nanalysis

QUANTITATIVE NUCLEAR MAGNETIC RESONANCE

BASIC

INTERNAL CALIBRANT

- Must be soluble and stable in solution, unreactive toward other analytes, high in a known purity, and its signals must not overlap with others in the spectrum

MASS AND VOLUME

- Ensure solids are weighed using an analytical balance and stock solutions are prepared using a volumetric flask

ACQUISITION PARAMETERS

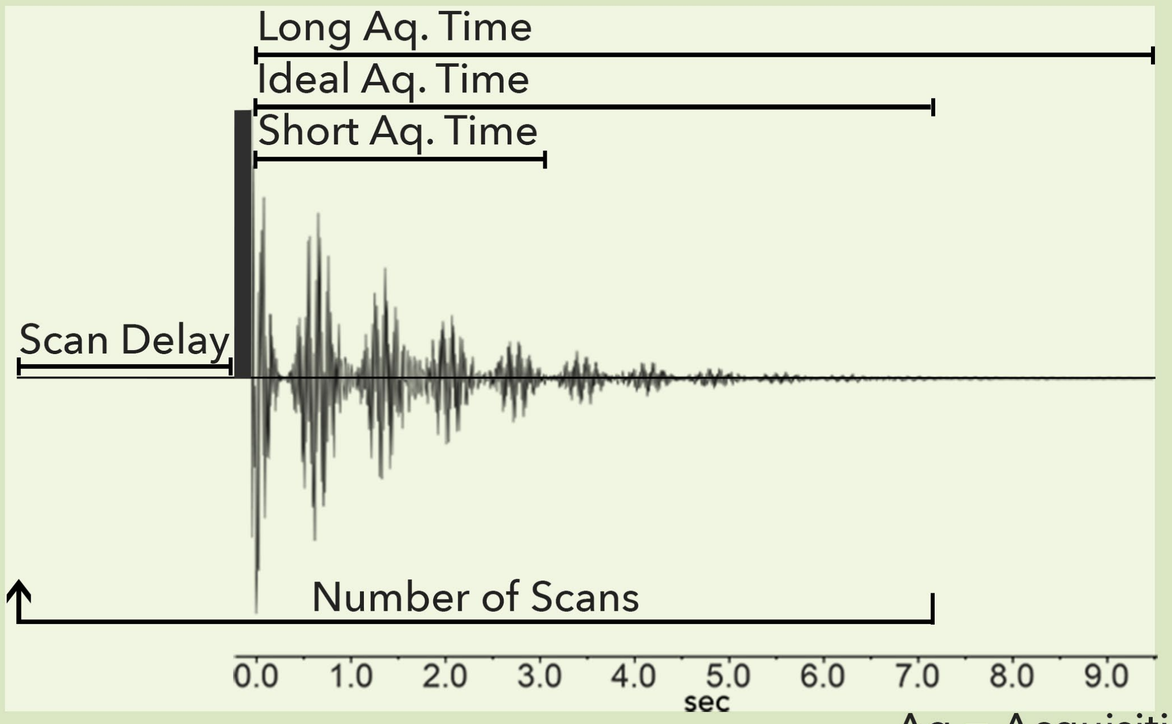
- Acquisition parameters vary from sample to sample, take a look at the right side of this infographic for a basic rundown!

REPRODUCIBILITY

- Collect data in triplicates (at a minimum) to ensure statistical significance

BASELINE & PHASE

- Ensure each spectrum is processed properly to avoid baseline and phase distortions



Aq = Acquisition

Acquisition Parameters

ACQUISITION TIME

$$\frac{\text{NUMBER OF POINTS}}{\text{SPECTRAL WIDTH}}$$

- Too long of an acquisition time can lead to unnecessary noise acquired
- Too short of an acquisition time can lead to FID truncation
- Ensure appropriate apodization parameters are used during data processing

SCAN DELAY

- Must be long enough to allow for full relaxation of spins
- Aim for 5-7 times the longest T_1 value for the signals of interest

NUMBER OF SCANS

- Aim for a high signal-to-noise ratio for more accurate quantitative results

1. G.F. Pauli, S. N. Chen, C. Simmler, D. C. Lankin, T. Gödecke, B. U. Jaki, J. B. Friesen, J. B. McAlpine, J. G. Napolitano, *J. Med. Chem.* **2014**, *57*, 9220.
2. P. Giraudeau, *Magn. Reson. Chem.* **2017**, *55*, 61.

https://www.nanalysis.com/nmready-blog/2021/6/21/nmr-acquisition-parameters-and-qnmr
https://www.nanalysis.com/nmready-blog/2019/2/27/beyond-structural-elucidation-introduction-to-qnmr-part-i