

Lipidomics

Lipidomics is the large scale identification and quantitation of the diverse repertoire of lipids in biologic samples that play critical roles in cellular function. Although the field of lipidomics using mass spectrometry has been practiced for over 30 years, recent robust advances in multiple integrated technologies have greatly expanded the scope and penetrance of the field. Through the synergistic utilization of a wide array of technological advances in ionization, fragmentation, high mass accuracy analysis and robust increases in resolution, the power of lipidomics-based investigations has greatly expanded facilitating the identification of biomarkers of disease, disease mechanisms and the efficacy of therapeutic approaches for disease entities. This Virtual Issue highlights recent articles published in *Analytical Chemistry* that have utilized innovative strategies and technologies that have and will continue to greatly impact progress in the field.

-From the editorial by Michal Holčápek and Richard W. Gross

Editorial

DOI: 10.1021/ac5027644

Review

Analytical Methods in Lipidomics and Their Applications

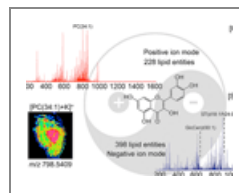
Min Li, Li Yang, Yu Bai, and Huwei Liu*

Anal. Chem., 2014, 86 (1), pp 161–175

DOI: 10.1021/ac403554h

2014 | 2013 | 2012 | 2011 | 2010 | 2009 | 2008

2014

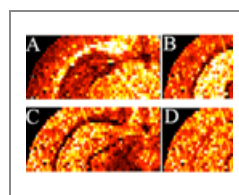


Comprehensive Imaging of Porcine Adrenal Gland Lipids by MALDI-FTMS Using Quercetin as a Matrix

Xiaodong Wang, Jun Han, Jingxi Pan, and Christoph H. Borchers*

Anal. Chem., 2014, 86 (1), pp 638–646

DOI: 10.1021/ac404044k



Shotgun Approach for Quantitative Imaging of Phospholipids Using Nanospray Desorption Electrospray Ionization Mass Spectrometry

Ingela Lanekoff*, Mathew Thomas, and Julia Laskin*

Anal. Chem., 2014, 86 (3), pp 1872–1880

DOI: 10.1021/ac403931r



X¹³CMS: global tracking of isotopic labels in untargeted metabolomics

Xiaojing Huang, Ying-Jr Chen, Kevin Cho, Igor Nikolskiy, Peter A. Crawford, and Gary J. Patti

Anal. Chem., 2014, 86 (3), pp 1632–1639

DOI: 10.1021/ac403384n

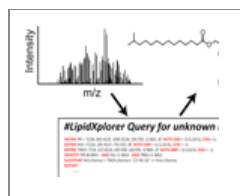
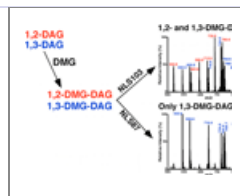
Characterization and Quantification of Diacylglycerol Species in Biological Extracts after One-Step Derivatization: A Shotgun Lipidomics Approach

Miao Wang, Jun Hayakawa, Kui Yang, and Xianlin Han*

Anal. Chem., 2014, 86 (4), pp 2146–2155

DOI: 10.1021/ac403798q

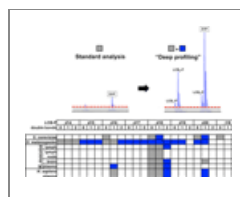




Systematic Screening for Novel Lipids by Shotgun Lipidomics

Cyrus Papan, Sider Penkov, Ronny Herzog, Christoph Thiele, Teymuraz Kurzchalia, and Andrej Shevchenko*
Anal. Chem., **2014**, 86 (5), pp 2703–2710

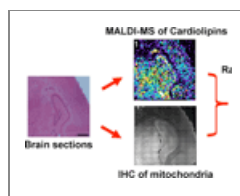
DOI: 10.1021/ac404083u



Lipidomic "Deep Profiling": An Enhanced Workflow to Reveal New Molecular Species of Signaling Lipids

Pradeep Narayanaswamy, Sudhirkumar Shinde, Robert Sulc, Rachel Kraut, Gregory Staples, Chung Hwee Thiam, Rudolf Grimm, Börje Sellergren, Federico Torta*, and Markus R. Wenk**
Anal. Chem., **2014**, 86 (13), pp 3043–3047

DOI: 10.1021/ac4039652



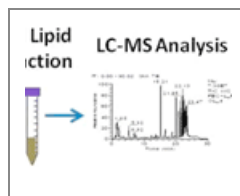
Imaging Mass Spectrometry of Diversified Cardiolipin Molecular Species in the Brain

A. A. Amoscato*, L. J. Sparvero, R. R. He, S. Watkins, H. Bayir*, and V. E. Kagan*

Anal. Chem., **2014**, 86 (13), pp 6587–6595

DOI: 10.1021/ac5011876

2013

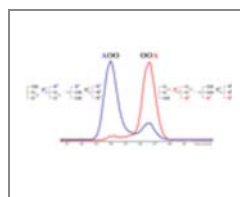


Method Development for Fecal Lipidomics Profiling

Katherine E. Gregory, Susan S. Bird, Vera S. Gross, Vasant R. Marur, Alexander V. Lazarev, W. Allan Walker, and Bruce S. Kristal*

Anal. Chem., **2013**, 85 (2), pp 1114–1123

DOI: 10.1021/ac303011k

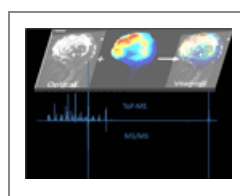


Characterization of Triacylglycerol Enantiomers Using Chiral HPLC/APCI-MS and Synthesis of Enantiomeric Triacylglycerols

Miroslav Líska* and Michal Holčápek

Anal. Chem., **2013**, 85 (3), pp 1852–1859

DOI: 10.1021/ac303237a

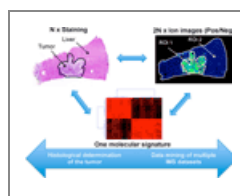


Single-Cell Lipidomics: Characterizing and Imaging Lipids on the Surface of Individual *Aplysia californica* Neurons with Cluster Secondary Ion Mass Spectrometry

Melissa K. Passarelli*, Andrew G. Ewing, and Nicholas Winograd*

Anal. Chem., **2013**, 85 (4), pp 2231–2238

DOI: 10.1021/ac303038j

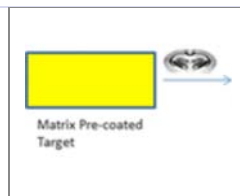


Histology-Driven Data Mining of Lipid Signatures from Multiple Imaging Mass Spectrometry Analyses: Application to Human Colorectal Cancer Liver Metastasis Biopsies

Aurélien Thomas, Nathan Heath Patterson, Martin M. Marcinkiewicz, Anthoula Lazaris, Peter Metrakos, and Pierre Chaurand*

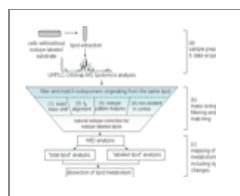
Anal. Chem., **2013**, 85 (5), pp 2860–2866

DOI: 10.1021/ac3034294



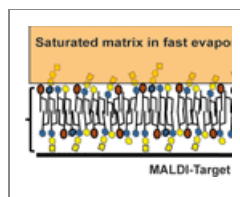
Matrix Precoated Targets for Direct Lipid Analysis and Imaging of Tissue

Junhai Yang and Richard M. Caprioli*
Anal. Chem., **2013**, 85 (5), pp 2907–2912
 DOI: 10.1021/ac303554e



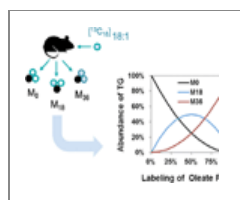
Stable Isotope-Assisted Lipidomics Combined with Nontargeted Isotopomer Filtering, a Tool to Unravel the Complex Dynamics of Lipid Metabolism

Jia Li, Miriam Hoene, Xinjie Zhao, Shili Chen, Hai Wei, Hans-Ulrich Häring, Xiaohui Lin, Zhongda Zeng, Cora Weigert, Rainer Lehmann*, and Guowang Xu*
Anal. Chem., **2013**, 85 (9), pp 4651–4657
 DOI: 10.1021/ac400293y



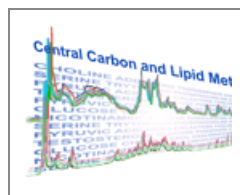
Quantitative Characterization of Tissue Globotetraosylceramides in a Rat Model of Polycystic Kidney Disease by PrimaDrop Sample Preparation and Indirect High-Performance Thin Layer Chromatography–Matrix-Assisted Laser Desorption/Ionization–Time-of-Flight–Mass Spectrometry with Automated Data Acquisition

Hermelindis Ruh, Roger Sandhoff, Björn Meyer, Norbert Gretz, and Carsten Hopf*
Anal. Chem., **2013**, 85 (13), pp 6233–6240
 DOI: 10.1021/ac400931u



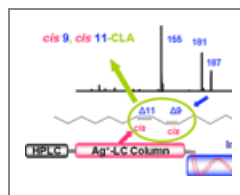
Use of [¹³C₁₈] Oleic Acid and Mass Isotopomer Distribution Analysis to Study Synthesis of Plasma Triglycerides In Vivo: Analytical and Experimental Considerations

David G. McLaren*, Helene L. Cardasis, Steven J. Stout, Sheng-Ping Wang, Vivienne Mendoza, Jose M. Castro-Perez, Paul L. Miller, Beth A. Murphy, Anne-Marie Cumiskey, Michele A. Cleary, Douglas G. Johns, Stephen F. Previs, and Thomas P. Roddy
Anal. Chem., **2013**, 85 (13), pp 6287–6294
 DOI: 10.1021/ac400363k



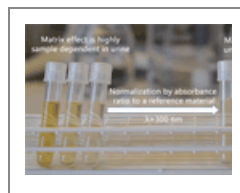
Toward 'Omic Scale Metabolite Profiling: A Dual Separation–Mass Spectrometry Approach for Coverage of Lipid and Central Carbon Metabolism

Julijana Ivanisevic, Zheng-Jiang Zhu, Lars Plate §, Ralf Tautenhahn, Stephen Chen, Peter J. O'Brien, Caroline H. Johnson, Michael A. Marletta, Gary J. Patti*, and Gary Siuzdak*
Anal. Chem., **2013**, 85 (14), pp 6876–6884
 DOI: 10.1021/ac401140h



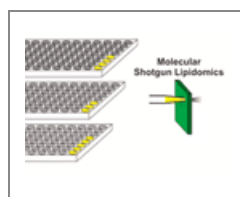
Identification of Conjugated Linoleic Acid (CLA) Isomers by Silver Ion-Liquid Chromatography/In-line Ozonolysis/Mass Spectrometry (Ag⁺-LC/O₃-MS)

Chenxing Sun, Brenna A. Black, Yuan-Yuan Zhao, Michael G. Gänzle, and Jonathan M. Curtis*
Anal. Chem., **2013**, 85 (15), pp 7345–7352
 DOI: 10.1021/ac401242z



Quantification of Lipid Mediator Metabolites in Human Urine from Asthma Patients by Electrospray Ionization Mass Spectrometry: Controlling Matrix Effects

David Balgoma*, Johan Larsson, Joshua Rokach, John A. Lawson, Kameran Daham, Barbro Dahlén, Sven-Erik Dahlén, and Craig E. Wheelock*
Anal. Chem., **2013**, 85 (16), pp 7866–7874
 DOI: 10.1021/ac401461b

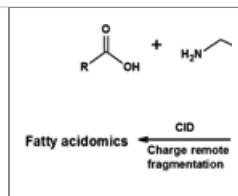


Long-Term Performance and Stability of Molecular Shotgun Lipidomic Analysis of Human Plasma Samples

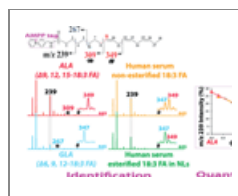
Laura A. Heiskanen, Matti Suoniemi, Hung Xuan Ta, Kirill Tarasov, and Kim Ekroos*
Anal. Chem., **2013**, 85 (18), pp 8757–8763
 DOI: 10.1021/ac401857a

Fatty Acidomics: Global Analysis of Lipid Species Containing a Carboxyl Group with a Charge-Remote Fragmentation-Assisted Approach

Miao Wang, Rowland H. Han, and Xianlin Han*

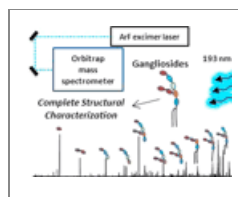


Anal. Chem.
, 2013, 85 (19), pp 9312–9320
DOI: 10.1021/ac402078p



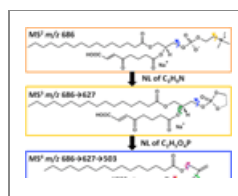
Identification and Quantitation of Fatty Acid Double Bond Positional Isomers: A Shotgun Lipidomics Approach Using Charge-Switch Derivatization

*Kui Yang, Beverly Gibson Dilthey, and Richard W. Gross**
Anal. Chem., 2013, 85 (20), pp 9742–9750
DOI: 10.1021/ac402104u



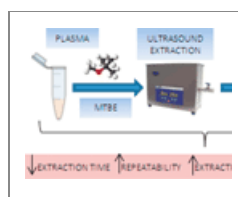
Structural Characterization of Gangliosides and Glycolipids via Ultraviolet Photodissociation Mass Spectrometry

*John P. O'Brien and Jennifer S. Brodbelt**
Anal. Chem., 2013, 85 (21), pp 10399–10407
DOI: 10.1021/ac402379y



Characterization of Phosphatidylcholine Oxidation Products by MALDI MSⁿ

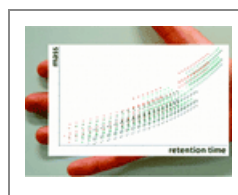
*Whitney L. Stutts, Robert F. Menger, András Kiss, Ron M. A. Heeren, and Richard A. Yost**
Anal. Chem., 2013, 85 (23), pp 11410–11419
DOI: 10.1021/ac402400f



Plasma Lipidomic Profiling Method Based on Ultrasound Extraction and Liquid Chromatography Mass Spectrometry

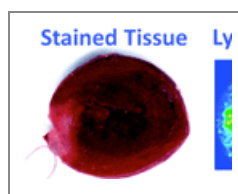
Consuelo Pizarro, Irene Arenzana-Rámila, Nuria Pérez-del-Notario, Patricia Pérez-Matute, and José-María González-Sáiz*
Anal. Chem., 2013, 85 (24), pp 12085–12092
DOI: 10.1021/ac403181c

2012



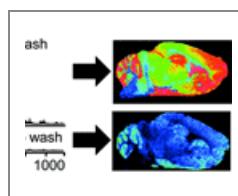
Profiling and Characterizing Skin Ceramides Using Reversed-Phase Liquid Chromatography-Quadrupole Time-of-Flight Mass Spectrometry

*Ruben t'Kindt, Lucie Jorge, Emmie Dumont, Pauline Couturon, Frank David, Pat Sandra, and Koen Sandra**
Anal. Chem., 2012, 84 (1), pp 403–411
DOI: 10.1021/ac202646v



MALDI Mass Spectrometric Imaging of Cardiac Tissue Following Myocardial Infarction in a Rat Coronary Artery Ligation Model

*Robert F. Menger, Whitney L. Stutts, Dhanalakshmi S. Anbukumar, John A. Bowden, David A. Ford, and Richard A. Yost**
Anal. Chem., 2012, 84 (2), pp 1117–1125
DOI: 10.1021/ac202779h



Enhanced Sensitivity for High Spatial Resolution Lipid Analysis by Negative Ion Mode Matrix Assisted Laser Desorption Ionization Imaging Mass Spectrometry

*Peggi M. Angel, Jeffrey M. Spraggins, H. Scott Baldwin, and Richard Caprioli**
Anal. Chem., 2012, 84 (3), pp 1557–1564
DOI: 10.1021/ac202383m

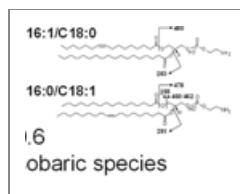


Sublimation of New Matrix Candidates for High Spatial Resolution Imaging Mass Spectrometry of Lipids: Enhanced Information in Both Positive and Negative Polarities after 1,5-Diaminonaphthalene Deposition

Aurélien Thomas, Jade Laveaux Charbonneau, Erik Fournaise, and Pierre Chaurand*

Anal. Chem., **2012**, 84 (4), pp 2048–2054

DOI: 10.1021/ac2033547

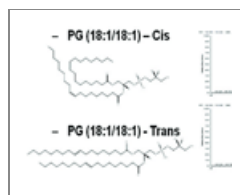


MALDI Imaging and Structural Analysis of Rat Brain Lipid Negative Ions with 9-Aminoacridine Matrix

Christopher D. Cerruti, Farida Benabdellah, Olivier Laprèvote, David Touboul*, and Alain Brunelle

Anal. Chem., **2012**, 84 (5), pp 2164–2171

DOI: 10.1021/ac2025317

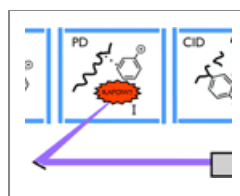


Separation of Cis–Trans Phospholipid Isomers Using Reversed Phase LC with High Resolution MS Detection

Susan S. Bird, Vasant R. Marur, Irina G. Stavrovskaya, and Bruce S. Kristal*

Anal. Chem., **2012**, 84 (13), pp 5509–5517

DOI: 10.1021/ac300953j

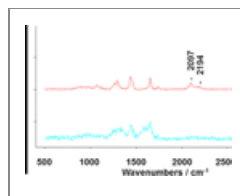


Differentiation of Complex Lipid Isomers by Radical-Directed Dissociation Mass Spectrometry

Huong T. Pham, Tony Ly, Adam J. Trevitt, Todd W. Mitchell, and Stephen J. Blanksby*

Anal. Chem., **2012**, 84 (17), pp 7525–7532

DOI: 10.1021/ac301652a

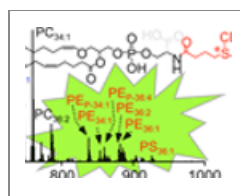


Noninvasive Imaging of Intracellular Lipid Metabolism in Macrophages by Raman Microscopy in Combination with Stable Isotopic Labeling

Christian Matthäus*, Christoph Krafft, Benjamin Dietzek, Bernhard R. Brehm, Stefan Lorkowski, and Jürgen Popp

Anal. Chem., **2012**, 84 (20), pp 8549–8556

DOI: 10.1021/ac3012347

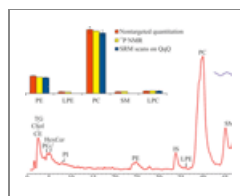


Comprehensive Lipidome Profiling of Isogenic Primary and Metastatic Colon Adenocarcinoma Cell Lines

Cassie J. Phaner, Sichang Liu, Hong Ji, Richard J. Simpson, and Gavin E. Reid*

Anal. Chem., **2012**, 84 (21), pp 8917–8926

DOI: 10.1021/ac302154g



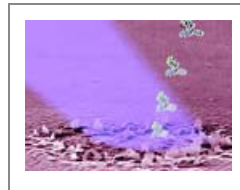
Nontargeted Quantitation of Lipid Classes Using Hydrophilic Interaction Liquid Chromatography–Electrospray Ionization Mass Spectrometry with Single Internal Standard and Response Factor Approach

Eva Cifková, Michal Holčápek*, Miroslav Lisa, Magdaléna Ovčáčíková, Antonín Lyčka, Frédéric Lynen, and Pat Sandra

Anal. Chem., **2012**, 84 (22), pp 10064–10070

DOI: 10.1021/ac3024476

2011

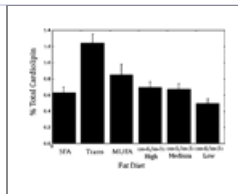


Nanostructure-Initiator Mass Spectrometry Metabolite Analysis and Imaging

Matthew P. Greving, Gary J. Patti, and Gary Siuzdak

Anal. Chem., **2011**, 83 (1), pp 2–7

DOI: 10.1021/ac101565f

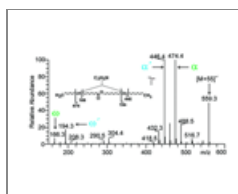


Characterization of Mitochondrial Cardiolipins and Monolysocardiolipins

Susan S. Bird, Vasant R. Marur, Matthew J. Sniatynski, Heather K. Greenberg, and Bruce S. Kristal

Anal. Chem., **2011**, 83 (3), pp 940-949

DOI: 10.1021/ac102598u

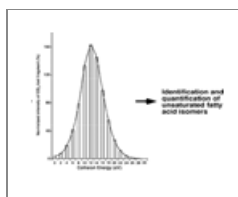


Localization of Double Bonds in Wax Esters by High-Performance Liquid Chromatography/Atmospheric Pressure Chemical Ionization Mass Spectrometry Utilizing the Fragmentation of Acetonitrile-Related Adducts

Vladimír Vrkoš, Martina Hájková, Karolína Pecková, Klára Urbanová, and Josef Cvačka

Anal. Chem., **2011**, 83 (8), pp 2978-2986

DOI: 10.1021/ac1030682

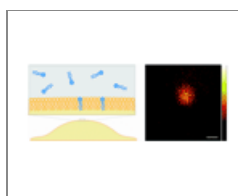


Identification and Quantitation of Unsaturated Fatty Acid Isomers by Electrospray Ionization Tandem Mass Spectrometry: A Shotgun Lipidomics Approach

Kui Yang, Zhongdan Zhao, Richard W. Gross, and Xianlin Han

Anal. Chem., **2011**, 83 (11), pp 4243-4250

DOI: 10.1021/ac2006119

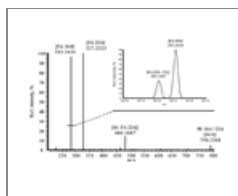


Relative Quantification of Phospholipid Accumulation in the PC12 Cell Plasma Membrane Following Phospholipid Incubation Using TOF-SIMS Imaging

Ingela Lanekoff, Peter Sjövall, and Andrew G. Ewing

Anal. Chem., **2011**, 83 (13), pp 5337-5343

DOI: 10.1021/ac200771g

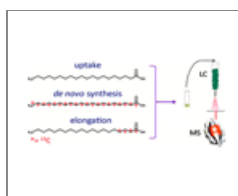


Bottom-Up Shotgun Lipidomics by Higher Energy Collisional Dissociation on LTQ Orbitrap Mass Spectrometers

Kai Schuhmann, Ronny Herzog, Dominik Schwudke, Wolfgang Metelmann-Strupat, Stefan R. Bornstein, and Andrej Shevchenko

Anal. Chem., **2011**, 83 (14), pp 5480-5487

DOI: 10.1021/ac102505f



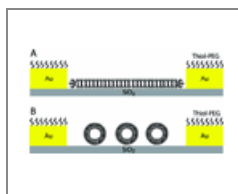
Liquid Chromatography-High Resolution Mass Spectrometry Analysis of Fatty Acid Metabolism

Jurre J. Kamphorst, Jing Fan, Wenyun Lu, Eileen White, and Joshua D. Rabinowitz

Anal. Chem., **2011**, 83 (23), pp 9114-9122

DOI: 10.1021/ac202220b

2010

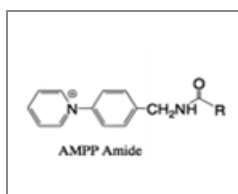


Spatial-Resolution Limits in Mass Spectrometry Imaging of Supported Lipid Bilayers and Individual Lipid Vesicles

Anders Gunnarsson, Felix Kollmer, Sascha Sohn, Fredrik Höök* and Peter Sjövall*

Anal. Chem., **2010**, 82 (6), pp 2426-2433

DOI: 10.1021/ac902744u



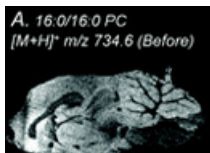
Improved Sensitivity Mass Spectrometric Detection of Eicosanoids by Charge Reversal Derivatization

James G. Bollinger, Wallace Thompson, Ying Lai, Rob C. Oslund, Teal S. Hallstrand, Martin Sadílek, Frantisek Turecek, and Michael H. Gelb

Anal. Chem., **2010**, 82 (16), pp 6790-6796

DOI: 10.1021/ac100720p

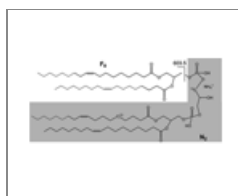
Relationship between MALDI IMS Intensity and Measured Quantity of Selected Phospholipids in Rat Brain Sections



Joseph A. Hankin and Robert C. Murphy

Anal. Chem., **2010**, 82 (20), pp 8476-8484

DOI: 10.1021/ac101079v



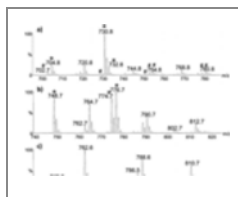
Simultaneous Quantification of Cardiolipin, Bis(monoacylglycero)phosphate and their Precursors by Hydrophilic Interaction LC-MS/MS Including Correction of Isotopic Overlap

Max Scherer, Gerd Schmitz, and Gerhard Liebisch

Anal. Chem., **2010**, 82 (21), pp 8794-8799

DOI: 10.1021/ac1021826

2009

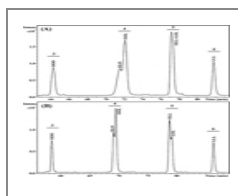


Identification of Abundant Alkyl Ether Glycerophospholipids in the Human Lens by Tandem Mass Spectrometry Techniques

Jane M. Deeley, Michael C. Thomas, Roger J. W. Truscott, Todd W Mitchell* and Stephen J. Blanksby*

Anal. Chem., **2009**, 81 (5), 1920–1930

DOI: 10.1021/ac802395d

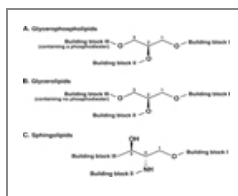


Regioisomeric Characterization of Triacylglycerols Using Silver-Ion HPLC/MS and Randomization Synthesis of Standards

Miroslav Lísá, Hana Velínská and Michal Holčápek*

Anal. Chem., **2009**, 81 (10), 3903–3910

DOI: 10.1021/ac900150j

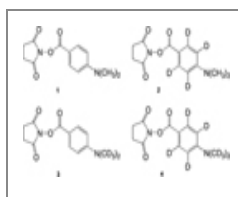


Automated Lipid Identification and Quantification by Multidimensional Mass Spectrometry-Based Shotgun Lipidomics

Kui Yang, Hua Cheng, Richard W. Gross and Xianlin Han*

Anal. Chem., **2009**, 81 (11), 4356–4368

DOI: 10.1021/ac900241u



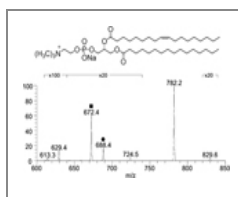
Stable Isotope Labeled 4-(Dimethylamino)benzoic Acid Derivatives of Glycerophosphoethanolamine Lipids

Karin A. Zemski Berry, William W. Turner, Michael S. VanNieuwenhze and Robert C. Murphy*

Anal. Chem., **2009**, 81 (16), pp 6633–6640

DOI: 10.1021/ac900583a

2008



Ozone-induced dissociation: Elucidation of double bond position within mass-selected lipid ions

Michael C. Thomas, Todd W. Mitchell, David G. Harman, Jane M. Deeley, Jessica R. Nealon, and Stephen J. Blanksby*

Anal. Chem., **2008**, 80 (1), pp 303–311

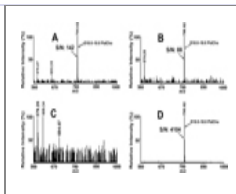
DOI: 10.1021/ac7017684

Matrix-Assisted Laser Desorption/Ionization Time-of-Flight Mass Spectrometric Analysis of Cellular Glycerophospholipids Enabled by Multiplexed Solvent Dependent Analyte–Matrix Interactions

Gang Sun, Kui Yang, Zhongdan Zhao, Shaoping Guan, Xianlin Han and Richard W. Gross*

Anal. Chem., **2008**, 80 (19), pp 7576–7585

DOI: 10.1021/ac801200w



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