World Academy of Science, Engineering and Technology
International Journal of Biotechnology and Bioengineering
Vol:10, No:01, 2016

Biosensor Design through Molecular Dynamics Simulation

Authors : Wenjun Zhang, Yunqing Du, Steven W. Cranford, Ming L. Wang

Abstract : The beginning of 21st century has witnessed new advancements in the design and use of new materials for biosensing applications, from nano to macro, protein to tissue. Traditional analytical methods lack a complete toolset to describe the complexities introduced by living systems, pathological relations, discrete hierarchical materials, cross-phase interactions, and structure-property dependencies. Materiomics – via systematic molecular dynamics (MD) simulation – can provide structure-process-property relations by using a materials science approach linking mechanisms across scales and enables oriented biosensor design. With this approach, DNA biosensors can be utilized to detect disease biomarkers present in individuals' breath such as acetone for diabetes. Our wireless sensor array based on single-stranded DNA (ssDNA)-decorated single-walled carbon nanotubes (SWNT) has successfully detected trace amount of various chemicals in vapor differentiated by pattern recognition. Here, we present how MD simulation can revolutionize the way of design and screening of DNA aptamers for targeting biomarkers related to oral diseases and oral health monitoring. It demonstrates great potential to be utilized to build a library of DNDA sequences for reliable detection of several biomarkers of one specific disease, and as well provides a new methodology of creating, designing, and applying of biosensors.

Keywords : biosensor, DNA, biomarker, molecular dynamics simulation
Conference Title : ICBST 2016 : International Conference on BioSensing Technology
Conference Location : Zurich, Switzerland
Conference Dates : January 12-13, 2016