PÔSTER - RESUMO - SENSORES E BIOSSENSORES

MERCURY(II) ION DETECTION USING A NOVEL FLUORENE-BASED FLUORESCENT CHEMOSENSOR: COMPUTATIONAL STUDIES, APPLICATION IN FISH LIVER AND BRAZILIAN CACHAÇA

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Mercury is a persistent and globally distributed contaminant of major environmental and toxicological concern. Classified by the World Health Organization[1] as a nonessential and harmful element at any level of bioaccumulation, mercury poses severe risks to ecosystems and human health, particularly in its inorganic and methylated forms. Its occurrence in water, soil and food systems is frequently associated with industrial effluents, mining activities, inadequate waste disposal and other anthropogenic processes. These issues highlight the urgent need for sensitive, selective and cost-effective detection systems capable of monitoring mercury in complex matrices, reinforcing the growing relevance of sustainable approaches to environmental and public-health surveillance[1]. In this context, fluorescent sensors and chemosensors have emerged as important tools due to their operational simplicity, high sensitivity and adaptability to real-sample analysis[2].

This study reports the synthesis, characterization and analytical evaluation of a new fluorene-based chemosensor, diethyl 2-(2,7-dibromo-9-oxo-9H-fluoren-9-ylidene)malonate (FDE), designed for the selective detection of HgII ions in ethanolic medium. The work presents an intrinsically multidisciplinary nature because it integrates concepts from organic chemistry (synthesis and structural modification), inorganic chemistry (metal–ligand interactions and coordination behavior), analytical chemistry (method validation, fluorescence quenching mechanisms and calibration studies) and theoretical chemistry (electronic-structure analysis via DFT calculations). The environmental and public-health relevance of mercury detection further aligns this research with principles of sustainability, emphasizing low-cost monitoring strategies capable of supporting safer water quality control, food assessment and exposure prevention.

The proposed sensor exhibits strong intrinsic fluorescence, which undergoes pronounced quenching in the presence of HgII ions, reaching 99 percent suppression. A linear analytical response was observed in the 0.1–0.9 μmol L?^{1} concentration range, with remarkably low limits of detection and quantification, 10.5 and 33.5 nmol L?^{1}, respectively, obtained by the least-squares method. Selectivity tests revealed no interference from 24 different metal ions even when analyzed in alcoholic medium, demonstrating the sensor's high specificity. Job's plot, Benesi-Hildebrand[3] and Stern–Volmer[4] treatments indicated formation of a highly stable complex with 1:2 metal:sensor stoichiometry. The association constant, 4.67x104 L mol?^{1}, is among the highest reported for mercury chemosensors, while the Stern–Volmer constant of 4.73x104 L mol?^{1} supports a static-quenching mechanism. Theoretical calculations[5] further corroborated these findings by indicating that the fluorescence suppression most plausibly occurs through ligand-to-metal charge transfer followed by intersystem crossing, favoring population of triplet states and reducing emissive pathways.

Method applicability was demonstrated through recovery assays using real matrices, including artisanal cachaça and the certified reference material DOLT-4 (fish liver). These experiments yielded satisfactory recovery values, proving that FDE can be employed reliably for mercury quantification in complex samples. Statistical validation confirmed the robustness and accuracy of the calibration model.

Overall, the developed fluorene-based chemosensor represents a promising sustainable, sensitive and low-cost alternative for HgII monitoring. Its multidisciplinary foundation and strong analytical performance contribute meaningfully to advances in sensor and chemosensor technologies aimed at environmental protection and public-health monitoring.

References

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Palavras-chave: fluorescence; mercury(ii) detection; quenching; chemosensor; sensor.