

# A semiparametric modeling approach for the development of metabonomic profile and biomarker discovery mechanism

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*Abstract:* The discovery and validation of biomarkers is an important step towards the development of criteria for early diagnosis of disease status. Recently electrospray ionization (ESI) and matrix assisted laser desorption (MALDI) time-of-flight (TOF) mass spectrometry have been used to identify biomarkers both in proteomics and metabonomics studies. Data sets generated from such studies are generally very large in size and thus require the use of sophisticated statistical techniques to glean useful information. Most recent attempts to process these types of data model each compound's intensity either discretely by positional (mass to charge ratio) clustering or through each compounds' own intensity distribution. Traditionally data processing steps such as noise removal, background elimination and m/z alignment, are generally carried out separately resulting in unsatisfactory propagation of signals in the final model. It is more intuitive to develop models for patterns rather than discrete points following the basic principle of "borrowing strength" for such a scenario.