**XCMS Output Files Description for Readme file**

**“XCMS-diffreport-MultiClass” -** Pair-wise (a direct comparison of two data sets) comparisons to investigate differences in metabolites for the high (without overt cytotoxicity) and low exposure concentrations for each compound. Used to identify significant metabolites that were different between the low and high exposure concentrations. This analysis was completed to determine whether expected changes in endogenous metabolites were occurring based on putative mode of action of the various test articles

**“XCMS-Report-annotaated-SingleClass” –** Data processed using a single data analysis method (all data were analyzed together without statistical comparisons). This method allows for multiple experimental conditions to be examined at a single time, in this case multiple exposure concentrations, instead of being limited to two experimental conditions as is the case with the pair-wise data analysis method.