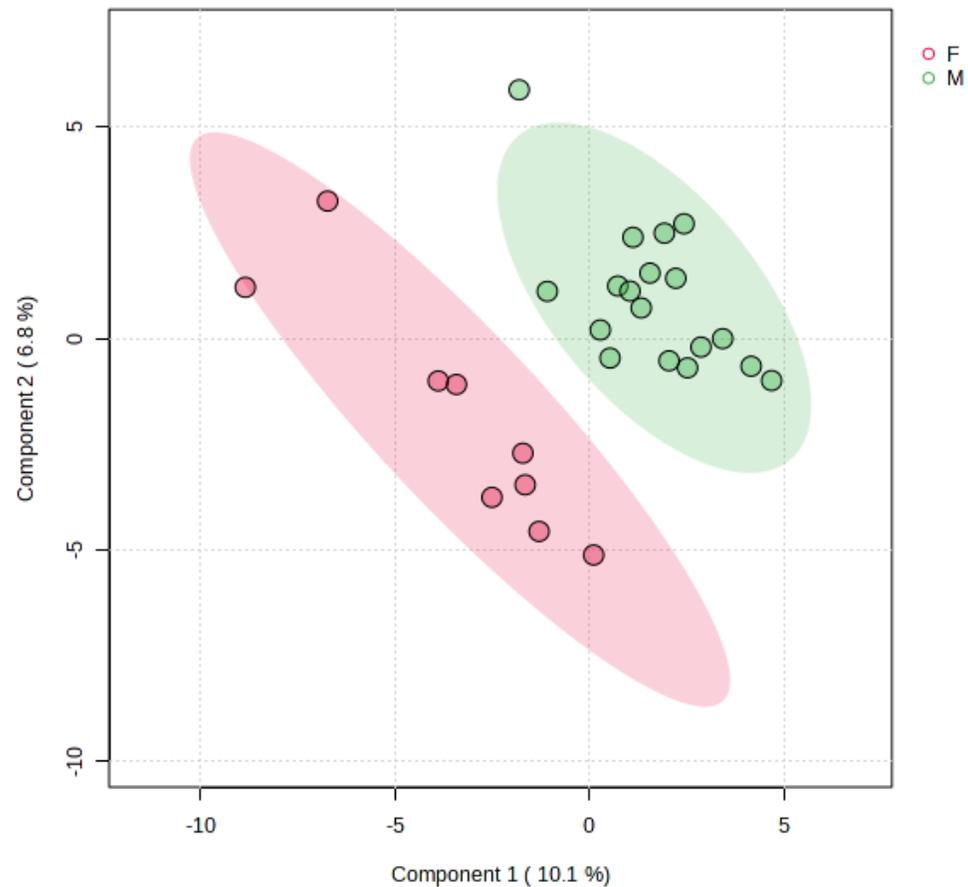


A**Scores Plot****B**

Butyrylcarnitine
 Malonylcarnitine
 Hexenoylcarnitine
 Propionic acid
 Lysophosphatidylcholine acyl C17:0
 Tiglylcarnitine
 Diacetylspermine
 Serine
 Hydroxyoctadecenoylcarnitine
 Hydroxytetradecenoylcarnitine
 Octadecadienylcarnitine
 Hippuric acid
 Methylglutaryl carnitine
 p-Hydroxyhippuric acid
 Serotonin

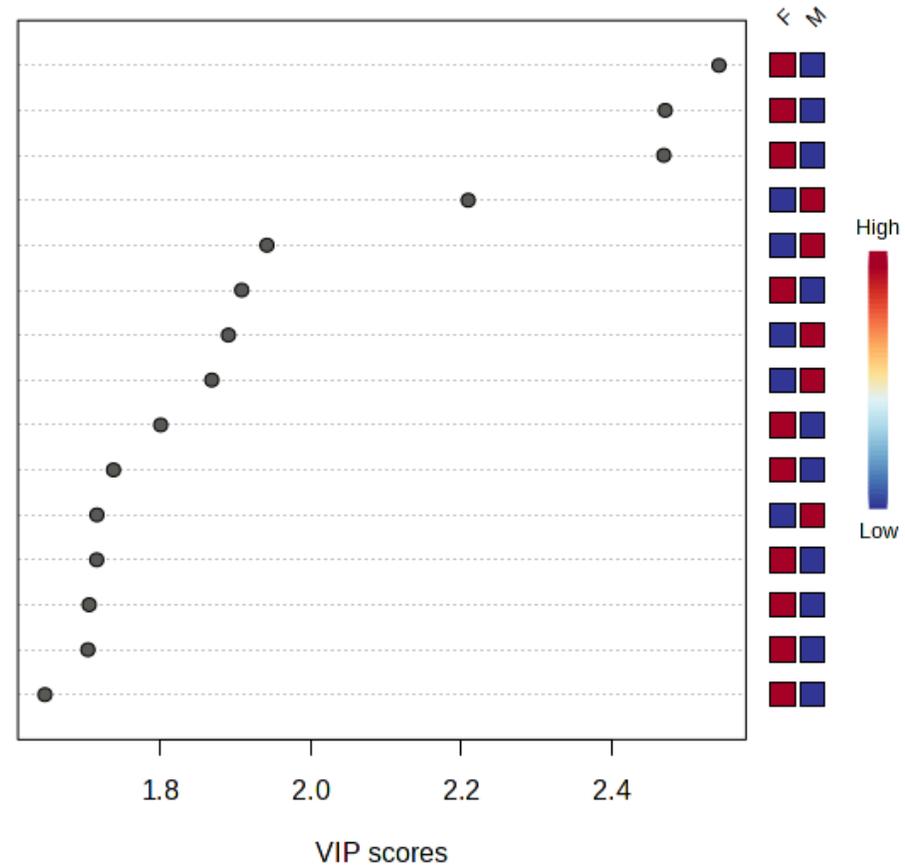


Figure S4. Biliary group – PLS-DA sex-based analysis. **A.** scores plot between the first 2 components and **B** important features identified by PLS-DA.