Elemental Composition Validation from Stored Waveform Inverse Fourier Transform (SWIFT) Isolation FT-ICR MS Isotopic Fine Structure

B.M. Ruddy (FSU, Chemistry), G.T. Blakney (NHMFL, Chemistry), R.P. Rodgers (FSU, NHMFL, Chemistry), C.L. Hendrickson (NHMFL, Chemistry), and A.G. Marshall (FSU, NHMFL, Chemistry)

Results and Discussion

Elemental composition assignment confidence in mass spectrometry is typically assessed by monoisotopic mass accuracy. For a given mass accuracy, resolution and detection of other isotopologues can further narrow the number of possible elemental compositions. However, such measurements require ultrahigh resolving power and high dynamic range, particularly for compounds containing low numbers of nitrogen and oxygen (both ^{15}N and ^{18}O occur at less than 0.4% natural abundance). Here, we demonstrate validation of molecular formula assignment from isotopic fine structure, based on ultrahigh resolution broadband Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS). Dynamic range is enhanced by external quadrupole and internal stored waveform inverse Fourier transform (SWIFT) isolation to facilitate detection of low abundance heavy atom isotopologues. Figure 1 demonstrates validation of the assignment of monoisotopic $^{12}C_{29}{}^{1}H_{43}{}^{16}O_2$ based on resolution and identification of the isotopologue, $^{12}C_{29}{}^{1}H_{43}{}^{16}O_1{}^{18}O_1$.

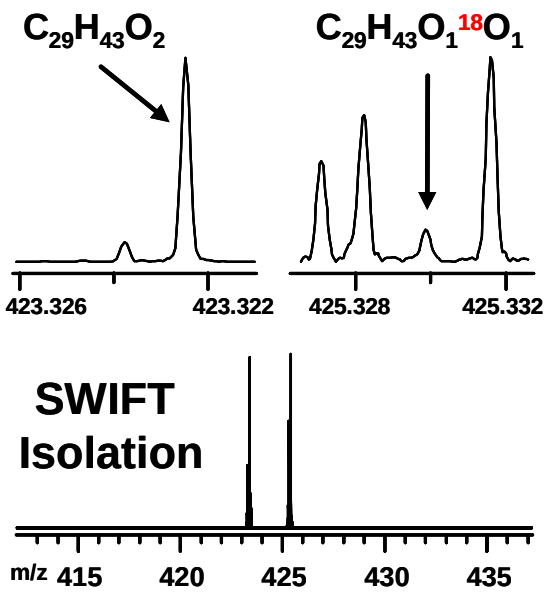

Figure 1. Bottom: SWIFT-isolated spectral segment, containing only ions of nominal mass 423 and 425 Da. Top Left: Monoisotopic isotopologue at nominal m/z 423. Top Right: Corresponding $^{18}O_1$ isotopologue at nominal m/z 425.

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References

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