Development and Validation of a Novel Breath Analysis and Machine Learning Platform for Non-Invasive Diagnosis of Heart Failure

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Currently, 6.2 million adults suffer from heart failure (HF), with 30-40% surviving one-year post-hospitalization and a 30-day readmission rate of 23%. The urgent need for an affordable, specific, non-invasive, and portable screening test to rapidly diagnose HF has led to a novel diagnostic approach using breath analysis and machine learning. In this study, twenty-seven HF patients and thirty healthy controls were enrolled and provided exhaled breath samples through a microfabricated microreactor chip coated with 2-(aminooxy) ethyl-N,N,N trimethylammonium to capture carbonyl compounds in the breath. Carbonyl compounds were then analyzed by ultra-high performance liquid chromatography-mass spectrometry. There were unique metabolic fingerprints associated with HF, indicated by the altered concentrations and patterns of twelve carbonyl compounds. Patients with HF showed significantly higher levels of compounds such as acetone, pentanal, acetic acid, caproic acid, acrolein, and 3,4 methylenedioxyamphetamine while exhibiting lower levels of others like 2-butanone, pentanone, ethyl propionate, cyclohexylacetone, methyl acrylate, and 4-hydroxy-2-hexenal compared to healthy controls. Sparse partial least squares discriminant analysis and 2D scores plot allowed complete differentiation of HF patients from healthy controls. Random forest machine learning algorithm achieved an average area under the curve of 0.99, validating the potential of breath analysis combined with machine learning as a non-invasive diagnostic tool for HF. Top 5 features in the machine learning algorithms were acetone, cyclohexylacetone, pentanone, 2-butanone and ethyl propionate. In conclusion, this study provides compelling evidence for the use of breath analysis and machine learning in diagnosing HF.

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