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Webinars

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Host-guest complexes based on p-sulfonatocalix[n]arenes and a pyranoflavylium-type dye for dynamic capture of biogenic amines

Ana Sofia Pires

LAQV REQUIMTE, Department of Chemistry and Biochemistry, Faculty of Sciences of the University of Porto

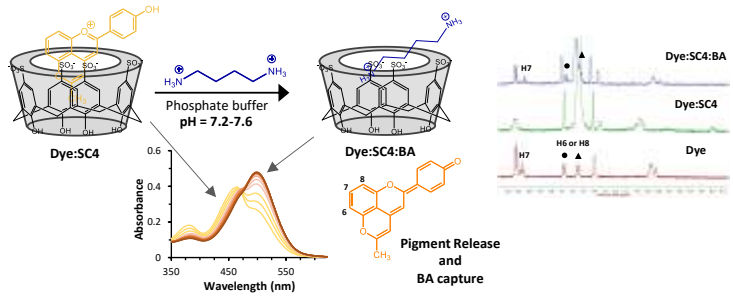
sofia_pires97@hotmail.com

Biogenic amines (BAs) are biologically active nitrogen-containing compounds, formed in the normal metabolism of living organisms, during food spoilage process and are key markers of food quality and safety. Since their presence in foods at high levels can cause significant health problems, researchers have been focused on developing novel strategies and methods for early detection/capture of these analytes. Host−guest chemistry is a subfield of supramolecular chemistry focused on molecular recognition (non-covalent binding) of small molecules or ions (guests) by larger receptors (hosts) to form a host−guest complex. These systems allow the modification and control of the physical-chemical properties of the guest molecules, potentially leading to applications in sensing field and drug delivery.

The main goal of this work was to develop new host-guest systems based on the complexation of water-soluble sulfonated calix[n]arenes host receptors with positively charged and pH-sensitive pyranoflavylium-based2 guests. The interactions between the hosts and the pigment towards BAs detection was evaluated by means of UV-Vis, fluorescence, 1H NMR, and ITC techniques.

The dye concentration, host-guest molecular ratio, and working pH was adjusted to promote the highest interaction between the free dye (pKa 6.72) and the macrocyclic receptors (e.g., pKa SC8-dye 8.45). Overall, the host-flavylium cation complexes were able to detect putrescine/tyramine in phosphate buffer solutions (pH 7.2 7.6) with the simultaneous release of the neutral quinoidal base

species of dye to the bulk, resulting in a colorimetric variation from yellow to pink-red. The BAs sensing was further established by fluorescence quenching for the calix[n]arene:dye complexes and fluorescence dye recovery upon the addition of BAs. 1H NMR spectroscopy was used to demonstrate the interaction mode, suggesting an encapsulation-driven process. Overall, these host-guest systems demonstrated significant potential for detecting BAs, one of the most important crucial markers of food deterioration.



Short Bio

Ana Sofia Pires graduated in Chemistry, in 2018, at Faculty of Sciences of University of Porto (FCUP). Her bachelor's internship, at CIQUP, was about Polymer/surfactant mixtures as dispersants and non-covalent functionalization agents of multiwalled carbon nanotubes. In 2020, obtained her Master's Degree in Chemistry at the Faculty of Sciences of University of Porto (FCUP). During that period she developed a thesis entitled "pH sensors for anthocyanin application in food packaging" at the FoodPolyphenolLab. Since October 2021, she is a PhD student of the Doctoral Programme in Sustainable Chemistry, LAQV-REQUIMTE where she aims to develop new colorimetric and fluorescent systems based on pyranoflavylium for selective recognition of metabolites resulting from food degradation.

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