Calculation of Solid Fat Content for Interestifications – Part II

Preface

This newsletter is again about the calculation of the SFC values of transesterification. We have significantly improved and simplified the practical calculation. On the other hand, there is a small but important detail, namely deleting of analytical parameters and components.

- Up to now it was possible – after a security prompt – to delete analytical parameters and components. This was rarely done, but in this case 'residues' were always left behind. These are parameters and components in datasheets and interesterifications that can no longer be assigned. As of the new version, it is checked whether the parameter or component can be deleted at all. We apologize for this error. For more information, see *Deleting Analytical Parameters and Components*

- There are major improvements and simplifications in predicting the SFC values of interesterification. With the new version, it is much easier to find suitable interesterifications for specified SFC values - keywords: target values and component mixers. In addition, we once again looked at the statistical data that form the basis for the calculation. The result was interesting. See *Predicting Interesterification SFC Values* for more information.

First we would like to point out our demo version.

Demo Version

We would be happy to provide you with a full-featured demo version. The demo version can be used for three months. If necessary, the term can be extended.

The demo version not only offers all functions of the full version, the data generated with the demo version can still be used with the full version. The database is compatible with both the demo and the full version.

And it's that quick and easy (time required approx. 15 minutes):

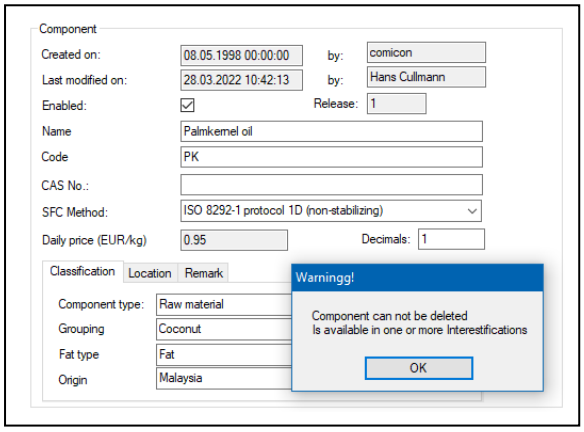
- Request download link info@oil-expert.net
- Download the software package from our website
- Install Oil-Expert software
- Start Oil-Expert.net and enter the registration code
- Finished!

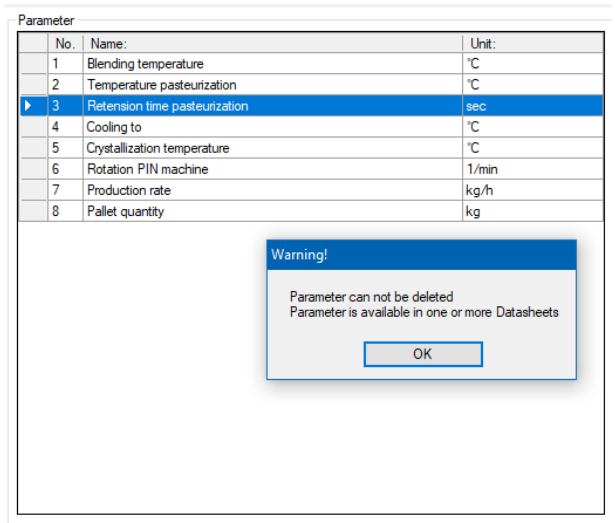
The software is supplied with around 40 standard components and some example projects. Using the example projects and the PDF manual, you can quickly and easily learn how to work with Oil-Expert.net. If you have any questions, please do not hesitate to contact us - by email, phone, Skype or any other medium of your choice.

Deleting Analytical Parameters and Components

Previously, it was possible to delete analysis parameters and components without any problems. Since each parameter and each component has a unique ID (identification number), the parameter or component can no longer be assigned. In practice, this has the following effect: In the parameter list or the component list, the number zero is displayed instead of the respective name. The only thing that helps is deleting and re-entering. However, important system parameters (SFC 10°C, SFC 20°C, etc.) cannot be deleted anyway.

The new version checks whether the parameter or component occurs in other tables in the database. In these cases, deletion is no longer possible.





Predicting Interesterification SFC Values – Part II

Introduction

There are different approaches to predict the SFC values of interesterifications. We use a statistical approach to estimate SFC values (see Newsletter No. 11). In chemical interesterification, after the interesterification is complete, all of the fatty acids are statistically distributed across the triglycerides. It is therefore possible to estimate the SFC values of the interesterification using the proportions of each individual fatty acid in the interesterification mixture. We have now expanded this procedure further in order to make the calculation as convenient as possible for the user. This includes the definition of target values (min, max, typical) and the component mixer, as is already used for calculating the SFC values of fat blends.

There is also an export function for fully calculated interesterifications, which exports almost all the data required for interesterifications as components. Annoying data entry is thus eliminated. And finally, we examined the data quality again.

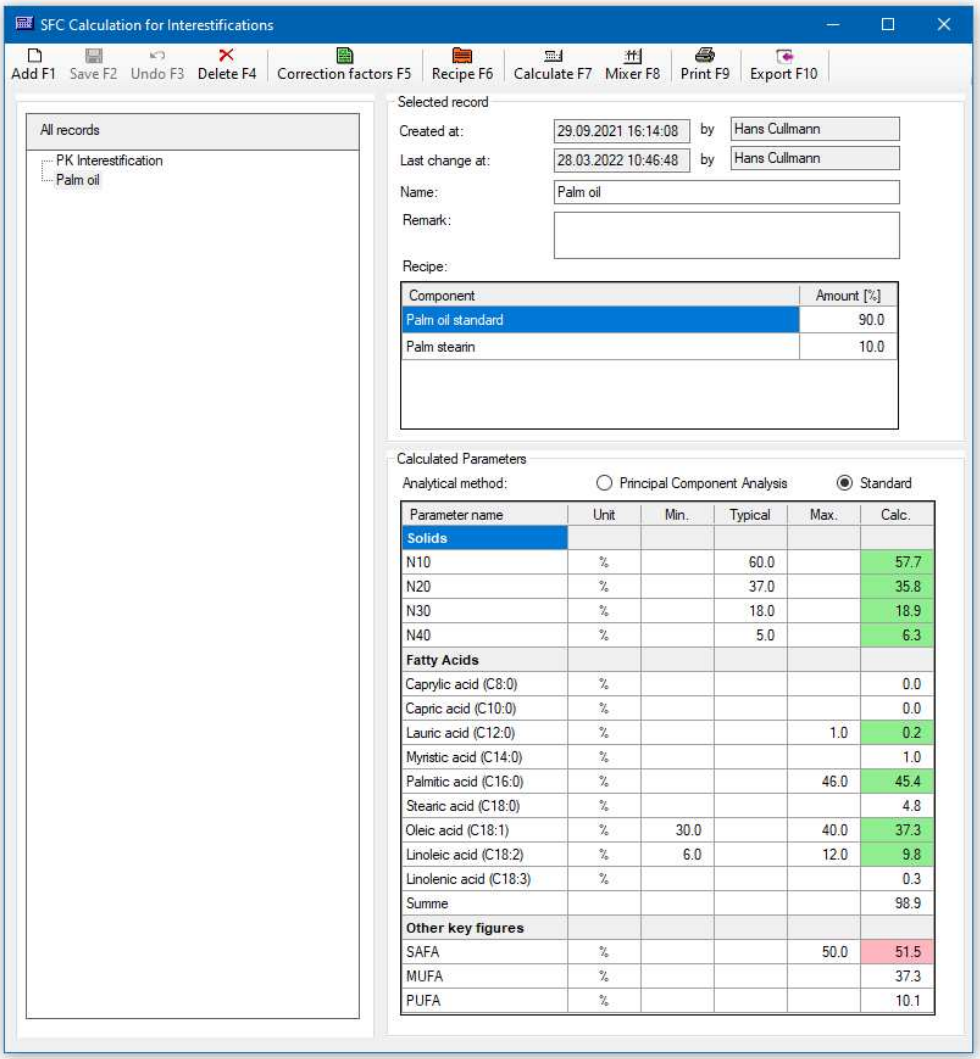
Target Values

From the new version - 7.5.8 - target values can be defined. Min/max values and/or typical values are possible (see figure on next page). All values can be combined as desired. A range of ± 3 is automatically used for the typical values.

All target values are entered directly into the table. Immediately after entering the calculated value is colored. Is it within the specifications with green, otherwise with red. To delete a target value, mark the field with the mouse and press the *Del* key. The background of the calculated value is then automatically reset to white.

In addition to the previous data, SFC values and fatty acids, the fatty acids are summed up and output as SAFA (Saturated fatty acids), MUFA (Mono unsaturated fatty acids) and PUFA (Poly unsaturated fatty acids). Target values can also be defined for these parameters.

With the help of the target values, predefined interesterifications can be simulated by calculation. It is also possible to improve already known interesterifications, e.g. if changes on the raw materials market make this necessary - replacing expensive raw materials with cheaper ones.



Dialog for calculation of interestifications

Export

Completely calculated interesterifications can now be exported directly as a new interesterification component. After clicking on the Export button (see dialog above), the component dialog opens with the calculated interesterification data. Only some additional data such as product code and SFC method then have to be entered.

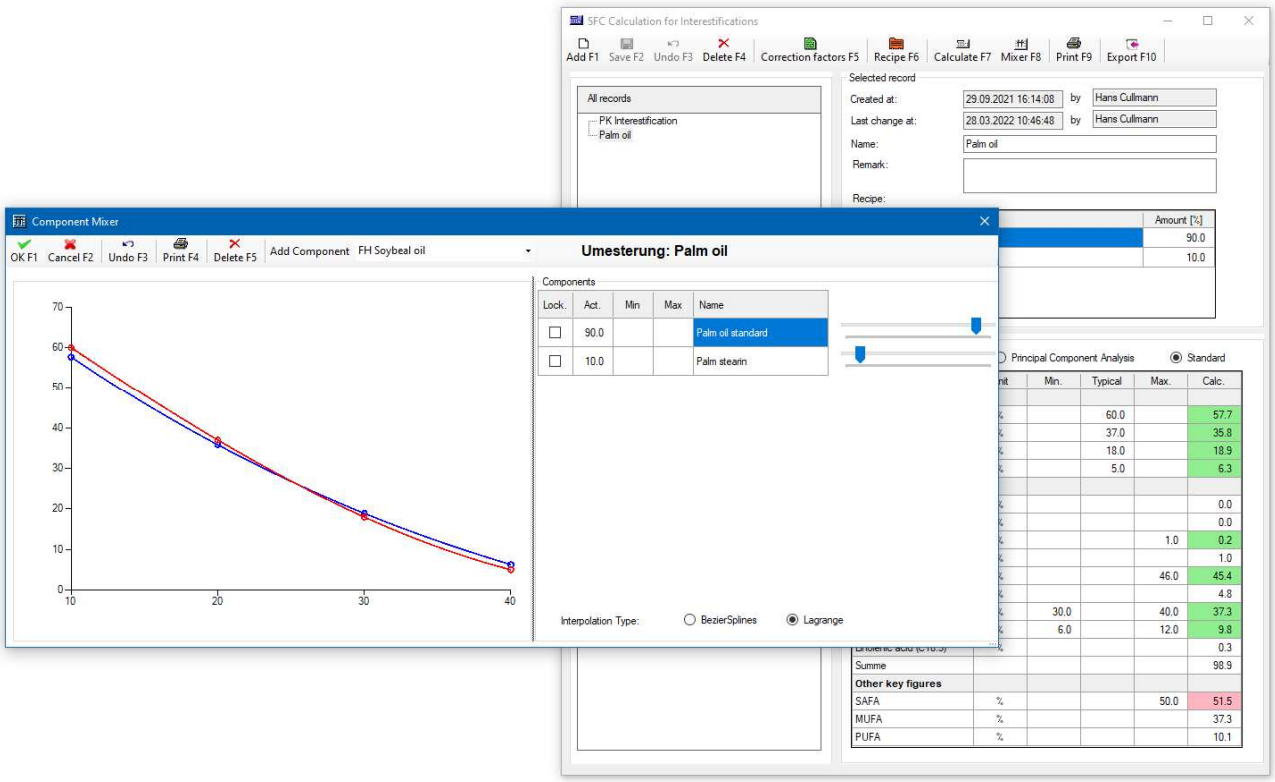
Component-Mixer

As of version 7.5.8, the component mixer is now also available. It has all the functions known from the calculation of fat blends. Calculations are made with typical values. If typical values are not available but min/max values are, then the typical values are calculated from the min/max values.

The functionality is identical to that of fat blends. The proportion of the components is changed by the sliders. The resulting parameters are immediately calculated and reflected in the SFC curve and displayed in the interesterification dialog (see figure below). Components can be added and deleted.

The interesterification components can also be blocked and min/max values are possible for each component. However, the defined values are not saved, they are only currently available.

After the calculation has been successfully completed, the component mixer is exited using the *OK* button. The calculated data are accepted in the interesterification dialog.

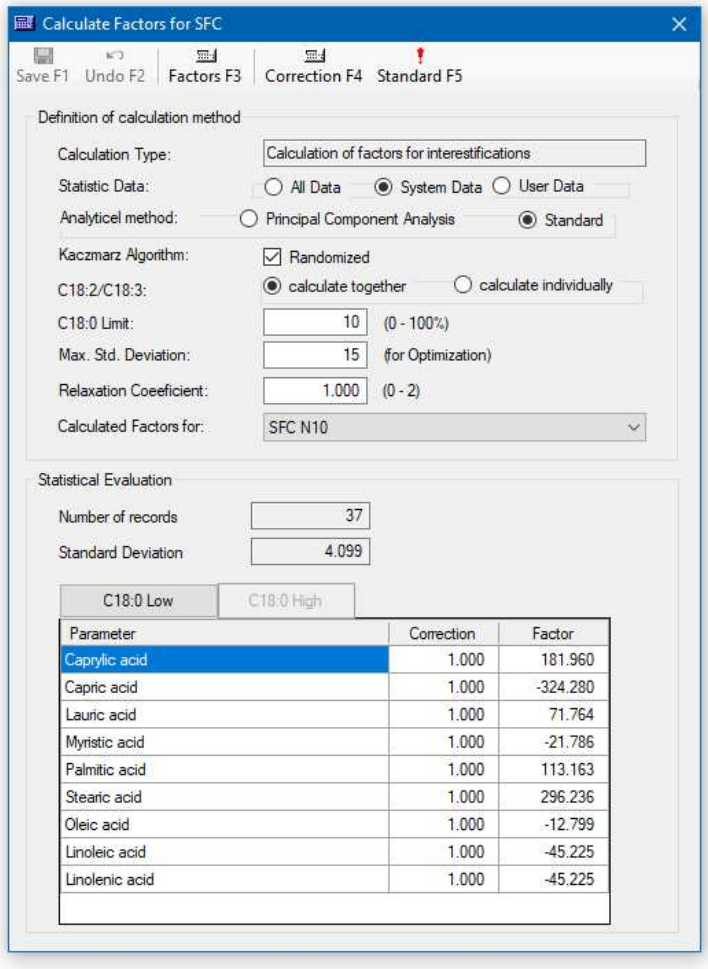


Component-Mixer with Interestification dialog

Optimization

Optimization is carried out when calculating the factors for interesterification from statistical data. All data sets that exceed a defined standard deviation are eliminated. A second calculation run is made with the remaining data sets, which results in a significantly better standard deviation.

The number of data sets available after optimization and the calculated standard deviation are now displayed in the calculation dialog. It's amazing how few records are left. In the figure below it is just 37 out of the original 130 for the SFC value at 10°C. At higher temperatures the ratio gets better, e.g. for 40°C: data sets = 59, standard deviation 2.656.



Dialog for statistical data analysis

Statistical Data

The use of statistical methods to calculate interesterification SFC values has revealed a major problem – the reliability of the data. There are four possible errors that play a role in the calculations:

- Inaccuracy of the measured values (SFC values, fatty acids)
- Incomplete interesterification
- Wrong recipes (e.g. palm oil instead of palm stearin)
- Differences in the SFC values and the fatty acids of the individual raw materials

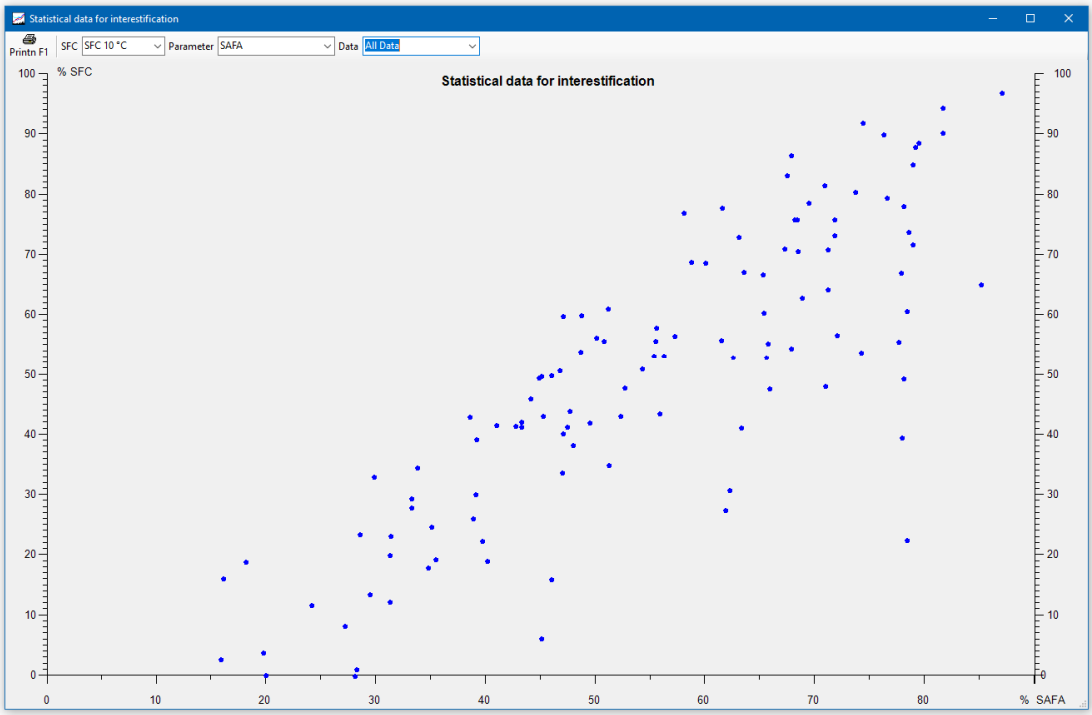
Taken together, these sources of error result in a large scattering of the experimental measured values. We have examined this in more detail. The following turned out to be the case (see also the following figures):

- A trend can be seen for SAFA – the more SAFA, the higher the SFC values..
- The same applies vice versa for PUFA - the more PUFA, the lower the SFC values.
- For MUFA there is no trend at all.

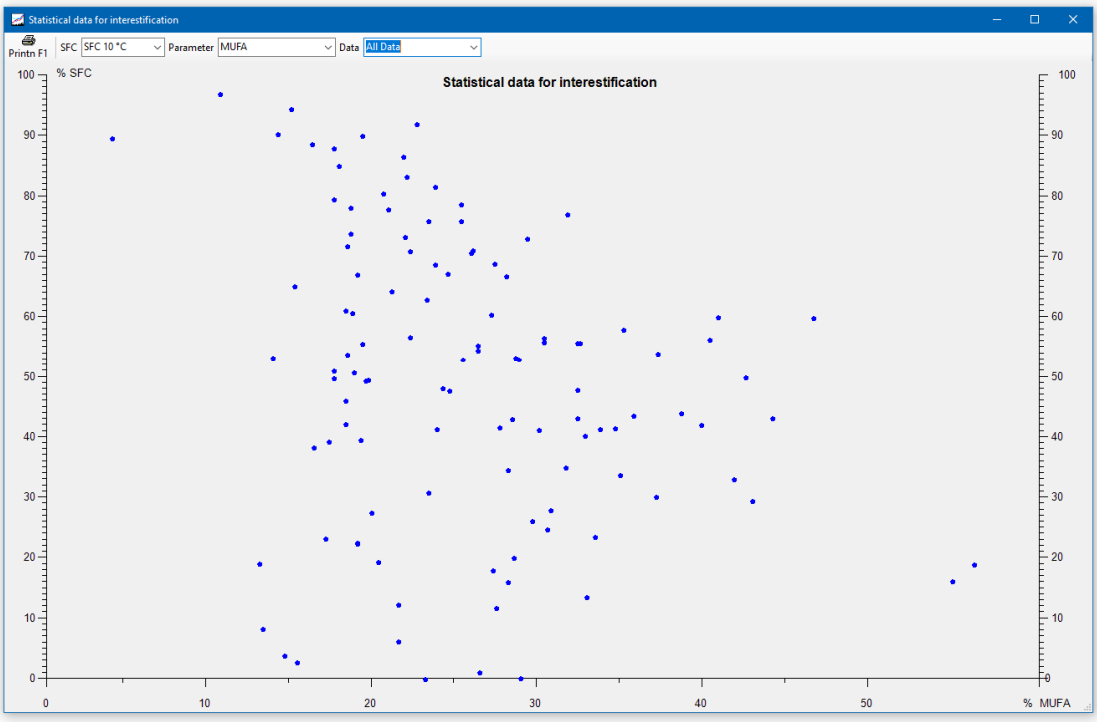
However, the spread is very large, as can be seen from the figures. This shows that the SFC values depend on the totality of the fatty acids and therefore a main component analysis does not provide good results. However, there is one exception: linoleic acid and linolenic acid. These two fatty acids have an identical impact on SFC values, so they can always be summed up for the prediction.

The research also shows why a distinction must be made between fat blends with a high and low C18:0 content. The boundary between high and low C18:0 content is around 10%. This is clearly evident from the graphs which show the correlation between C18:0 content and SFC values for all temperatures.

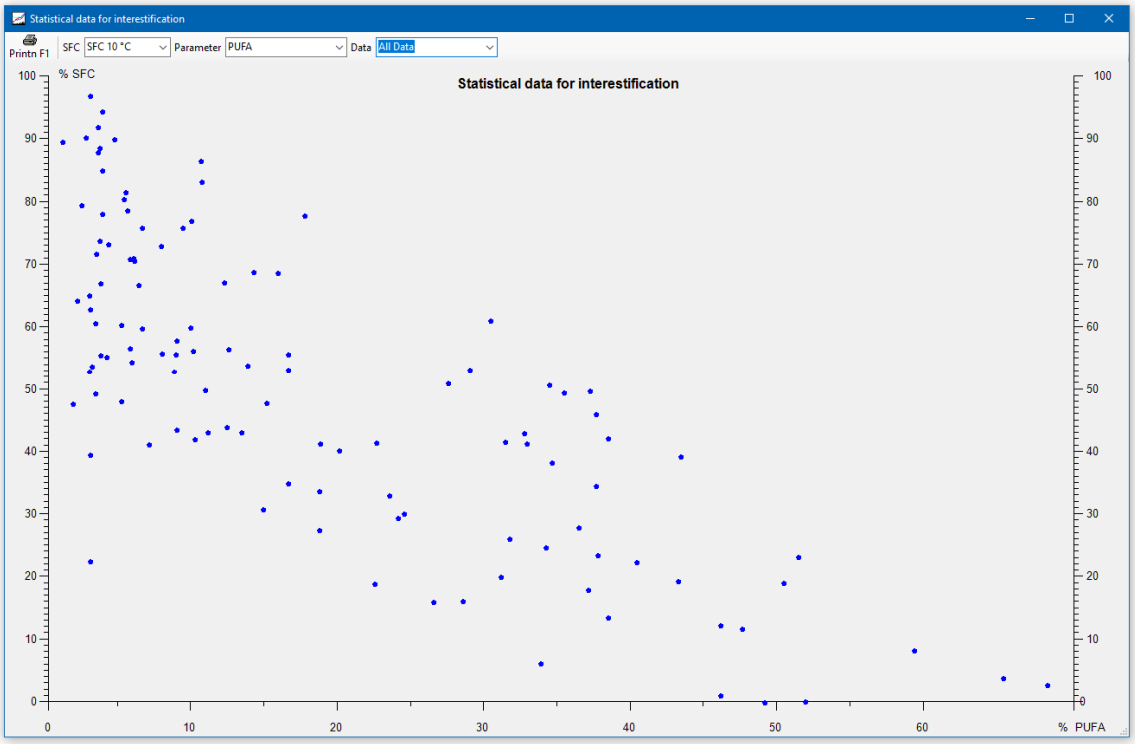
Oil-Expert users can understand this with the new version 7.5.8. In addition to the relationships shown and discussed, there are others, e.g. C8:0-C12:0 content, C16:0-C18:0 content, etc. The dialog allows the selection of the SFC value and the selection of different fatty acid combinations. The choice of statistical data between system data, user data and system data + user data is also provided. And finally, the graphic can be printed.



Correlation between SFC 10°C and SAFA content



Correlation between SFC 10°C and MUFA content



Correlation between SFC 10°C and PUFA content

Outlook

What's next? Next, we'll look at the recipes. Until the next big update we want to expand and improve the recipe management as follows:

- Assemblies (fat assembly, water assembly, vitamin assembly, etc.)
  Editing and saving of assemblies
- Calculation of nutritional values for declarations (initially only for Germany)
- Creation of lists of ingredients for declarations (initially only for Germany)

Imprint

We would be glad to provide you with further information. Please feel free to contact one of our distributors.

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