Scan-Centric, Frequency-Based Method for Characterizing Peaks from Direct Injection Fourier transform Mass Spectrometry Experiments

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**Abstract:** We introduce a novel, scan-centric method for characterizing peaks from direct injection multi-scan Fourier transform mass spectra of complex samples that utilizes frequency values derived directly from the spacing of raw m/z points in spectral scans. Our peak characterization method utilizes intensity independent noise removal and normalization of scan level data to provide a much better fit of relative intensity to natural abundance probabilities for low abundance isotopologues that are not present in all of the acquired scans. Moreover, our method calculates both peak- and scan-specific statistics incorporated within a series of quality control steps that are designed to robustly derive peak centers, intensities and intensity ratios with their scan-level variances. These cross-scan characterized peaks are suitable for use in our previously published peak assignment methodology, Small Molecule Isotope Resolved Formula Enumeration (SMIRFE).

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### Deleteme

*frequency* = a + x \* *mz*-1/2 + y \* *mz*-1/3

mz = a + x \* *frequency*-1 + y \* *frequency*-2 + z \* *frequency*-3

ln(*intensity*) = a + x \* *position* + y \* *position*2

ln(*NAP*P1 / *NAP*P2) - ln(*Int*P1 / *Int*P2) 0