Supplemental information S1

Lipidomics reagents. All Liquid chromatography mass spectrometry (LC-MS) grade reference compounds, water (H2O) and methanol (MeOH) were from VWR International (Plainview, NY). LC grade ammonium formate, chloroform (CHCl3), 2-propanol (IPA) and formic ac-id were from Sigma-Aldrich (Saint Quentin Fallavier, France). All internal standards (IS) used in lipidomic approach were purchased from Avanti Polar Lipids, Inc. (Alabaster, Alabama, USA).

Metabolomics reagents. Ultra-high performance liquid chromatography/mass spectrometry reference grade solvents (acetonitrile and methanol) were purchased from VWR International (Plainview, NY, USA). Analytical-grade ammonium hydroxide and ammonium carbonate were obtained from Sigma-Aldrich (Saint-Quentin-Fallavier, France). The stable isotope-labeled mix (Algal amino acid mixture-13C,15N) that was used as an internal standard for the metabolomic approach was purchased from Sigma-Aldrich (Saint-Quentin-Fallavier, France). Deionized water came from a Milli-Q Elix system fitted with an LC-PaK and a MilliPak filter at 0.22 µm (Merck Millipore, Guyancourt, France).

Sample preparation for lipidomics. Plasma samples were extracted using adapted methods reported in Seyer et al., 2016 [1]. A volume of 100 µL of plasma was added to 490 µL of CHCl3/MeOH 1:1 (v/v) and 10 µL of internal standard mixture. Sam-ples were vortexed for 60 s and then sonicated for 30 s using a sonication probe. Extraction was performed after 2 h at 4°C with mixing. In addition, 75 µL of H2O was added and samples were vortexed for 60 s before centrifugation at 15000 rpm for 10 min at 4°C. The upper phase (aqueous phase), containing ganglioside species and several lysophospho-lipids, was transferred into a glass tube and then dried under a stream of nitrogen. The protein disk interphase was discarded and the lower rich-lipid phase (organic phase) was pooled with the dried upper phase. Samples were reconstituted with MeOH/IPA/H2O 65:35:5 (v/v/v) and one hundred-fold diluted from the initial plasma volume (100 µl), then vortexed for 30 s and sonicated for 60 s before injection.

Sample preparation for metabolomics. Eight volumes of frozen acetonitrile (–20 °C) containing internal standards (labeled mix of amino acids at 10 µg/mL) were added to 100 µL of heparin plasma samples from fasting patients (collected in the Nucleipark study) and vortexed. The resulting samples were then sonicated for 10 minutes and centrifuged for 2 minutes at 10,000 × g at 4 °C. Supernatants were incubated at 4 °C for 1 hour for the slow protein precipitation process. Samples were centrifuged for 20 minutes at 20,000 × g at 4 °C. Supernatants were transferred to another series of tubes, and then dried and stored at –80 °C prior to the liquid chromatography/mass spectrometry analyses.

Référence

1. Seyer, A.; Boudah, S.; Broudin, S.; Junot, C.; Colsch, B. Annotation of the Human Cerebrospinal Fluid Lipidome Using High Resolution Mass Spectrometry and a Dedicated Data Processing Workflow. *Metabolomics* **2016**, *12*, 91, doi:10.1007/s11306-016-1023-8.