

PEAK SEARCH

The commands [AFPEAK](#) (to mark and list peaks) and [FPEAKS](#) (to define Gaussian or Lorentzian peaks as fit function) are provided for an automatic search of any number of peaks within a displayed spectrum.

As a first step, the peak structure in the spectrum which is not attributed to statistical fluctuations is taken to deduce a guess value of the full width at half maximum (FWHM) of the peaks by an automatic procedure. The displayed data are smoothed internally over the specified width and convoluted with a bipolar function to a spectrum, in which zero crossings correspond with relative minima and maxima of the original spectrum.

The net peak area estimated from the convolution function is divided by the square root of the corresponding contents of the smoothed spectrum to define the statistical peak significance. Peaks with a significance smaller than the specified value are ignored; if more peaks than desired are found, only the most significant ones are considered.

A reasonable start value for the full peak width at half maximum (FWHM) is essential. If the automatically determined value is not adequate, the value has to be given as input parameter. A small value may overestimate statistical fluctuations; if chosen too large, sharp peaks or peaks located in a shoulder may be smoothed off.