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DNA Breath Sensor Array using Molecular Dynamics Simulation

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ABSTRACT
DNA biochemical sensors can be utilized to detect certain disease biomarkers present in individuals' breath, for instance, acetone and ethanol for diabetes and H2S for cardiovascular diseases. We have developed a wireless sensor array based on single-stranded DNA (ssDNA)-decorated single-walled carbon nanotubes (SWNT) and successfully detected the trace amount of methanol and acetone in vapor. Various chemicals can also be differentiated by pattern recognition of DNA array. We conducted steered molecular dynamics (SMD) simulation of the interactions between different DNA sequences with acetone to screen out the best sensing-performance sequences. Using the Brownian dynamics fluctuation-dissipation-theorem (BD-FDT), we were able to accurately compute the free-energy landscapes of interaction between four single DNA nucleotides (consisting one of the four nucleobases- Adenine (A), Guanine (G), Cytosine (C), and Thymine (T)) on both single-stranded DNA (ssDNA) and double-stranded DNA (dsDNA) with acetone. We found that dsDNA react differently than ssDNA to the acetone, requiring more energy to move the molecule close to DNA as indicated by the potential of mean force (PMF). Comparing the PMF values of the different systems, we obtained the affinity strength rank of DNA nucleotide-acetone systems: A>C=T>G for ssDNA, and A>G>T>C for dsDNA. In the same way, we can generate a library of DNA sequences for the detection of a wide range of chemicals. Thus, a DNA-SWNT sensor array built with selected optimal DNA sequences differentiating many disease biomarkers can be used in breath analysis for disease diagnosis and monitoring.

KEYWORDS: *DNA biochemical sensors, wireless sensor array, Brownian dynamics fluctuation-dissipation theorem (BD-FDT)*