A computational framework for integration of lipidomics data into metabolic pathways

ID 2420143
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Year 2014
Title A computational framework for integration of lipidomics data into metabolic pathways
Journal Metabolic engineering
Volume 23
Pages / **Article-Number** 1-8
Keywords Phospholipids, Database, Bioinformatics, Bis(monoacylglycero)phosphate (Bmp)

Lipids are important compounds for human physiology and as renewable resources for fuels and chemicals. In lipid research, there is a big gap between the currently available pathway-level representations of lipids and lipid structure databases in which the number of compounds is expanding rapidly with high-throughput mass spectrometry methods. In this work, we introduce a computational approach to bridge this gap by making associations between metabolic pathways and the lipid structures discovered increasingly thorough lipidomics studies. Our approach, called NICELips (Network Integrated Computational Explorer for Lipidomics), is based on the formulation of generalized enzymatic reaction rules for lipid metabolism, and it employs the generalized rules to postulate novel pathways of lipid metabolism. It further integrates all discovered lipids in biological networks of enzymatic reactions that consist their biosynthesis and biodegradation pathways. We illustrate the utility of our approach through a case study of bis(monoacylglycero)phosphate (BMP), a biologically important glycerophospholipid with immature synthesis and catabolic route(s). Using NICELips, we were able to propose various synthesis and degradation pathways for this compound and several other lipids with unknown metabolism like BMP, and in addition several alternative novel biosynthesis and biodegradation pathways for lipids with known metabolism. NICELips has potential applications in designing therapeutic interventions for lipid-associated disorders and in the metabolic engineering of model organisms for improving the biobased production of lipid-derived fuels and chemicals.

Publisher Elsevier
ISSN/ISBN 1096-7176
edoc-URL http://edoc.unibas.ch/dok/A6243434
Full Text on edoc No;
Digital Object Identifier DOI 10.1016/j.ymben.2013.12.007
PubMed ID http://www.ncbi.nlm.nih.gov/pubmed/24395008
ISI-Number WOS:000335385500001
Document type (ISI) Journal Article