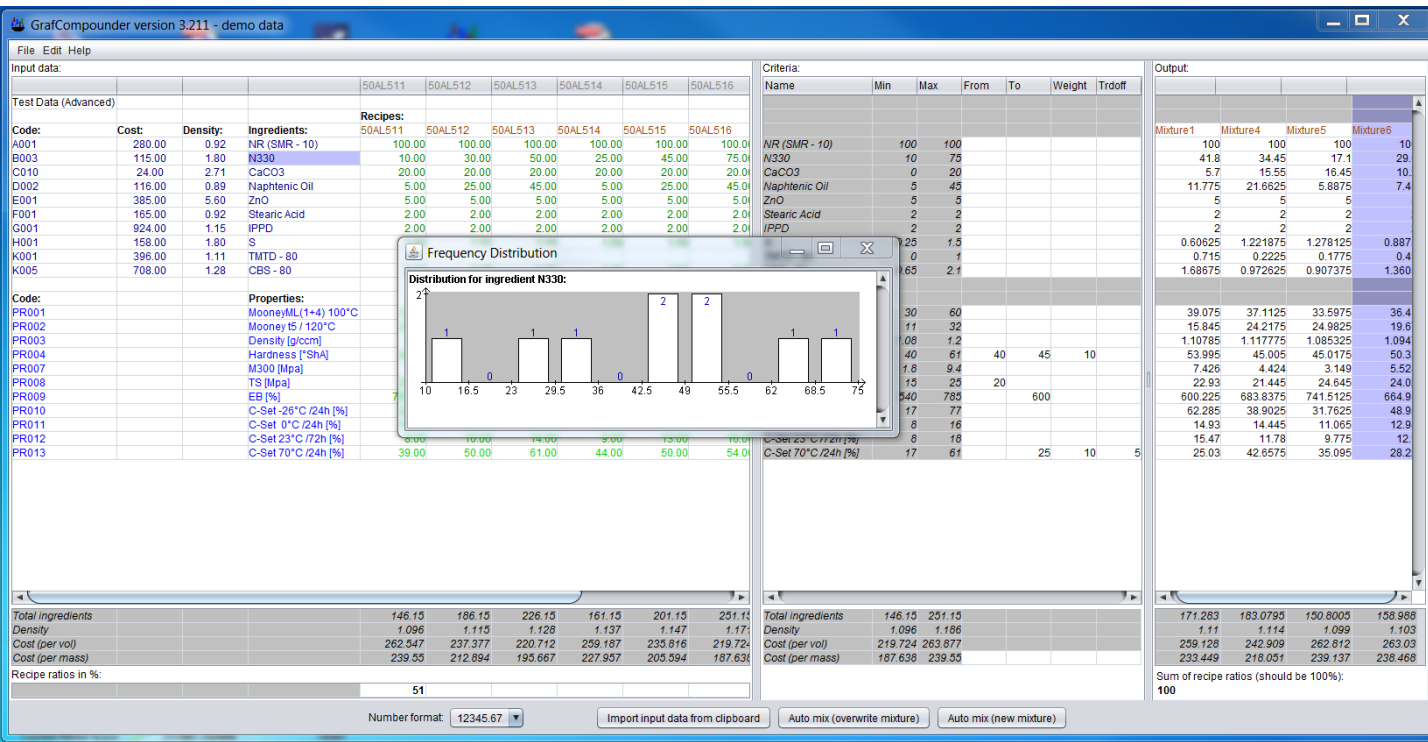
At the bottom of the interface, there are buttons for "Import input data from clipboard", "Auto mix (overwrite mixture)", and "Auto mix (new mixture)".

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 menu select "frequency distribution for row"

# Database Tools

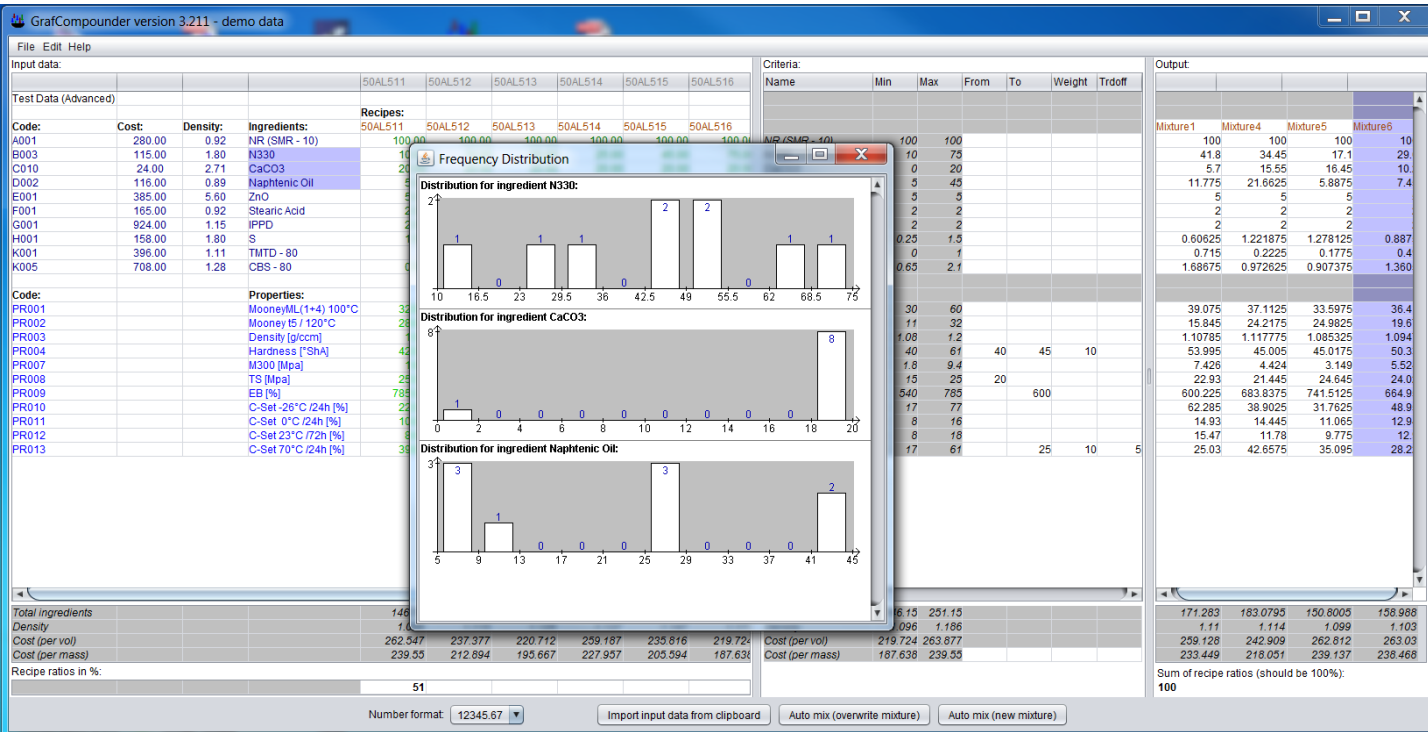


“frequency distributio for row”

- 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



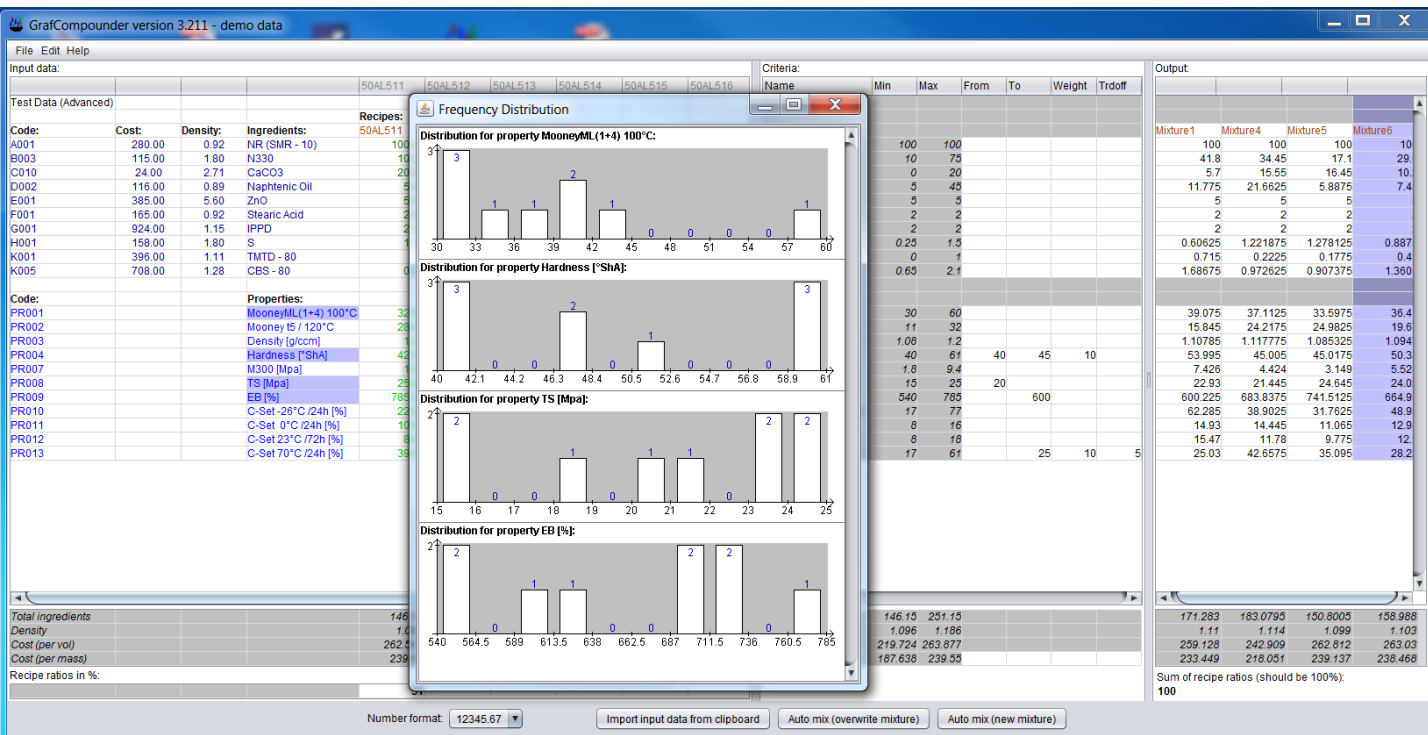
# Database Tools



## “frequency distribution for x rows”

- Example frequency distribution for more than one ingredient:
- Highlight all ingredients you want to see:  
Example: N330, CaCO3 and Naphtenic Oil
- Pull Down menu with right click
- Select “frequency distribution for 3 rows”

# Database Tools



“frequency distribution for x rows”

- Example frequency distribution for more than on Property:
- Highlight all properties you want to see:  
Example: Mooney, Hardness, TS-Tensile, EB-Elongation
- Pull Down menu with right click
- Select “frequency distribution for 4 rows”

As in our previous example distributions are uneven (*what is expected with a small sample database*)

# Database Merger of Data Tables

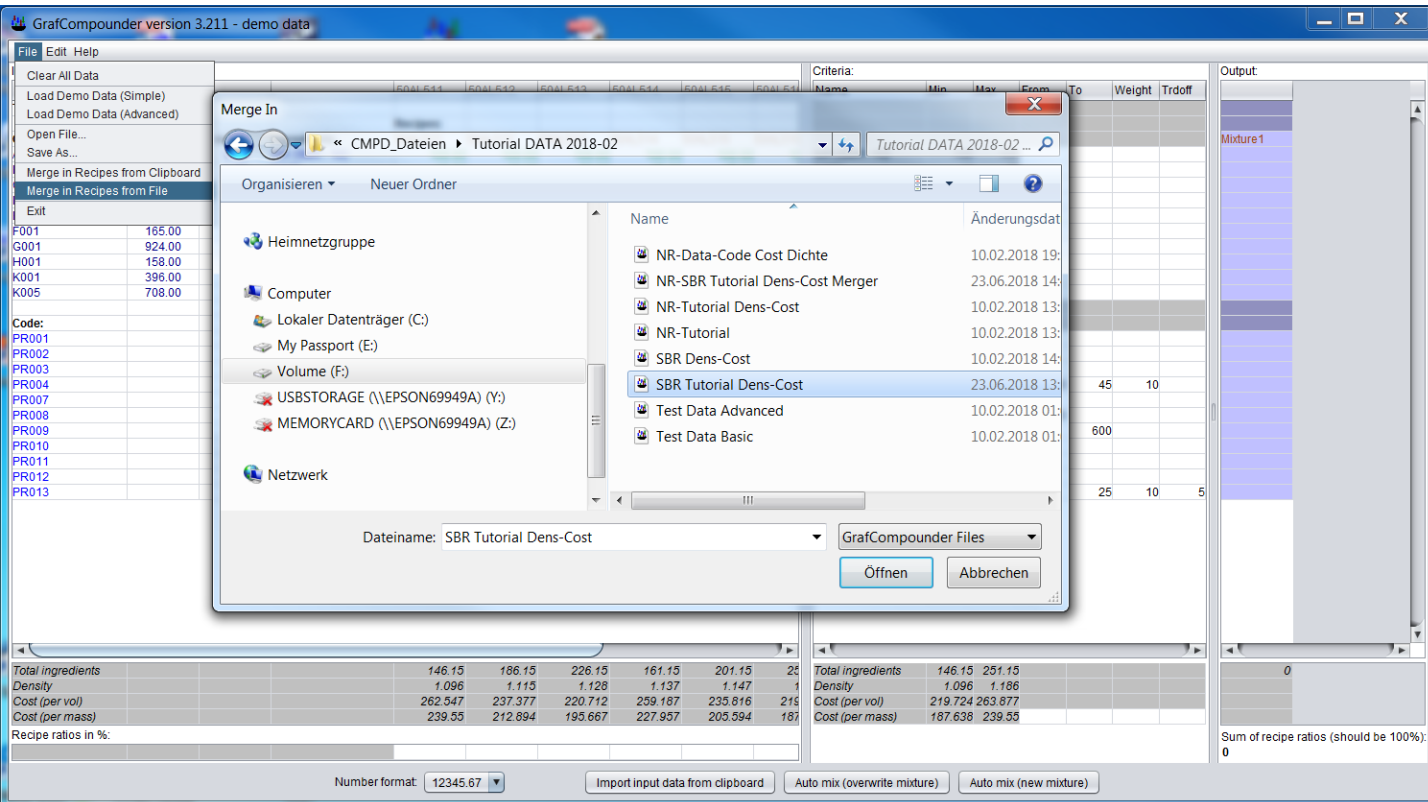
The screenshot shows the GrafCompounder version 3.211 - demo data interface. The main window displays a table with columns for ingredients and recipes (50AL511 to 50AL516). A right-hand pane shows a list of criteria with columns for Name, Min, Max, From, To, Weight, and Tdroff. An 'Output' pane on the far right shows a list of ingredients and their weights. At the bottom, there are summary statistics for ingredients and recipes, and a 'Recipe ratios in %' section.

Ingredients	50AL511	50AL512	50AL513	50AL514	50AL515	50AL516
Density	0.92	1.80	2.71	0.89	5.60	0.92
NR (SMR - 10)	100.00	100.00	100.00	100.00	100.00	100.00
N330	10.00	30.00	50.00	25.00	45.00	25.00
CaCO3	20.00	20.00	20.00	20.00	20.00	20.00
Naphtenic Oil	5.00	25.00	45.00	5.00	25.00	25.00
ZnO	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
IPPD	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
TMTD - 80	1.11	1.11	1.11	1.11	1.11	1.11
CBS - 80	0.65	0.65	0.65	0.65	0.65	0.65

- Because of insufficient Data base you want to expand and add more data
  - Click File
  - Right click pull down menu:
    - 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

The screenshot shows the GrafCompounder version 3.2111 - demo data interface. It features a main data table with columns for Code, Cost, Density, Ingredients, and Recipes (50AL511 to 50AL516). A 'Criteria' table is visible on the right, listing various ingredients like NR (SMR - 10), N330, CaCO3, etc., with columns for Name, Min, Max, From, To, Weight, and Trdoff. A dialog box titled 'Merge in Recipes From File' is overlaid on the main table, displaying an information icon and the text: '22 recipes have been added. 26 new ingredient rows have been added.' with an 'OK' button.

- 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

The screenshot shows the GrafCompounder software interface. The main window displays a table with columns for 'Code', 'Cost', 'Density', 'Ingredients', and several recipe columns (50AL511 to 50AL516). A context menu is open over the 'Ingredients' column, with the option 'Sort selected ingredient rows' highlighted. The right side of the interface shows a 'Criteria' table and an 'Output' window displaying 'Mixture 1'. The bottom of the window shows summary statistics for ingredients and costs.

- 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

GrafCompounder version 3.211 - demo data

Input data:				50AL511	50AL512	50AL513	50AL514	50AL515	50AL516
Code:	Cost:	Density:	Ingredients:	50AL511	50AL512	50AL513	50AL514	50AL515	50AL516
A001	280.00	0.92	NR (SMR - 10)	100.00	100.00	100.00	100.00	100.00	100.00
A011	178.00	0.94	SBR 1500						
A013	178.00	1.12	SBR 1618 (50II/50CB)						
A015	178.00	0.94	SBR 1711 (37.50II/...						
A016	178.00	0.94	SBR 1707 (37.50II/...						
A018	178.00	1.14	SBR 1808 (47.50II/...						
A019	178.00	1.20	SBR 1843 (150II/10...						
A021	200.00	0.92	Buna CB 10						
A902	105.00	1.25	Recycled Tread						
B002	115.00	1.80	N 220						
B003	115.00	1.80	N330	10.00	30.00	50.00	25.00	45.00	
B005	115.00	1.80	N550						
B901	55.00	1.25	Ground Rubber						
C010	24.00	2.71	CaCO3	20.00	20.00	20.00	20.00	20.00	
C021	172.00	2.70	Clay						
C022	125.00	2.00	Silittin N						
D002	116.00	0.89	Naphtenic Oil	5.00	25.00	45.00	5.00	25.00	
D003	128.00	0.98	Aromatic Oil						
E001	385.00	5.60	ZnO	5.00	5.00	5.00	5.00	5.00	
F001	165.00	0.92	Stearic Acid	2.00	2.00	2.00	2.00	2.00	
F002	250.00	0.98	Benzoic Acid						
F101	130.00	0.90	Paraffin Wax						
F102	280.00	1.05	Koresin						
F103	187.00	1.10	Cumar Resin						
F104	55.00	1.30	Durant B						
F105	125.00	1.40	Struktol 40 MS						
F106	2.20	1.20	Strukto W 33						
G001	924.00	1.15	IPPD	2.00	2.00	2.00	2.00	2.00	
G002	891.00	1.15	PBN						
G011	579.00	1.33	TMQ						
H001	158.00	1.80	S	1.50	1.50	1.50	1.50	1.50	
K001	396.00	1.11	TMTD - 80						

Criteria:	Name	Min	Max	From	To	Weight	Trdoff
	NR (SMR - 10)	0	100				
	SBR 1500	0	100				
	SBR 1618	0	155				
	SBR 1711	0	100				
	SBR 1707	0	137.5				
	SBR 1808	0	223.5				
	SBR 1843	0	140				
	Buna CB 10	0	20				
	Recycled Tread	0	90				
	N 220	0	60				
	N330	0	80				
	N550	0	50				
	Ground Rubber	0	20				
	CaCO3	0	20				
	Clay	0	100				
	Silittin N	0	50				
	Naphtenic Oil	0	45				
	Aromatic Oil	0	25				
	ZnO	1	7				
	Stearic Acid	0	3				
	Benzoic Acid	0	0.5				
	Paraffin Wax	0	3				
	Koresin	0	5				
	Cumar Resin	0	9				
	Durant B	0	10				
	Struktol 40 MS	0	20				
	Strukto W 33	0	7.5				
	IPPD	0	2				
	PBN	0	3				
	TMQ	0	3				
	S	0	2.4				
	TMTD - 80	0	4				

Output:	Mixture1
	0

Total ingredients	146.15	186.15	226.15	161.15	201.15	251.15
Density	1.096	1.115	1.128	1.137	1.147	1.157
Cost (per vol)	262.947	237.377	220.712	259.167	235.816	215.181
Cost (per mass)	239.55	212.894	195.667	227.957	205.594	181.181

195.667 (this is a value calculated from input data of recipe 50AL513)

Number format: 12345.67

Import input data from clipboard    Auto mix (overwrite mixture)    Auto mix (new mixture)

### 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

The screenshot shows the GrafCompounder software interface. A central dialog box titled "Exit Confirmation" with a question mark icon asks "Have you saved your data?". Below the question are two buttons: "Yes, Exit" and "No, Cancel". The background shows a data table with columns for material names and various properties. The table is partially obscured by the dialog box.

Code	Name	50AL511	50AL512	50AL513	50AL514	50AL515	50AL516
A021	Buna CB 10						
A902	Recycled Tread						
B002	N 220						
B003	N330	10.00	30.00	50.00	25.00	45.00	
B005	N550						
B901	Ground Rubber						
C010	CaCO3	20.00	20.00	20.00	20.00	20.00	
C021	Clay						
C022	Silittin N						
D002	Naphtenic Oil	5.00	25.00	45.00	5.00	25.00	
D003	Aromatic Oil						
E001	ZnO	5.00	5.00	5.00	5.00	5.00	
F001	Stearic Acid	2.00	2.00	2.00	2.00	2.00	
F002	Benzoic Acid						
F101	Paraffin Wax						
F102	Koresin						
F103	Cumar Resin						
F104	Duranti B						
F105	Strukto 40 MS						
F106	Strukto W 33						
G001	IPPD	2.00	2.00				
G002	PBN						
G011	TMQ						
H001	S	1.50	1.50				
K001	TMTD - 80						
K002	MBTS						
K003	CBS						
K004	DPG						
K005	CBS - 80	0.65	0.65	0.65	0.65	0.65	

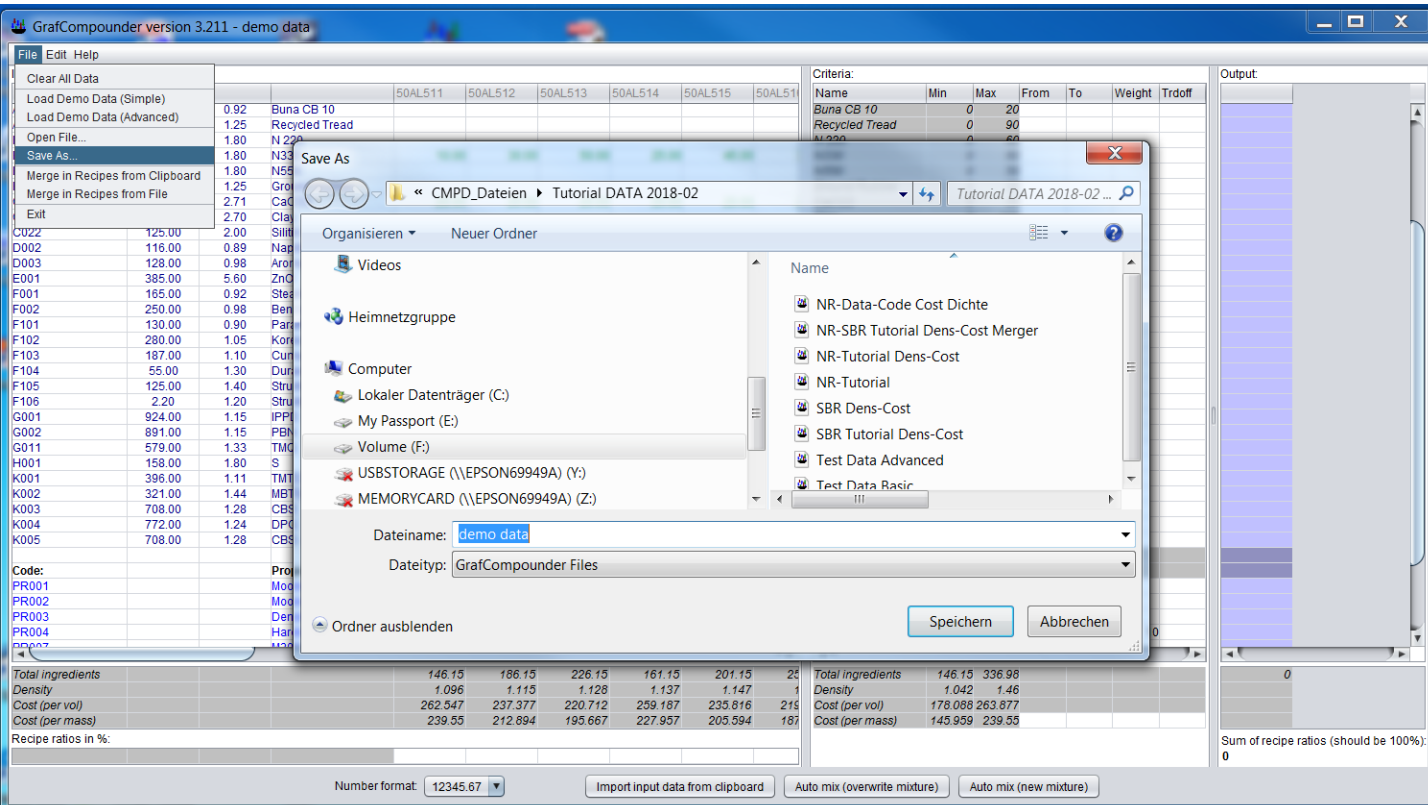
## Store your results before closing the program

- 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 2<sup>nd</sup> 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

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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](http://www.grafcompounder.com) FAQ page**

# Summary

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- ⌋ **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.**