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Fruit-extracted thiols as tools for mercury removal in contaminated water sources

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Over the years, extensive research has focused on the bioremediation and synthetic remediation of water contaminated with mercury and mercury-containing compounds because of their high toxicity. Functionalizing adsorbent materials optimizes their ability to adsorb Hg (II), due to the strong interactions between sulphur-containing molecules (such as thiols) and mercury [1]. However, the currently available thiols are expensive and unsuitable for application in developing countries. In this project, we aim to develop new technologies based on the sustainable exploitation of local resources. These resources include fruits as sources of sulphur molecules with the presence of thiol groups (*e.g.* glutathione (GSH) and cysteine (CYS)) for functionalizing materials such as iron magnetic nanoparticles (NP) cheaply and sustainably.

This work develops novel techniques for the extraction of thiol molecules from four different perennial fruits from local Colombian crops, using a reliable, low-cost, and easy-to-implement methodology. Thiol extraction is carried out for the three main parts of the fruits: pulp, peel, and seeds. Our work is based mainly on the separation of naturally produced organic thiols such as CYS and GSH. We quantify the thiol concentrations (GSH and cysteine in particular) using spectrophotometry and HPLC analysis. Showing a higher concentration of these molecules in the pulp of the fruits compared to the concentrations of the seeds and the peel Furthermore, we discuss the durability and degradation factors affecting these thiols, as well as their possible outsourcing from Colombian crops. Additionally, we complement our studies with the results of computational quantum chemical modelling of the properties of candidate thiols and their interactions with Hg. It is expected that the effectiveness of these materials can be proven in simulated aqueous media contaminated with mercury species and subsequently they could be used as remediation mechanisms in real bodies of water.

[1] R. Liang, H. Zou, Removal of aqueous Hg(ii) by thiol-functionalized nonporous silica microspheres prepared by one-step sol-gel method, RSC Advances. 10 (2020) 18534–18542. https://doi.org/10.1039/d0ra02759f