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Synthesis and anion recognition studies of new ureylbenzamide-based receptors

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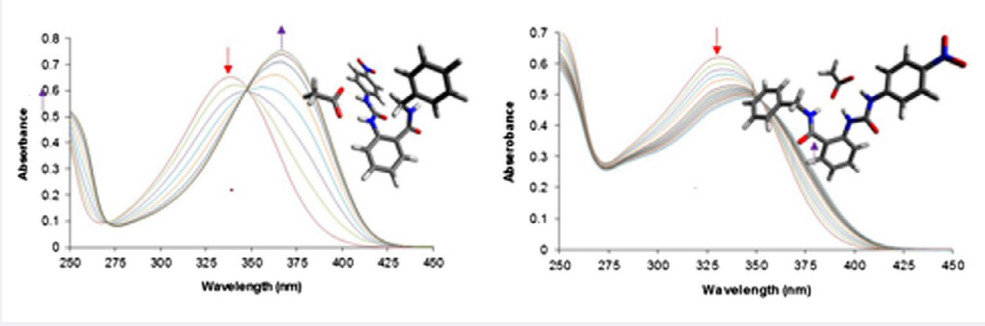
ABSTRACT

A new group of ureylbenzamide-based receptors (**1**–**4**) has been synthesized; its binding affinity and capacity to form supramolecular complexes in solution with different anions have been investigated. For designing these receptors, it was considered a combination of the positions of the urea and amide groups (*ortho* and *meta*), and the chromophore groups naphthyl and nitrophenyl, yielding four receptors. The position and chromophore structure affected the acidity of the urea and amide hydrogens in the order **4**>**3**>**2**>**1**. All the spectroscopic studies showed a significant change of **1** and **2** compared with **3** and **4** in the presence of different TBAX salts in acetonitrile. The ^{1}H-NMR spectra show a preferential interaction of the anions with the urea group in receptors **1** and **2** due to the less steric hindrance, while there is a cooperative interaction of amide group in receptors **3** and **4** due to the closeness of both groups.



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Introduction

In recent years, research in supramolecular chemistry has experienced tremendous growth under the significant roles played by common anions in the biological and environmental world, and therefore, the development of effective methods for detecting anions is very important (*1–6*). Due to many possible applications, neutral receptor molecules for different anions have attracted much attention (*7–10*). Moreover, among the anion analytes of biological and environmental importance, fluoride is one of the most significant due to its crucial role in dental health, since most of the drinking water comes from processing plants that add fluorides before sending by the water systems to be consumed. Hence, damages both the environment when discarded and reach rivers and seas, and it is also involved in dental and bone health when fluoride is consumed (*11*).

Despite all efforts, attempts to increase the receptor's affinity and specificity for fluoride ion have mostly led to a complexity of design and synthesis, and therefore there is a challenge to make an effective sensor that is sensitive and has a high association constant for fluoride ion (*12–15*). Ureas and thioureas are neutral receptors providing H-bond donors, which bind to anions by hydrogen bonding interactions regardless of solution pH (*16, 17*). A molecule with one or more preorganised urea or thiourea groups can provide H-bond donors for an anion which increases its capability to form supramolecular complexes (*18–23*). Other functional groups capable to

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