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### Drug monitoring using integrated approaches

**Statement of the Problem:** The high consumption of drugs unavoidably leads to their release into the environment and this has been a subject of interest for many years. A vast number of reports in the last decade have highlighted the occurrence of drugs and their metabolites in aquatic systems, waste waters and water treatment plants. Their presence in aquatic environment and drinking waters is a result of unsuccessful elimination during sewage treatments. Majority of these compounds are in polar nature; therefore, soluble in water, with a molecular mass ranging between 0.2 and 1 kDa. They have been detected in concentrations from the ng L<sup>-1</sup> to the µg L<sup>-1</sup> in water sources. The monitoring and detection of drugs and their metabolites are both very crucial before and after water treatments for manufacturing effective filtration systems against them. This will prevent their contamination of drinking water, as traces of these chemicals in water can result in increased resistance and tolerance or toxic effect which can directly cause health problems due to the loss of effective treatment.

**Methodology & Theoretical Orientation:** Artificial affinity receptors (nanoMIPs) were developed by employing molecular modelling and then used in combination with surface plasmon resonance (SPR) based biosensors and liquid chromatography-mass spectrometry (LC-MS) for the monitoring and detection of drugs from water. Diclofenac, metoprolol and vancomycin specific nanoMIPs were synthesized using recipes based on the molecular modelling results and in house know-how. The nanoMIPs were characterized by employing dynamic light scattering (DLS) and transmission electron microscopy methods to determine the size, quality and uniformity of the produced nanoMIPs. These molecular receptors were then covalently immobilized on the SPR sensors and the affinity interaction between drugs and their corresponding receptors were investigated. As an alternative detection method, LC-MS was employed where nanoMIPs were packed in solid phase extraction (SPE) columns and the water samples contaminated with three drugs were loaded throughout the columns and the samples were measured in LC-MS before and after filtration.

**Findings:** The DLS size measurements of the nanoMIPs were found to be ~ 132.3±3.2 nm, 169.4±3.5 nm and 233±8 nm for diclofenac, metoprolol and vancomycin with a polydispersity index of ~0.3 which highlights the high quality of the synthesized affinity receptors. The dissociation constants were determined as 4.27 x 10<sup>-10</sup>, 1.68 x 10<sup>-11</sup>, 2.86 x 10<sup>-11</sup> for diclo-, meto- and vanco-nanoMIPs, respectively. The detection limits of nanoMIP-SPR sensors were 1.2 ng mL<sup>-1</sup>, 1.9 ng mL<sup>-1</sup> and 0.06 ng mL<sup>-1</sup>, respectively. NanoMIPs integrated SPE columns coupled with LC-MS was developed for three drugs and their monitoring were investigated in the concentration ranges of 1-5000 ng mL<sup>-1</sup> for diclofenac and vancomycin; and 1-160 ng mL<sup>-1</sup> for metoprolol with a detection limits of 18 ng mL<sup>-1</sup>, 4.4 ng mL<sup>-1</sup>, 1 ng mL<sup>-1</sup>. The achieved results show the excellent success of nanoMIPs by employing integrated approaches that tightly connected computational simulations, biosensors and LC-MS for drug monitoring. These simple, cost-effective and user-friendly techniques can provide promising future technology for the routine analysis of water samples.

### Biography

Zeynep Altintas has her expertise in the fields of biosensors, biomimetic materials and diagnostics. She is the Head of Biosensors and Receptor Development Group in Technical University of Berlin. Prior to her current position, she worked in Cranfield University as a Faculty Member as well as in other institutes as Visiting Professor and Researcher. She pioneered nanoMIPs-based SPR sensors for the detection and removal of pharmaceuticals, toxins and viruses using a novel solid phase synthesis method. Her research on virus imprinting area creates new pathways for virus sensing and removal by providing strong alternatives to natural antibodies. Her works have received several awards from international organizations in recent years. She is serving as an Expert Reviewer for EU and Wisconsin Groundwater Coordinating Council (USA) funded projects in addition to acting as the reviewer for several important journals in her areas of expertise.

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