Supplementary information for:

Liquid Chromatography Quadrupole Time-of-Flight Mass Spectrometry Characterization of Metabolites Guided by the METLIN Database

Andrew W. Schultz¹, Junhua Wang¹, Zheng-Jiang Zhu¹, Caroline H. Johnson¹, Steven M. Yannone², Gary J. Patti³,* and Gary Siuzdak¹,*

¹Scripps Center for Metabolomics and Mass Spectrometry, The Scripps Research Institute, 10550 North Torrey Pines Road, La Jolla, CA 92037

²Life Sciences Division, Lawrence Berkeley National Lab, One Cyclotron Road, Berkeley, CA 94720

³Departments of Chemistry, Genetics, and Medicine, Washington University, 660 South Euclid Ave, St. Louis, MO 63110

Corresponding authors: Gary Siuzdak (siuzdak@scripps.edu) phone (858) 784-9415 fax (858) 784-9496
Gary J. Patti (gjpattij@wustl.edu) phone (314) 362-8358

Supplemental Figure 1: Example of in source fragmentation. Two species, m/z 480.3084 and m/z 339.2892 are observed to coelute (A), with both species observed in MS (B). Comparison of the high resolution parent ion and the MS/MS fragment (D) supports the characterization of m/z 480.3084 as a lysoPE(18:1). Note the prominent fragment at m/z 339.2892. m/z 339.2892 is observed in the MS scan (D). Fragmentation of this species provides the MS/MS spectrum (C) which is characteristic of a dehydrated oleoyl (18:1) glycerol, a major fragment of lysoPE(18:1).