

Differences in Rounded Values in Empower Software

Depending on a variety of factors, both software-calculated or manually-entered values may be rounded differently when displayed in Empower™ software. Note that, throughout this document, Empower refers to Empower 3 Build 3471, Empower 2 Build 2154, and Empower Build 1154.

The differences in rounding are due to the different ways in which Microsoft and Oracle define double-precision floating-point numbers. Empower use the Microsoft format to display data prior to saving results and then uses the Oracle format after saving results. Two examples of this behavior are described in this document. The first involves peak area calculations made on chromatographic data. The second involves manually entering values via the Component Editor.

Internal Number Representation in Empower Software

Empower uses double-precision floating-point numbers to internally represent the results (such as Area) calculated by the software.

In certain circumstances, the results for some fields displayed in the Review window before they are saved may be slightly different from the same fields and results after they are saved. This is due to the fact that before results are saved, they are governed by Microsoft's operating system rules; after saving, they are governed by Oracle's rules.

Microsoft uses the Institute of Electrical and Electronics Engineers, Inc. (IEEE) floating-point format for floating-point number representation. Oracle uses the Binary Coded Decimal (BCD) format for floating-point number representation. This directly affects the representation and rounding of numbers:

- **Representation** – The IEEE format represents numbers in Base 2, which makes it difficult to express certain numbers. For example, a number ending in xxxxx.5 is actually less than XXXXX.5 in Base 2. This is similar to the way in which 1/3 (0.33333333...) is difficult to represent in Base 10. In comparison, the BCD format expresses a number as a sequence of decimal digits and then each decimal digit is encoded as a four-bit binary number. This approach allows Oracle to represent xxxxx.5 more accurately.
- **Rounding** – Microsoft defines double-precision floating-point numbers as 15 digits. Oracle defines stored double-precision numbers as being rounded from the 17th digit.

Example 1: Peak Area Calculation

A peak's Area may round to xxxxx.5 or xxxxx.0 if the peak is integrated with a flat baseline, which causes the sum of the height counts for all the points across the peak to be an integer. The sampling rate has an effect on the area calculated for a peak. A specific sampling rate of 2 points/second exhibits a higher probability of producing peak areas which round to xxxxx.5.

For peaks whose areas end in xxxxx.5, the 5 is used as a decision point for rounding for display purposes (for example, when a peak whose area rounds to xxxxx.5, but its area is actually less than xxxxx.5 due to the Microsoft method for expressing numbers). Following the Microsoft rules, the peak is not (and should not be) rounded up to xxxxx+1 when it is displayed with no decimal places. After being stored and fetched in the Oracle database, that same peak has an area that rounds to xxxxx.5. The peak is (and should be) rounded up to xxxxx+1 when it is displayed with no decimal places.

The following table contains examples of how Area count values are rounded differently, depending on whether the result has been saved to the database. Note that the numbers are different in their 17th significant digit.

Peak	Area Calculated in Review (Microsoft Number Format)		Area After Saving Result (Oracle Number Format)	
	Full Value (Not Viewable)	Displayed Value in Review (Data Precision = 0)	Full Value (Not Viewable)	Displayed Value (Data Precision = 0)
1	25614.49999999999600	25614	25614.50000000000000	25615
2	35199.49999999999300	35199	35199.50000000000000	35200
3	15987.49999999999600	15987	15987.50000000000000	15988
4	15976.49999999999800	15976	15976.50000000000000	15977
5	4462956.49999999910000	4462956	4462956.50000000000000	4462957

Example 2: Manual Data Entry in the Component Editor

You can enter amounts for one or more components in a variety of places within Empower; typically, you do this using the Component Editor from the Samples table. In the Component Editor, the default precision setting is 6 digits after the decimal point. You can see the effects of the rounding behavior described in this document when entering values where the number of digits entered exceeds the precision specified for the column (for example, entering a value ending in .95 when the precision is set to 1 digit). Depending on the precise number, the representation may cause an apparent rounding error. Because Empower uses the entire number in each calculation rather than the rounded and displayed number, the effect of this behavior is minimal.

Example 3: Calculations in Report Methods

A report method uses a field stored in the database with only one digit after the decimal point (Precision = 1). For example:

Field Type	CField Id	Type	Width	Precision	Minimum	Maximum	Default	Source	Required	Formula
Sample	135	Real (0.0)	4	1	0	100		Keyboard	<input type="checkbox"/>	

Two samples values (100 and 99.7) are stored for this field. However, when the mean is calculated in a report method table and rounded to one decimal point, the value is reported as 99.8 as opposed to the expected value of 99.9.

This is because the sample value of 99.7 is represented as 99.69999694824210 when converted from Oracle's BCD format. This causes the mean to be calculated as 99.84999847412105, which then becomes 99.8 when rounded to one decimal point.

The solution is to display at a higher Precision of 2 to avoid the rounding inaccuracy. In this case, the returned mean would be calculated correctly as 99.85.

NOTE: *It is not possible to predict whether a number conversion will result in a rounding up or a rounding down event.*

Conclusion

Due to the fact that this behavior is related to the differences in how Microsoft and Oracle define double-precision floating-point numbers, Waters is not planning on changing the way numbers are represented in Empower software. However, you may be able to reduce the likelihood of encountering these differences by employing one or more of the following:

- Increase the displayed Data Precision value in the Review window, Component Editor, and other places that Empower uses numeric data. A minimum of 1 additional digit is recommended. If you are attempting to confirm mathematical calculations made by Empower, we recommend that you temporarily increase to the full precision.
- Change the acquisition sampling rate (for example, from 2 to 1 or 5).
- Report results after storing them in the database

NOTE: *When making any changes to a system, you should consider the applicable Standard Operating Procedures (SOPs) and complete the appropriate documentation and validation.*