\* MALDI mMass pre-processed raw data \*

Attached msd data files (MALDI\_RCC\_data.zip) were obtained from raw data files using clipboard exact mass export function of Qual Browser of Thermo XCalibur 4.0.27.10 software (Thermo Fisher Scientific). Each spectrum was obtained by averaging of 2.2 minutes TIC record and then exported to open-source mass spectrometry tool mMass (free available at www.mmass.org). All attached .msd files can be open using this software.

Workflow for the data evaluation:

1. Open all files corresponding to one sample (e.g., DV018a, DV018b, DV018c, DV018d, DV018e). It is sufficient to copy these files to opened mMass window
2. Now, you will see overlaid mass spectra. All values of m/z together with their intensities can be further copied to attached LipidQuant excel script: Click to individual sample name at the bottom right window and then select all ions (columns) in bottom left window and transfer m/z with particular intensities to “LipidQuant\_MALDI\_RCC.xlsm” file using Ctrl C and Ctrl V (place it on the B10 position). Repeat this step and copy all binary data (m/z, intensities) for other files within the sample (second binary data set place on the D10 position, third set on the F10, forth on the H10, and fifth on the J10).
3. When all binary data within selected sample are copied to START-NEG list of LipidQuant\_MALDI.xlsm, click to Calculate button for the matching of copied m/z with the lipids in the database including internal standard. You will be now redirect to List Database\_NEG, where you can select all matched intensities together with standard deviations and copy them to another excel file where calculations of molar or relative intensities can be done.
4. Repeat all steps for other samples

This peak assignment resulted in the generation of the list of present m/z of the studied lipids with the median intensities and relative standard deviations of repetitions for each measured sample, which was used for further calculations of relative and molar concentrations.

Resulted lists of all m/z together with their median intensities for all studied samples are presented in „Results\_all.xlsx” (sheets plasma \_raw\_INT, urine\_raw\_INT, tissue\_raw\_INT). All intensities below the threshold 8000 (minimum intensity for reproducible quantitative results) are replaced there by 8000. Only lipids, which met two inclusion criteria, have been further used for the calculation of relative concentrations. The first criterion (inclusion criterion 1) is that the evaluated lipid must be present at least in case of 50% of samples within both groups (control x cancer) of individual datasets (plasma, urine, tissue). The second criterion (inclusion criterion 2) is that the coefficient of variance of the raw intensities (Supplementary Data 1-3) of the lipids in the measured QC samples must be less than 35%. In case of urine samples, we have also excluded 27 selected subjects (24 patients and 3 controls) because more than 50% of the lipids were below LOQ or the IS signal was below LOQ due to the high matrix effect (inclusion criterion 3). For relative quantitation, the zero values (sheets plasma \_raw\_INT, urine\_raw\_INT, tissue\_raw\_INT) were replaced by the value corresponding to lowest reproducible intensity (8000) for all lipids and the signal intensities of one specie were related to the sum of all intensities for all lipid species within a particular class (SM, sulfatides and sterol sulfates) and multiplied by 100 for each sample separately to calculate relative % (the percentage abundance of lipid species within individual lipid classes).

For the calculation of molar concentrations, values of raw intensities below the threshold 8000 were not replaced and first the intensity of lipid species was divided by the intensity of a particular IS and multiplied by the concentration of IS (except tissue samples, for which these ratios were multiplied by 100). Then zero values were replaced by 80% of the minimum of concentrations within all samples for each corresponding lipid species (each column).

In this exel file, all-important information including the mMass file ID, article sample ID, gender, BMI, or sample type, can be found. Manual check of lipid overlaps was performed before the IS normalization (List 1) because used mass resolution was not sufficient to completely resolve some peaks of very closed masses (Mass analyzers with higher mass resolving power can solve this problem).