

# Statistical criteria for quality control of XAS - fluorescence data

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Quality control of XAS fluorescence data is often a time-consuming and difficult process based on subjective judgment. Fluorescence data recorded by multi-element detectors can be divided into scans and channels. With each scan one spectrum for each detector element is recorded. A channel includes all spectra from one detector element for the whole measurement. While it is possible that individual spectra from a certain scan and channel are affected by errors, in most cases whole scans or channels are corrupted.

For scans these errors can result from temporary glitches of the detector electronics. For corrupted channels which are more common two potential sources for errors exist. On the one hand, sample preparation (e.g. inhomogenous distributions of the sample) or the formation of ice can be responsible. On the other hand electronic problems affecting the data collection of one detector element may be the cause.

Corrupted data from affected channels and scans must be excluded from the final EXAFS data. Therefore careful selection of the spectra is required. For biological samples this selection is often complicated by the usually low concentration of the material and the resulting high noise level. For fast and reliable screening of fluorescence data a system called CHAOS (*Channel Analyzing and Omitting System*) was developed. CHAOS compares each channel with a reference which is derived from the data. After calculating the difference spectrum of the channel and the reference a number of useful statistical criteria are used for the evaluation of deviations.

Several statistical criteria were tested. Different types of errors were classified and characterized by their effect on these criteria. Through the use of appropriate statistical criteria an objective and reliable system for quality control has been developed allowing on-site screening of the data and eventually the automatization of the whole procedure.