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NMR Based Metabolomics in Respiratory Diseases

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Respiratory diseases represent a complex manifestation of heterogeneous infection, inflammation and pathogenesis which results in prolonged treatment and therapeutic response. Interstitial lung disease, asthma, chronic obstructive pulmonary disease (COPD), cystic fibrosis, pneumonia, acute respiratory distress syndrome (ARDS) with complex clinical disparity and heterogeneity accounts for high mortality and hospital care. They comprise a complex spectrum of aetiology and pathobiology with varying clinical disposition and hence predicting outcome poses a significant challenge for clinicians worldwide. Earlier clinical decision-making and prognosis requires high throughput and high content analytical methods that can provide sensitive and specific biomarkers. Disease specific biomarkers will aid in better understanding of disease, the underlying pathobiology, disease onset and progression. The existing diagnostic criteria is rather generic in terms of patient heterogeneity, risk stratification and characterizing disease sub-phenotypes.In this respect metabolomics complements current clinical assays and other omics technologies by redefining the disease in terms of clinical, physiological and biochemical abnormalities. Metabolomics is defined as dynamic and comprehensive measure to quantify and detect the small molecular weight molecules/metabolites in different biological matrices in response to environmental, pathological and physiological stimuli.

The ability to provide a real time snapshot of metabolic perturbations in response to drug and disease state with readout of existing physiological state due to both endogenous and exogenous insult makes metabolomics preferable to other omics technologies. Presently nuclear magnetic resonance (NMR) and mass spectrometry are the most instrumental analytical platforms in metabolomics. Reproducible, non-invasive with minimal sample preparation and short analytical run makes NMR a robust and high throughput approach than Mass Spectrometry (MS). The ease of data interpretation, unbiased analysis and generating multidimensional dataset from just single sample makes it a promising approach in identifying and characterizing respiratory metabolome under stress and environmental insult. The application of NMR based metabolomics in airway obstructive diseases is trailing behind when compared to other life threatening ailments like cancer and cardiovascular diseases. Although principal biomatrices like exhaled breath condensate (EBC), sputum, lung tissue, bronchoalveolar lavage fluid (BALF), blood and urine have been employed but substantial biomarker credentials are yet to be established for personalised medicine and therapy. Urine metabolite signature between exacerbated asthmatics and stable asthmatics with 94% accuracy has been established using NMR. Similarly, NMR serum profile has discriminated moderate and severe COPD. Extensive biomarker characterization in ARDS has led to discrimination between acute lung injury/ARDS with respect to healthy control providing both systemic and lung specific metabotype using both serum and mBALF. Meanwhile EBC endotyping of cystic fibrosis patients led to a diagnostic model with 96% accuracy.NMR based studies helped in distinguishing Streptococcus *pneumonia* strains distinctive of community-acquired *pneumonia*.

All the approaches till now in NMR based respiratory-omics have made efforts to develop and standardize the analytical platform in identifying metabolic signatures in different biofluids and hence establish biomarker model based on the disease sub-phenotypes. But the diagnostic accuracy of the model is yet to be established as per the requisite international standards both on prospective cohorts and on retrospective scale. This necessitates the need to integrate the metabolomics generated datasets with other omics driven data to quantify disease severity and progression. Metabolomics holds the potential to establish diagnostic pattern based on streamlining thousands of analytes (hexose, amino acids, lipids, peptides, organic acids) interlinked to metabolic pathway. Bringing metabolomics in application to clinical medicine requires large clinical studies and validation of large datasets generated worldwide and integrated at acommon platform for initiating follow up studies and clinical trials to develop system based medicine.

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