

06-04: Oxylipidomics – large scale determination of oxidized lipids using high res MS and MS/MS

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Lipid oxidation is a process ubiquitous in life, but the direct and comprehensive analysis of oxidized lipids has been limited by available analytical methods. We applied high-resolution liquid chromatography-mass spectrometry (LC-MS) and tandem mass spectrometry (MS/MS) to quantify oxidized lipids (glycerides, fatty acids, phospholipids, lysophospholipids, and galactolipids) and implemented a platform-independent high-throughput-amenable analysis pipeline for the high-confidence annotation and acyl composition analysis of oxidized lipids. Lipid contents of 90 different naturally aged wheat (*Triticum aestivum*) seed stocks were quantified in an untargeted high-resolution LC-MS experiment, resulting in 18,556 quantitative mass-to-charge ratio features. In a posthoc liquid chromatography-tandem mass spectrometry experiment, high-resolution MS/MS spectra (5 mD accuracy) were recorded for 8,957 out of 12,080 putatively monoisotopic features of the LC-MS data set. A total of 353 nonoxidized and 559 oxidized lipids with up to four additional oxygen atoms were annotated based on the accurate mass recordings (1.5 ppm tolerance) of the LC-MS data set and filtering procedures. MS/MS spectra available for 828 of these annotations were analyzed by translating experimentally known fragmentation rules of lipids into the fragmentation of oxidized lipids. This led to the identification of 259 nonoxidized and 365 oxidized lipids by both accurate mass and MS/MS spectra and to the determination of acyl compositions for 221 nonoxidized and 295 oxidized lipids. Analysis of 15-year aged wheat seeds revealed increased lipid oxidation and hydrolysis in seeds stored in ambient versus cold conditions.

References

[1] RIEWE, D., et al., 2017: Plant Physiology, **175**, 600-618.