Evaluation of Metabolic Profiling of Urine Metabolites at Urosepsis using J-resolved NMR Spectroscopy

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Introduction: *Native urine ^1H NMR spectra suffer from spectral congestion due to presence of plethora of metabolites that contribute more than 5000 transitions. It can routinely be resolved by observing decoupled 1D projection spectra of 2D J-resolved spectroscopy. The objective of study was to evaluate the perturbation in determining the concentration of gravimetrically prepared solution of 26 known metabolites in J-resolved spectra. To perform multivariate analysis of urine sample in order to identify additional biomarker when compared with normal ^1H NMR counterpart for differentiation of urosepsis.*

Methodology: *A standard stock solution having 2.8 mM concentration of 26 metabolites was prepared. Recording of NMR data was carried out on 800 MHz FT-NMR spectrometer. T_1 and T was calculated using Inversion Recovery and CPMG pulse experiment. For urine sample, 1D ^1H and J-resolved NMR spectra was recorded or healthy (n=32) and urosepsis (n=28) cases. The normalized bins of 0.01ppm of spectra data further subjected for multivariate analysis (PCA,PLSDA).*

Results: *Concentration comparison in J-resolved NMR spectra form ^1H NMR spectra were found to be equivalent for aliphatic signal region of metabolites while for aromatic signals, a value upto 60% perturbation was observed. Statistical analysis J-resolved spectra of control (Healthy subject) and diseased (Urosepsis subject) using PLS-DA model resulted in value of R^2 is 0.948 and Q^2 is 0.812. Additional peaks observed in PC1 loadings of J-resolved NMR spectra were identified as lysine, cadavarine and acetate. These metabolites are correlating the pathway for the formation of previously identified butyrate as a confounder in urosepsis cases.*

Conclusion: *The J-resolved NMR spectra provide a complementary data with ^1H NMR based metabolomic studies.*