Whether deployed as two, three, or even four distinct sequences, this strategy marks a pivotal advancement. Leveraging Density Functional Theory (DFT) and Molecular Dynamics (MD), we constructed a computationally-optimized peptide library, calibrated for maximum specificity. This database serves as the foundation for selecting peptides that form the most stable binding complexes with targeted small molecules. We initially demonstrated this approach's efficacy using tripeptides proline-cysteine-histidine (PCH) and γ-L-glutamyl-L-cysteinyl-glycine (glutathione, GSH) for mercury detection, adsorbed onto 20 nm gold nanoparticles (AuNPs). The heteroligand PCH/GSH-AuNPs outperformed its monoligand counterparts, doubling its Hg2+ detection capabilities to a limit of detection (LOD) of 25 ppb. Notably, the heteroligand system minimized the entropy of the binding complex, thereby enhancing specificity. Extending our methodology, we targeted branched-chain amino acids (BCAAs) for predictive diabetes diagnostics. Our library-driven heteroligand strategy demonstrated exceptional adaptability, promising a versatile pathway for early disease detection by targeting a broad spectrum of small molecules.

Keywords

Heteroligand
Plasmon Coupling
Metabolites
Biomarker

12:00 - 12:10

RC.04 Novel cost-effective electrochemical systems for sensing cancer biomarkers

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Abstract

Development of point-of-care (POC) biosensors for detection of cancer biomarkers is a crucial topic for enabling early detection of cancer occurrence and monitoring its progression. Our results showcase cost-effective solutions for detection of human epidermal growth factor receptor 2 (HER2) based on custom-made gold leaf electrodes (GLEs) and Matrix proteinase 2 (MMP2) detection based on graphene-functionalized commercial screen-printed gold electrodes. Overexpressed HER2 biomarker has been classified as both a prognostic and predictive biomarker for breast cancer while MMP-2 is a protein that is typically overexpressed in tumor tissues, with important roles in tumor invasion, metastasis as well as in tumor angiogenesis. Different novel strategies are employed for optimization of the surface functionalization with suitable proteins, antibodies, and aptamers to achieve highly sensitive and specific interaction with cancer biomarkers. Electrochemical characterization was performed using cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) and the potential of biomarker-sensing was examined in phosphate buffer saline (PBS) and in a cell culture medium. The proposed solution showed good specificity and high sensitivity of HER2 detection without any enrichment steps, achieving a limit of detection (LOD) of 0.02 ng/mL in PBS and 0.03 ng/mL in cell culture medium, making the proposed sensor a cost-effective and sensitive candidate for detection in complex biological matrices. In case of the MMP-2 sensor, based on impedimetric measurements, we could detect as low as 3.32 pg/mL of MMP-2 in PBS with a wide dynamic range of 1 pg/mL – 10 ng/mL. Besides high specificity, rGO-based aptasensor showed a potential for reuse due to demonstrated successful signal restoration after experimental detection of MMP-2. These novel cost-effective biosensing systems represent a promising step toward future application for POC detection of HER2 and MMP2 cancer biomarkers.

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Keywords

cancer biomarkers
electrochemical biosensors
MMP-2
HER2

12:10 - 12:20

RC.05 Shining light on cancer biomarkers with fluorescent peptide biosensors : Profiling kinase activity signatures in tumour biopsies

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Abstract