

In-Depth Characterization of Structurally Diverse Targets

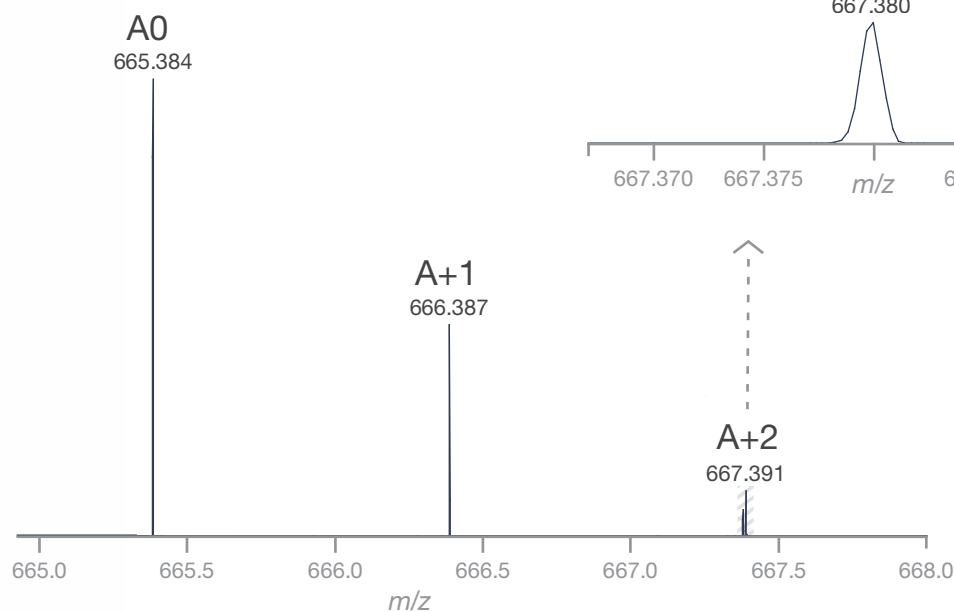
Superior Elemental Composition Determination

The Thermo Scientific™ Orbitrap Fusion™ Lumos™ Tribrid™ mass spectrometer with 1M provides fine isotope information with high isotopic fidelity on a time scale amenable to liquid chromatography. Resolving fine isotope structure allows confident assignment of the elemental composition of small molecule analytes. Ultra-high resolution, along with MSⁿ capability and the availability of multiple fragmentation modes, opens up new opportunities for the characterization of various analytes.

ULTRA HIGH RESOLUTION FOR RESOLVING IRGANOX 1035 FINE ISOTOPE STRUCTURE

Shown below is a mass spectrum of Irganox 1035 acquired at the 1,000,000 (1M) resolution setting (*m/z* 200) with a 2 s transient.

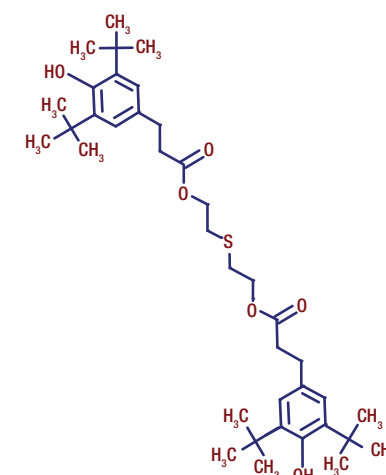
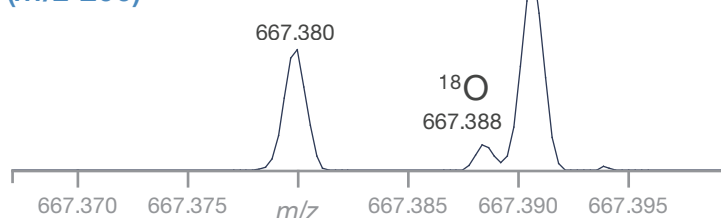
The zoom-in on the right panel shows the fine structure for the A+2 isotope acquired at the 500,000 versus 1,000,000 resolution setting. The ¹⁸O and ²¹³C isotopes can be resolved using the Orbitrap Fusion Lumos with 1M.



Orbitrap Resolution 500,000
(*m/z* 200)



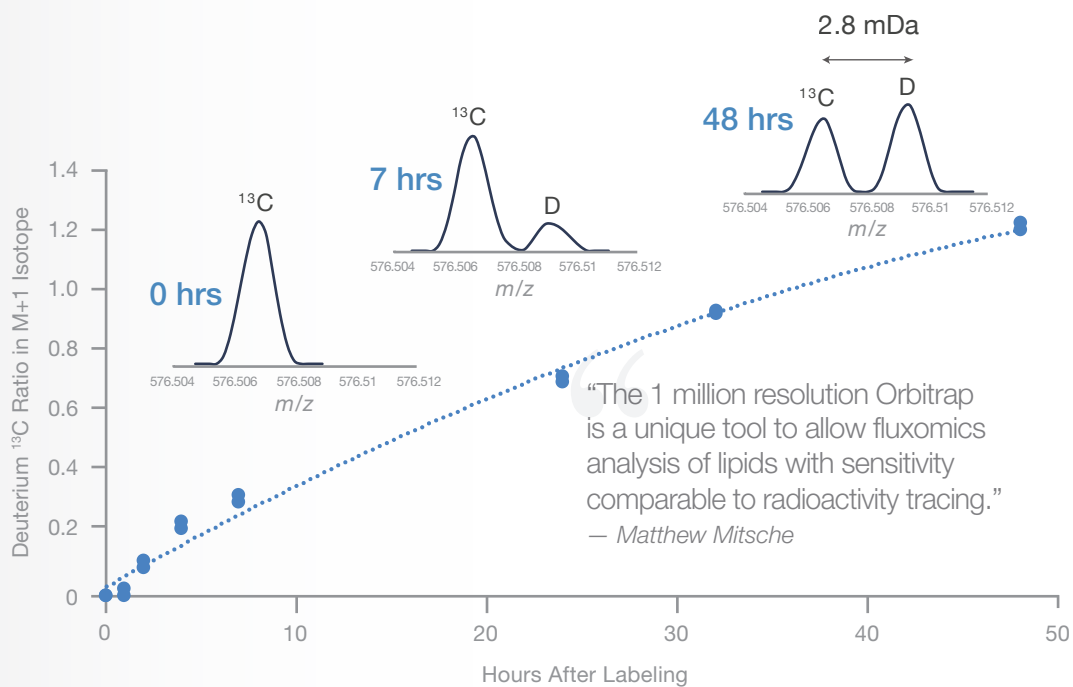
Orbitrap Resolution 1,000,000
(*m/z* 200)



Enabling Lipid Metabolic Flux Analysis

The determination of lipid turnover rates based on stable isotope labeling and isotope dilution analysis is a challenging task. Deuterated water is a commonly used reagent for these experiments as it is easily incorporated into metabolic pathways and simplifies the peak assignments compared to using heavier isotopes like ^{18}O . However, the abundance of naturally occurring ^{13}C overlaps and often eclipses the D isotope owing to the small difference in mass defect between these isotopes, thereby complicating accurate quantitation. Using ultra-high resolution it is possible to baseline-resolve these two peaks, greatly improving the selectivity and detection limit of this quantitative technique.

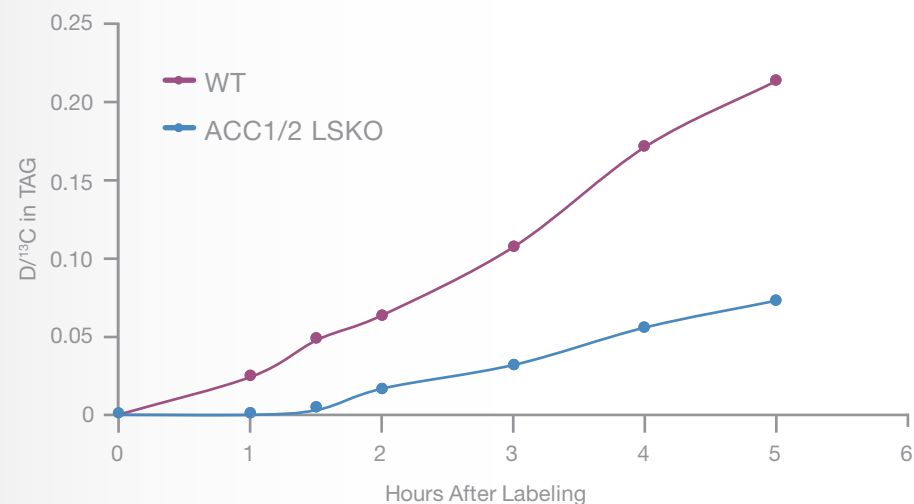
RESOLVING NATURAL ^{13}C FROM LABELED DEUTERIUM



Rate of deuterium incorporation for TAG52:3 in human hepatoma cells (HuH7) labeled with 5% D_2O . The triacylglyceride precursor ion was fragmented using high energy collisional activation and deuterium levels were plotted for the fragment ion at m/z 576.5.

Data Courtesy: Dr. Matthew Mitsche, University of Texas Southwestern Medical Center

DEUTERIUM UPTAKE LEVELS IN WILD TYPE VS. ACC1/2 KNOCK-OUT CELLS



Rate of deuterium incorporation for TAG52:3 in ACC1/2 liver-specific knockout and wild type mouse-derived primary hepatocyte cells labeled with 5% D_2O . Deuterium uptake levels were measured for the TAG52:3 fragment ion at m/z 576.5.

Specifications:

- Max resolution 1,000,000 (1M) at m/z 200 in 2 s
- S/N \geq 1000 for ^{34}S peak in the MRFA A+2 peak family with fine structure resolved at 1M
- Isotope ratios in spec up to resolution 500,000 in SIM mode
- Isotope ratios in spec up to resolution 1,000,000 in SIM mode

Find out more at thermofisher.com/lumos