AbstractID: 14142 Title: Evaluation of Metabolomics Data using Univariate and Multivariate Statistical Analysis Techniques

Purpose: To quantify urinary metabolic changes in experimental animals as they transitioned from healthy to tumor bearing. Univariate and multivariate statistical tests were used to identify patterns of metabolic behaviour that changed in a significant manner. Receiver operator characteristic (ROC) curve analysis was used to evaluate the utility of the tests.

Method and Materials: Human GBM cells were grown as xenografts in NIH iii nude mice at 6 weeks of age. Urine samples were collected daily beginning one week prior to cell injections and lasting four weeks after injection. Selected samples were run on an Oxford 800MHz cold probe NMR Spectrometer (Oxford, England) utilizing a 1-D NOESY pulse sequence. The acquired spectra were analyzed by targeted profiling using Chenomx Suite 5.1 (Chenomx Inc, Edmonton, Canada). The paired t-test was used to evaluate changes in metabolite concentrations in the pre-injection population compared to the post-injection population. The same test was also applied to metabolite ratios. Principal component analysis (PCA) and partial least squares discriminant analysis (PDS-DA) were used to search for more complicated relationships in the data.

Results: Application of the t-test to the ratios of metabolites revealed 20 ratios that were significant beyond the Bonferroni correction threshold and 152 more ratios were significant under the FDR condition. Of the significant ratios, 7 had an AUC greater than 0.9 and 68 had an AUC between 0.8 and 0.9. After correcting for changes found in the control animals, 12 and 36 ratios that satisfied the Bonferroni and FDR thresholds respectively. 6 ratios had an AUC exceeding 0.9 and a further 16 having an AUC greater than 0.8.

Conclusion: Metabolic profiling of urine samples in animal models demonstrates that this technique has the potential to serve as a screening tool for certain types of cancers.

Conflict of Interest (only if applicable):