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Untargeted approach for breath markers of chronic kidney disease through TD-GC/MS (Thermal Desorption Gas chromatography Mass-spectrometry)

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Objectives: Volatile Organic Compounds (VOCs) can vary depending on a person's health state. The pattern of breath VOC of CKD patients would change with decreasing kidney function. Therefore, we aimed to explore breath markers to identify CKD patients from normal healthy controls.

Methods: Untargeted breath analysis using thermal desorption-gas chromatography mass-spectrometry (TD-GCMS) was performed on breath samples from normal healthy controls (n=18) and non-dialysis CKD patients (n=21), and end-stage renal disease (ESRD) patients on hemodialysis (n=12). A total of 378 VOCs (MW 41.027-393.397 amu) were measured and identified, of which 14 VOCs belonging to the siloxane group were excluded. We conducted the statistical analysis with 364 VOCs along with clinical variables to find significant VOCs related to CKD.

Results: Metabolomic analysis revealed fifty-eight significantly different VOCs in breath of CKD patients (non-dialysis CKD + ESRD) compared to normal healthy controls by using T-test. Thirty-six VOCs and two clinical parameters showing significant associations with CKD in univariate analysis were chosen for further analysis. The spectra of breath VOCs from normal group to two CKD groups were different, which can be shown by the heat map and principal component analysis. We extracted the main VOCs and clinical parameters in the first step of multivariate analysis through a hundred times repeated training and test set analyses. Final multivariate model which incorporated age [OR 0.18 (95% CI: 0.07-2.49), p = 0.013], 2-methyl-pentane (alkane) [OR 2.10 (95% CI: 0.94-2.24), p = 0.025] and cyclohexanone (ketone) [OR 2.31 (95% CI: 0.88-2.64), p = 0.008] showed high performance in identifying CKD patients (accuracy = 86%).

Conclusions: This study showed that renal dysfunction induces a characteristic pattern of breath VOCs that can be used as non-invasive potential biomarkers in screening tests of CKD.

Fig 1. Heat plot of breath VOCs related to CKD in the univariate analysis.