Supporting Information

An intelligent mobile electronic nose system comprising hybrid polymer-functionalized quartz crystal microbalance sensor array

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1 Temperature effect on data acquisition system

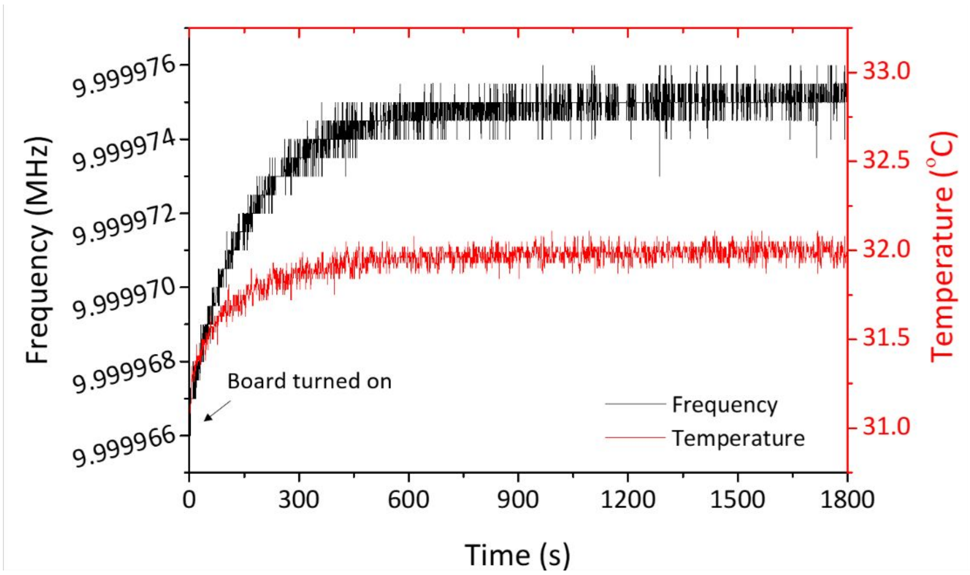

Figure S1 Dependence of the frequency from the data acquisition (DAQ) system on the board temperature measured for 30 min after the board has been turned on.

2 Comparison of different gate times for data acquisition system

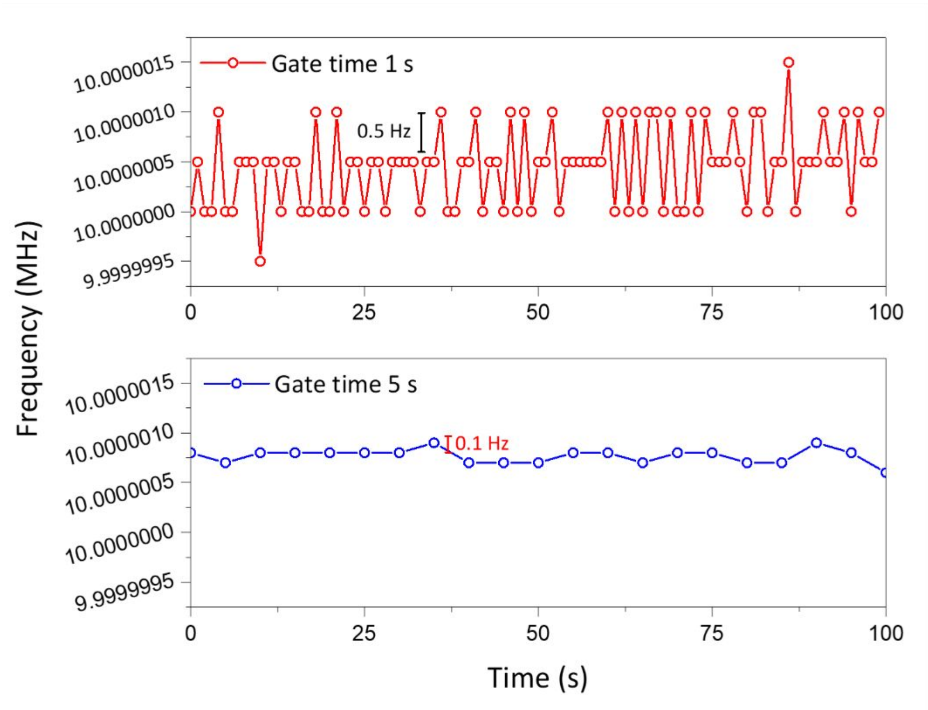

Figure S2 Measured frequency by data acquisition system with 10 MHz input for different parameters of gate time (1 s and 5 s). Longer gate time results in fewer data points over time, which can then reduce data number and response time.

3 Frequency measurement results of polymer-coated QCM sensors

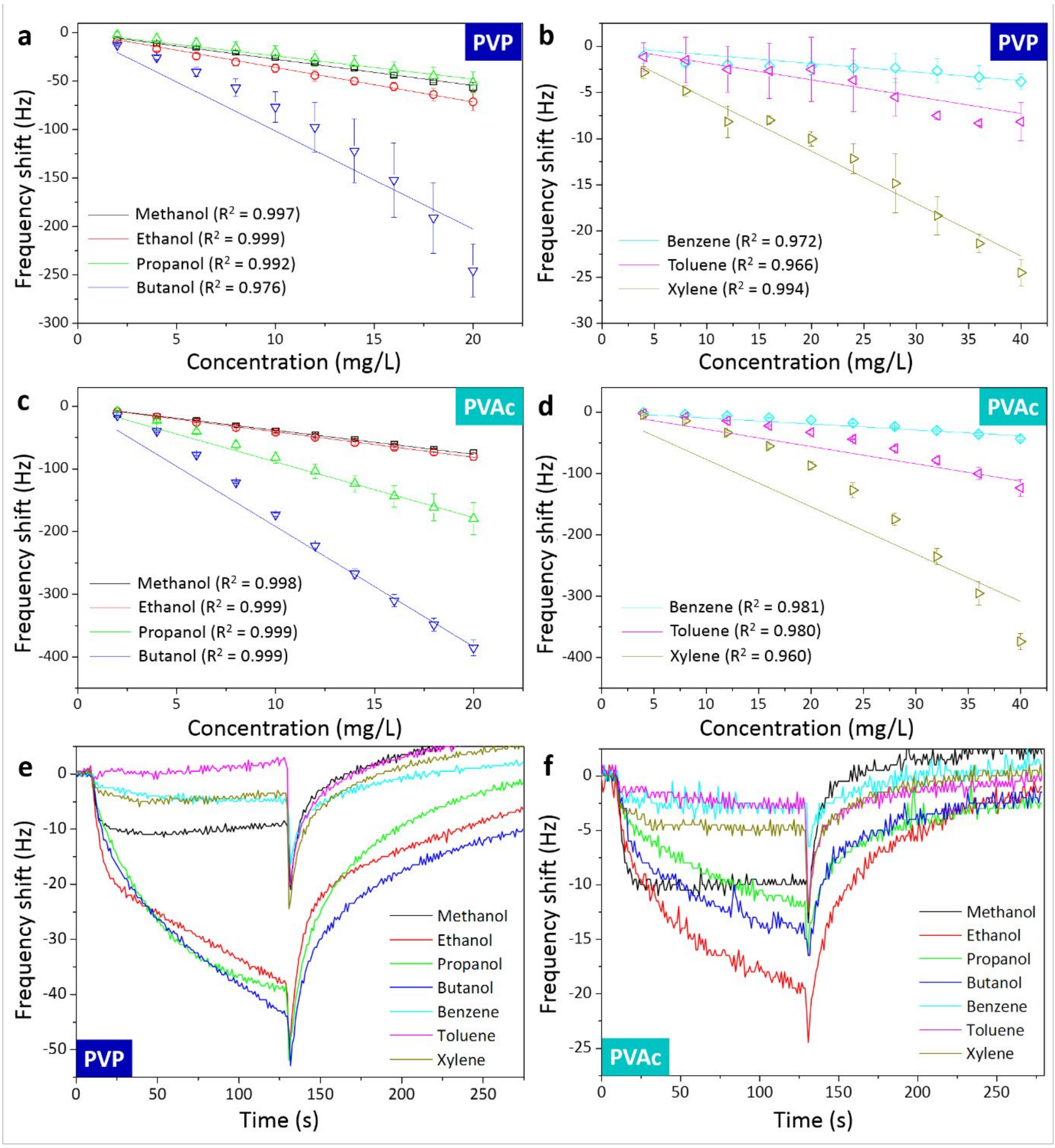

Figure S3 Frequency shifts of QCM sensors functionalized with (a,b) polyvinyl pyrrolidone (PVP) and (c,d) polyvinyl acetate (PVAc) thin films under exposure to different volatile organic compounds (VOCs, i.e., methanol, ethanol, propanol, butanol, benzene, toluene, and xylene) at incremental concentrations of up to 20 and 40 mg/L for alcohol and BTX samples, respectively. Full-cycle dynamic responses of the QCM sensors functionalized with (e) PVP and (f) PVAc thin films under influence of various VOCs at a concentration of 1 mg/L. These QCMs belong to the sensor array inside the e-nose system.

4 Principal component analysis

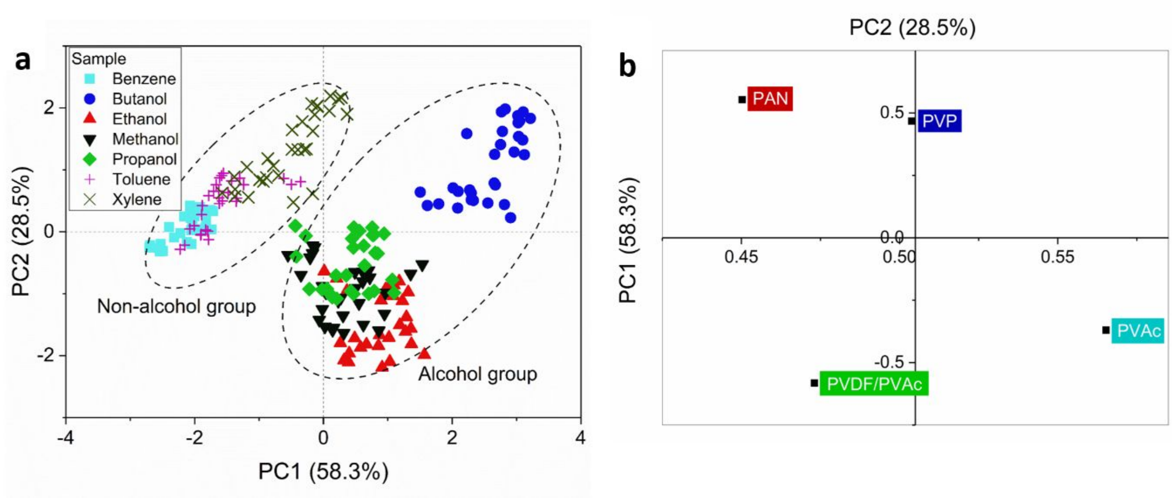

Figure S4 (a) Score plot of the first two principal components (PC1 and PC2) and (b) principal component analysis (PCA) loading plot of the VOC samples resulted from QCM-based e-nose signal profiles.

Principal component analysis (PCA), an unsupervised pattern recognition method, was used to investigate data variability. PCA reduced the dimensionality of the data by orthogonal transformation into principal components (PCs). By decreasing order, the first PC represented the highest variability of data that provided the most relevant information. The PCA applied to the data matrix demonstrated that three PC functions explained 96.6% of the total data variance. **Figure S4(a)** shows the score plot of the first two principal components (PC1 and PC2) allowed to explain 86.8% of the data variability. It presents the established matrix data for two clusters according to the functional groups, i.e., non-alcohol group (benzene, toluene, and xylene) and alcohol group (butanol, ethanol, methanol, and propanol). **Figure S4(b)** depicts the loading plot of the first two principal components allowed to strongly explain the contribution of each sensor influencing the principal component. Loadings close to -1 or 1 indicate that the variable strongly influences the component. All sensors contributed to separate data into two functional sample groups, in which they had relative similar influence. PAN and PVP sensors were positively correlated resulting in positive contribution for the PC2. Meanwhile, PVDF/PVAc and PVAc sensors were positively correlated having negative contribution for the PC2. They contributed to separate Xylene from alcohol group (ethanol, methanol, and propanol). It was also interpreted that all sensors delivered strong contributions to separate butanol from all other samples. Moreover, from the natural distribution of all samples, the replicates of each sample were located close to each other, showing good precision. Although several samples still exhibited overlapping, they could clearly establish clusters based on the VOC types. These results demonstrated that the signal profiles recorded by the QCM-based e-nose contained representative information that could be further employed to classify each sample using supervised multivariate statistical techniques (i.e., linear discriminant analysis (LDA) and support vector machine (SVM) models).

5 Block diagram of chemometric method used in mobile e-nose

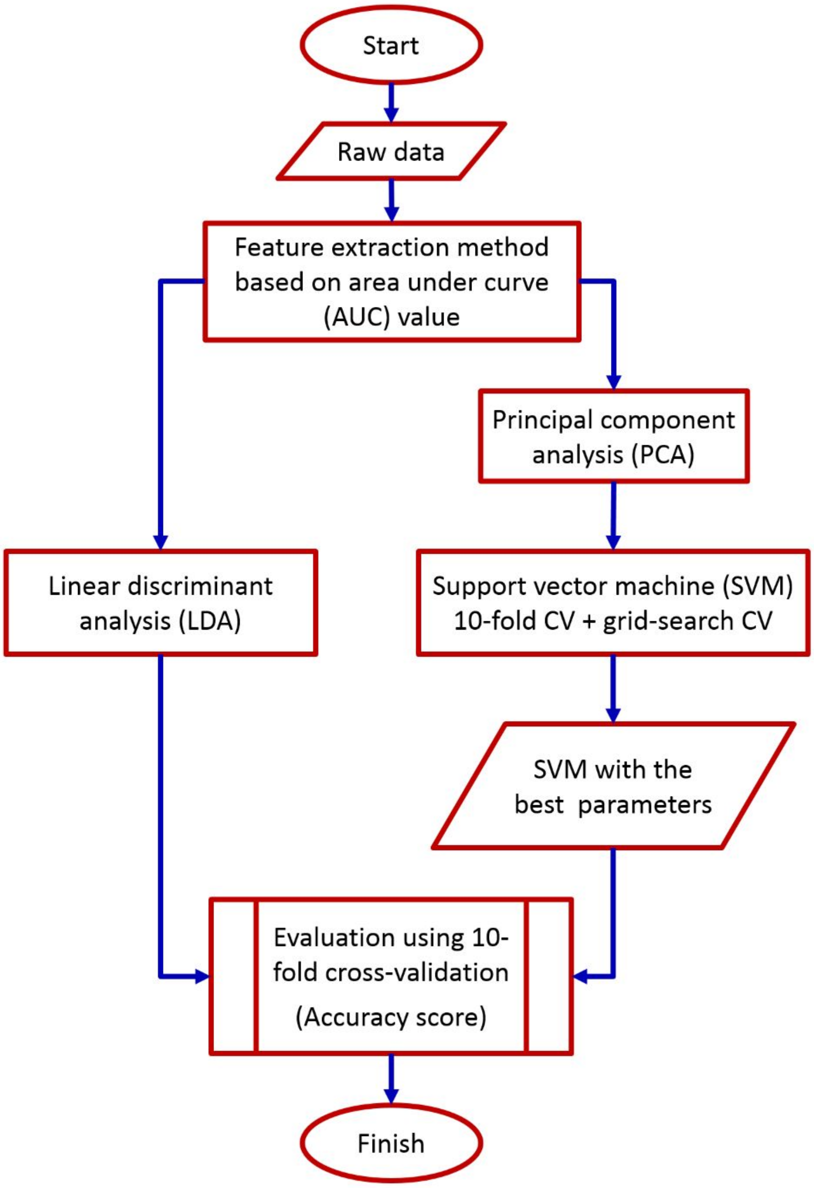

Figure S5 Block diagram of the chemometric method used in smart mobile electronic nose (e-nose). Two types of machine learning algorithms (i.e., linear discriminant analysis (LDA) and support vector machine (SVM) models) were employed to differentiate and classify the tested analytes. Principal component analysis (PCA) was used to investigate data variability.