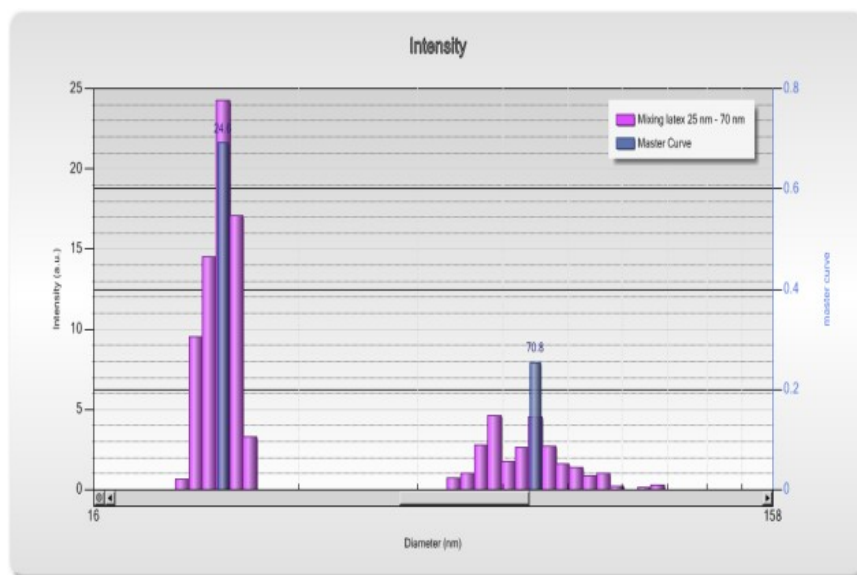


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FAQ on particle size data and representation with NanoQ



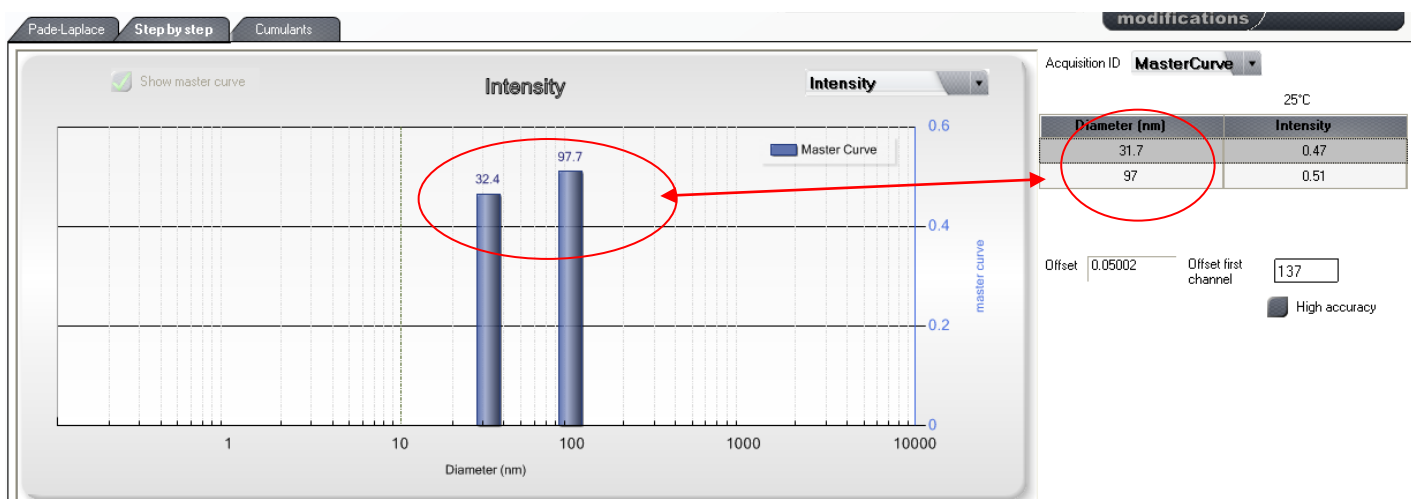
FAQ on particle size data and representation with NanoQ: how to read and interpret your results

Key Words: NanoQ, Pade Laplace, Cumulants, Dynamic Light Scattering (DLS), Particle size analysis, size distribution, master curve.

This FAQ intends to explain how to read and interpret the particle size data results provided by NanoQ

- [Question : with the Pade Laplace analysis, in the ANALYSIS folder, why the « step by step » size results displayed in the table on the right side are not exactly the same as those displayed on the histogram?](#)
- [Question: what is the histogram binning and how is it defined?](#)
- [Question : what is the peak analysis based on and what is the definition of the peak information?](#)
- [Question : how is the master curve calculated and what is the meaning of it?](#)
- [Question : what are the differences between the Cumulant and Padé Laplace analysis and is Cumulant relevant for multi-acquisition analysis?](#)

Question: with the Pade Laplace analysis, in the ANALYSIS folder, why the « step by step » size results displayed in the table on the right side are not exactly the same as those displayed on the histogram?



The size histogram is a graphic representation of all the particle size solutions found by the Pade analysis. Indeed, this histogram is built by sorting-out these solutions into size bins. One size bin of the histogram is defined by an average size and a size width and the histogram is made of a certain number of bins (typically 250 for the default factory setting). The values displayed above the bars on the histogram are the average size of these bins; The values displayed in the table on the right side are the exact solutions given by PADE. The consequence of this representation for multiacquisition results is that one bar of the histogram could correspond to several PADE solution if they differ by less than a bin width and will appear just as one averaged size value in the histogram. The second consequence is that the Pade solutions and the histogram values may slightly differ (typically by less than +/- 3%). To illustrate this, let's take an example (see figure above): if PADE finds two solutions, 31.7 nm and 97 nm, in the histogram these solutions will be stored in the 32.4 and 97.7 bins respectively. Similarly, if PADE finds one solution at 96.5 nm and then 98.5 nm at the next acquisition, these two solutions will appear under the same bin centered at 97.7 nm .

Question: what is the histogram binning and how is it defined?

In order to represent the size solutions found by the Pade-Laplace analysis on a histogram (Peak intensity vs particle size) in a readable and understandable manner, a logarithmic size scale is used to cover on the same graph the entire size range spanned by VASCO (1 nm to 10 μ m). The Pade solutions are then sorted with their intensity into size classes along the size axis. The size classes are defined by a binning set by three parameters: Size class number (=number of BINS), Max and Min size classes (=span range) which default values are preset from factory (see Parameters-> Algorithm settings menu). These values are set to give the best representation of the results across the entire size range; It is recommended not to change them because they can strongly impact the histogram. With the default binning settings, the maximum size difference between the PADE step by step values and the histogram binned values should not exceed +/-3%.

Binning settings

Size Class Number: 250

Max Size Class: 10000.0

Min Size Class: 0.1

Important to Notice :

- The exact values given by Pade Laplace can be read in the table on the right side of the histogram, in the step by step folder.
- The particle size results displayed in the pdf report in the **statistical distribution** table (see example below) corresponds to the histogram values and not the exact Pade Laplace solutions.

Statistical distribution

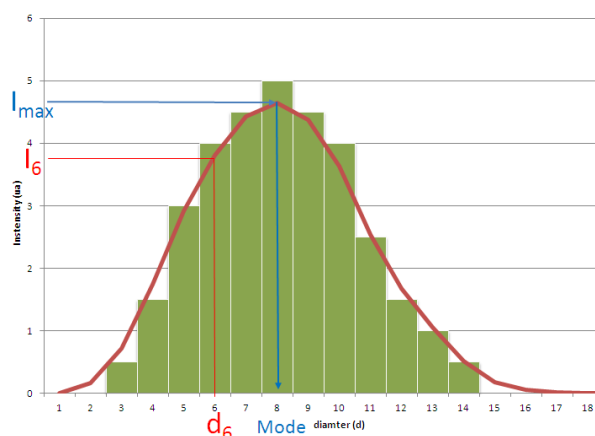
Size	Intensity	Number	Volume
30,91	0,23	0,56	0,50
32,37	0,24	0,44	0,45
97,75	0,52	0,00	0,05

Question : what is the peak analysis based on and what is the definition of the Peak information?

In order to help the users to identify some population modes within a size histogram, a linear peak Interpolation is generated using a sliding averaging filter applied on the raw size histogram data. It is purely a mathematical/statistical approach. The peaks generated are defined by 4 characteristics: **peak Mode**, **peak Mean**, **peak StdDev**, **peak Intensity** displayed on the right side of the histogram in the Analysis folder.

Peak 1 informations

Mode	245.5 nm
Mean	250.2 nm
StdDev	2.3%
Intensity	45.2%



- **Peak Mode value:** corresponds to the size for which the peak amplitude is maximum:

$$\text{Mode} = d_{I_{\max}}$$

- **Peak Intensity:** it is the integral of the intensity of a peak and is equal to the total area below the peak; is it usually express in % of total intensity

$$I = \sum_k I_k$$

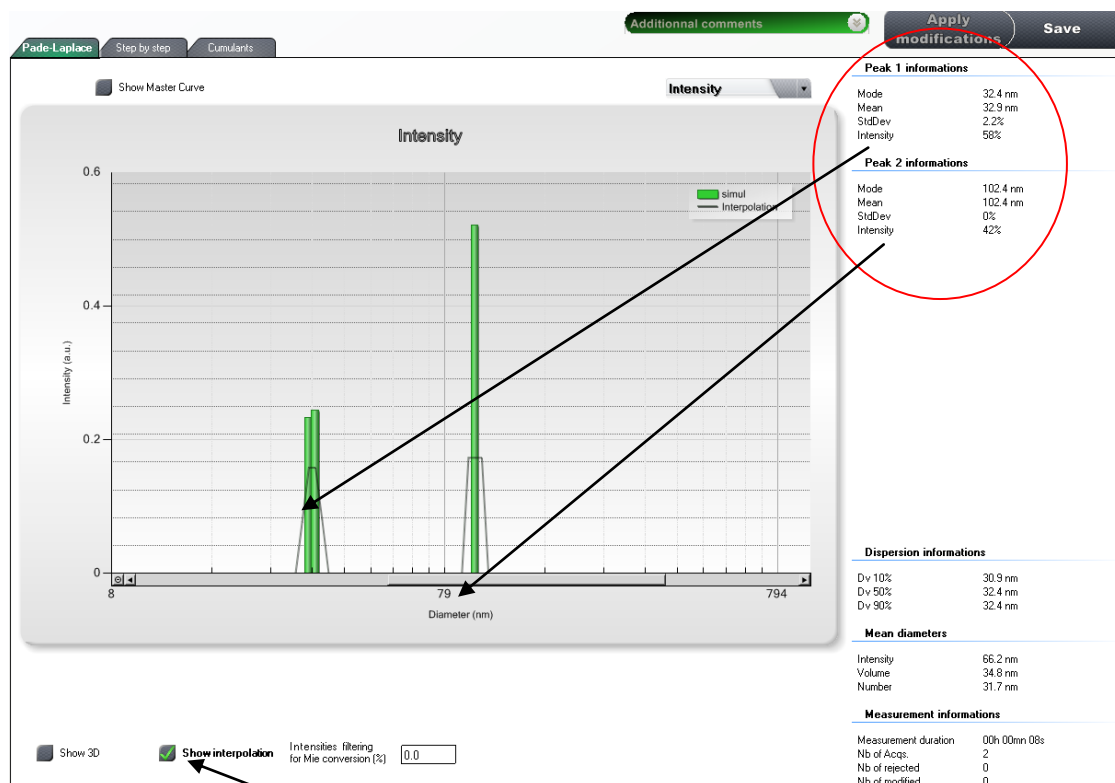
Nota bene: the summation of the peak intensities on all the peaks is equal to one (100%)

- **Peak Mean value:** corresponds to the intensity weighted average size value.

$$\bar{d} = \sum_k \frac{d_k \times I_k}{I}$$

- **Peak StdDev:** it is equivalent to the RMS width of the peak;

$$\text{StdDev} = \sqrt{\sum_k \frac{d_k^2 \times I_k}{I} - \bar{d}^2}$$



Remark: selecting « Show interpolation » box below the histogram displays the interpolated peaks on the histogram.

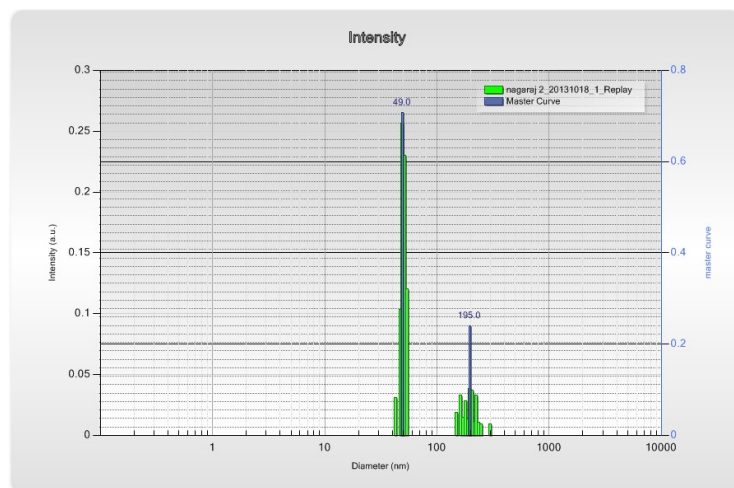
Caution: in case of complex sample multi-acquisition measurements, the peak analysis mode can be tricky to interpret since the interpolation algorithm can generate a large number of “calculated” peaks.

Question : How is the master curve calculated and what is the meaning of it?

When you have achieved a statistical acquisition, several autocorrelation functions have been acquired. Pade-Laplace is applied on each acquisition and results can be displayed individually in the Step-by-Step Tab of the analysis page. The master curve is the autocorrelation function averaged from the whole captured correlogram of the sequence.

$$G_{master}(\tau) = \frac{\sum_1^n G_k(\tau)}{n}$$

This averaging allows to increase the signal to noise ratio of the measurement (by a factor \sqrt{n}) if n is the number of successive acquisition of the sequence. The master curve is also an improved/complementary indicator about the average size of the size modes of the histogram (see example below)

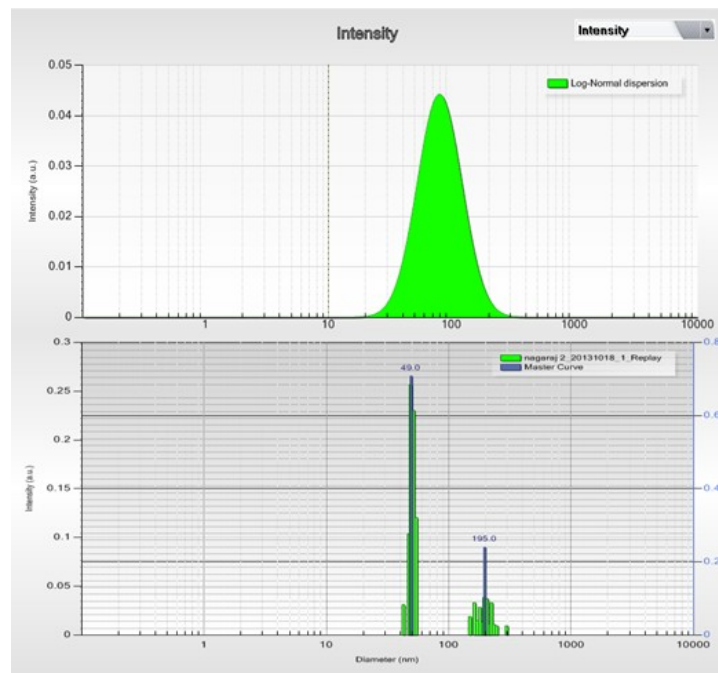


Example of Master curve vs histogram analysis; Blue bar: master curve results; green bars: multi-acquisition results.

Nota Bene: the use of the master curves analysis with the multi-acquisition makes sense only if the sample/measurement is stable all along the multiple-acquisition sequence. This can be confirmed by a small envelop of the accumulated autocorrelation functions of the sequence.

Question : What are the differences between the Cumulant and Padé Laplace analysis and is Cumulant relevant for multi-acquisition analysis?

Padé Laplace results are based on a multi-exponential (SVD) analysis. It is recommended for complex and/or polymodal sample analysis. Padé gives discrete size values associated to intensity values. Distribution information can be obtained by a statistical multi-acquisition measurement. The Cumulant analysis is based on a single exponential decay model. Cumulant result is defined by an intensity weighted harmonic average size value (Z average) and a polydispersity index (PDI). Cumulant is only relevant and accurate for monodispersed and monomodal samples. When used in the multi-acquisition mode, Cumulant is only applied to the master curve. In case of a polymodal sample, Cumulant will give an averaged value with a distribution centered in between the modes given by Padé (see below).



Nota Bene: for a Log Normal/Gaussian particle size distribution, the PDI of the Cumulant is proportional to the distribution width.

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