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**KAREN A KOPCIUK**, Alberta Health Services - Cancer Care  
*Sample Size Estimation Methods for NMR Metabolomics Data*

Typical projection-based methods used to analyze metabolomics data, such as Partial Least Squares Regression, do not have statistical inference methods or the corresponding sample size methods. To overcome this study planning limitation, we investigated sample size estimation approaches for high dimensional microarray data for their suitability with NMR metabolomics data. Simulation studies compared three methods across a number of relevant data features. Simulation study results and an application to a pancreatic cancer data set suggested two methods could be used for sample size estimation of NMR metabolomics data. Future work will investigate these methods with mass spectrometry metabolomics data.