Baseline Correction of Absorption-Mode Fourier Transform Ion Cyclotron Resonance Mass Spectra

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Results and Discussion

An absorption-mode Fourier transform ion cyclotron resonance (FT-ICR) mass spectrum exhibits two types of baseline distortion: a slow periodic oscillation even where no signal peaks are present, and additional distortion near signal peaks and proportional to signal magnitude. These distortions interfere with automated peak-picking, unless the baseline systematic variation is much less than baseline rms random noise. We previously showed that the slow oscillation is removed by low-pass filtering. Here, we present a fast, robust, and automated algorithm that flattens the absorption-mode spectral baseline, even in the vicinity of signal peaks. The method begins by defining baseline data values, followed by linear interpolation to generate baseline data values between the defined values, then boxcar smoothing to generate a final baseline spectrum, and final subtraction of that baseline from the original spectrum to yield a baseline-flattened absorption-mode spectrum. We apply the algorithm to a crude oil spectrum (with 8,000 peaks) and to a ribonuclease A protein spectrum (with multiply-charged ion isotopic distributions—see **Figure 1**). We identify many more peaks (crude oil) without loss of mass accuracy, and obtain more accurate isotopic distributions (RNase A).[1]

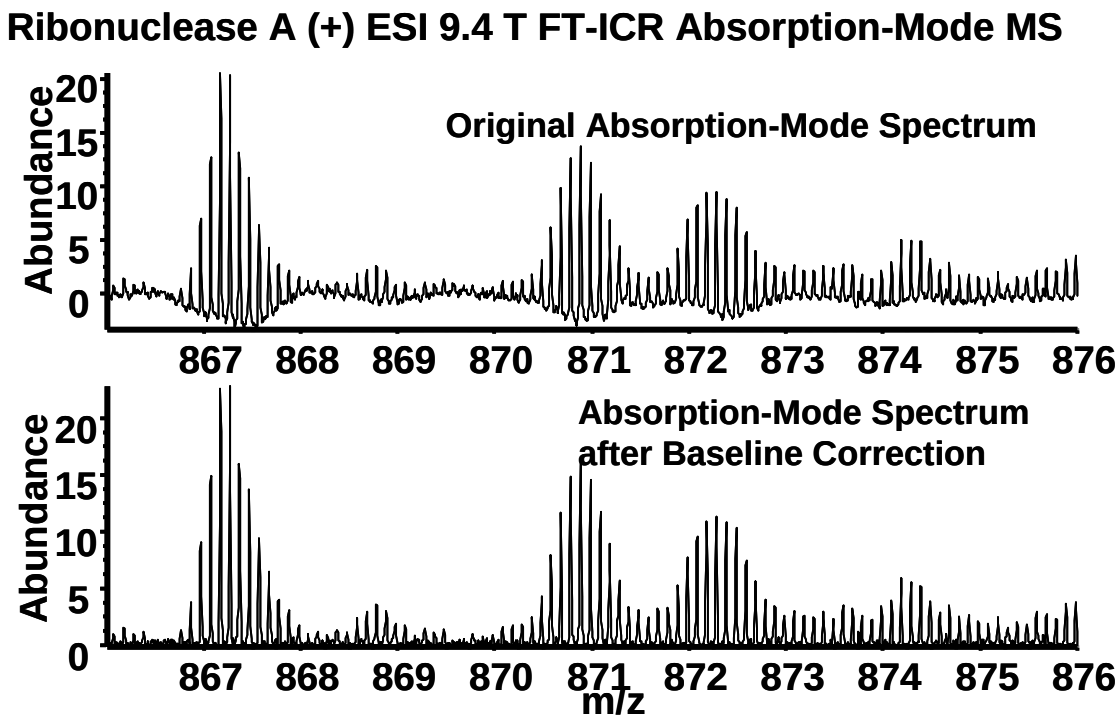

Figure 1. RNase A positive ESI FT-ICR absorption-mode mass spectral segments, demonstrating the performance of the baseline correction algorithm.

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References

[1] Xian, F., *et al.*, Int. J. Mass Spectrom., **325-327**, 67-72 (2012).