

MS Summary

Samples were ionized using Electron Spray Ionization (ESI) in both the modes. The various MS parameters used for the present study are as discussed. The gas flow, GS1 and GS2 were kept at 50 psi, curtain gas flow (CUR) at 30 psi and capillary voltage (ISVF) at 5500 V for positive and -4500 V for negative ionization mode with source temperature 400⁰C for both ionization modes. The MS calibration was performed through CDS (calibrant delivery system). For MS/MS fragmentation of metabolites, collision energy was set at 35 eV with a collision energy spread of ± 15 eV and declustering potential of 60 eV. Mass range was set at 100-1200m/z. Metabolites were identified by matching with company provided library and Metlin public database (<https://metlin.scripps.edu>).