Green synthesis of biomass-derived Carbon Quantum Dots for metal ion sensing: optimization, characterization, and binding affinity studies

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Carbon Quantum Dots (CQDs) are photoluminescent carbonaceous nanomaterials characterized by a particle size smaller than 10 nm and the presence of hybridized sp^2 carbon and oxygen-containing groups on their surface [1]. The existence of these functional groups makes CQDs prone to interaction with metal cations, leading to the photoluminescence quenching even at low metal concentrations, often showing good selectivity [2]. Consequently, extensive research has been conducted on the potential application of CQDs in metal ion sensing.
One of the main advantages of CQDs is the possibility to synthetize them from green sources, such as biomasses, offering a promising alternative for agricultural and food waste management [1]. Among the various preparation strategies, the hydrothermal approach is the most commonly used. However, there is considerable variation in the literature regarding the synthesis conditions. When using water as solvent, temperature, time, and initial concentration of precursors have the main influence on the particle size, surface functionalization and, consequently, photoluminescence properties and stability of the CQDs [3].
The first part of this work exploits the chemometric tool of experimental design [4] to optimize the synthesis of biomass-based CQDs using citrus waste bergamot pomace as a precursor. An initial hydrothermal synthesis was carried out using 250 mg of pomace in 25 mL of water, heated in an autoclave at 180 °C for 6 hours [5]. The experimental design was then conducted according to a 2^k full factorial design while varying the initial amount of precursor, the temperature, and the reaction time. After purification, the quantum yield was evaluated using quinine sulfate as a reference. The results were used to construct the experimental surface, allowing for the determination of the optimal synthesis conditions.
In the second part, the CQDs with the highest quantum yield were characterized by ATR-FTIR spectroscopy to identify the surface functional groups potentially able to interact with metal cations. Finally, the ability of different metals to quench the CQDs fluorescence was tested. The binding ability of the most selective candidates was further evaluated through spectrofluorimetric titrations.

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