Electronic Supplementary Material (ESI) for Analyst.

SUPPLEMENTARY INFORMATION FOR THE MANUSCRIPT:

A Two-Phase Approach to Fourier Transform Ion Mobility Time-of-Flight Mass Spectrometry

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The experimental and algorithmic approach to signal reconstruction for the FT-IMMS experiment is outlined in Figure 1 of the primary manuscript, however, to add clarity to benefits afforded by the two-phased approach to signal reconstruction we have added the following 3 figures for clarity. There is a well-defined consequence to the data product through the FFT for signals that are not periodic. Because the FT-IMMS experiment is conducted through the on and off pulsing of the ion gate there are a number of areas in which the ion signal approaches or is 0 (See Figure 1b and 1d in the primary manuscript). This is because the ion gate was closed during such times which effectively preventing the ion beam from reaching the detector. Stated differently, the on/off pulsing of the ion gate establishes a situation where the ion signal reaching the detector is not "periodic" from the perspective of the Fourier transform. The combined-phase approach is an attempt to minimize the impacts of operating the instrument in such a fashion. Figure S1 highlights the high-level transform of the combined and individual phases collected with the IM-TOF configuration. However, a zoomed view of the data with a focus on the noise that arises (Figure S2) demonstrates that the non-periodic nature of the single-phase data yield a number of side lobes common for the FT of non-periodic data. The green trace in Figure S2 highlights the benefits of pulling the two phases together prior to transformation—the noise from the individual phases is largely removed in its entirety. It should be noted that no smoothing or additional signal processing steps were performed for the data shown. Finally, to aid future researchers we have included a zoomed view of the raw data following the initial multiplication by the pulsing sequence in Figure S3. This figure serves to show that two phases complement each other and when summed give rise to the data structures in Figures 1c and Figure 2 in the original manuscript.

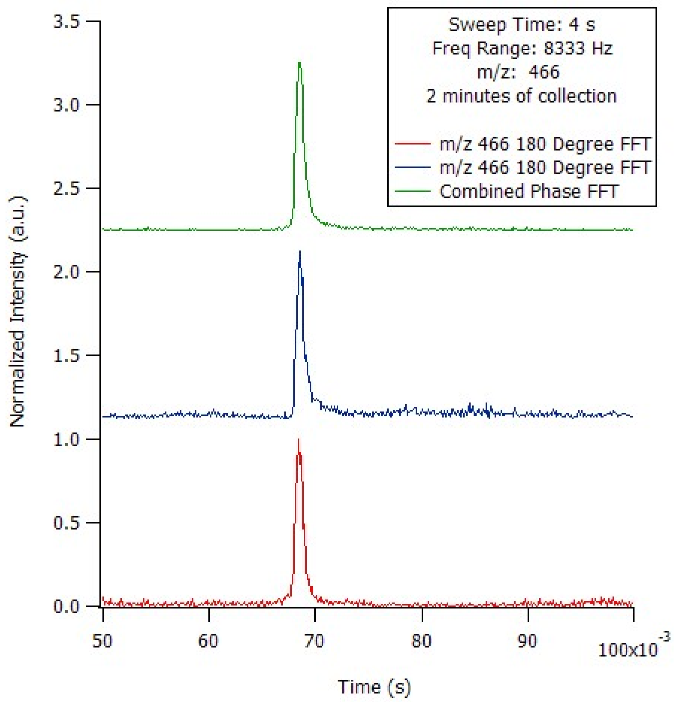

Figure S1. High-level view of the transformed data from the combined phase approach and the individual phases. Though subtle, there are noticeable signal to noise ratio gains afforded by the combined phase technique.

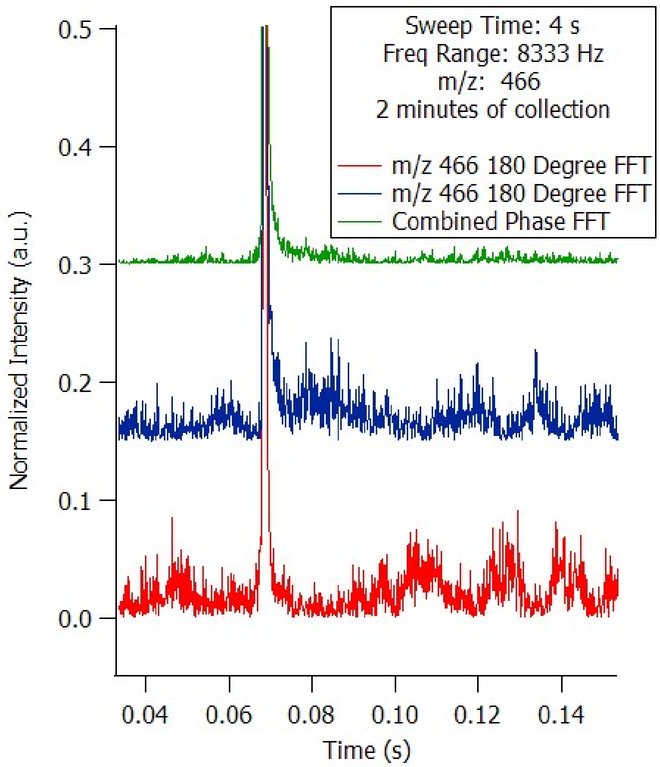

Figure 2S. Zoomed view of the transformed data from the individual data and after combining the phases. The top green trace highlights the lower noise achieved, while the red and blue traces correspond to the transformed data of the individual phases. It is interesting to note location of the ringing artifacts between the two phases. In many ways the ringing effects are 180 out of phase. These artifact arise specifically due to the areas in which the recorded ion counts approach zero.

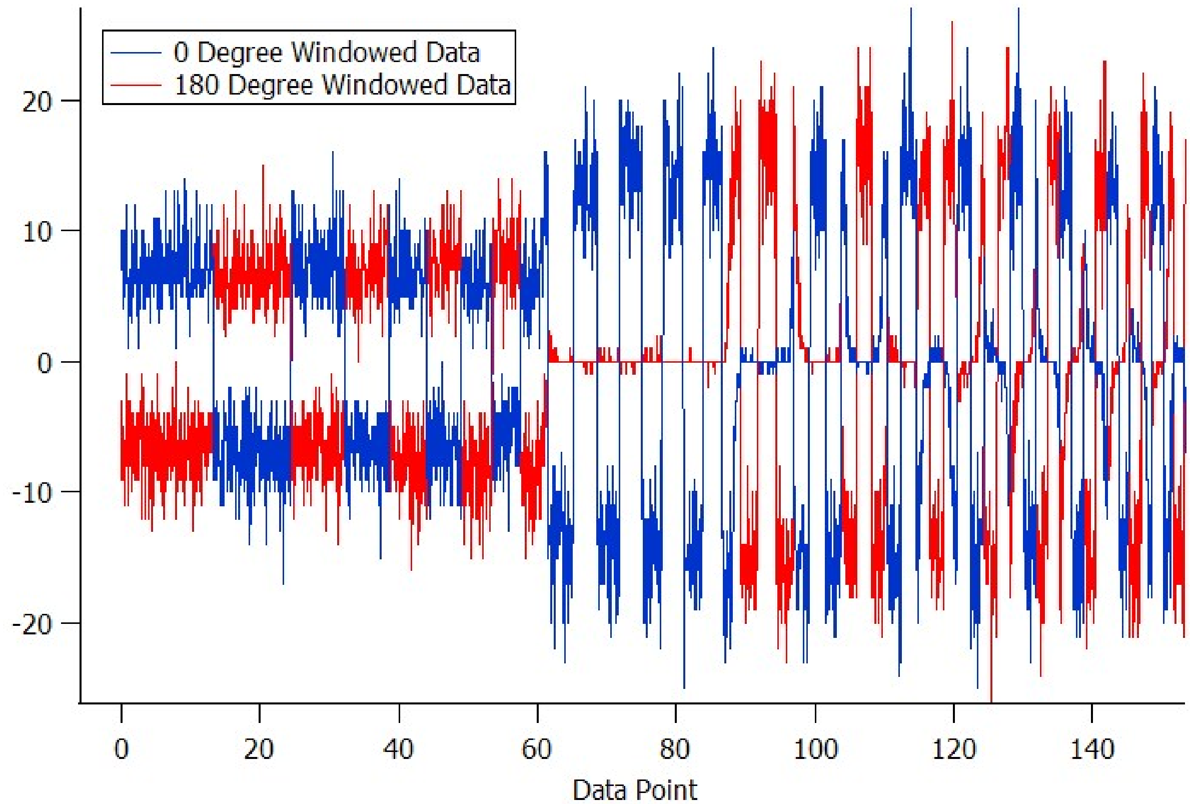

Figure 3S. Figure 1 in the manuscript outlines the two-phased approach to signal reconstruction. A critical step is multiplying the raw data by the gating function used. To highlight the consequence of this step this figure highlights the result of multiplying the two raw data sets by their respective pulsing schemes. It is most apparent for data points 0-60 that the two phases complement each other and through their combination can produce a more complete dataset suitable for FFT processing. The final step of the outlined approach in the manuscript is to sum these two signals prior to performing the FFT.