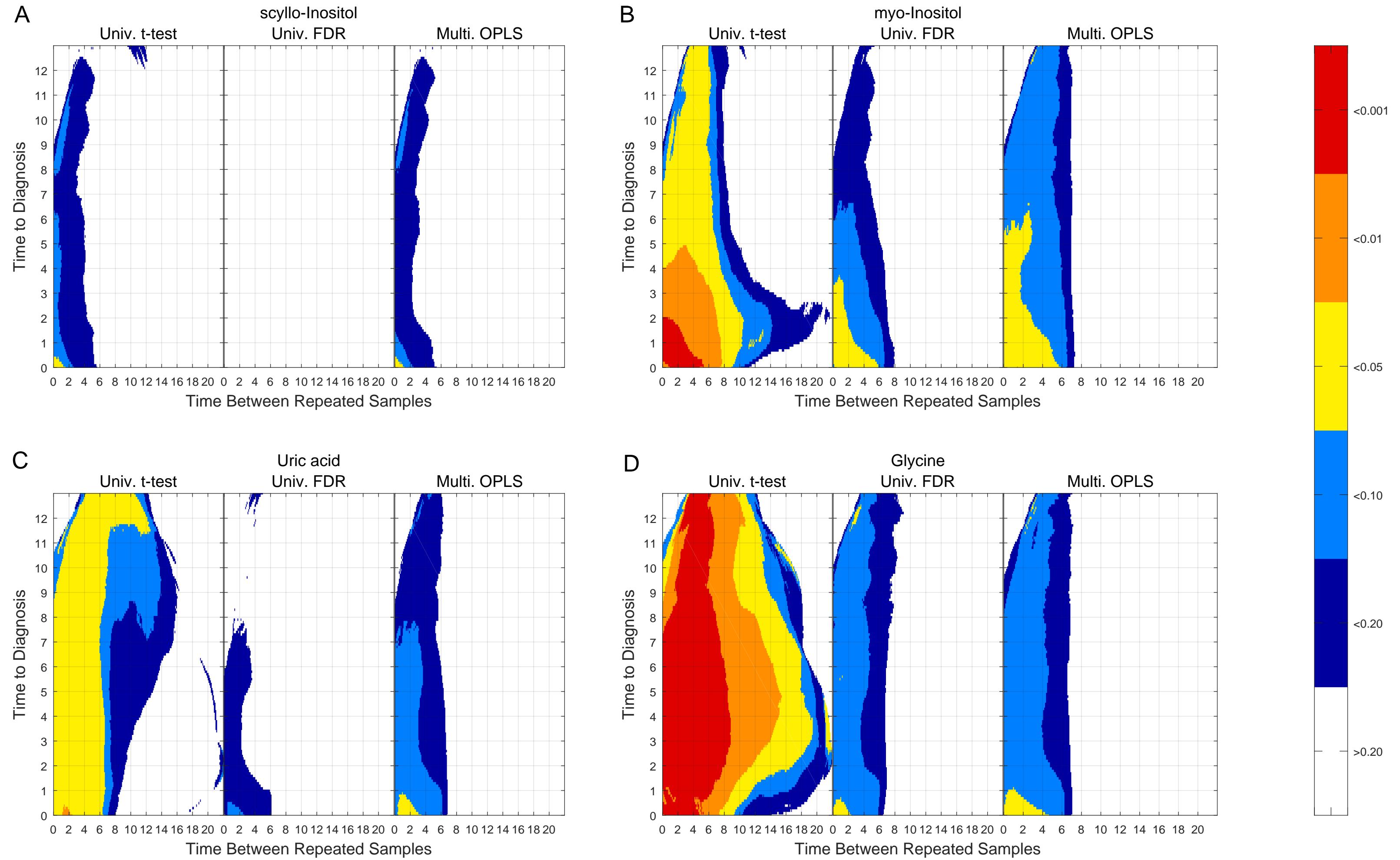
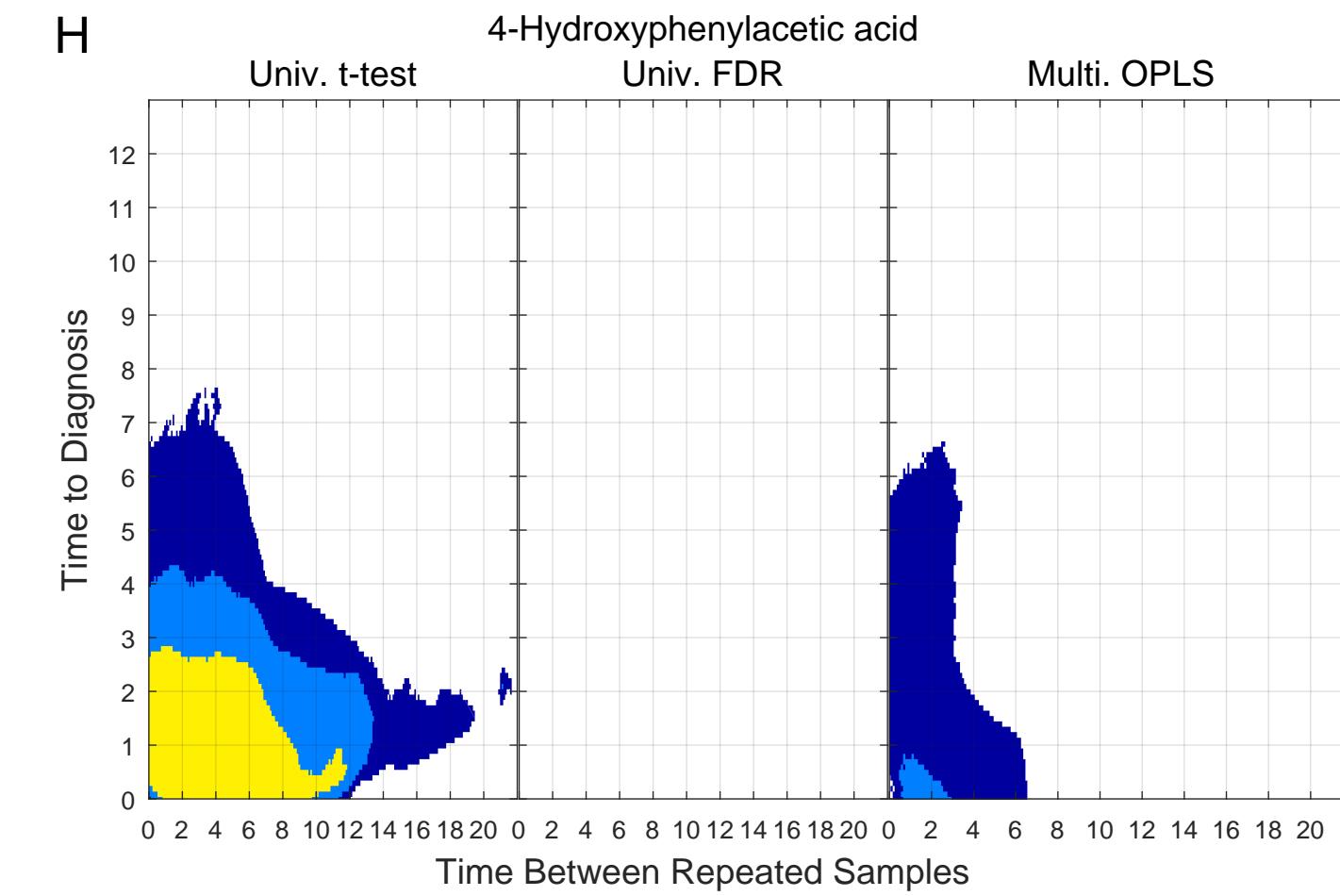
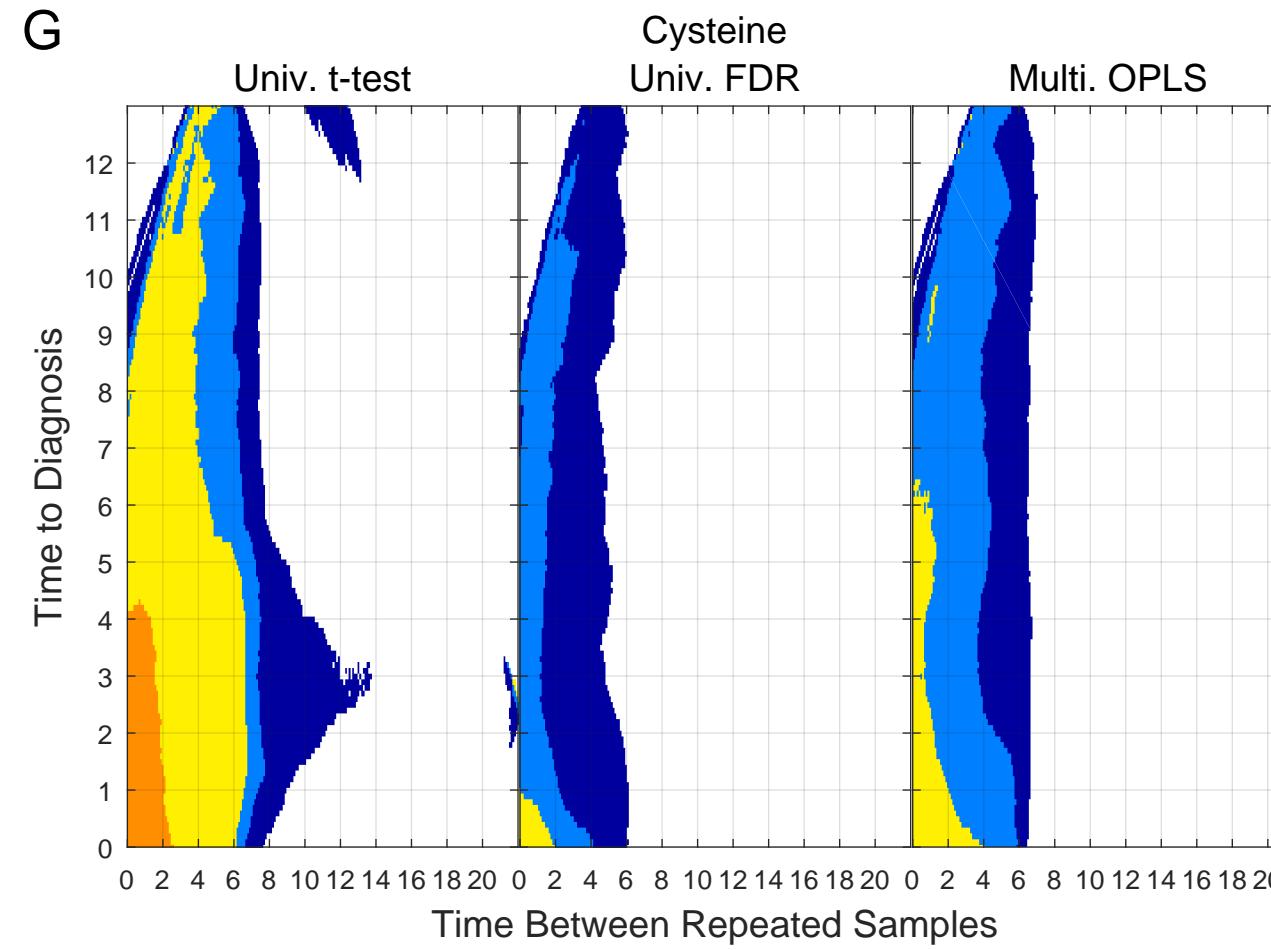
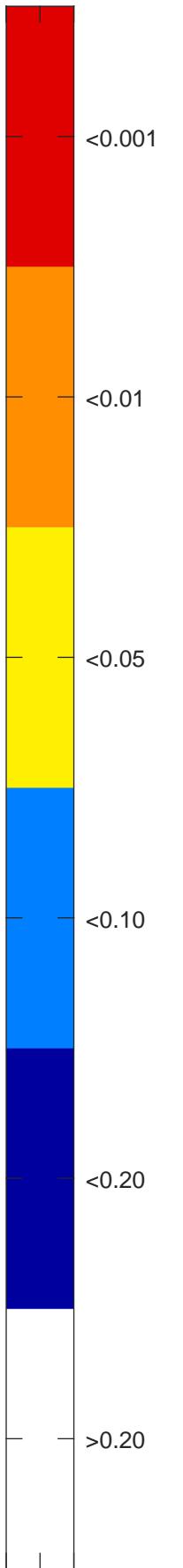
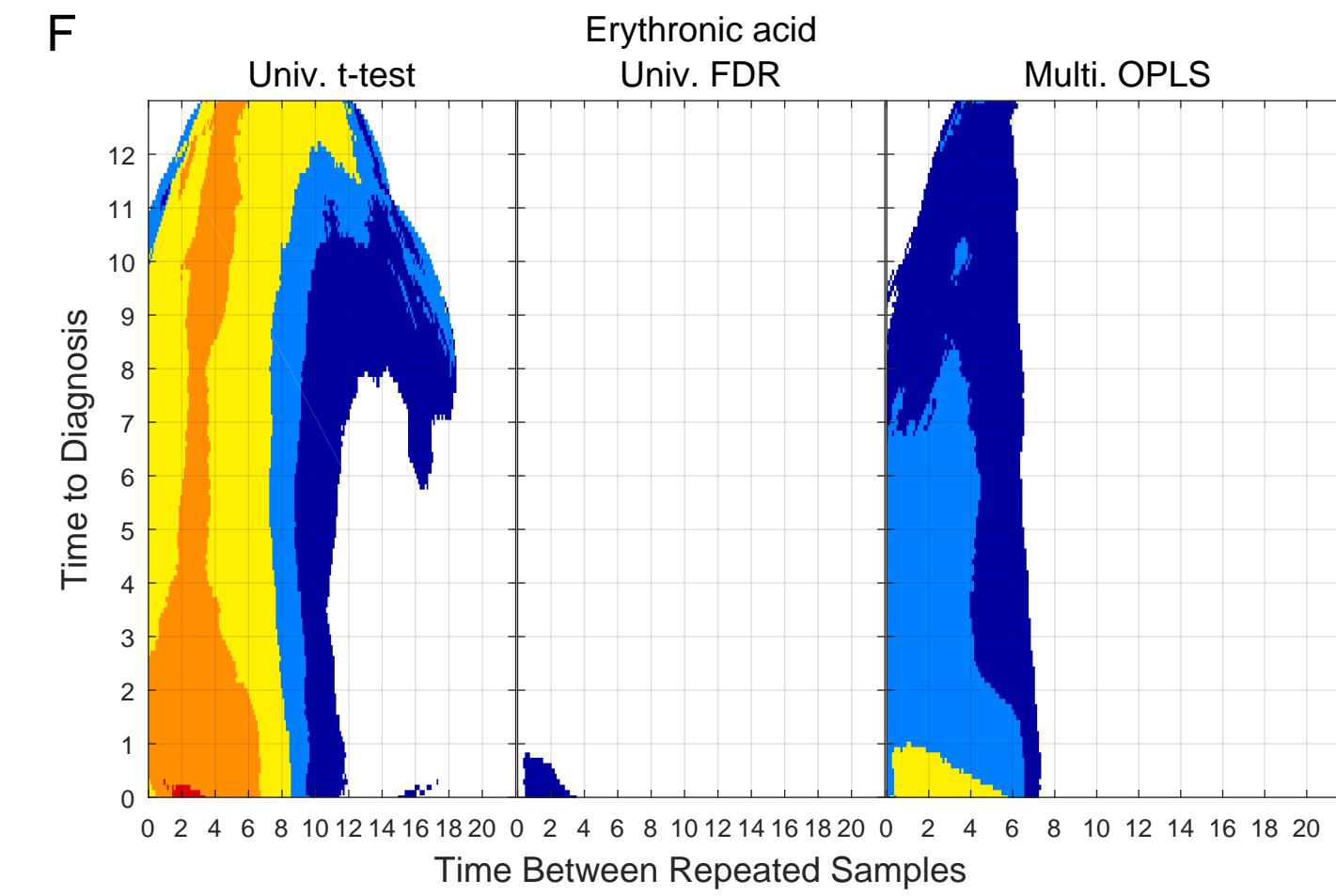
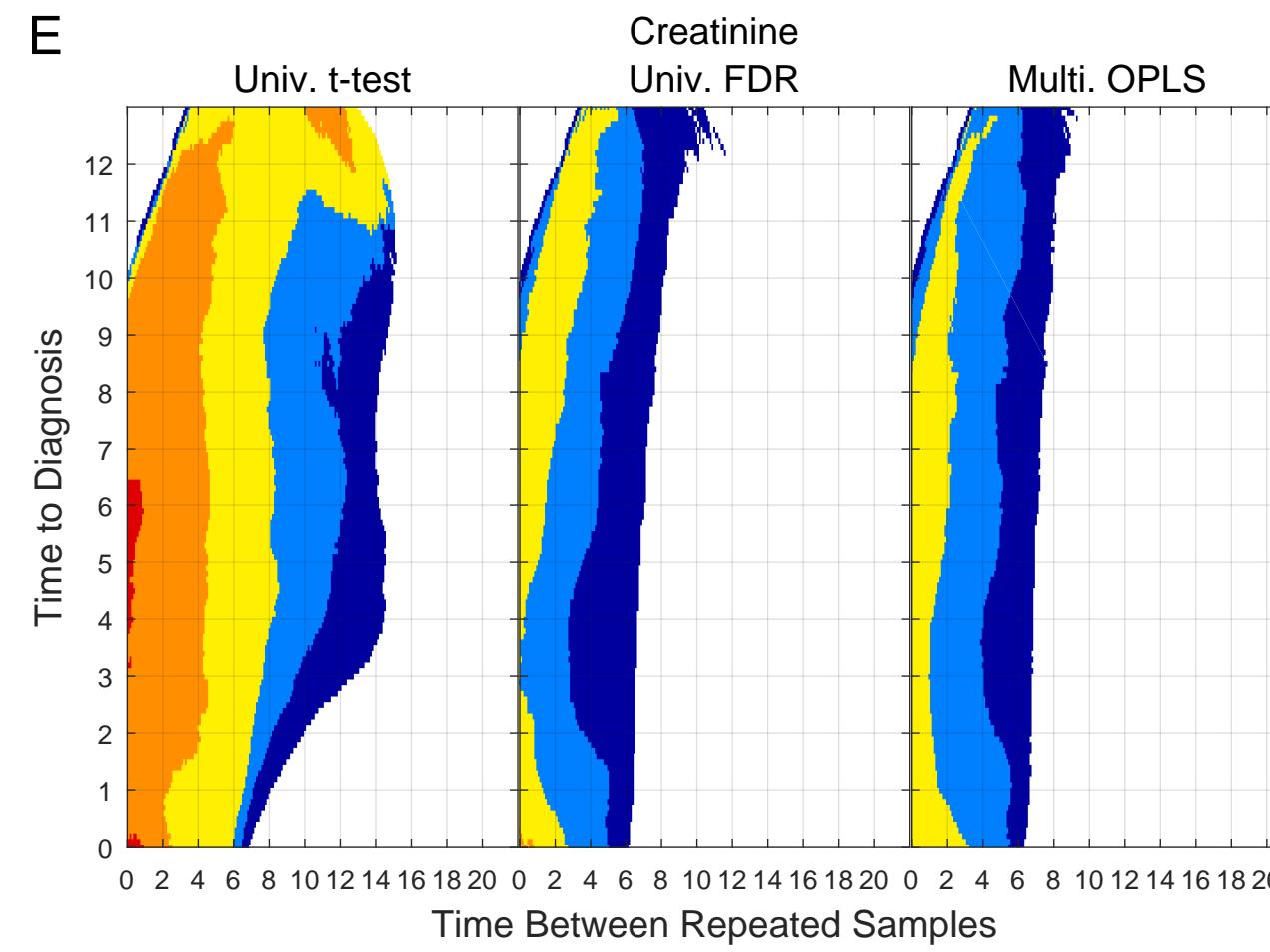
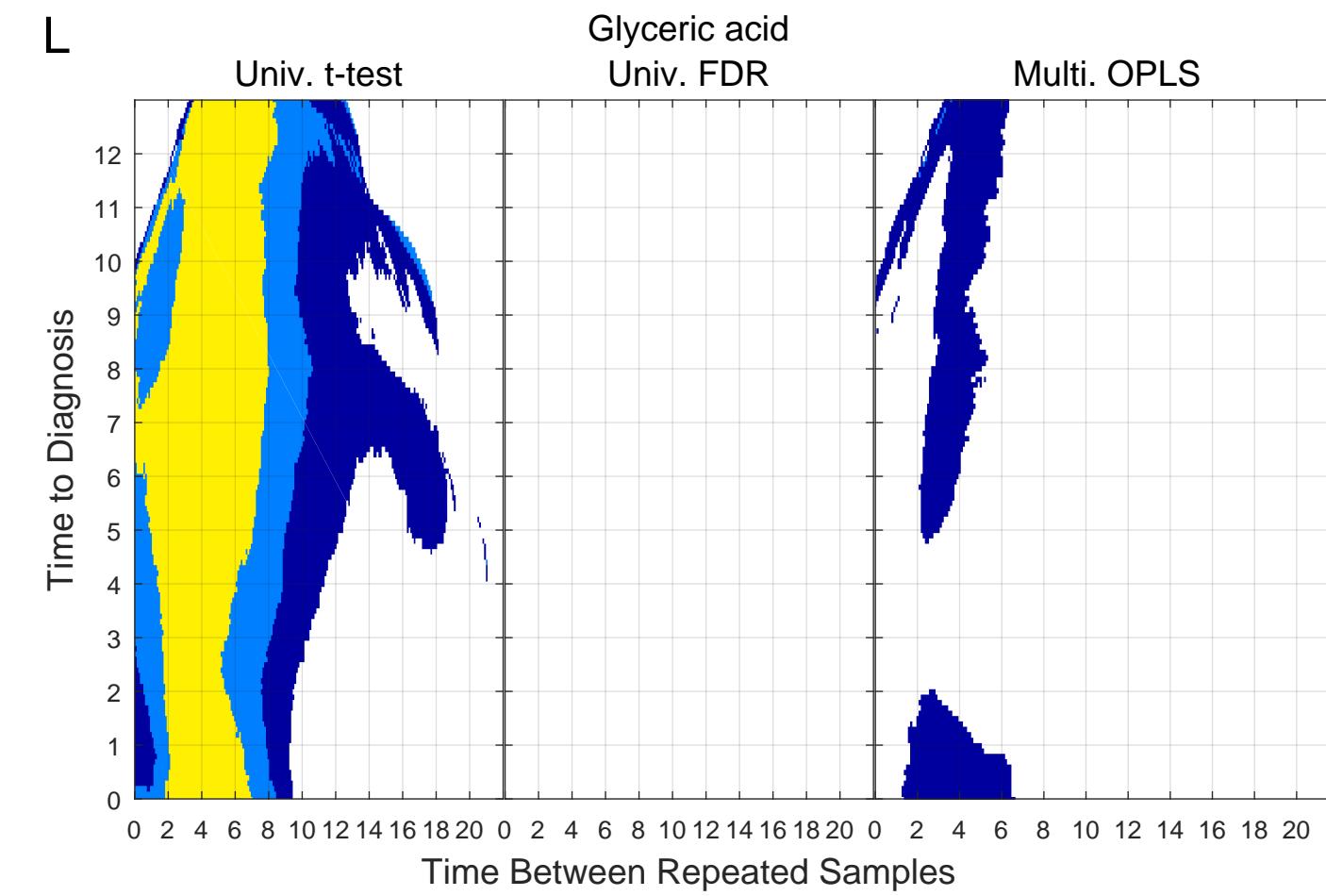
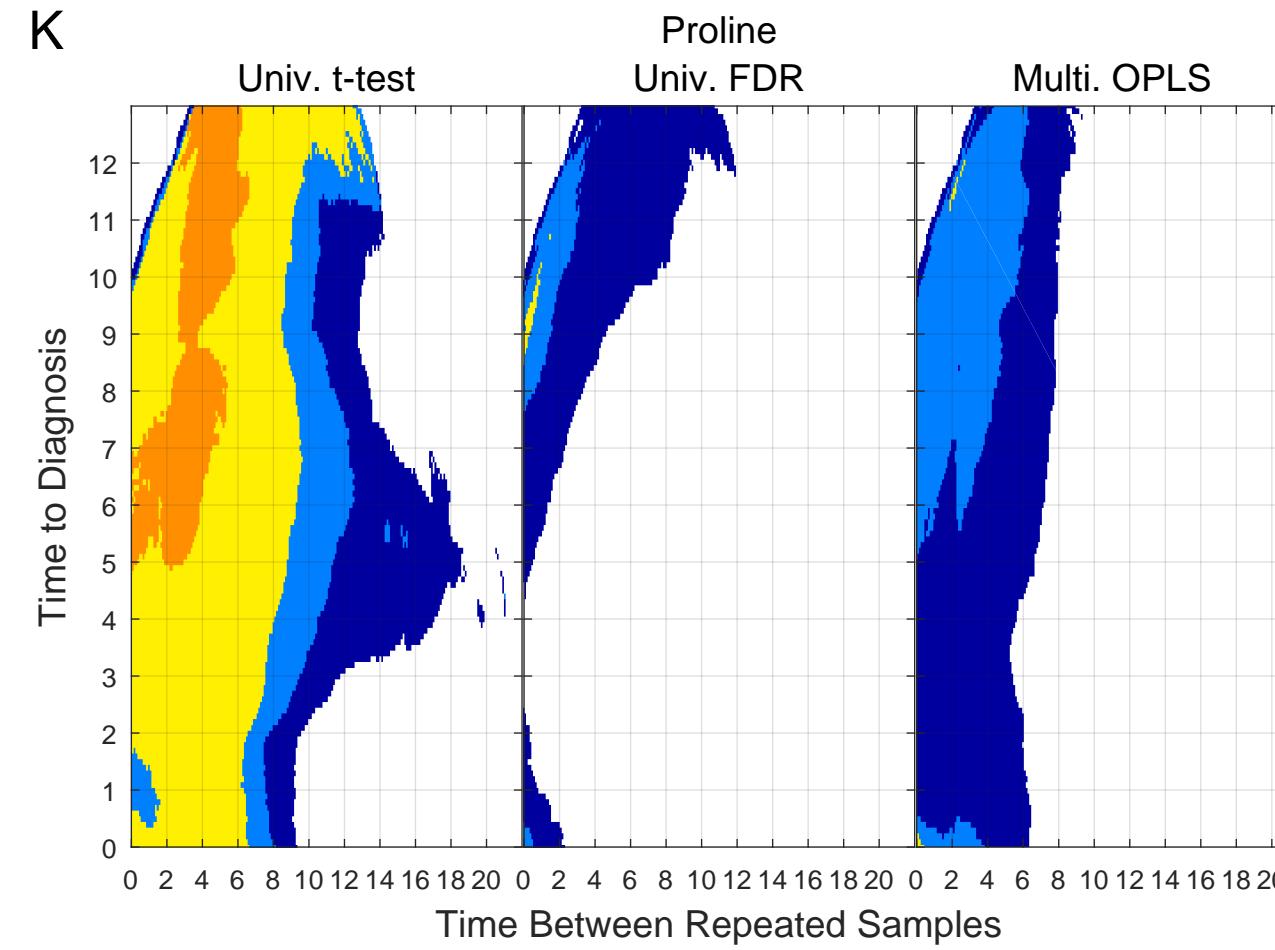
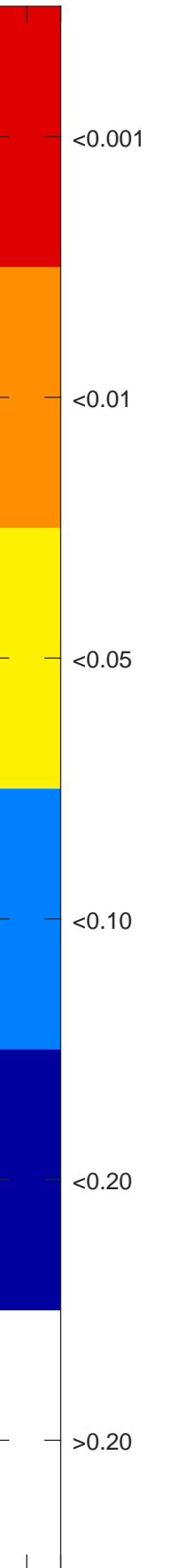
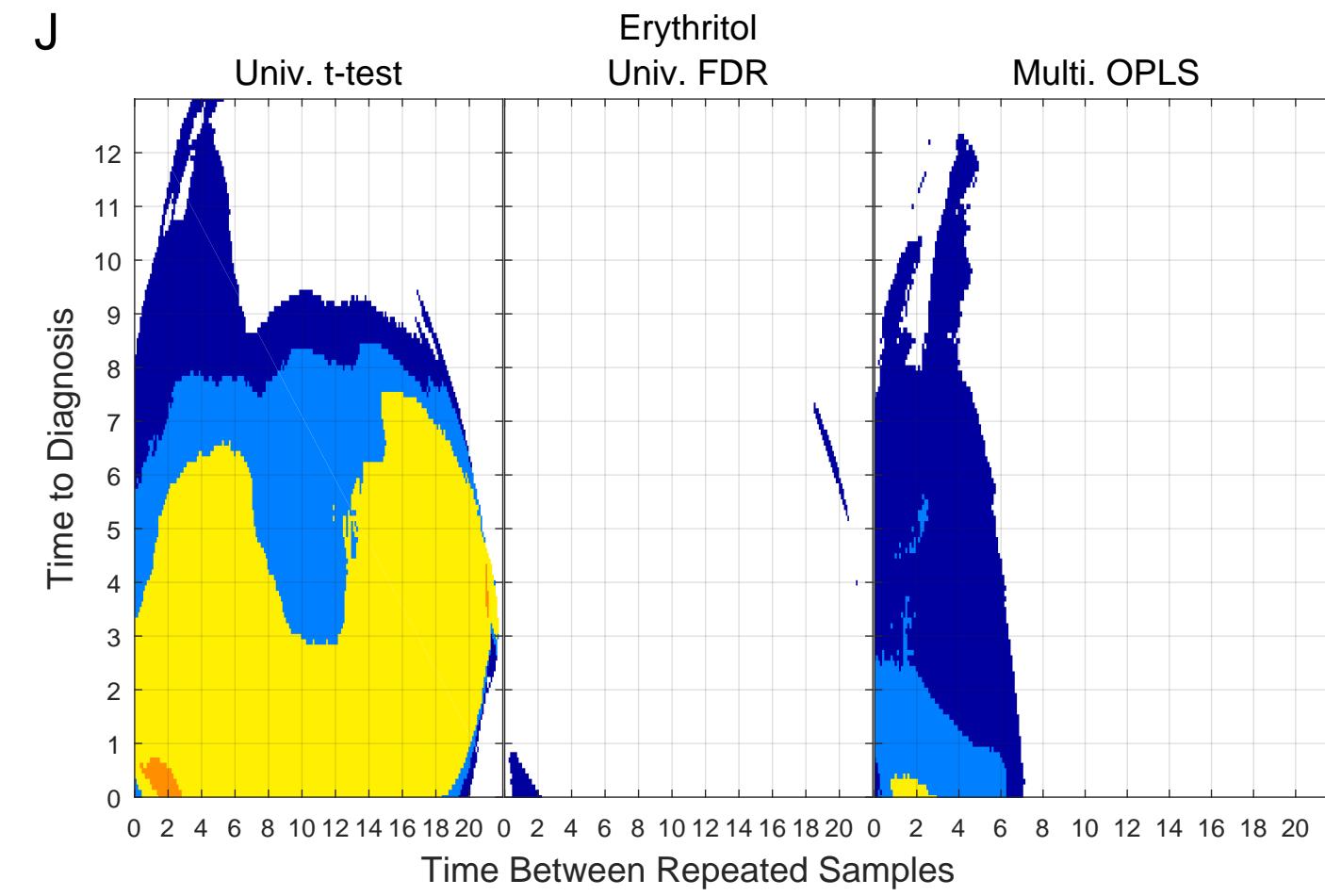
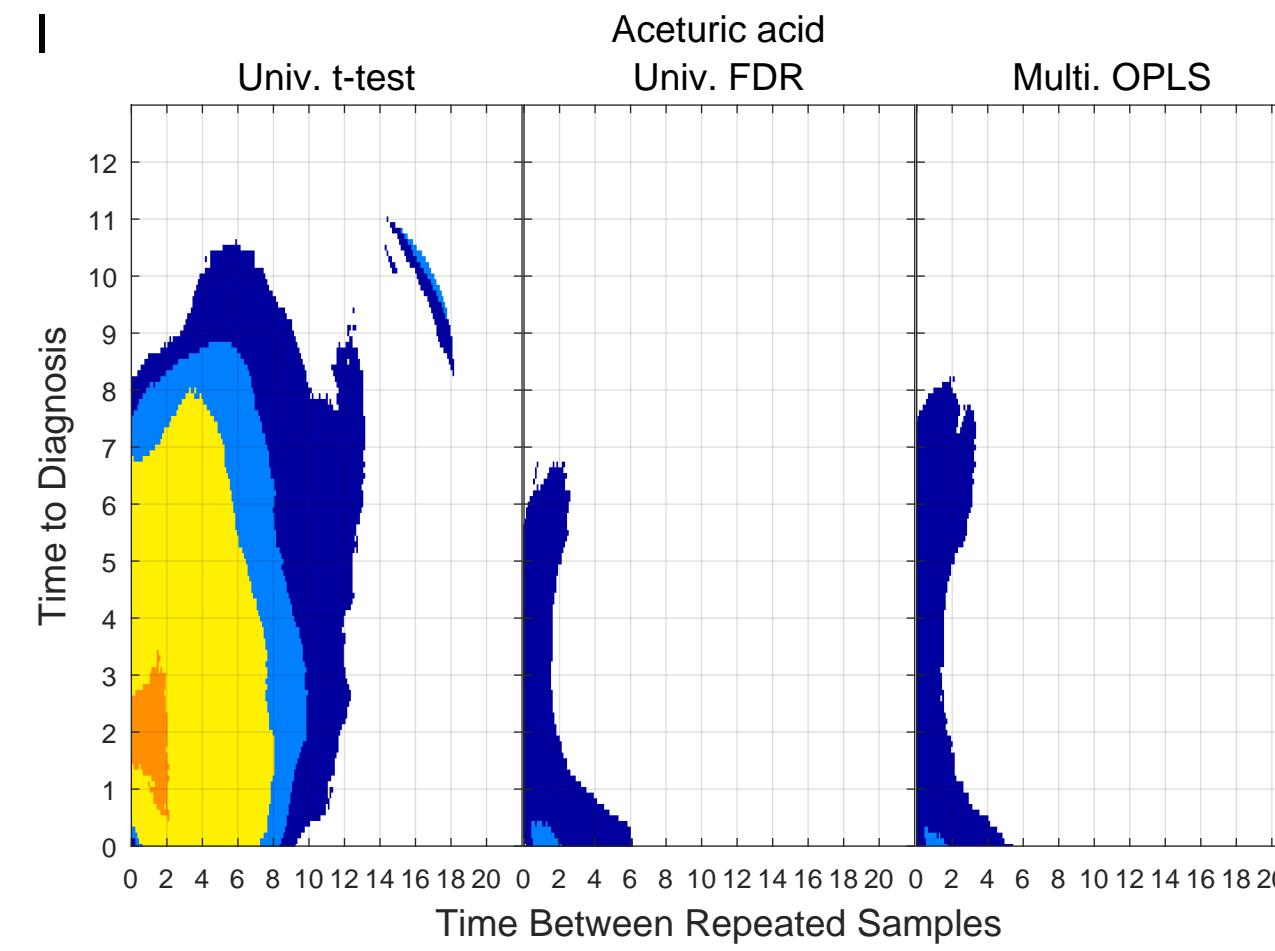
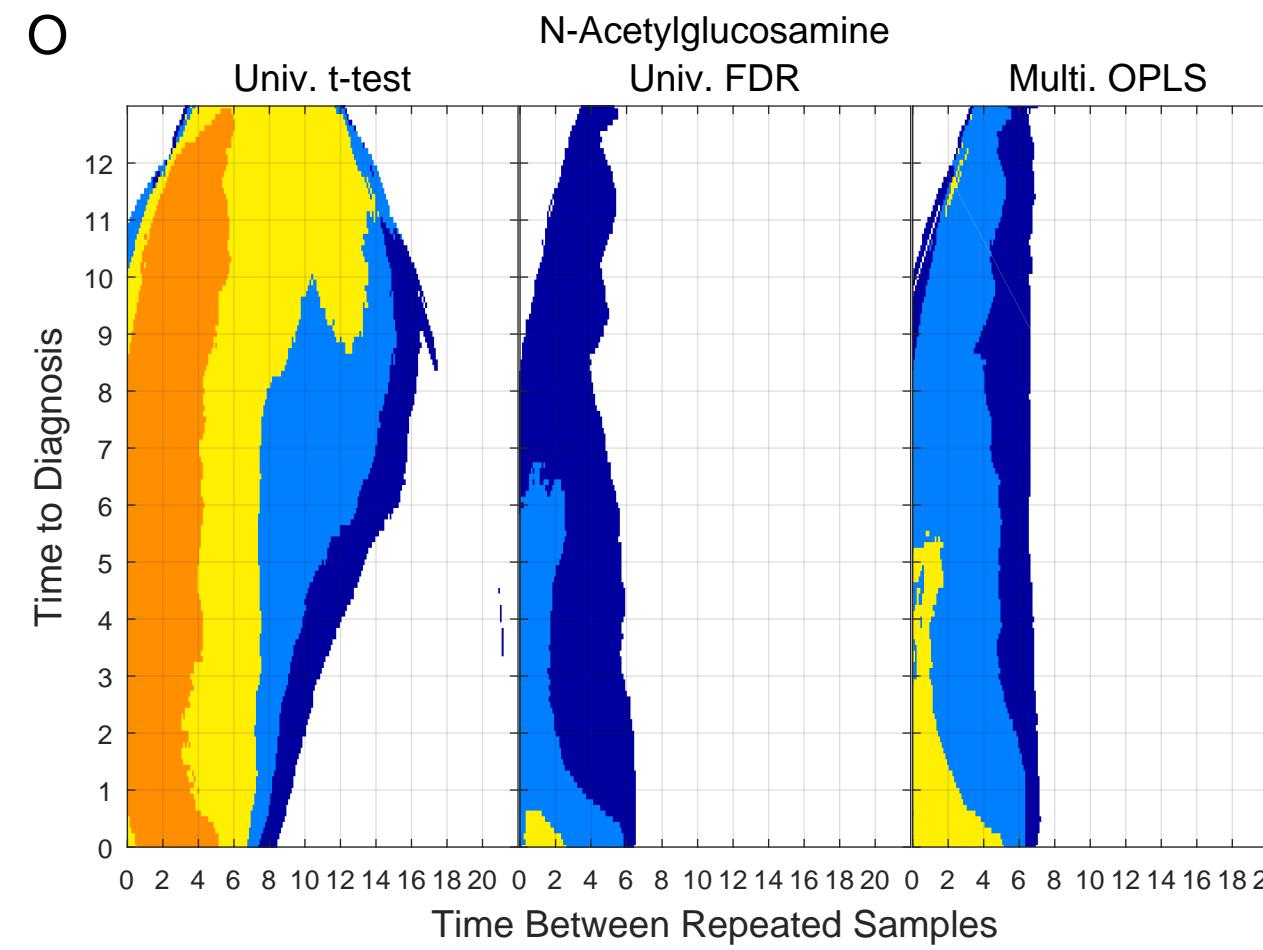
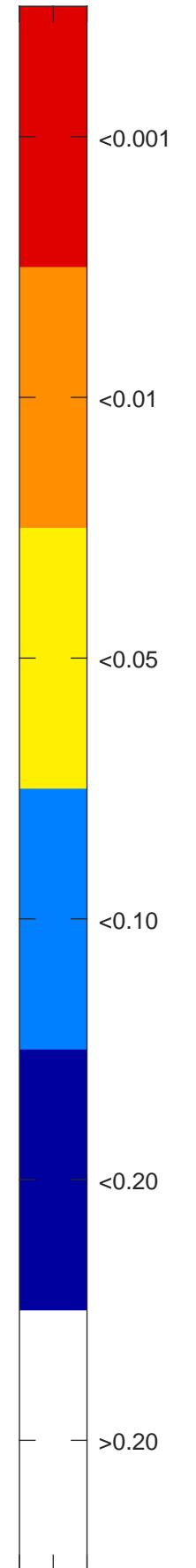
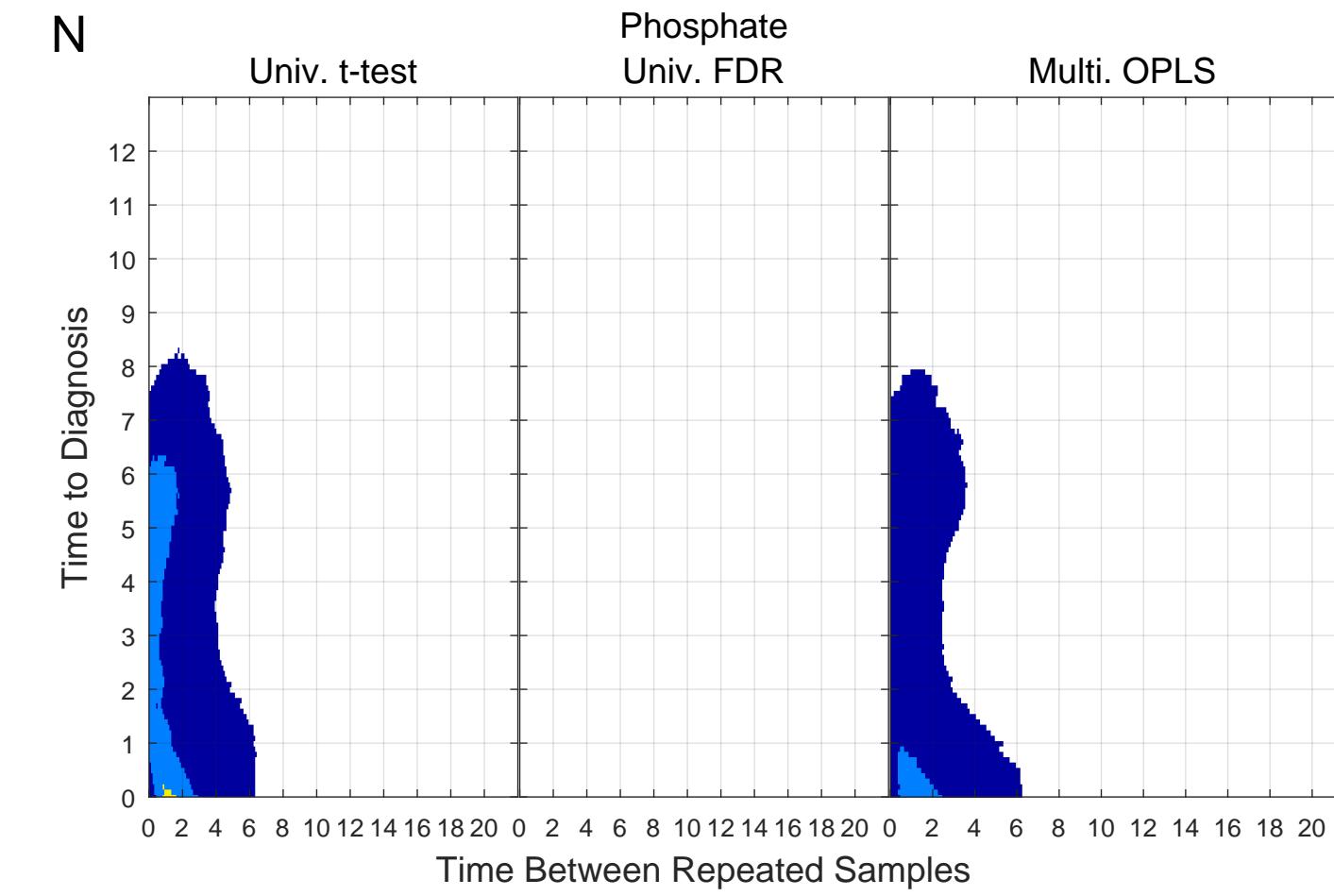
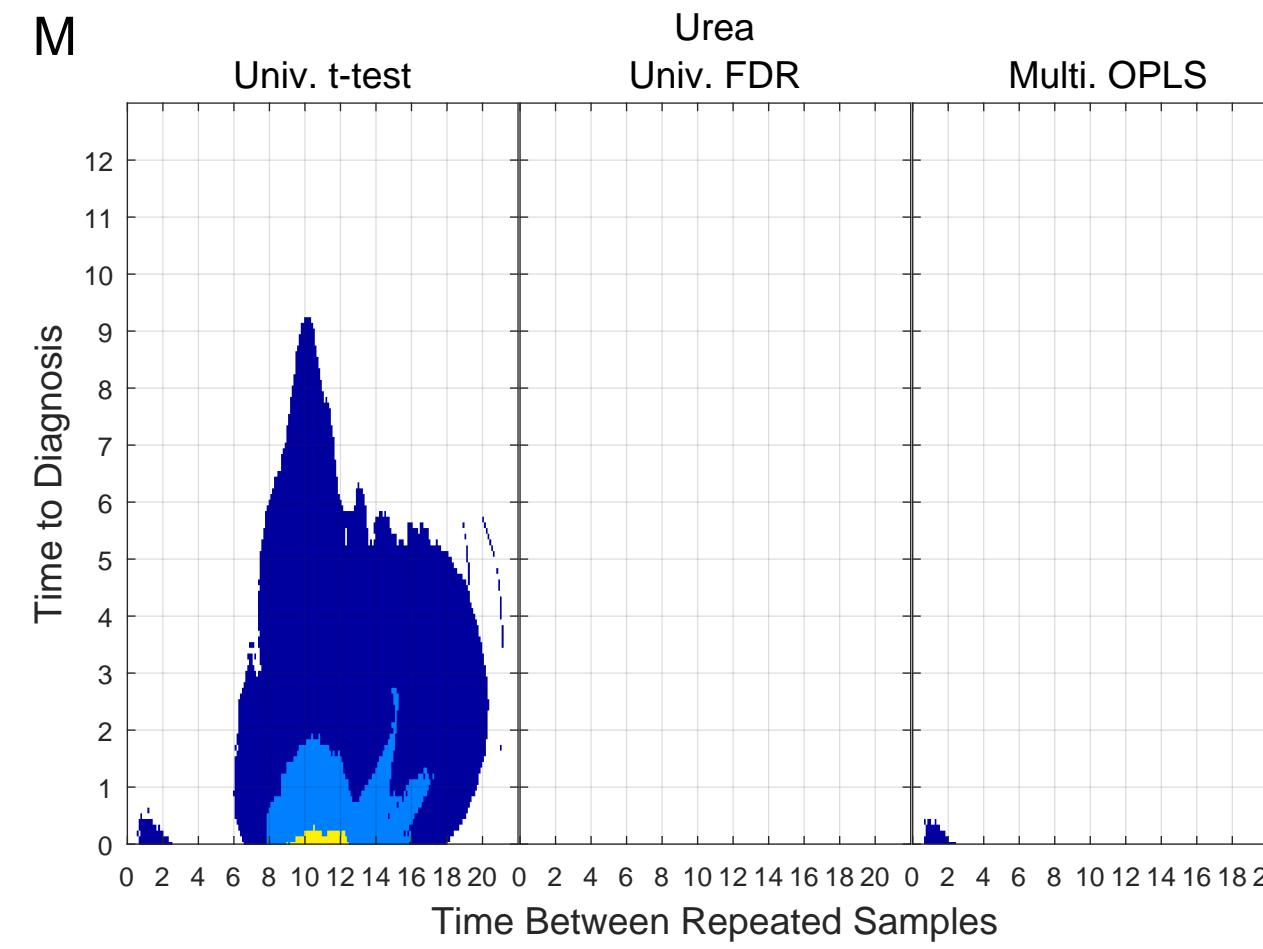


Supplementary Figure S1









Supplementary Figure S1 description:

To validate the statistics for the 15 metabolites found to be significant in the region of interest for biomarker pattern detection, we compared their individual SMART-observation distribution pattern to simulated random data. (A-O) SMART-observation plots for the 15 metabolites highlighting estimated probability of the intensities when comparing the individual metabolite to the 95 percentile for the simulated data. An estimated probability of < 0.05 means that the probability of getting this results as a random event, is less than 5%. For each metabolite the estimated probability was shown for univariate t-test (left panel), univariate t-test with FDR < 0.2 (center panel) and using multivariate OPLS significance (right panel). The plots shows that the region of interest is also highlighted for individual metabolites.