

## **Description of Additional Supplementary Files**

File Name: Supplementary Data 1

Description: Cardiolipins metadata contains spectral data and associated data (Nano-ESI-MS/MS) used to identify metabolites relevant for hypothesis generation.

File Name: Supplementary Data 2

Description: Ceramides/sphingomyelins metadata contains spectral data and associated data (Nano-ESI-MS/MS) used to identify metabolites relevant for hypothesis generation.

File Name: Supplementary Data 3

Description: Fatty acids metadata contains spectral data and associated data (Nano-ESI-MS/MS) used to identify metabolites relevant for hypothesis generation.

File Name: Supplementary Data 4

Description: GPLs Metadata contains spectral data and associated data (Nano-ESI-MS/MS) used to identify metabolites relevant for hypothesis generation.