Tutorial
GrafCompounder 5.0

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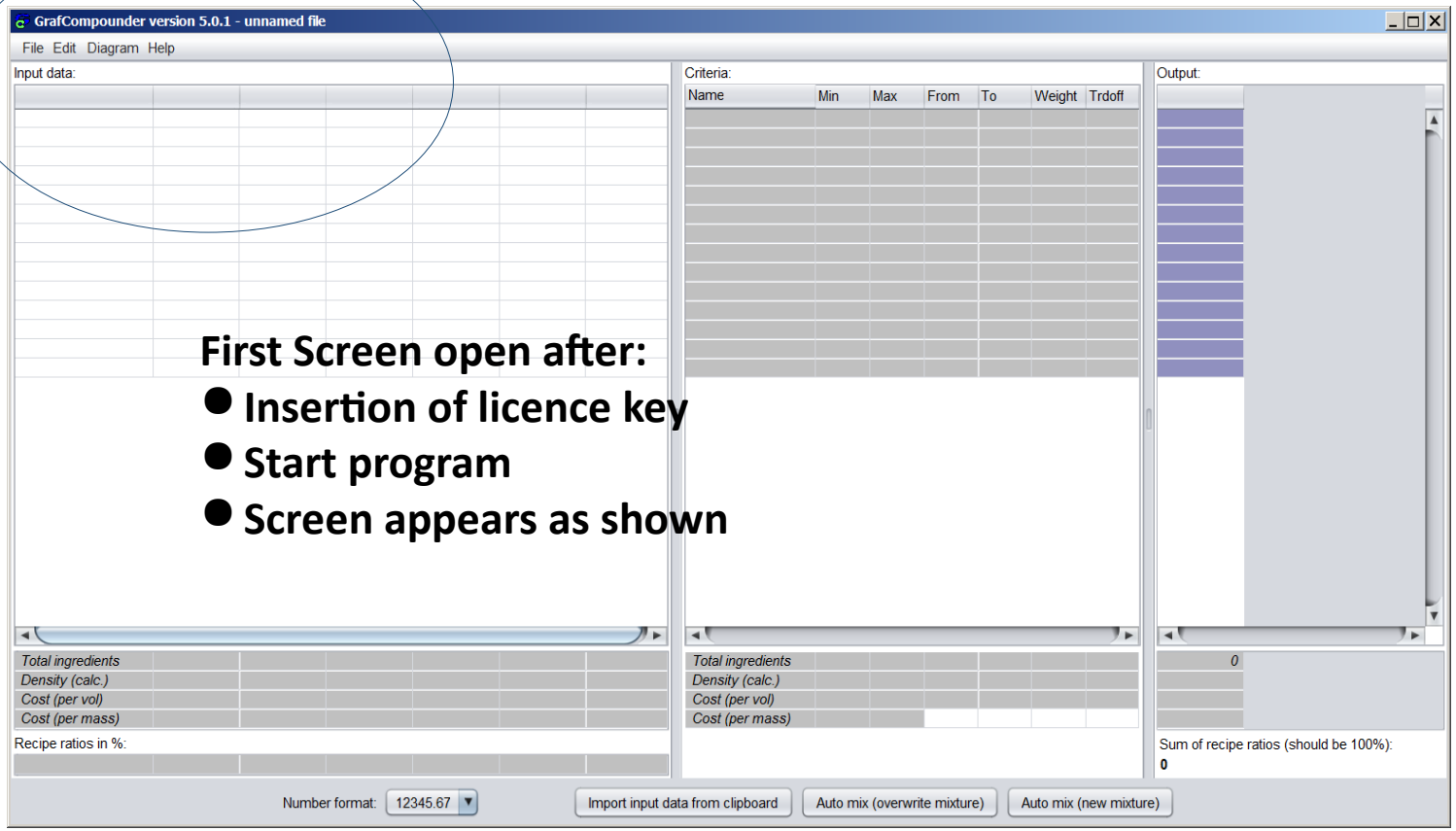
Content :

GrafCompounder 5.0

Step by Step
with
Screen Shots
From Start
to first calculated
Compound

Closing Remarks

Start G[raf]Compounder 5.0

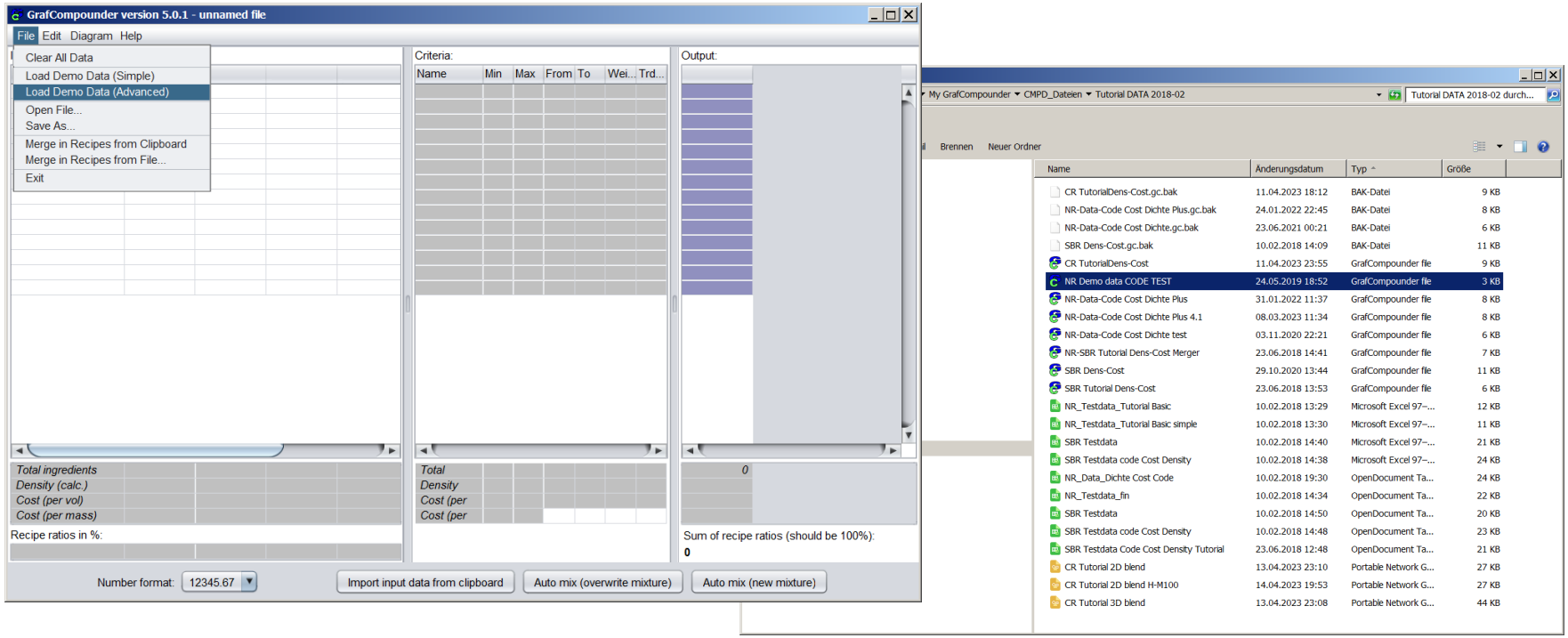


First Screen open after:

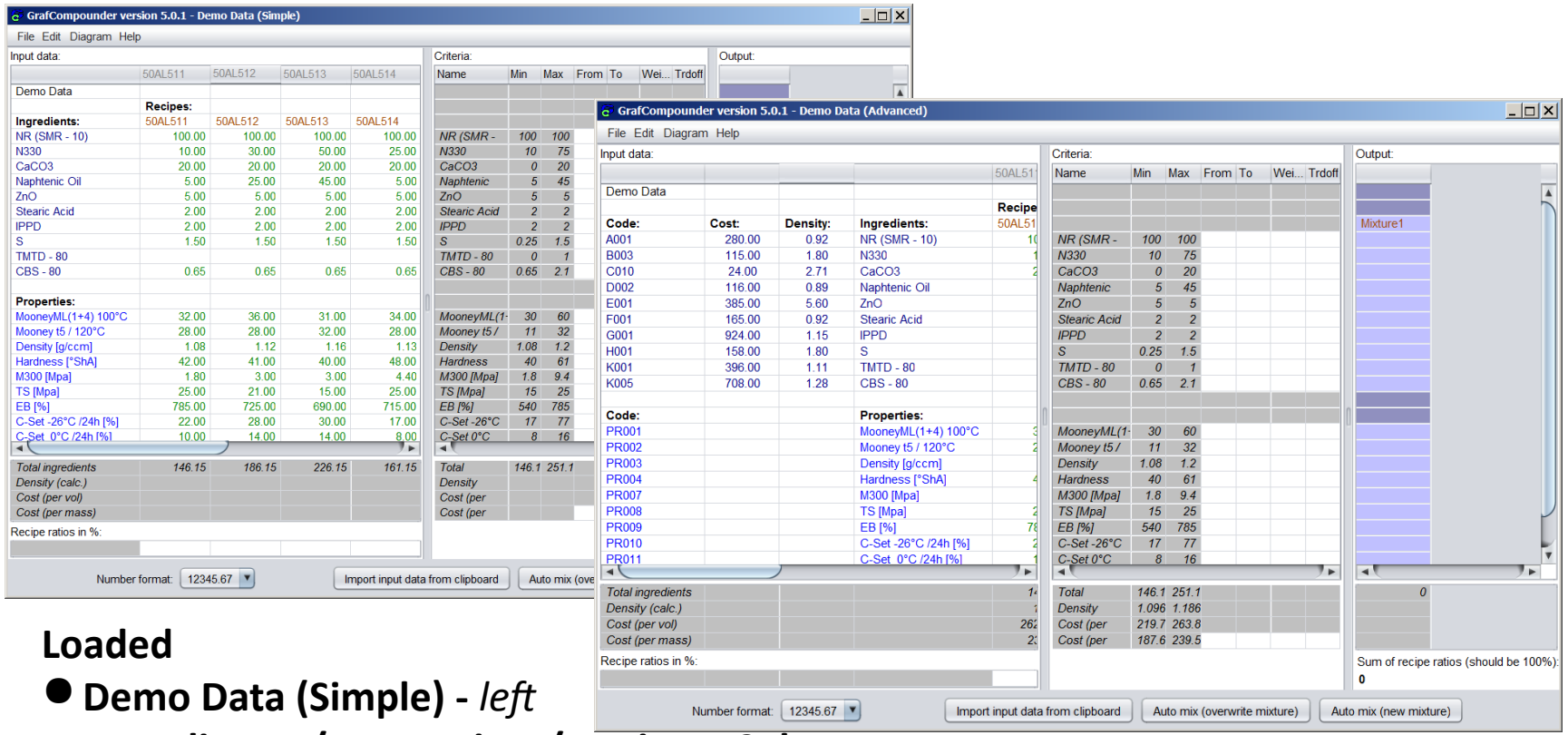
- **Insertion of licence key**
- **Start program**
- **Screen appears as shown**

Start GrafCompounder 5.0

- **Open pull down menue „Load Demo Data (Simple)**
  - **Open File “compound.gc”**
  - **Any other table files: “Copy / Paste” for incorporation**



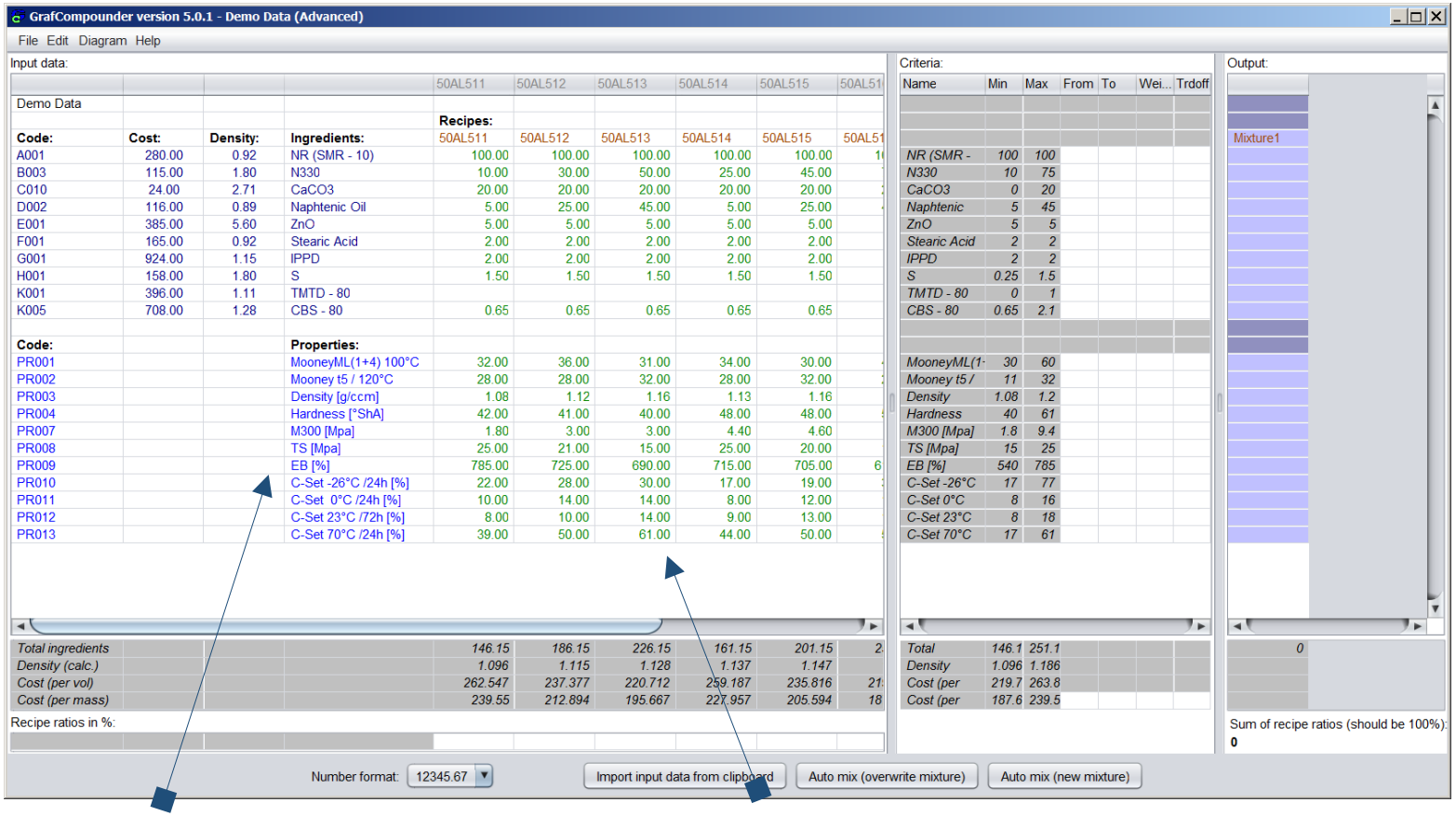
Start G[raf]Compounder 5.0



Loaded

- **Demo Data (Simple)** - *left*
  Ingredients: / Properties: / Recipes: Column
- **Demo Data (Advanced): With additional columns Code: / Cost: / Density:** - *right*

Start G[raf]Compounder 5.0



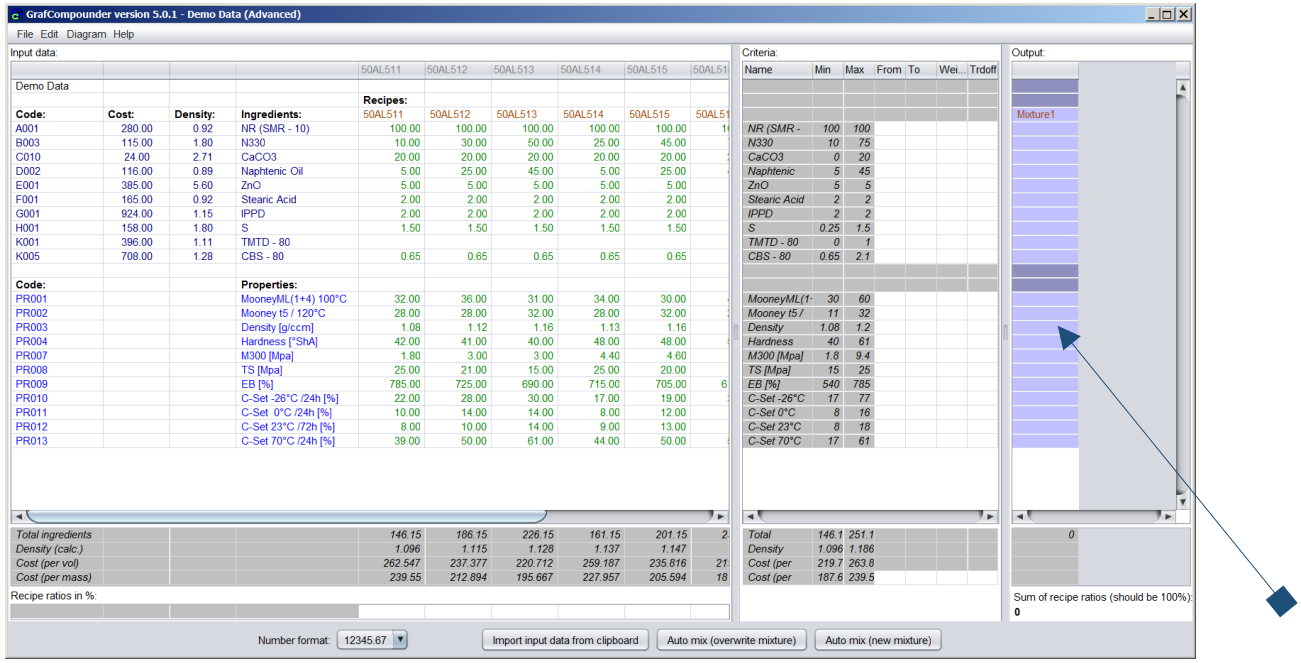
Columns: Numbers in Blue

Recipes: Numbers in Green

Start G[raf]Compounder 5.0

- **Empty Cell in Properties: Column = Data not recognized; Criteria fields empty.**
- **Number in yellow field: Wrong number format, excluded from calculation**

Start G[raf]Compounder 5.0 – Predict a compound

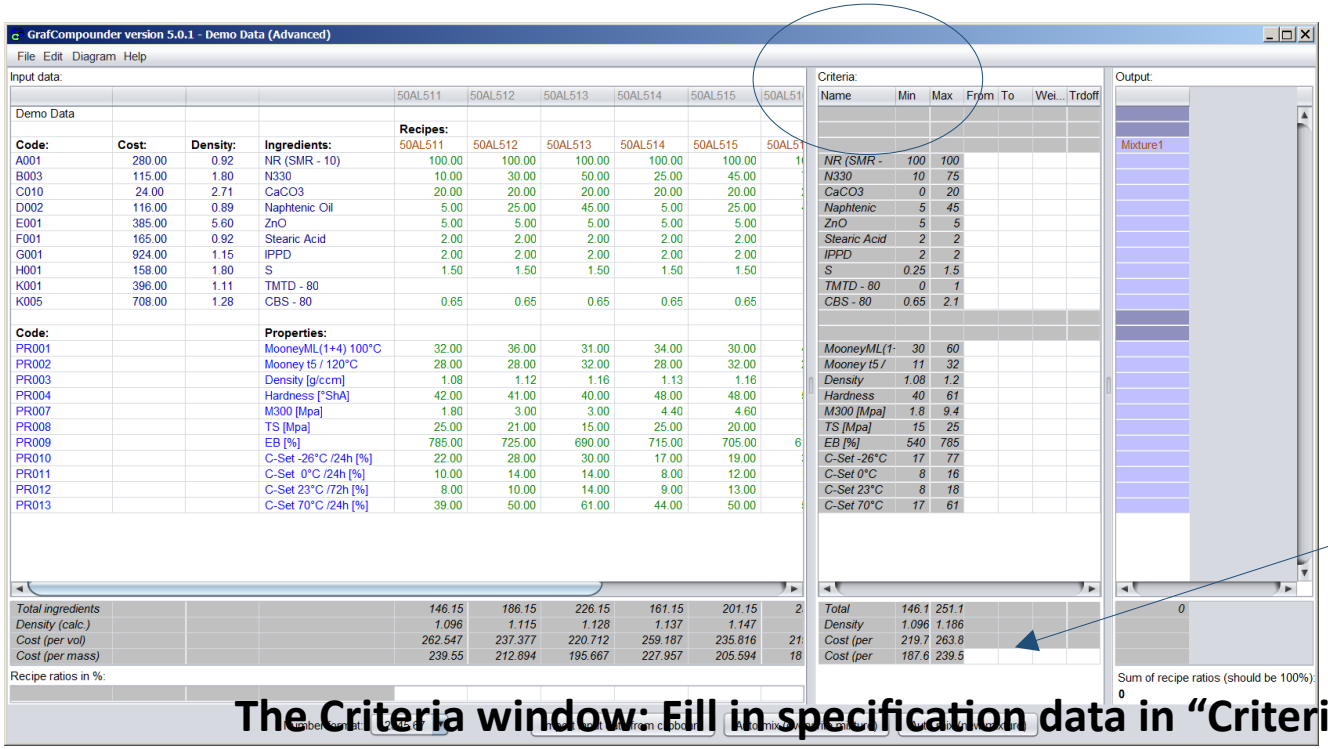


Program Screen with Data ready for calculation:

Option 1: Automix (overwrite mixture): writing result in “mixture 1” column
Overwrites „mixture n“ column (*cells in blue color*)

Option 2: Automix (new mixture): creates “mixture 2” column
creates new “mixture n” column

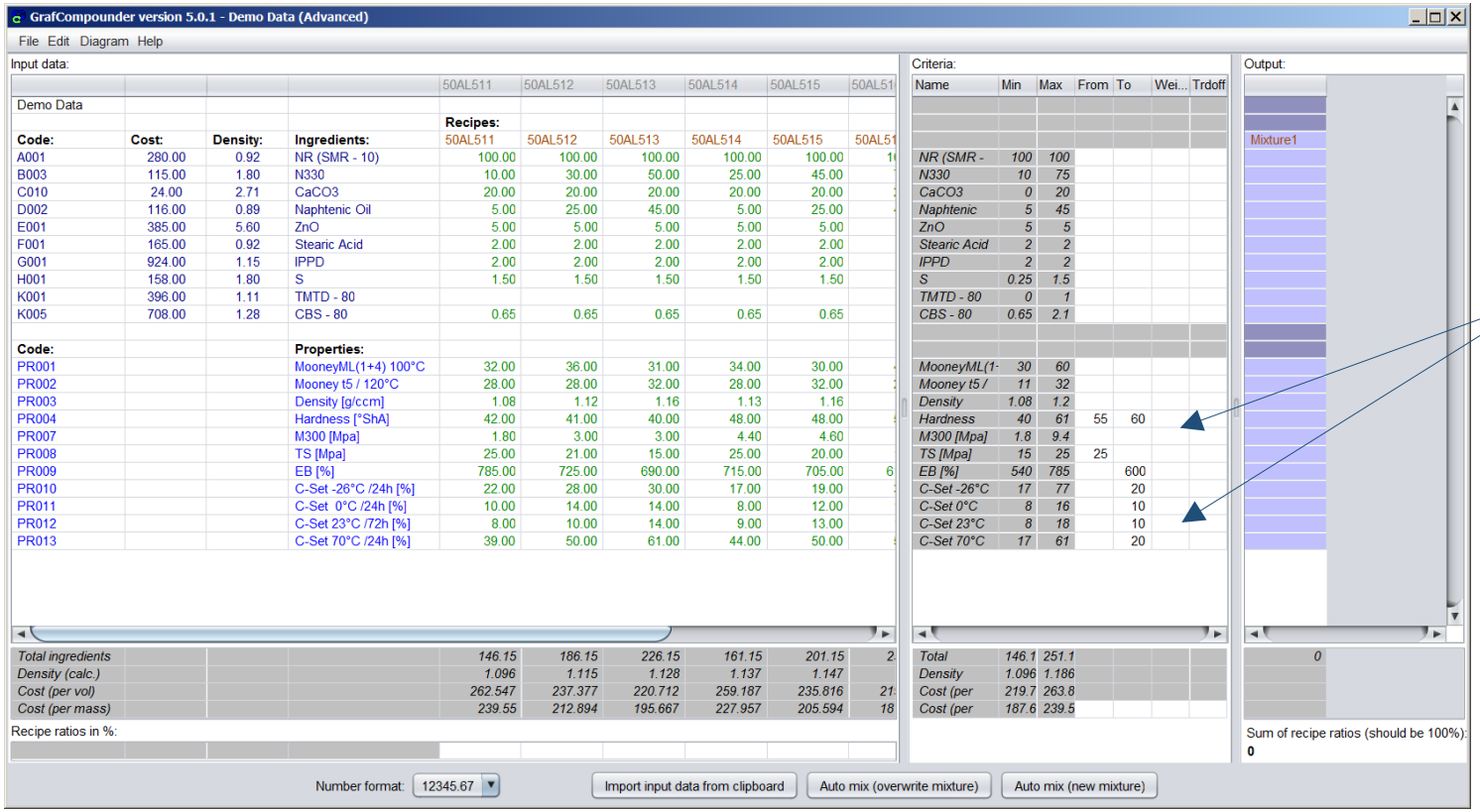
Start G[raf]Compounder 5.0 – Predict a compound



The Criteria window: Fill in specification data in “Criteria” window

*(**Remark**: “cost per vol” can not be a target = **grey cell**:*
{there is no compound yet, therefore no density}
*”cost per mass” can be targeted = **blanc cell**)*

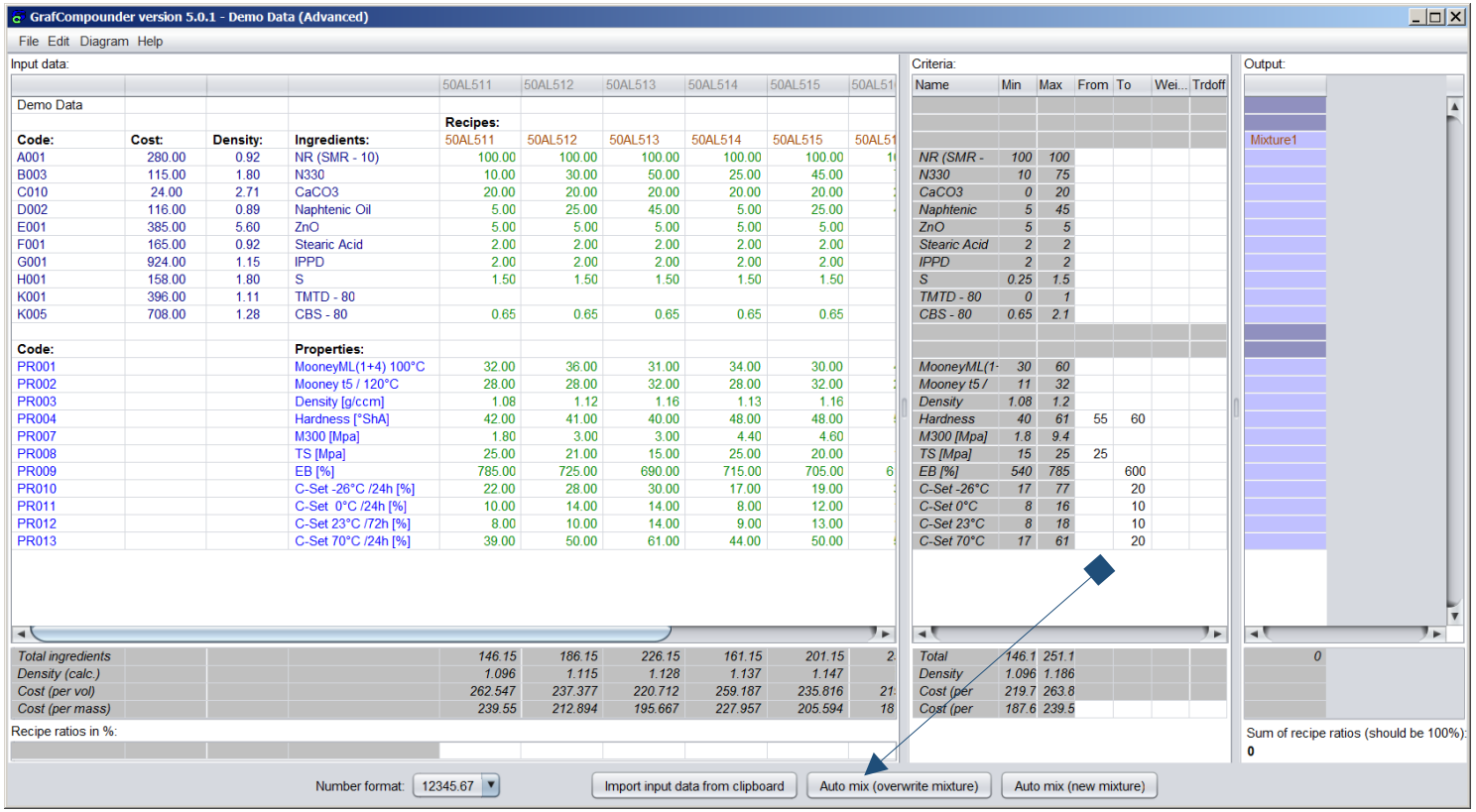
Start G[raf]Compounder 5.0 – Predict a compound



Chose criteria values and put them in the "**Criteria**" Window

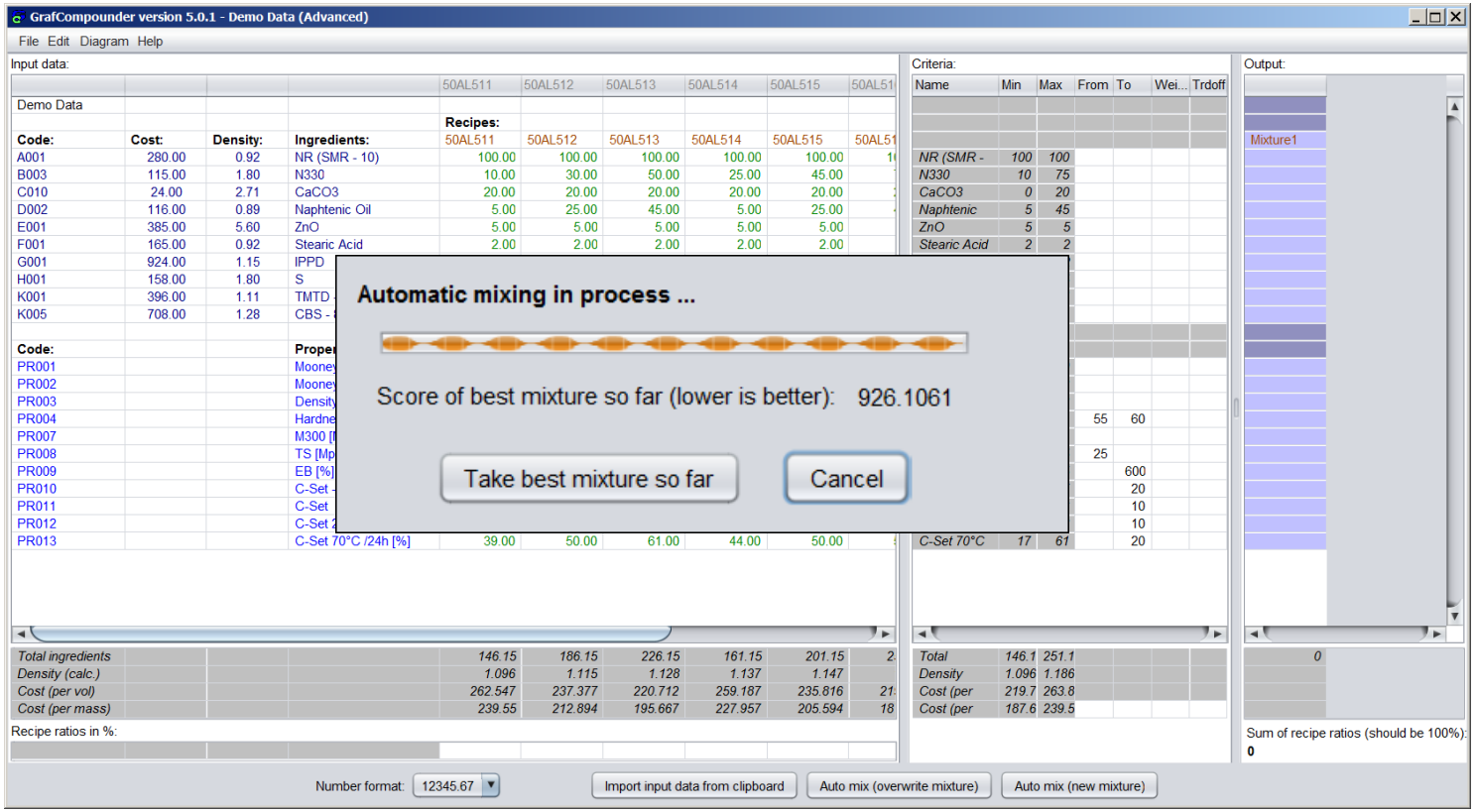
(*You can also copy / paste data from a specification if it is organized similar)*

Start G[raf]Compounder 5.0 – Predict a compound



Click on Button: “**Auto mix (overwrite mixture)**”

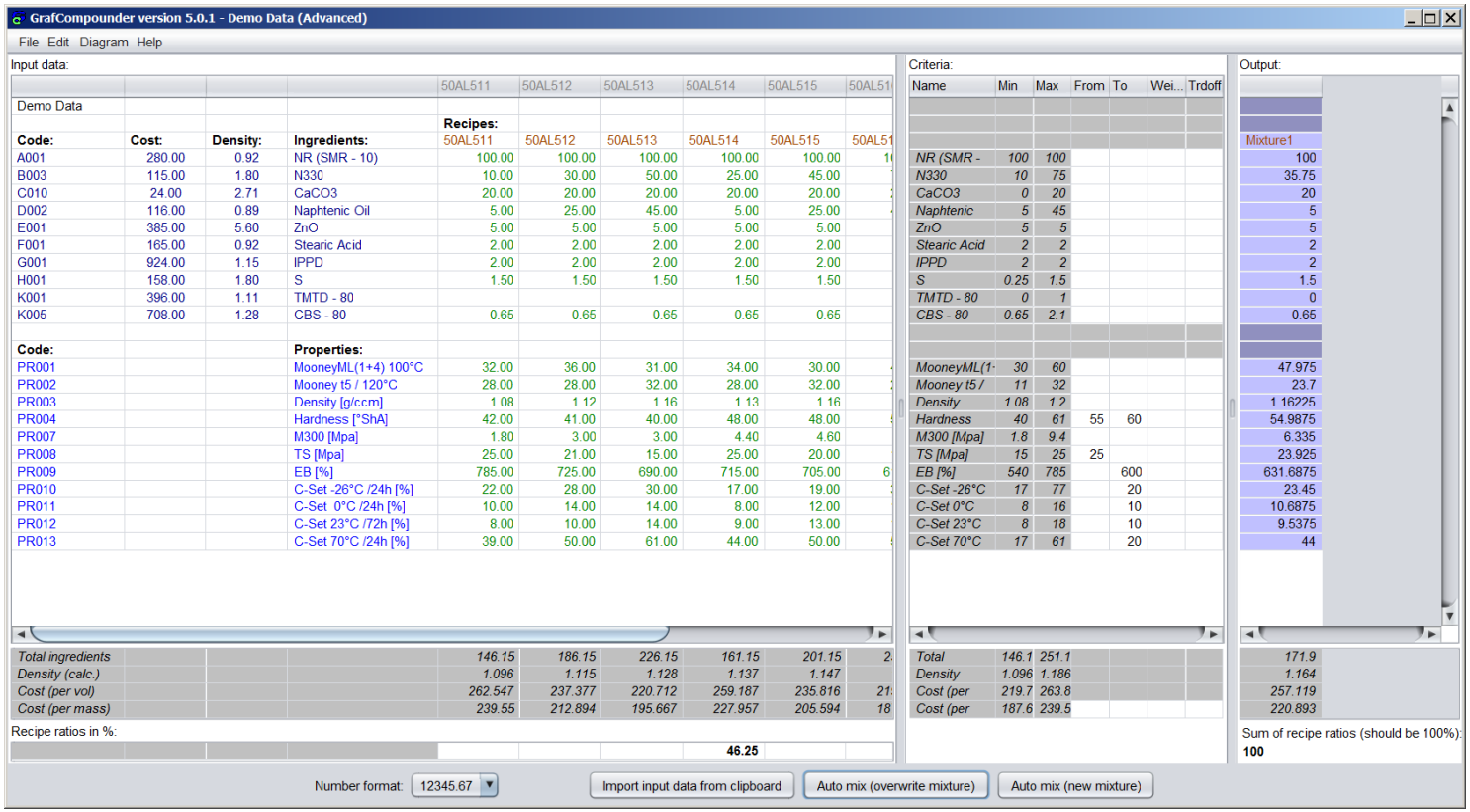
Start G[raf]Compounder 5.0 – Predict a compound



Accept: "**Take best mixture so far**"

(*Value of Fitness Function = 926.. shows, not all criteria could be met*)

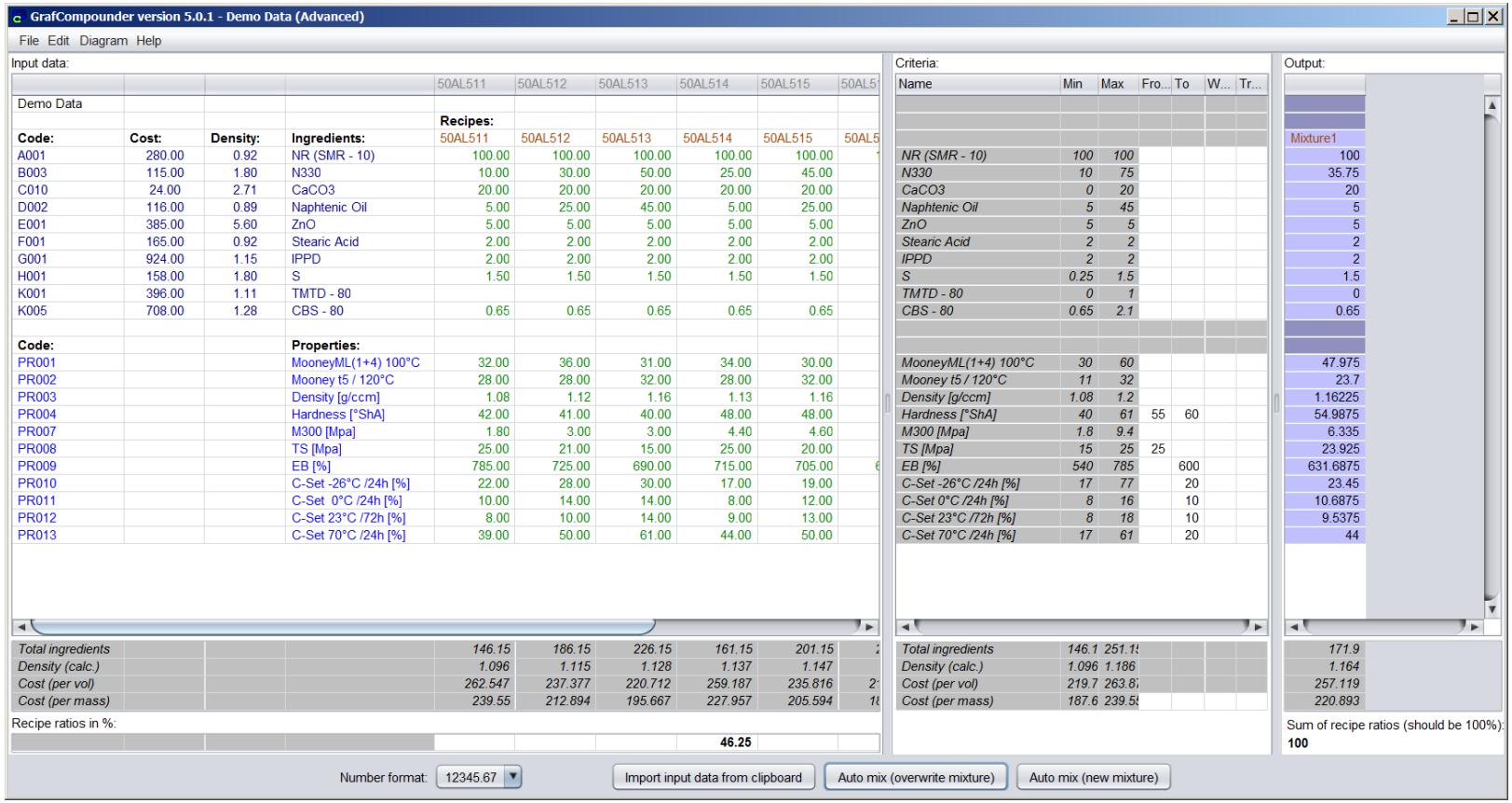
Start G[raf]Compounder 5.0 – Predict a compound



First prediction of a compound is finished.

View result in “Output” window.

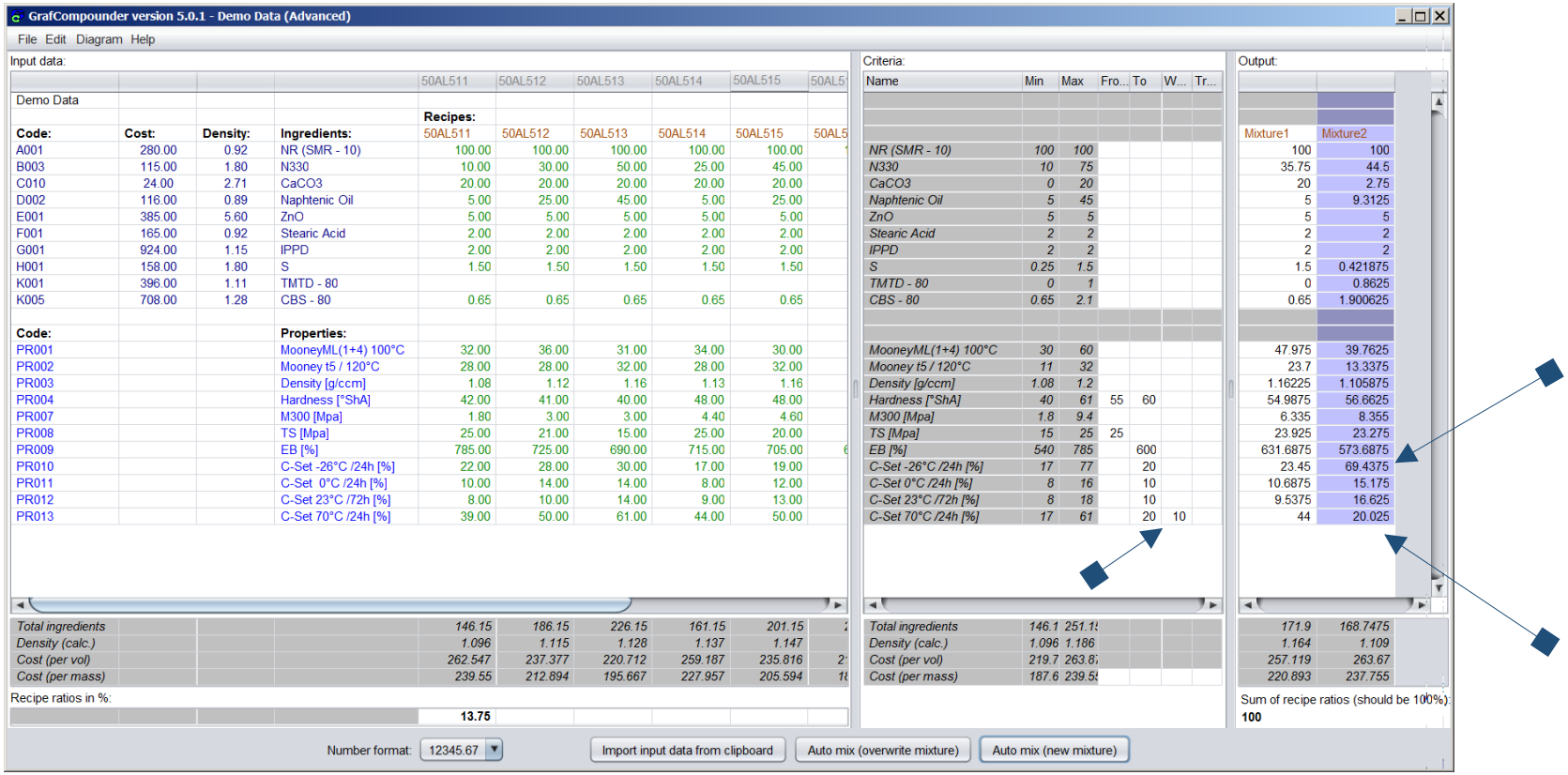
G[raf]Compounder 5.0 – Tune Prediction of a compound



Refine Result: C- 70°C seems to high

Criteria window: Put in "**Weight**" (*select any number: 10 for demonstration*)

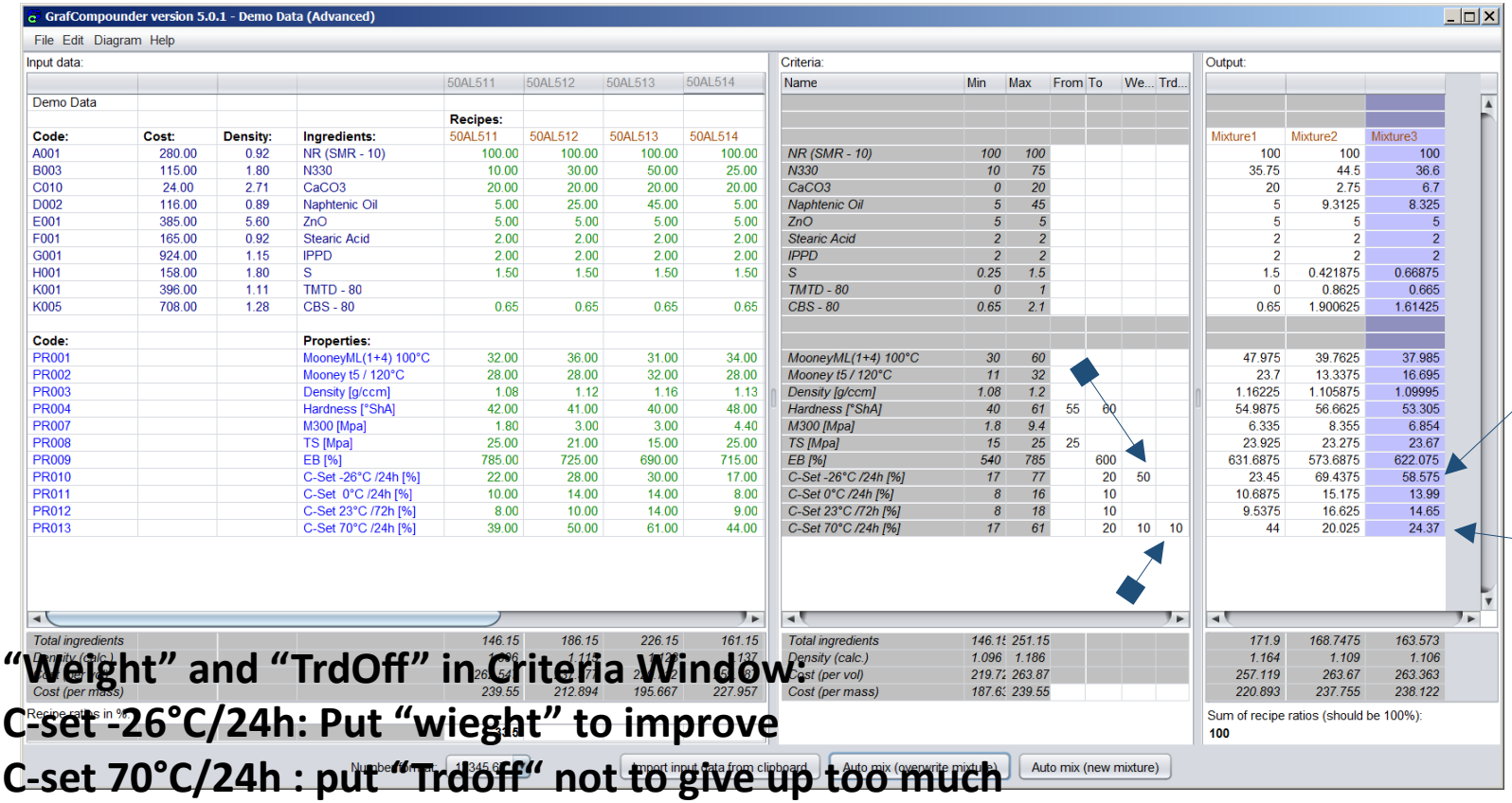
G[raf]Compounder 5.0 – Tune Prediction of a compound



Button “**Automix (new mixture)**” to watch changes

Accept result and evaluate: *C-set 70°C/24h improved at the expense of C-Set-26°C/24h*

GrafCompounder 5.0 – Tune Prediction of a compound



"Weight" and "TrdOff" in Criteria Window:

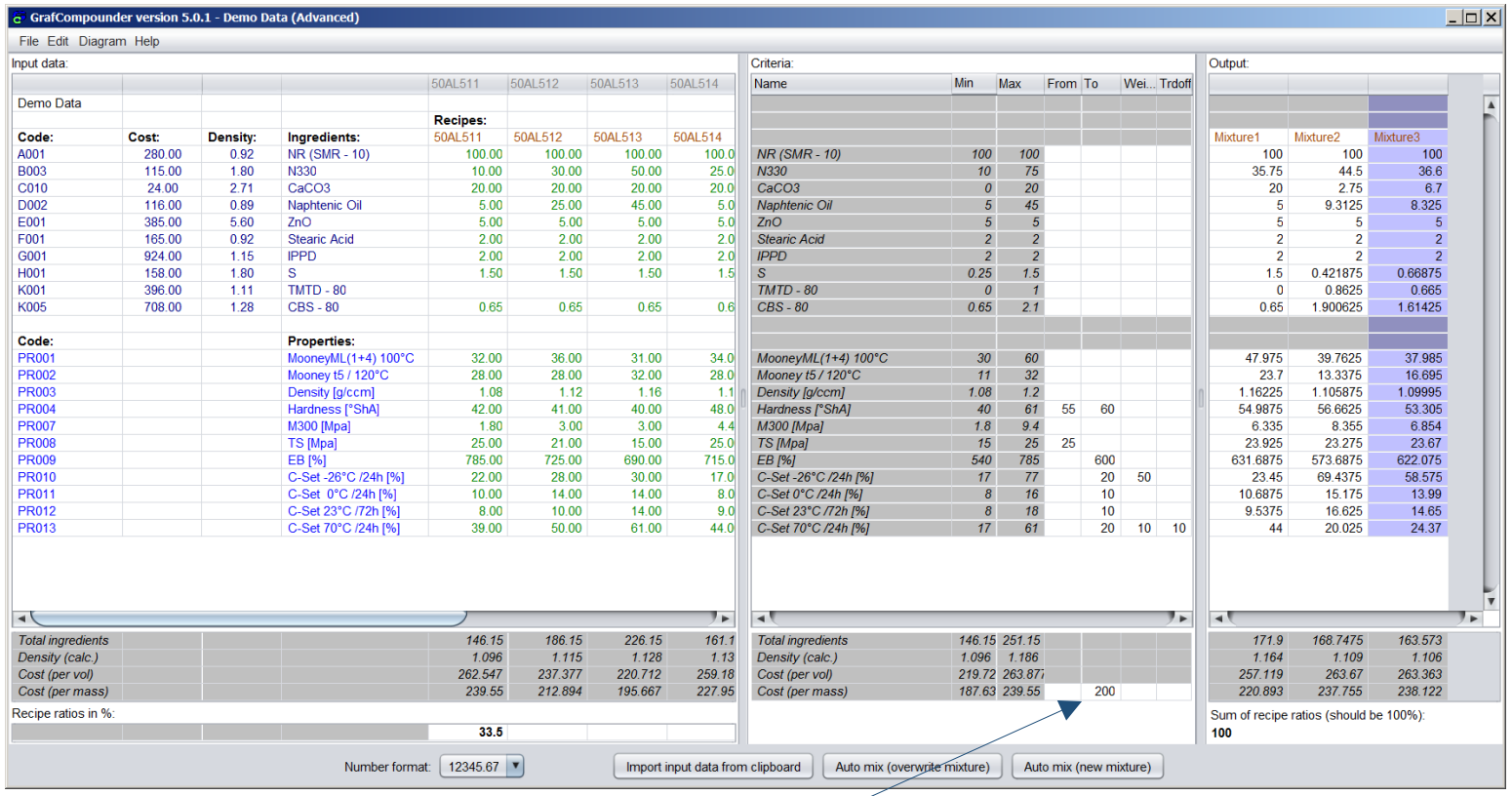
C-set -26°C/24h: Put "wieght" to improve

C-set 70°C/24h : put "Trdoff" not to give up too much

Choose "Auto mix (new mixture)", evaluate results side by side!

(*Play with the numbers of „weight" and "Trdoff" to study effect***)**

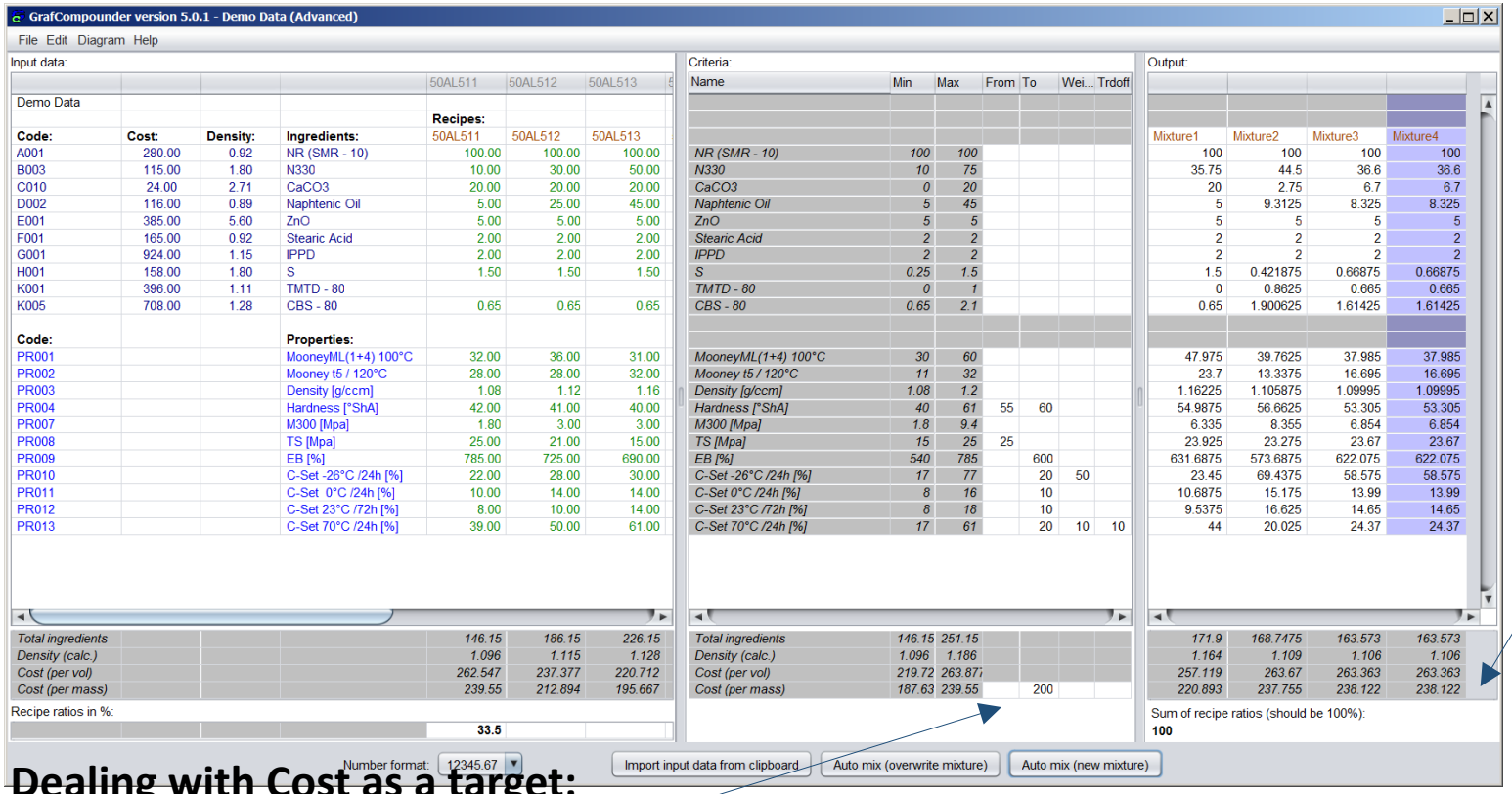
GrafCompounder 5.0 – Tune Prediction of a compound



Dealing with Cost as a target:

Criteria window: Put in **“cost”** target in “Cost per mass” cell

GrafCompounder 5.0 – Tune Prediction of a compound



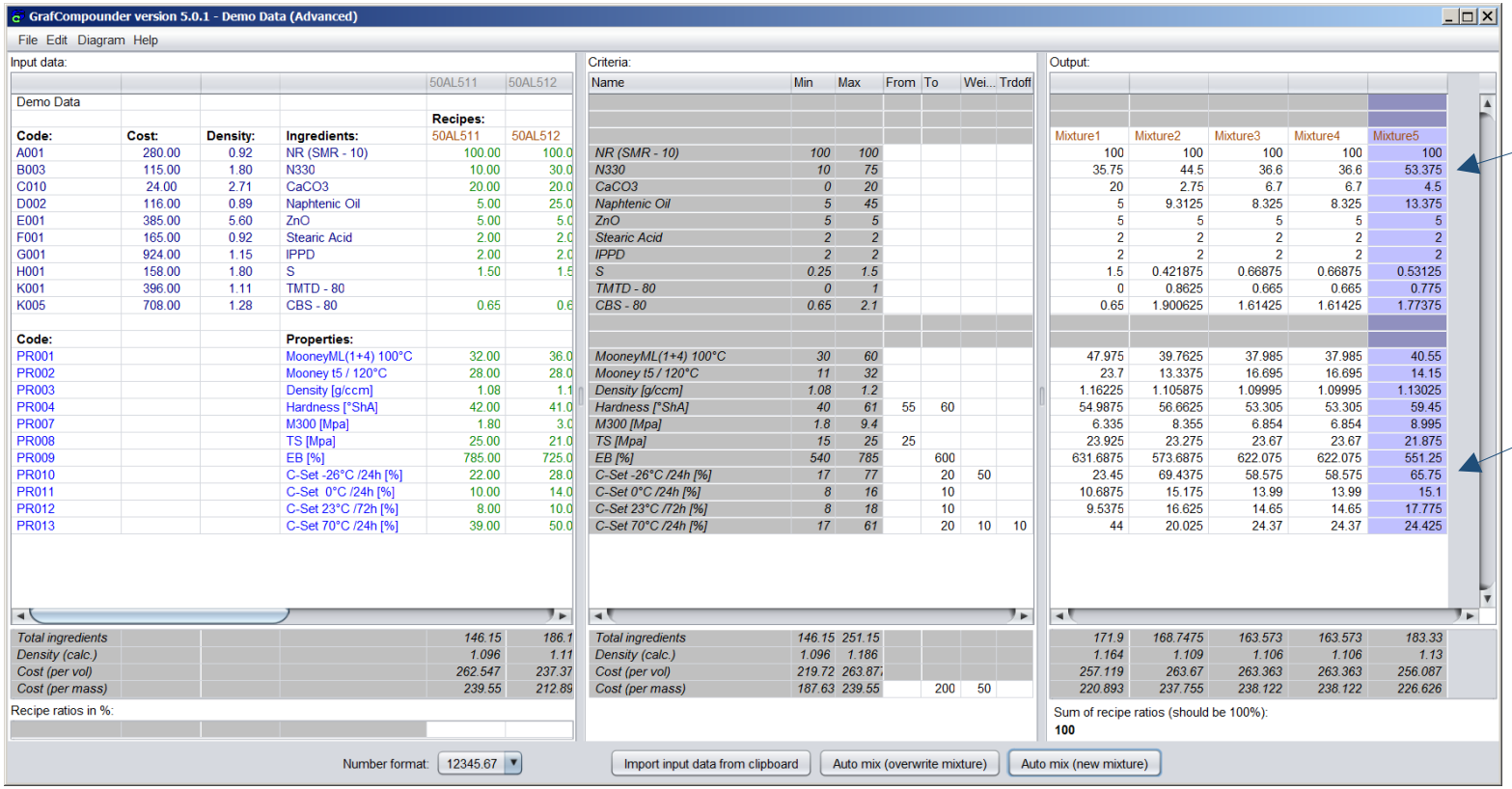
Almost no Change!

~~Dealing with Cost as a target:~~

Output window: **“cost”** target no match.

Chose **„Automix (new mixture)“, evaluate influence on compound and properties**

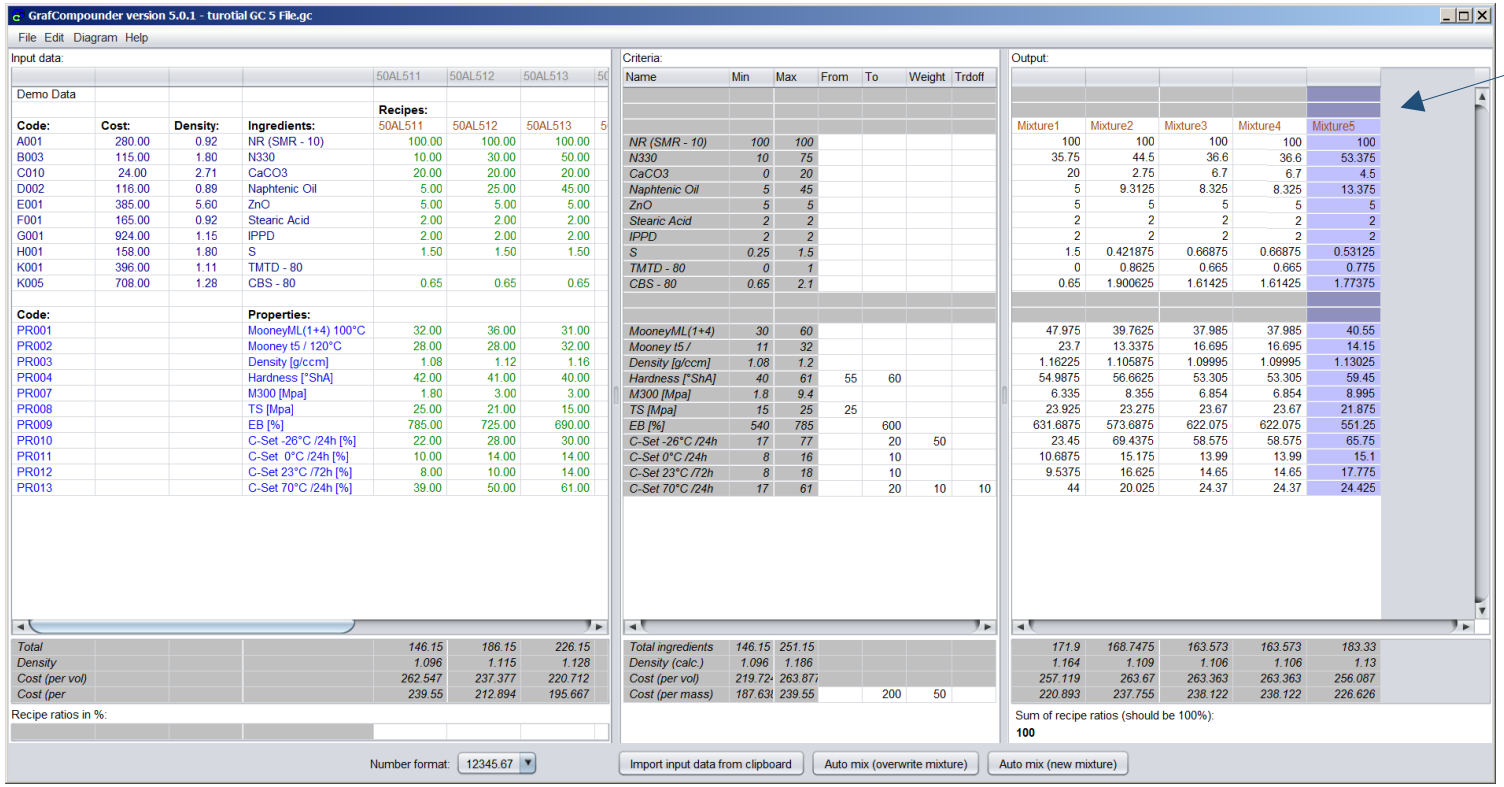
G[raf]Compounder 5.0 – Tune Prediction of a compound



Dealing with Cost as a target:

Put a "Weight" on „Cost per mass": Effect on CB (*Up*) at expense of C-Set-26°C/24h

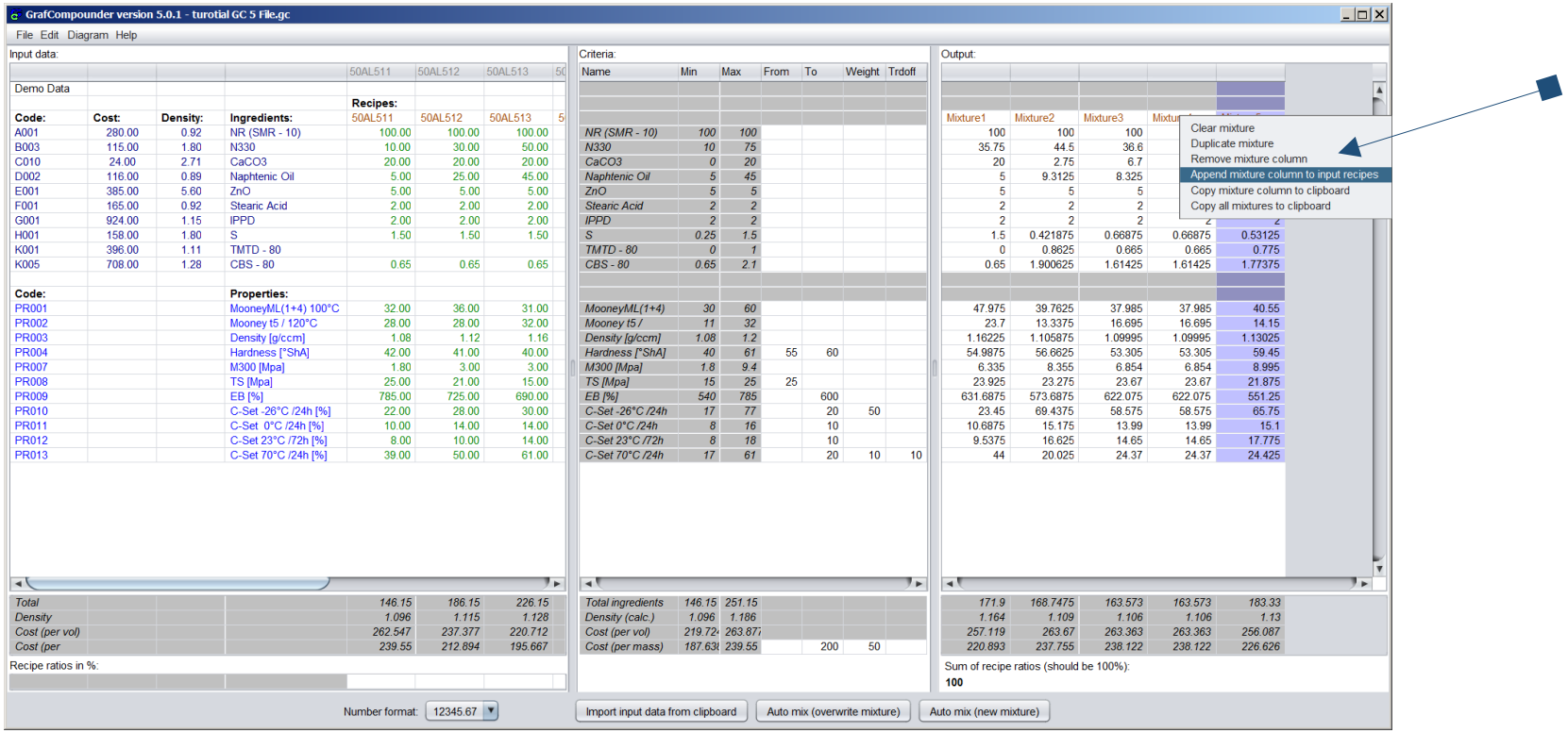
GrafCompounder 5.0 – Confirmation trial



Preparing Confirmation Trial

- **Select a Compound for confirmation (*Example mixture 5*)**
- **Highlight column mixture ..**

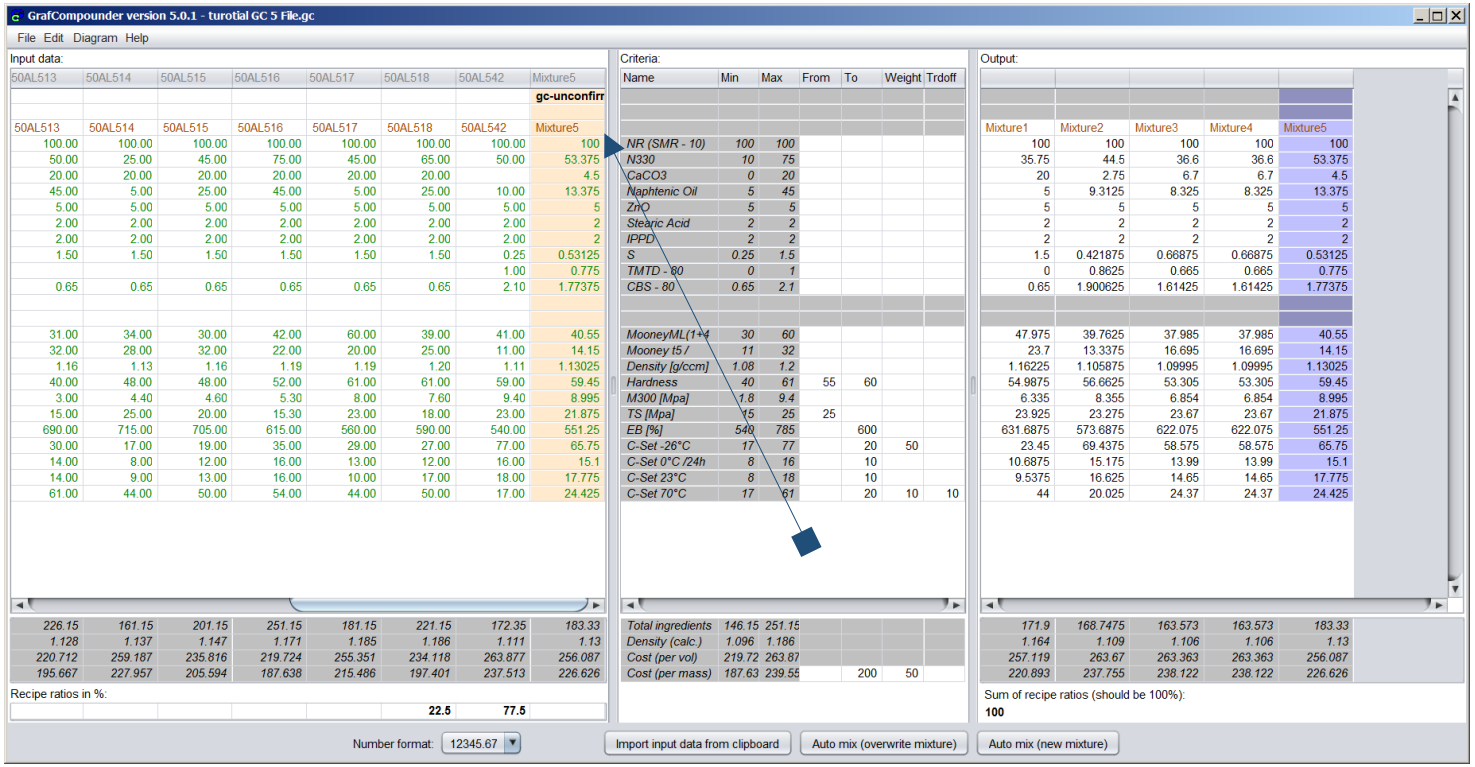
G[raf]Compounder 5.0 – Confirmation trail



Preparing Confirmation Trial

- Select a Compound for confirmation (*Example mixture 5*)
- **Pull down menue, select "Append mixture column into Input recipes"**

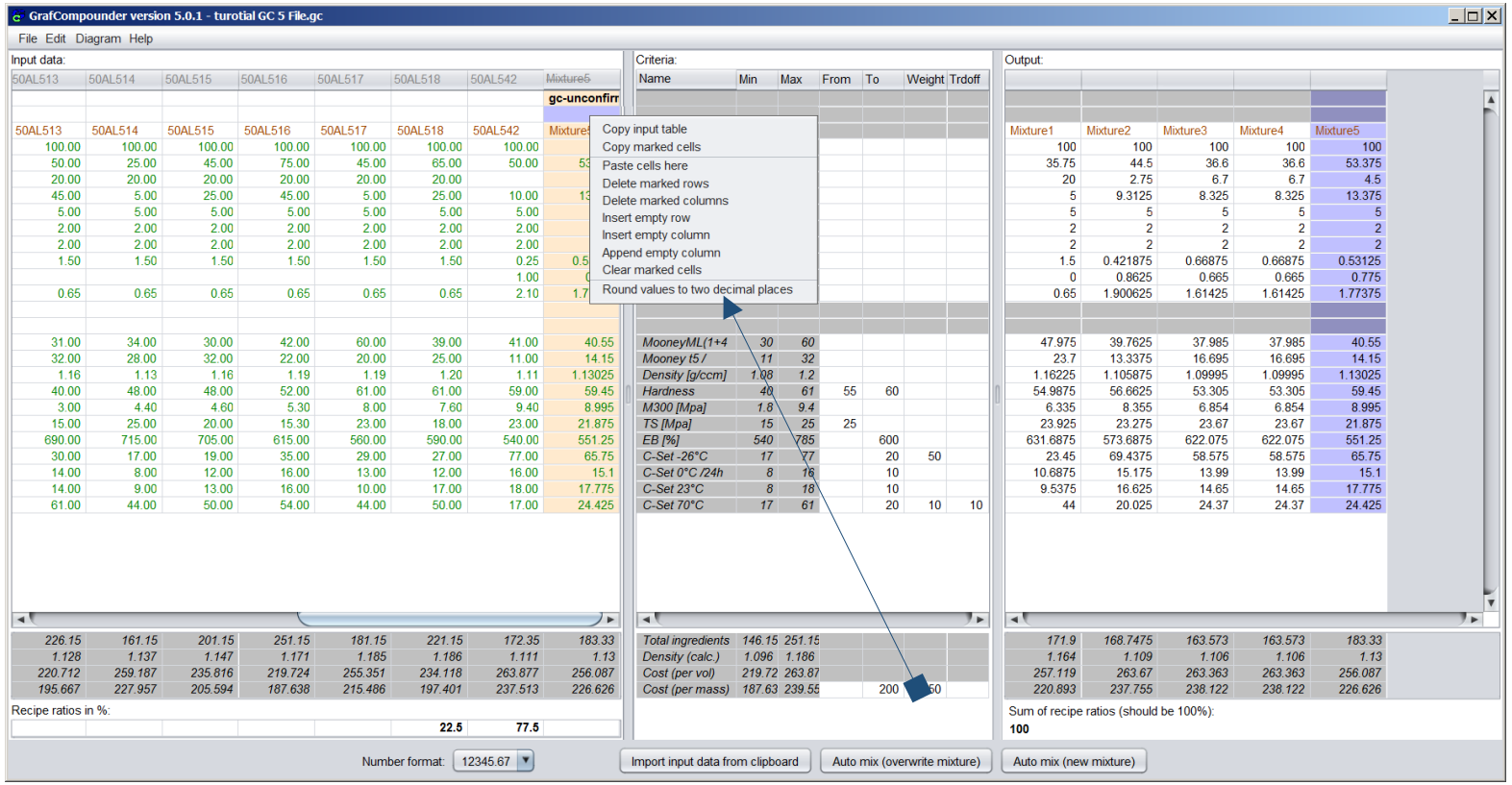
G[raf]Compounder 5.0 – Confirmation trail



Preparing Confirmation Trial

- after “Append mixture column into Input recipes” selected, compound appears in “Input data“ window as “gc-unconfirmed“

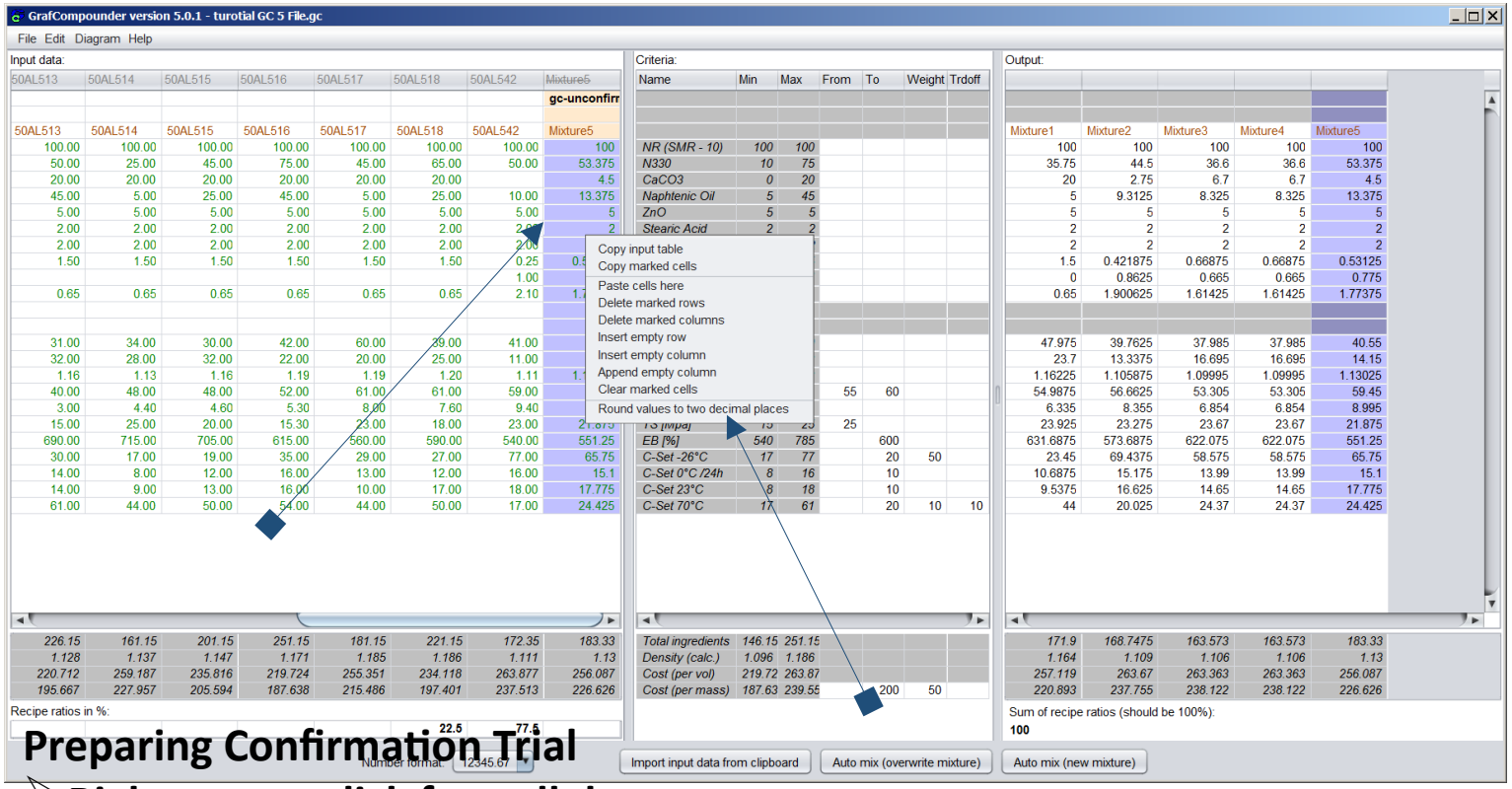
GrafCompounder 5.0 – Confirmation trail



Preparing Confirmation Trial

- Left Mouse click cell, Right mouse click for Pull down Menue
- Select: “Round values to two decimal places”

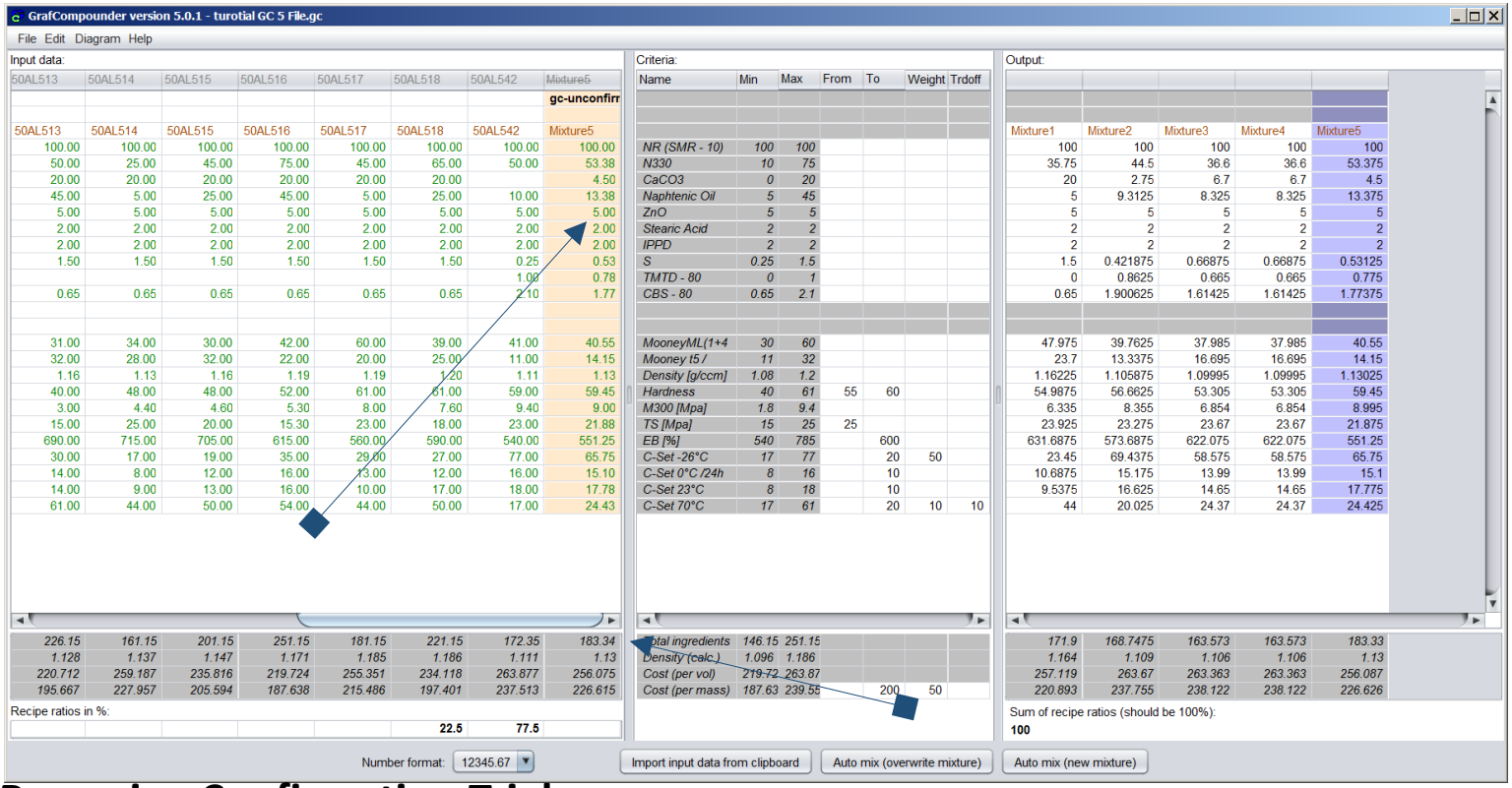
G[raf]Compounder 5.0 – Confirmation trail



Preparing Confirmation Trial

- Right mouse click for pull down menue
- Left Mouse click: highlight cells turningn blue for change values
- Select: “Round values to two decimal places”

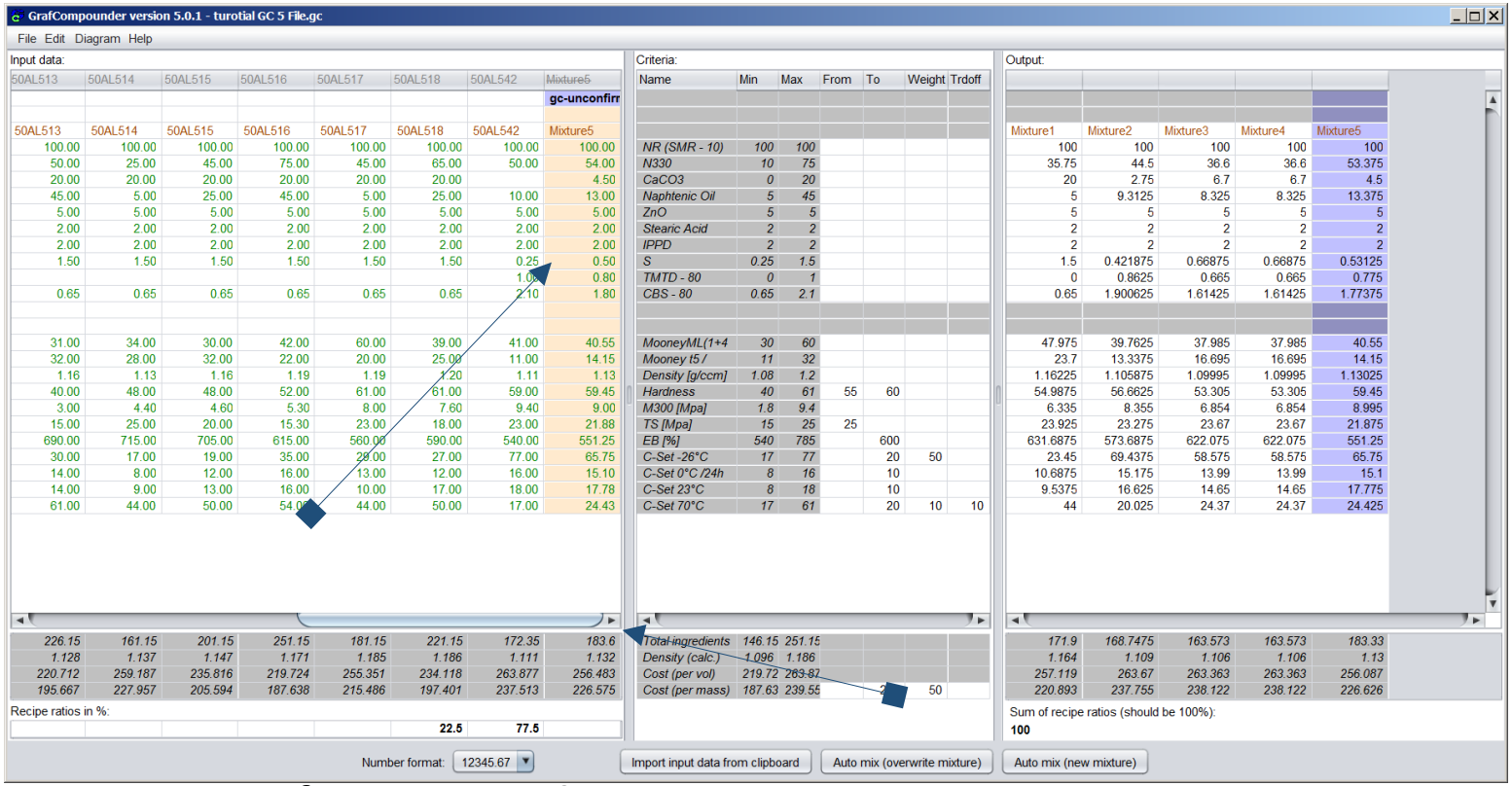
G[raf]Compounder 5.0 – Confirmation trail



Preparing Confirmation Trial

- **Review ingredient values: Round up / down values / even eliminate ingredients with small amoount according your experience**

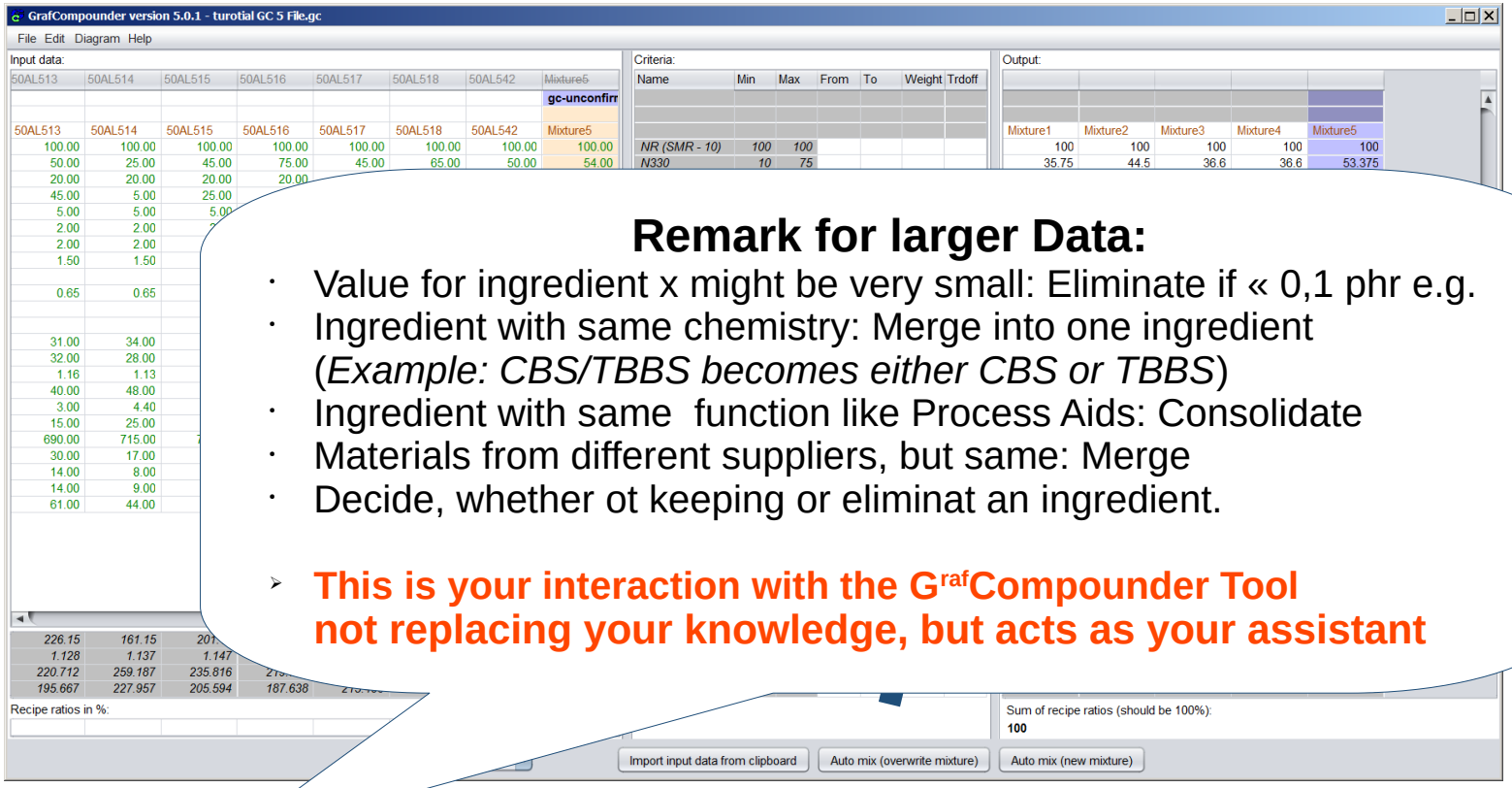
G[raf]Compounder 5.0 – Confirmation trail



Preparing Confirmation Trial

- After operation is done:
- "Total Ingredients" corrected automatically

G[raf]Compounder 5.0 – Confirmation trail



Remark for larger Data:

- Value for ingredient x might be very small: Eliminate if « 0,1 phr e.g.
- Ingredient with same chemistry: Merge into one ingredient (*Example: CBS/TBBS becomes either CBS or TBBS*)
- Ingredient with same function like Process Aids: Consolidate
- Materials from different suppliers, but same: Merge
- Decide, whether ot keeping or eliminat an ingredient.

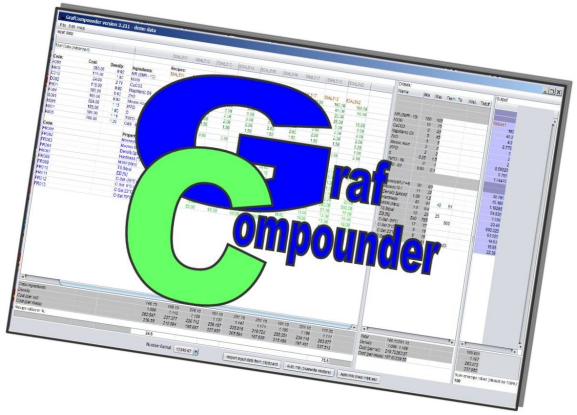
➢ **This is your interaction with the G[raf]Compounder Tool not replacing your knowledge, but acts as your assistant**

Preparing Co…mation Trial

- ➢ **Review ingredient values: Round up / down values according your experience**
- ➢ **“Total Ingredients” corrected automatically**

G[raf]Compounder 5.0 – What is learned

- **Prediction Calculation of a Compound**
  - Starting G[raf]Compounder
  - Open / Input Compound data
    - Auto mix (overwrite / new)
  - Targets, Criteria
  - Fine Tune Criteria
    - Wheight
    - Trdoff
    - Cost target
- Compound Preparation for
  - Confirmation Experiment



Release „Graf Compounder“ Version 5.0
July 2023

Upgrades from earlier versions upon request

Send us your:

Questions, Remarks, Doubts?

www.grafcompounder.com