Supporting Information

LipPy software

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A database of known lipid structures, fragmentation patterns, and neutral losses^{2,3} was created in silico 3 4 using Lipid MAPS nomenclature. Lipids were identified by matching the observed precursor/fragment mass pairs with entries in the database. LipPY® applied a set of filters to the data set to eliminate low abundance 5 6 fragment signals with no analytical significance and to remove the isotopic contributions of lower mass 7 peaks. With this approach, the number of false positive identifications was dramatically reduced. Identified 8 lipids were normalized to their corresponding internal standard (i.e. each lipid of a specific class was normalized to its correspondent lipid class internal standard). When the appropriate internal standard was 9 10 missing, identified lipids were normalized to cholesterol ester (CE) or PE for positive and negative

ionization mode, respectively. Results were expressed in mean±standard error format.