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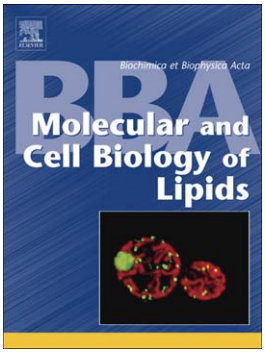

Common cases of improper lipid annotation using high-resolution tandem mass spectrometry data and corresponding limitations in biological interpretation

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Common Cases of Improper Lipid Annotation using High-Resolution Tandem Mass Spectrometry Data and Corresponding Limitations in Biological Interpretation

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Common Cases of Improper Lipid Annotation using High-Resolution Tandem Mass Spectrometry Data and Corresponding Limitations in Biological Interpretation

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Introduction:

Lipids have a wide-range of biological functions enabled by enormous diversity in lipid structure. Combinations of structural motifs (e.g., fatty acids and head group moieties linked to various backbones), linkages (e.g., ester, ether, vinyl ether), and complexes with non-lipid species (e.g., carbohydrates and proteins) result in countless possible structures. The lipidome - the entire collection of individual lipid species in cells, tissues or biofluids - has been estimated to be composed of 1,000 to more than 180,000 molecular lipid species [1,2], but many of these species are likely very low in abundance or have not been observed [3]. These estimations do not consider isomeric lipid species with different fatty acyl double-bond positions and configurations (*cis* or *trans*), positional isomers (e.g., *sn*1, *sn*2), and stereoisomers (*R* or *S*). Ekroos et al. determined that the number of phosphatidylcholine (PC) positional isomers in Madin-Darby canine kidney II cells nearly doubled the total number of individual lipid species [4], which highlights the substantial presence of lipid isomers in nature. Furthermore, these lipid isomers can also exhibit a variety of specific biological roles. For example, the acyl position of membrane lipids can impact the enzymatic activity that occurs within cellular membranes [5]. Shinzawa-Itoh et al. [6] found biological specificity of acyl chain

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