HOW TO PROPERLY ROUND
WITH CHROMELEON™

QPLIANCE

#1: THE DEFINITION OF SIGNIFICANT DIGITS

The individual digits of a number are referred to as significant digits if this number is within the limits of the deviation of the last measurement (or similar). This includes all meaningful numbers without the leading zeros. Ending zeros are significant if they are obtained by the measurement as a definite result. By appropriate spelling and the correct transfer of results, this can be clearly defined.

Example: 01.3060 g

The zero before the 1 is not significant as leading zero, the other two probably already. The zero between 3 and 6 is definitely significant as clearly related to the measurement result. For the last zero, it would have to be checked whether it was included in the measurement result (e.g. the initial weight) or attached. Assuming that the zero is part of the initial weight, there are 5 significant digits for this result, whereby the following calculations can only calculate with 4 digits, since the last digit for subsequent calculations always has one error (measurement uncertainty).

#2: SIGNIFICANT DIGITS

In general, it should be noted that the number of permissible significant digits of the total calculations is defined by the value with the lowest number. Although all measurements can be given in their number of significant digits unchanged, but in the calculation, the value with the least number is the determining factor. It is therefore wrong to rate the frequently used method of multiplication with more digits than justify the measurement results and does not correspond to the correct calculation with significant digits according to DIN EN ISO 80000-1.

Example: 10,1436 g   1,4092 g   0,0366 g

If the 3 sample weights mentioned in the example were taken into account, there are 6, 5 and 3 significant digits. However, since in this case 3 is the lowest value, it is possible to work with a maximum of 3 significant digits, whereby the fourth decimal place is subject to an error and may no longer be used in further calculations. Important for further consideration, however, is that it depends on which calculation action is performed. If a line calculation is carried out, then the number of the smallest decimal places is decisive, with all other calculations the number of the smallest significant digits counts.

In a multiplication only with 3 digits in the result should be calculated further, the fourth decimal place is fraught with uncertainty. If an addition took place, the number of the smallest decimal places would be 4 for all 3 measured values and the results could all be displayed with 4 decimal places, whereby according to the measurement uncertainty it would have to be checked whether the fourth one may be displayed in the result or not.

#3: THE ROUNDING ALGORITHM IN CHROMELEON™

Chromeleon™ uses a rounding algorithm that uses commercial rounding to show results. This means that if at the first position, which is omitted according to the rounding is a digit from 0 to 4, the number is simply cut off at the desired location, the digit before the cut remains unchanged. If there is a 5 to 9 in the first position, it will also be cut, but the last digit will be increased by 1 before the cut. In addition, the algorithm in Chromeleon is set so that trailing zeros are not represented after the comma, but of course relevant for further calculations and consideration of significant digits.

Example: 1.0340 g is represented as: 1.034 g

Rounding is a weak point in the presentation of results because rounding always loses a certain precision of the value, so rounding should always be done as late and as rarely as possible. Repeated rounding leads to a significant measurement error. Chromeleon™ always offers the possibility to select the desired number of decimal places, but calculates with 16 decimal places, therefore the proposal made by Qpliance GmbH for an SOP for rounding in Chromeleon™ only concerns the actual result that is output. All measured values and intermediate results are processed with the raw data, which only contains the measurement-related errors.

#4: CUSTOMIZE DECIMAL PLACES

In Chromeleon™ there is the possibility to determine the number of decimal places for each column. For example, you can choose more for the Amount, as shown in Figure 1. In addition to the classic option of selecting the desired number of decimal places, an exponential output of the results can also be set here. For measured values where a time format must be selected, this could also be con-figured here according to the needs or requirements.
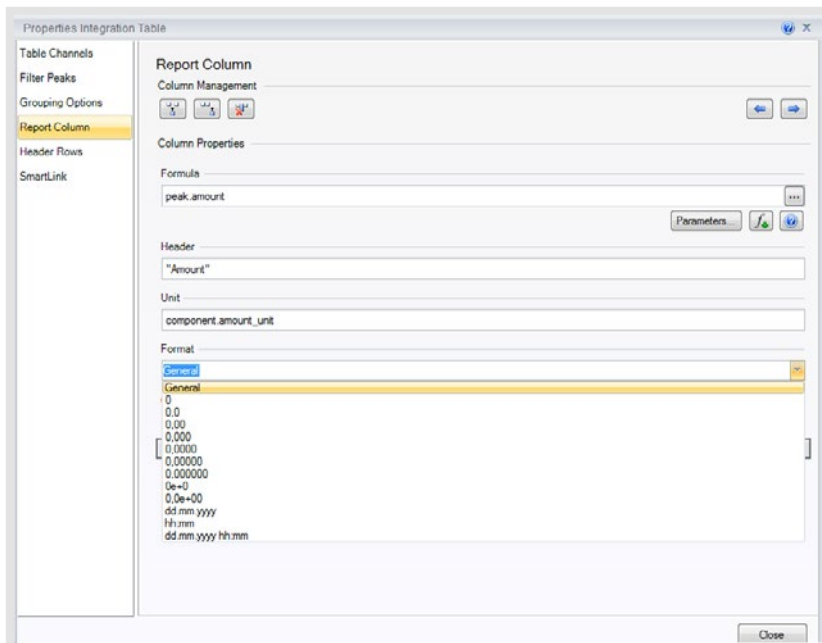

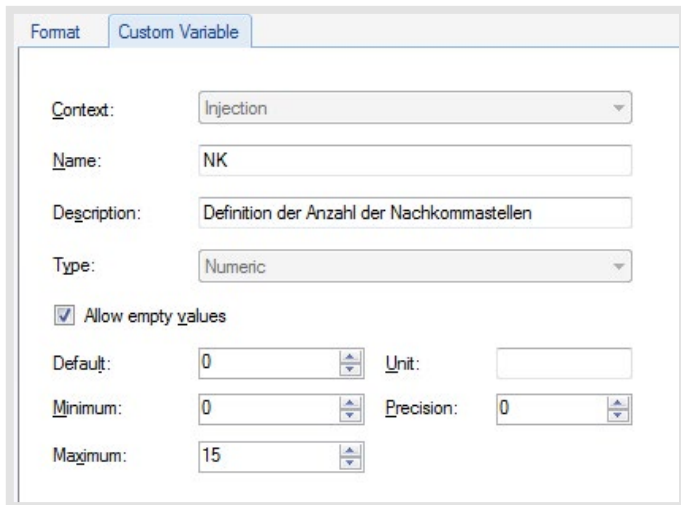**Figure 1:** The number of decimal places can be set in the properties of the column under Format.

In addition, it is possible to define the number of decimal places in a column, depending on the injection. In this case, for example, the "Amount" could receive a different number of decimal places for each entry. Thus, depending on the previously correctly determined significant digits, the result could always represent the correct amount of decimal places.

To achieve this goal, a custom variable must first be created. This must be a numeric injection variable. It is possible to define the default value as well as the minimum and maximum value. Figure 2 shows an example. Thus, a separate column is created in the injection list, in which integers can be entered.

	A	B	C	D	E
1	Inj.	Injection Name	Type	Ref.Time	Amount
2	No.	Selected Peak:		min	
3				UV_VIS_1	UV_VIS_1
4				Component	Component 1
5	1	Cal Standard 1 (0.010 m	Calibration	0,628	0,08107
6	2	Cal Standard 1 (0.010 m	Calibration	0,632	0,08057
7	3	Cal Standard 1 (0.010 m	Calibration	0,630	0,07864
8	4	Cal Standard 2 (0.050 m	Calibration	0,632	0,497
9	5	Cal Standard 2 (0.050 m	Calibration	0,628	0,495
10	6	Cal Standard 2 (0.050 m	Calibration	0,632	0,493
11	7	Cal Standard 3 (0.100 m	Calibration	0,632	1,04
12	8	Cal Standard 3 (0.100 m	Calibration	0,633	1,04
13	9	Cal Standard 3 (0.100 m	Calibration	0,632	1,03
14	10	Cal Standard 4 (0.200 m	Calibration	0,632	2
15	11	Cal Standard 4 (0.200 m	Calibration	0,630	2
16	12	Cal Standard 4 (0.200 m	Calibration	0,630	2
17	13	Sample 1	Unknown	0,632	0,08057
18	14	Sample 2	Unknown	0,632	1,03
19	15	Blank	Blank	n.a.	n.a.
20	Maximum			0,633	2,0000
21	Average			0,631	0,8533
22	Minimum			0,628	0,0786
23	Standard Deviation			0,001	0,7260
24	Relative Standard Deviation			0,22%	85,09%

Figure 2: Example of a custom variable that can define the number of decimal places.

These represent the number of decimal places via the table columns in the report or screen report if the formula is used correctly. The input in the injection list directly controls the exact number of decimal places. A possible result is shown in Figure 3 using column E "Amount".
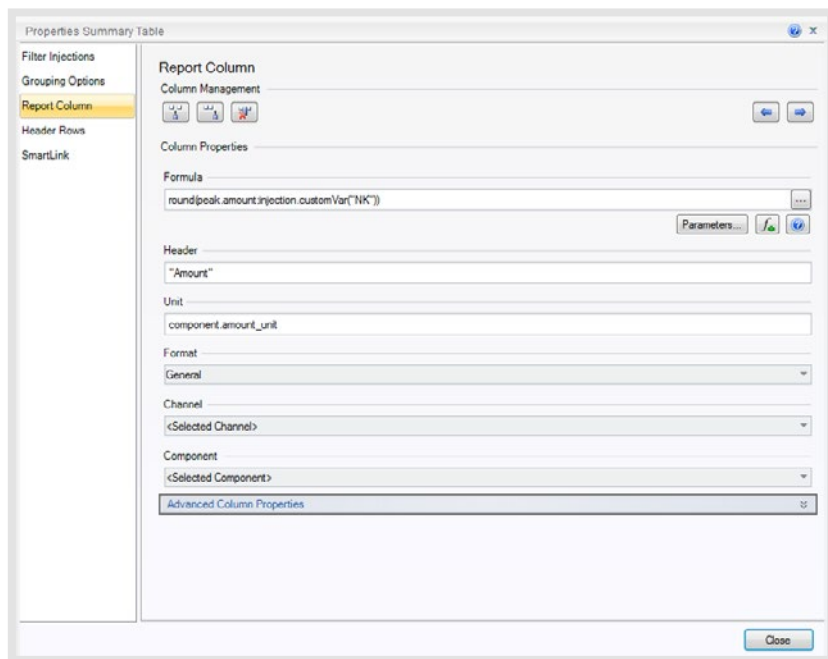
The formula necessary for this is shown in Figure 4. It can be seen that the main formula is the Round Value and the actual variable as well as the created custom variable have been inserted in the parenthesis.

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