NMR peak picking through wavelet transform and volume filtering

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Abstract

Nuclear magnetic resonance (NMR) has been widely used as a powerful tool to determine the three-dimensional structures of proteins in vivo. However, the post-spectra stage of NMR structure determination usually involves a tremendous amount of time and expert knowledge, which includes peak picking, chemical shift assignment, and structure calculation steps. We propose WaVPeak, a fully automatic peak detection method. WaVPeak applies wavelet smoothing and then use volumes around its smoothed peaks to filter out the false peaks. WaVPeak can detect weak peaks which are the ones the NMR spectroscopists need the most help to deal with. Experimental results demonstrate that WaVPeak achieves better results than some alternatives. We will also discuss how to employ Benjamini-Hochberg procedure to determine how many peaks to select automatically.

The work is jointly conducted with Prof. Xin GAO and others.