TITLE: ROUNDING FOR THE ANALYTICAL TEST RESULTS

1.0 PURPOSE:

To lay down the procedure for rounding the Analytical test results.

2.0 SCOPE:

This procedure is applicable to round off the calculated results of the test parameter / specification related to quality control analysis.

3.0 RESPONSIBILITY:

3.1 Analyst-QC is responsible to follow this SOP.

3.2 Head-QC/Designee is responsible for ensuring implementation of this SOP.

3.3 Head-QA/Designee is responsible for monitoring overall compliance of this SOP.

4.0 DEFINITIONS:

4.1 Rounding: Mathematical reduction of numerical values to the digit required according to the significant figure or tolerance established for the particular calculation.

4.2 Significant Figure: The number of digits necessary to express the results of a measurement consists with the measured precision.

4.3 Recorded data: The initial record of the output from the measuring system.

4.4 Reported value: A reportable is often a summary Value for several individual determinations. It is the end result of a completed measurement, method as document. It is the value compared with the acceptance criterion. In most cases, the reportable value is used as documentation for internal or external users.

4.5 Decimal Places: The number of digits following the decimal point.

4.6 Derived Numeral Value : The numeral value calculated from the recorded or reported

5.0 PROCEDURE:

5.1 Specified limits in quality documents such as BPR, ATR documents are always appropriate for their purpose and are specified with appropriate number of decimals.

5.2 Interpretation of process parameters in Manufacturing :

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Process parameters like temperature, pressure & vacuum and input quantities during material dispensing/charging for a batch is recorded to the last significant decimal place that the measuring instrument is capable of. Examples are tabulated below (refer table-1):

Table-1
Reporting format for process parameters –do's and don'ts

Description	Measuring Unit	Example		Conforms	Remarks
		Instrument Reading	Reporting Format		
Process parameter-Temperature	°C	**45.0**	**45.0**	**Yes**	**..**
		45.0	45	No	Reading not entered as read
		65.2	**65.2**	**Yes**	**..**
		65.2	65.20	No	Reading not entered as read
		65.2	65	No	Rounding of decimal places not permitted
Process parameter-Pressure	Kg/Cm^2	**5.0**	**5.0**	**Yes**	**..**
		5.0	5	No	Reading not entered as read
		3.5	**3.5**	**Yes**	**..**
		3.5	3.50	No	Rounding of decimal places not permitted
		3.5	4	No	Rounding of decimal places not permitted
		3.5	4.0	No	Rounding of decimal places not permitted
Process parameter-Vacuum	mm Hg	**680**	**680**	**Yes**	**---**
		680	680.0	No	Reading not entered as read
Input Quantity - Weight	Kg	**1.250**	**1.250**	**Yes**	**---**
		1.250	1.25	No	Reading not entered as read
		10.20	**10.20**	**Yes**	**---**
		10.20	10.2	No	Reading not entered as read
		124.0	**124.0**	**Yes**	**---**
		124.0	124	No	Reading not entered as read
Input Quantity - Volume	L	**10.0**	**10.0**	**Yes**	**---**
		10.0	10	No	Reading not entered as read

5.2.1 **Reporting Molecular weight and Batch yield:**

5.2.1.1 The number of decimal places for reporting molecular weight and batch yield follows 2 decimal places unless and otherwise stated.

5.2.2 **Rounding off policy:**

5.2.2.1 Rounding off is required, when observed/calculated/derived value has more decimal places than the number of significant decimal places in the limit of expression or required in the reported value.

5.2.2.2 Only one digit is considered in the decimal place to the right of the last place in the limit of expression or required in the reported value.

5.2.2.3 Accepted rule of rounding off is:

5.2.2.3.1 If this digit is smaller than 5, it is eliminated and the preceding digit is unchanged.

5.2.2.3.2 If this digit is greater than or equal to 5, it is eliminated and the preceding digit is increased by one.

5.2.2.4 If the actual values is not having the significant figures at decimal places as per the specifications, then the vacant decimal value is reported as ‘0’ (zero) at decimal places.

5.2.2.5 Examples are shown in table-2 for illustration purposes:

Table-2

Rounding off decimals- do's and don'ts

Description	Measuring Unit	Significant decimal places	Example		Conforms	Remarks
			Un-Rounded Value	Rounded Value		
Molecular weight	g	2	196.145	196.15	Yes	..
			196.145	196.14	No	Rounding off not applied
			256.1446	256.14	Yes	..
			256.1446	256.15	No	One decimal place to the right of significant decimal place is considered. Since 4 are ≤ 5, the 2nd decimal cannot be increased by one.
			256.1446	256.1	No	Required number of decimal place is not considered.
Batch Yield	Kg	2	**100.995**	**101.00**	**Yes**	**..**
			100.995	100.99	No	Since 9 is ≥ 5, the 2nd decimal should be increased by one.
			100.995	100.9	No	Required number of decimal place is not considered.
			64.545	64.54	No	Since 5 is ≥ 5, the 2nd decimal should be increased by one.
			64.545	64.5	No	Required number of decimal place is not considered.

5.3 Interpretation of requirements in Quality Control

5.3.1 Analytical results are observed in the QC (calculated from the experimental measurements) are compared with stated limits to determine whether there is conformance with compendia assay or test requirements.

5.3.2 The observed or calculated values usually contain more significant figure than there are in the stated limit, and a reportable result is rounded off to the number of places that is in agreement with the limit expression by following the procedure expecting for reporting of impurities.

5.3.3 If no response (% are) is found /recorded, result shall be reported as “Not Detected”.

5.3.4 If LOD & LOQ values information is not available, the calculated value rounded at least up to **two decimals**.

5.3.5 If LOD & LOQ values are established the reporting shall be based on level of calculated values as indicated in the following table.

LOD & LOQ values are established, reporting the result as mentioned below	
Calculated Value	**Reportable Value**
<LOD	'Below Limit of Detection’ and LOD levels of the method shall be written in the bracket
≥LOD, But < LOQ	Less than LOQ' and LOQ levels of the method shall be written in the bracket.

5.3.6 Where the calculated result is less tha n (Where the calculated result is less than (<) the Limit of Detection (LOD), then result shall be reported as **‘'Below Limit of Detection’ and LOD levels of the method shall be written in the bracket**.

5.3.7 Where the calculated result is less than (<) Limit of Quantification but above or equal (>) to the limit of Detection, then result shall be reported as **'Less than LOQ' and LOQ levels of the method shall be written in the bracket.**

5.3.8 Where the calculated result is equal to or greater (>) than LOQ value, then same result shall be reported as mentioned below.

Where the calculated value is more than the LOQ value the reported value should be as below.		
Specification limit	**Calculated Value**	**Reportable Value**
0.2%	0.1597	0.16
	0.2345	0.23
0.50%	0.5013	0.50
	0.5058	0.51
1.0%	1.0052	1.0
	1.0523	1.1
1.5%	1.5146	1.5
	1.5678	1.6
1.50%	1.5146	1.51
	1.5688	1.57

5.3.2 If the specification for impurities is ≤ 0.1% the result is reported to two decimals or reported as per the specification/ requirement.

Example: If, the obtained value for impurity A is 0.02% then the result is reported as 0.02% only but not rounded off.

5.3.3 If the specification limit is above or equal to (>) 1.0%, then the calculated value shall be reported to the number of decimal places in line with the specification or limit of expression as illustrated in above table

5.3.4 For total impurities, rounding off shall be applied by summing of all **calculated (unrounded)** impurities as defined test procedure.

5.3.5 In case of reporting Water Content, Loss on Drying, Loss on Ignition, Limit tests and Sieve analysis where the results becoming 'Zero (0)' after rounding, the result shall be reported up to the value to get the significant number.

Test parameter	Specification	Calculated value	Shall be reported as
Water content	1.0	0.0047	0.005
Loss on Drying	0.5	0.0026	0.003

5.3.6 For reporting the TLC and limit test result, it shall be reported as complies /does not comply.

5.3.7 The residual solvent data shall be reported only in whole number i.e. 315 ppm & not 314.6 ppm

5.3.8 Relative retention time (RRT), Relative response factor (RRF) and Correction factor shall be recorded up to 2 decimals. In chromatographic analysis rounding off the ratio of respective peak area to internal standard shall be up to 4 decimals.

5.3.9 Intermediate calculations (e.g. slope for linearity in validation of compendia methods) are rounded for reporting purposes, but the original values (not rounded) are used for any additional required calculations. Rounding off is not done until the final calculations for the reportable values has completed.

Note: The calculations are always retaining an extra significant figure over the significant ones. Rounding off is done only at the end of the correct significant figures.

Example: In the assay calculation of standard, if, the obtained value of water (by KF) is 0.19%, then the same value is considered in the calculation, but not rounded off.

5.4 Procedure for rounding off of Numerical in chemical Analysis & Reporting.

5.4.1 When rounding off is required, only one digit is considered in the decimal place to right of the last place in the limit expressions.

5.4.2 If the digit is smaller than 5, then the result is rounded off as per number of digits in specification and the preceding digit is unchanged.

5.4.3 If the digit is greater than 5, then the result is rounded off as per number of digits in specification and the preceding digit is increased by one.

5.4.4 If the digit is equals 5, the 5, then the result is rounded off as per number of digits in specification and the preceding digit is increased by one.

Examples of rounding off numerical are given in table

Illustration of rounding numerical values for comparison with Requirements				
S.No.	**Requirement**	**Unrounded value (in %)**	**Rounded result (in%)**	**Conforms to specification**
1	Assay Limit ≥ 98.0%	97.96	98.0	Yes
		97.92	97.9	No
		97.95	98.0	Yes
2	Assay Limit ≤ 101.5%	101.55	101.6	No
		101.46	101.5	Yes
		101.45	101.5	Yes

3	Limit test ≤ 0.02%	0.025	0.03	No
		0.015	0.02	Yes
		0.027	0.03	No
4	Limit test ≤ 0.0003%	0.00035	0.0004	No
		0.00025	0.0003	Yes
		0.00028	0.0003	No

Note: The example illustrated in S.No. 3 & 4 is for quantitative test but if the limit test is qualitative or comparative test, the value is given as per the standard requirement.

5.5 Rounding of shall not be done in following cases:

5.5.1 No rounding off shall be applied for the relative response factors indicated in the test procedure/Monograph.

5.5.2 No rounding off is applicable (ie) the observed/displayed value shall be reported as it is, in case of Identification test, where maxima has to be reported (either in UV Spectrophotometry)

5.5.3 Only rounded analytical test results are reported on Analytical Test Report (ATR), and Certificate Of Analysis (COA), however Analytical Register/ Analytical Work Sheet shall contain both “calculated value” and “rounded value”.

5.5.4 All the readable values, for the example pH meter readings or specific optical rotation values are not rounded off; the displayed/obtained value is reported as such. Note: Limits, which are fixed numbers, are not rounded off.

5.5.5 While calibrating the weighing balance with standard weights, the weight displayed to the last decimal by the balance shall be recorded without rounding off.

5.5.6 While weighing the test sample and / or a working standard in QC laboratory, actual weight to the last decimal as displayed by the balance shall be recorded as per the least count of the balance without rounding off.

5.5.7 System suitability parameters such as RSD, tailing factor and Resolution, Similarity factor, etc., are recorded as per the limit after rounding off.

5.6 Volumetric solution strength should be rounded with maintaining 4 decimals places

5.7 The reporting of pH, Water content, Loss on Drying, Residue on ignition, Sulphated ash, Bulk density, Individual Impurities and Total impurities two digits after the decimal.

5.8 For calculating the water content consider KF Factor in four decimals by rounding the fifth decimal.

5.9 The reporting of Residual solvents is rounding the number without decimal.

5.10 RSD and other statistical presentation. One significant figure to the right of the decimal point.

5.11 No rounding is applicable for light absorption (color of solution) % T (Transmittance) test in case of UV spectrophotometer shall be reported as it is.

5.12 Test like results to be given as less than 1% if the limit is less than 1.0%

5.13 For cleaning samples, one significant figure after decimal value.

5.14 Melting range results shall be reported as observed value.

5.15 Peak areas shall be recorded as it is.

5.16 Relative retention tine (RRT), Relative response factor (RRF) and Correction factors shall be recorded / reported two digits after the decimal.

5.17 Other than the above tests reporting the results based on specification.

7.0 CHANGE HISTORY:

Revision No.	Effective Date	Details of Revision	Ref CCF No.
00	03.03.2015	New SOP introduced	-----
01	05.08.2017	1) SOP formate changed in make to inline with SOP-QA-001-05. 2) All together procedure has been repharsed for better clarity.	CCF/GEN/17022

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