Abstract

Life as we know it is not possible without lipids. Changes in lipid homeostasis can lead to various diseases, raising the importance of reliable identification and measurement of lipids. For example, oxidized lipids have been connected to age-related and chronic diseases, atherosclerosis, inflammation and immune responses and galactolipids play important parts in structural integrity of plant membranes. Due to its sensitivity, liquid chromatography coupled mass spectrometry (LC-MS) has become the *de facto* standard in lipidomics research, leading to a rise in bioinformatics tools to analyze the recorded data. However, due to the enormous diversity of lipids, most tools cover only a marginal range of lipid classes. In an effort to reduce this shortcoming, this work aims to extend the lipid species covered by the Lipid Data Analyzer (LDA). Tools including LipidMatch, LipidMatch Flow and LPPtiger were used to survey lipids over a total of four different datasets to get an overview of LDA implementation gaps. Appropriate mass lists were generated for MS^1-identifications and the proprietary decision rulesets were extended for MS^2-identifications of important galactolipids and oxidized lipids, according to lipid-species-specific fragmentation patterns. Furthermore, LDA source code was extended to enable identification of (oxidatively) modified fatty acyl chains. LDA now reliably identifies monogalactosyldiacylglycerol (MGDG), digalactosyldiacylglycerol (DGDG), trigalactosyldiacylglycerol (TriGDG), tetragalactosyldiacylglycerol (TetraGDG) and sulfoquinovosyldiacylglycerol (SQDG), as well as oxidatively modified versions of all thirty implemented lipid classes with very low false positive rates. Comparison with LipidMatch, LipidMatch Flow and LPPtiger showed that LDA has a better coverage of the newly implemented lipids, providing researches with a powerful platform to elucidate diseases caused by perturbations in the oxidized lipidome.

Keywords: *lipidomics, bioinformatics, oxidized lipids, galactolipids, mass spectrometry, cheminformatics*