## Tutorial <br> $\mathbf{G}^{\text {raf }}$ Compounder 5.0

## 01. September 2023

## Content :

## Grampounder 5.0

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


Closing Remarks
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## Start $\mathbf{G}^{\text {rat }} \mathbf{C o m p o u n d e r} 5.0$



## Start G ${ }^{\text {raf }}$ Compounder 5.0

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

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## Start $\mathbf{G}^{\text {rat }}$ Compounder 5.0


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Start G ${ }^{\text {rat }}$ Compounder 5.0


Columns: Numbers in Blue
Recipes: Numbers in Green
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Start G ${ }^{\text {raf }}$ 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 ${ }^{\text {raf }}$ 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 ${ }^{\text {raf }}$ Compounder 5.0 - Predict a compound

(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 Grampounder 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 Graf ${ }^{\text {raf }}$ Compounder 5.0 - Predict a compound


Click on Button: "Auto mix (overwrite mixture)"

## Start Grampounder 5.0 - Predict a compound



Accept: "Take best mixture so far"
(Value of Fitness Function = 926.. shows, not all criteria could be met)

## Start Grampounder 5.0 - Predict a compound



First prediction of a compound is finished.
View result in "Output" window.
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## G ${ }^{\text {raf }}$ Compounder 5.0 - Tune Prediction of a compound



Refine Result: $\mathrm{C}-70^{\circ} \mathrm{C}$ seems to high
Criteria window: Put in "Weight" (select any number: 10 for demonstration)

Grampounder 5.0 - Tune Prediction of a compound


Button "Automix (new mixture)" to watch changes
Accept result and evaluate: C -set $70^{\circ} \mathrm{C} / 24 \mathrm{~h}$ improved at the expense of C -Set- $26^{\circ} \mathrm{C} / 24 \mathrm{~h}$
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Grampounder 5.0 - Tune Prediction of a compound

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G $^{\text {raf Compounder } 5.0 \text { - Tune Prediction of a compound }}$


Dealing with Cost as a target:
Criteria window: Put in "cost" target in "Cost per mass" cell
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## G ${ }^{\text {raf }}$ Compounder 5.0 - Tune Prediction of a compound


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## G ${ }^{\text {raf }}$ 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- $26^{\circ} \mathrm{C} / \mathbf{2 4 h}$

G ${ }^{\text {raf }}$ Compounder 5.0 - Confirmation trial


Preparing Confirmation Trial
$>$ Select a Compound for confirmation (Example mixture 5)
$>$ Highlight column mixture ..
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G ${ }^{\text {raf }}$ 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"
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G ${ }^{\text {raf }}$ 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"
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G ${ }^{\text {raf }}$ Compounder 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"
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G ${ }^{\text {raf }}$ Compounder 5.0 - Confirmation trail

> Right mouse click for pull down menue
Left Mouse click: highlight cells turningn blue for change values
> Select: "Round values to two decimal places"
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G ${ }^{\text {raf }}$ Compounder 5.0 - Confirmation trail

| c GrafCompounder version 5.0.1-turotial GC 5 File.gc |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | - - $\square$ \| $x$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| File Edit Diagram Help |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| Input data: |  |  |  |  |  |  |  | Criteria: |  |  |  |  |  |  | Output: |  |  |  |  |  |
| 50AL513 | 50AL514 | 50AL515 | 50AL516 | 50 LL 517 | 50AL518 | [50AL542 | Mixture5 gc-unconfirr | Name | Min | Max | From | To | Weight Trdoff |  |  | Mixture2 | Mixture3 | Mixture 4 | Mixture 5 | $\wedge$ |
|  |  |  |  |  |  |  | gc-unconfirr |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 50AL513 | 50AL514 | 50AL515 | 50AL516 | 50AL517 | 50AL518 | 50AL542 | Mixture5 |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | NR (SMR - 10) | 100 | 100 |  |  |  |  | 100 | 100 | 100 | 100 | 100 |  |
| 50.00 | 25.00 | 45.00 | 75.00 | 45.00 | 65.00 | 50.00 | 53.38 | N330 | 10 | 75 |  |  |  |  | 35.75 | 44.5 | 36.6 | 36.6 | 53.375 |  |
| 20.00 | 20.00 | 20.00 | 20.00 | 20.00 | 20.00 |  | 4.50 | CaCO3 | 0 | 20 |  |  |  |  | 20 | 2.75 | 6.7 | 6.7 | 4.5 |  |
| 45.00 | 5.00 | 25.00 | 45.00 | 5.00 | 25.00 | 10.00 | 13.38 | Naphtenic Oil | 5 | 45 |  |  |  |  | 5 | 9.3125 | 8.325 | 8.325 | 13.375 |  |
| 5.00 | 5.00 | 5.00 | 5.00 | 5.00 | 5.00 | 5.00 | 5.00 | ZnO | 5 | 5 |  |  |  |  | 5 | 5 | 5 | 5 | 5 |  |
| 2.00 | 2.00 | 2.00 | 2.00 | 2.00 | 2.00 | 2.00 | < 2.00 | Stearic Acid | 2 | 2 |  |  |  |  | 2 | 2 | 2 | 2 | 2 |  |
| 2.00 | 2.00 | 2.00 | 2.00 | 2.00 | 2.00 | 2.00 | 2.00 | IPPD | 2 | 2 |  |  |  |  | 2 | 2 | 2 | 2 | 2 |  |
| 1.50 | 1.50 | 1.50 | 1.50 | 1.50 | 1.50 | 0.25 | 0.53 | S | 0.25 | 1.5 |  |  |  |  | 1.5 | 0.421875 | 0.66875 | 0.66875 | 0.53125 |  |
|  |  |  |  |  |  | 1.08 | 0.78 | TMTD - 80 | 0 | 1 |  |  |  |  | 0 | 0.8625 | 0.665 | 0.665 | 0.775 |  |
| 0.65 | 0.65 | 0.65 | 0.65 | 0.65 | 0.65 | 2.10 | 1.77 | CBS -80 | 0.65 | 2.1 |  |  |  |  | 0.65 | 1.900625 | 1.61425 | 1.61425 | 1.77375 |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 31.00 | 34.00 | 30.00 | 42.00 | 60.00 | 39.00 | 41.00 | 40.55 | MooneyML (1+4 | 30 | 60 |  |  |  |  | 47.975 | 39.7625 | 37.985 | 37.985 | 40.55 |  |
| 32.00 | 28.00 | 32.00 | 22.00 | 20.00 | 25.00 | 11.00 | 14.15 | Mooney 5 / | 11 | 32 |  |  |  |  | 23.7 | 13.3375 | 16.695 | 16.695 | 14.15 |  |
| 1.16 | 1.13 | 1.16 | 1.19 | 1.19 | 1.20 | 1.11 | 1.13 | Density [g/cmm | 1.08 | 1.2 |  |  |  |  | 1.16225 | 1.105875 | 1.09995 | 1.09995 | 1.13025 |  |
| 40.00 | 48.00 | 48.00 | 52.00 | 61.00 | 61.00 | 59.00 | 59.45 | Hardness | 40 | 61 | 55 | 60 |  |  | 54.9875 | 56.6625 | 53.305 | 53.305 | 59.45 |  |
| 3.00 | 4.40 | 4.60 | 5.30 | 8.00 | 7.60 | 9.40 | 9.00 | M 300 [Mpa] | 1.8 | 9.4 |  |  |  |  | 6.335 | 8.355 | 6.854 | 6.854 | 8.995 |  |
| 15.00 | 25.00 | 20.00 | 15.30 | 23.00 | 18.00 | 23.00 | 21.88 | TS [Mpa] | 15 | 25 | 25 |  |  |  | 23.925 | 23.275 | 23.67 | 23.67 | 21.875 |  |
| 690.00 | 715.00 | 705.00 | 615.00 | 560.00 | 590.00 | 540.00 | 551.25 | EB [\%] | 540 | 785 |  | 600 |  |  | 631.6875 | 573.6875 | 622.075 | 622.075 | 551.25 |  |
| 30.00 | 17.00 | 19.00 | 35.00 | 29,00 | 27.00 | 77.00 | 65.75 | C-Set $-26^{\circ} \mathrm{C}$ | 17 | 77 |  | 20 | 50 |  | 23.45 | 69.4375 | 58.575 | 58.575 | 65.75 |  |
| 14.00 | 8.00 | 12.00 | 16.00 | $\not 13.00$ | 12.00 | 16.00 | 15.10 | C-Set $0^{\circ} \mathrm{C} / 24 \mathrm{~h}$ | 8 | 16 |  | 10 |  |  | 10.6875 | 15.175 | 13.99 | 13.99 | 15.1 |  |
| 14.00 | 9.00 | 13.00 | 16.00 | 10.00 | 17.00 | 18.00 | 17.78 | C-Set $23^{\circ} \mathrm{C}$ | - | 18 |  | 10 |  |  | 9.5375 | 16.625 | 14.65 | 14.65 | 17.775 |  |
| 61.00 | 44.00 | 50.00 | 54.00 | 44.00 | 50.00 | 17.00 | 24.43 | C-Set $70^{\circ} \mathrm{C}$ | 17 | 61 |  | 20 | 10 | 10 | 44 | 20.025 | 24.37 | 24.37 | 24.425 |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 4 |  |  | V |  |  |  | $3 *$ | 4 |  |  |  |  |  | $\cdots$ | 4 |  |  |  |  | $\cdots$ |
| 226.15 | 161.15 | 201.15 | 251.15 | 181.15 | 221.15 | 172.35 | 183.34 | ptal ingredients | 146.15 | 251.15 |  |  |  |  | 171.9 | 168.7475 | 163.573 | 163.573 | 183.33 |  |
| 1.128 | 1.137 | 1.147 | 1.171 | 1.185 | 1.186 | 1.111 | 1.13 | Vensity (calc) | 1.096 | 1.186 |  |  |  |  | 1.164 | 1.109 | 1.106 | 1.106 | 1.13 |  |
| 220.712 | 259.187 | 235.816 | 219.724 | 255.351 | 234.118 | 263.877 | 256.075 | Cost (per vol) | 219.72 | 263.87 |  |  |  |  | 257.119 | 263.67 | 263.363 | 263.363 | 256.087 |  |
| 195.667 | 227.957 | 205.594 | 187.638 | 215.486 | 197.401 | 237.513 | 226.615 | Cost (permass) | 187.63 | 239.55 |  |  |  |  | 220.893 | 237.755 | 238.122 | 238.122 | 226.626 |  |
| Recipe ratios in |  |  |  |  |  |  |  |  |  |  |  |  |  |  | Sum of recipe | ratios (should | be $100 \%$ ): |  |  |  |
|  |  |  |  |  | 22.5 | 77.5 |  |  |  |  |  |  |  |  | 100 |  |  |  |  |  |
|  |  |  |  | Numb | er format | 12345.67 - |  | Import input data fro | clipbo | oard | Auto | mix (over | write mi | xture) | Auto mix (new | v mixture) |  |  |  |  |

Preparing Confirmation Trial
$>$ Review ingredient values: Round up / down values / even eliminate ingredients with small amoount according your experience
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Grat ${ }^{\text {rat }}$ Pounder 5.0 - Confirmation trail


Preparing Confirmation Trial
After operation is done:
"Total Ingredients" corrected automatically
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G ${ }^{\text {raf }}$ Compounder 5.0 - Confirmation trail


Preparing Co mation Trial
Review ingredient values: Round up / down values according your experience
"Total Ingredients" corrected automatically

G ${ }^{\text {raf }}$ Compounder 5.0 - What is learned

- Prediction Calculation of a Compound
, Starting G ${ }^{\text {raf }}$ Compounder
> Open I Input Compound data
> Auto mix (overwrite I new)
, Targets, Criteria
> Fine Tune Criteria
, Wheight
, Trdoff
> Cost target
, Compound Preparation for
, Confirmation Experiment
 ompounder
" Release „GrafCompounder" Version 5.0 July 2023
$\Rightarrow$ Upgrades from earlier versions upon request
Send us your:
Questions, Remarks, Doubts?

