Experimental Design and Sample Description:

A set of [***sample description***: XXX human urine samples] was analyzed by UPLC-TOF MS in a single instrument run following the [***QC protocol***: protocol XXX (add reference if applicable)]. The QC procedure was applied for [***purpose***: assessing the validity of the data from an analytical standpoint.] Analysis was performed using an [***instruments &******manufacturer***:Acquity UPLC system (Waters, Elstree, UK), connected to an LCT Premier Time of Flight (ToF) mass spectrometer (Waters Micromass)], using an [***ion source***: electrospray ion- ization (ESI) source.] The analysis was performed in [***ionization mode*:** positive (ESI+) mode]. Data were recorded for the [***m/z region***: m/z region of 50–1000 in V-mode] with a [***scan time***: scan time of 0.20s] and [***dwell time***: dwell time of 0.01s] between scans. [***chromatographic separation***:Chromatographic separation was performed on an Acquity UPLC HSS T3C18 (1.8 m, 2.1mm×100mm) column, at 40◦C.] [***injection volume*:** The injection volume was 5 L.] [***replicates***: The samples were analyzed in random order and QC samples were analyzed every XX samples. Run the QC sample a minimum of 5.] The batch comprised XXX (total sample number) analyses with XX conditioning QC samples injected at the beginning and XX QC samples placed regularly in between samples. [***batch duration***: The duration of the analytical batch was 45h.] Samples were kept at 4◦C in the auto-sampler during analysis The acquired chromatographic data were processed by [***analyze******software & parameters*:** XCMS using optimized parameters]. [***allowable m/z***: 10ppm was set as the maximum allowable m/z variation between two successive scans], and the [***SNR***: signal-to-noise ratio was set at 10]. [***normalization method***: Normalization of the data was done using the median fold change algorithm.]