SYNTHESIS AND SPECTROSCOPIC CHARACTERIZATION OF NOVEL 1,2,3-TRIAZOYL-BENZOTHIAZOLES

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INTRODUCTION

Benzothiazole is an attractive building block in the design of novel fluorescent dyes because of its π-bridging and electron-withdrawing properties as well as high chemical and photophysical stability [1]. In addition, 1,2,3-triazoles have great potential in chemical sensing as they can act as a covalent linker between benzothiazole and corresponding functional group or can participate in binding of the target analyte [2]. Introduction of different electron donating and/or electron withdrawing substituents in the benzothiazole core can significantly affect the optical characteristics of the resulting molecule. In this work we present the synthesis of novel benzothiazole-1,2,3-triazole conjugates as novel donor-π-acceptor (D-π-A) systems using click-chemistry approach and their basic spectral characterisation in solution.

MATERIALS AND METHODS

Chemistry. New benzothiazole-1,2,3-triazole conjugate were synthesised by click-chemistry approach. First step included preparation of 2-azido-benzothiazole (A) via diazotation reaction. 2-azido-benzthiazole (A) reacted with corresponding alkynes to gain desired products (1-7).

Spectroscopic characterization.
The interaction of benzothiazole-1,2,3-triazoles 1-7 with different metal ions, effect of solvent and pH have been studied by UV/Vis absorption and fluorescence spectroscopy.

OBJECTIVES AND RESULTS

1) Synthesis of novel benzothiazole based chemosensors with 1,2,3-triazole as π-linker (D-π-A molecular systems)
2) Characterization of basic photophysical properties and effect of pH and metal ions in different solvents in order to develop new sensing molecular systems

Figure 1. Typical solvatochromic behaviour of D-π-A chromophore. a) Absorption and b) emission spectra of 4 (λem=λabs,max); c) dependence of the Stokes shift on the empirical polarity parameter E_{\text{r}}(30).

Figure 2. Emission spectra of 2 in DMSO, dichloromethane and H_{2}O (λem=λabs,max).

Figure 3. Effect of pH on spectral properties. a) Emission spectra of 4 in pH 1.0, 7.0 and 13.0; b) pH titration of 7 in pH range 1.0–13.0. pK_{w} were calculated by Boltzman sigmoidal fitting to be 3.1 and 11.4.

Figure 4. Emission spectra of 3 in the presence of metal ions (1 eq.)

CONCLUSIONS

Novel benzothiazole based D-π-A molecular systems were prepared. Spectral characterization showed that fluorescence properties of studied compounds can be altered by solvent polarity or binding an analyte. 2 and 4 exhibited red shifted emission maxima in polar solvents. 4 and 7 are presented as potential pH sensors. Compound 4 showed fluorescence intensity quenching in the presence of Fe^{3+} ions. All compounds showed similar behaviour in the presence of studied metal cations.

References:

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