

Breath Markers of Disease Identifiers for Portable Mass Spectrometry

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Breath capture chemistry is a rising method of examining physiological information as a means to discover and track biomarkers and metabolites for clinical applications. Previous studies have highlighted the ability of breath samples to indicate presence of respiratory viral infections, such as Influenza A, MERS, SARS-CoV-1, and in our group SARS-CoV-2, through the detection of volatile chemical markers via mass spectrometry (MS). Due to its noninvasive sample collection and unlimited supply, further exploration of this volatile chemistry in the breath for a more detailed understanding of its connection to disease, diet, and general lifestyle is incredibly beneficial for the medical field, among others. Here we will present a rapid non-invasive breath capture techniques for direct analysis with MS/MS to initially exact the chemicals of interest. We then coupled this data with the analytics of Partial-Least Squared Discriminant Analysis and K-Nearest Neighbor, and check with K-Fold Cross Validation to confirm chemical assignments. These experiments are designed to finalize the chemistry of the breath biomarker and metabolites, and help train more portable instruments on the chemicals of interest. Data will be shown as to the efficacy of this direct inlet mass spectrometry technique. For disease states, presence of drug metabolites, and lifestyle biomarkers, limits of detection and mass accuracy of this direct inject mass spectrometry screen will be presented.