Metabolomics method

Metabolomics analysis for 100 metabolites was performed as previously described (Nikkanen et al. Mitochondrial DNA Replication Defects Disturb Cellular dNTP Pools and Remodel One-Carbon Metabolism. Cell Metab. 2016 Apr 12;23(4):635-48. doi: 10.1016/j.cmet.2016.01.019.). For 11 additional metabolites in this study, the same extracted samples from 100 metabolites analysis were injected under different chromatography and mass spectrometry conditions for the analysis of methionine cycle metabolites together with calibration curve. Instrumental and analytical conditions were same as for 100 metabolites analysis except that metabolites were separated in 5.6 min of run time using 10 mM ammonium formate, pH 3 in the mobile phase A and B. The detection system, a Xevo® TQ-S tandem triple quadrupole mass spectrometer was operated in only positive polarity and optimized mass dependent parameters like declustering potential (DP) and collision energy (CE) were used for detection of the methionine cycle metabolites.