ANALYTICAL SEMINAR

Reactive Mass Spectrometry for Bioanalysis

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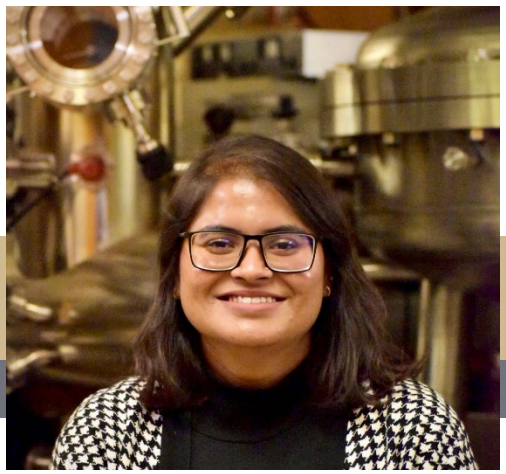

The rapid quantitative analysis of complex samples by mass spectrometry (MS) has proven useful for applications in both point-of-care (POC) and laboratory-based testing. Use of tandem MS for rapid identification and quantification without separation and with minimal sample preparation has garnered considerable interest as it can reduce the analysis time and increase sample throughput significantly. This presentation will highlight into designing molecular probes to capture and quantify small molecules by reactive tandem MS. For example, quantitation of biologically important thiols will be demonstrated by utilizing reactive MS directly from various biological matrices without extensive sample workup. A new derivatizing reagent has been developed combining a thiol-selective unit to capture biological thiols from complex matrices, and a pre-charged pyridinium unit to maximize sensitivity in MS, eliminating the need for separation steps. This method is applicable over a wide concentration range (1 µM to 10 mM) and is demonstrated for complex biological matrices, including blood sera, plasma and tissue samples. This experiment requires limited sample preparation (< 4 min) and short analysis time (< 1 min). High precision and accuracy (both better than 8%) are validated using independent HPLC-MS analysis. Additionally, it is suitable for monitoring redox homeostasis of Cys-Cystine. By enabling precise thiol quantification in biological samples with minimal sample preparation and rapid analysis, this method has potential for POC applications where quick results are essential.

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PURDUE UNIVERSITY

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ANALYTICAL SEMINAR

Molecular Logic and Computing

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Molecular Logic Gates (MLGs) are inspired by traditional semiconductor circuits and offer new possibilities for chemical-based computation. Unlike silicon-based circuits, which face physical limitations as they shrink, MLGs could enable smaller, efficient computing devices that overcome these challenges. MLGs are especially promising in fields that require ultra-miniaturized computing and sensing, as they can perform complex functions in tiny, adaptable forms. This study focuses on creating a new type of MLG that can detect multiple types of chemicals in a reusable, or resettable, format. Traditional “single molecule – multi-analyte” MLGs have several limitations, such as their inability to detect diverse chemicals and the need for distinct MLGs for each analyte. These designs are often non-resettable, meaning they cannot be reused. To address these limitations, we developed a fluorescent molecule based on oxazinoindoline (OZ), which can switch between different states in real time, allowing for repeated use. Our OZ-based MLGs use different solvents, bio-thiols, and metal ions as inputs, producing a binary output (YES or NO) based on the emission intensity at 595 nm. We also constructed a sensing network to distinguish between similar molecules, such as Cysteine and Homocysteine, using copper ions. Our MLGs are termed SMART (Single Molecule Activable in Real Time) because they can reset through reversible changes in their structure. Additionally, we added a chloride handle to the OZ molecules, allowing for potential attachment to solid supports for further applications. This work introduces a flexible, resettable MLG design that can detect and process various chemicals. The SMART MLGs could pave the way for advanced molecular computing and more efficient biochemical sensors in the future.

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