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Optical chemosensory studies of novel amphiphilic D-A-π-A benzothiadiazoles for cyanide detection

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INTRODUCTION & AIM

In recent years, donor-π-acceptor benzothiadiazole molecules have drawn significant attention due to their tunable optical and electronic properties. These benzothiadiazole derivatives are particularly interesting in the fields of optical chemosensing due to their easy functionalization, high photostability and biocompatibility. [1-4]

Cyanide ions are highly toxic to humans and the environment, as they interfere with oxygen use. This can lead to cellular death and negatively impact multiple physiological systems such as the vascular. Symptoms of cyanide poisoning include vomiting and, in severe cases, death. Despite its toxicity, cyanide remains in use across several industries, such as plastic manufacturing. [5-7]

This report aims to study two positively charged amphiphilic benzothiadiazole derivatives as effective cyanide-selective optical chemosensors in DMSO.

METHOD

- **Synthesis** and **photophysical characterization** of precursor **1** and benzothiadiazole derivatives **2** and **3** (**Figure 1**) have been reported recently by our research group. [8]

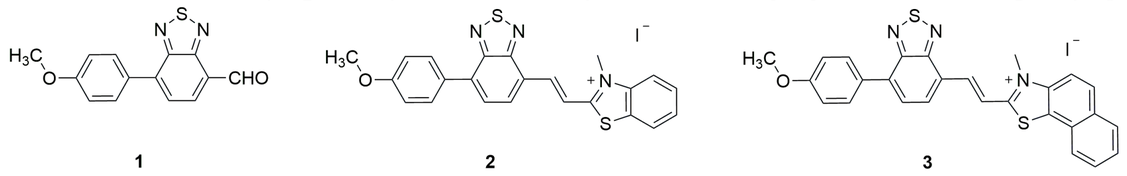
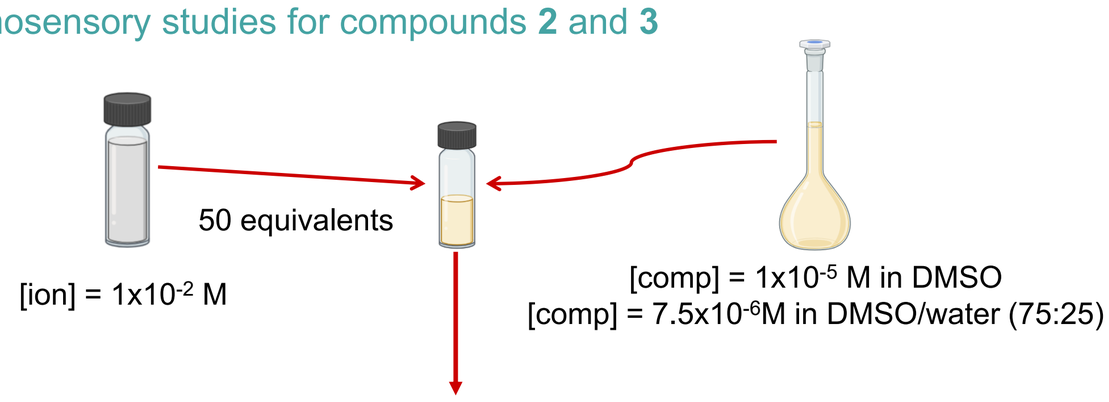


Figure 1. Chemical structures of precursor **1** and benzothiadiazoles **2** and **3**.

Chemosensory studies for compounds **2** and **3**



CONCLUSION/ FUTURE WORK

- Compound **2** and **3** are highly sensitive to cyanide in DMSO.
- In aqueous media, cyanide detection through compounds **2** and **3** is not as effective probably due to solvation effects that hinder the interaction between the probes and the anion.
- In the future, more selectivity test, NMR titrations and binding stoichiometry of the complexes using a Job's plot should be carried out.

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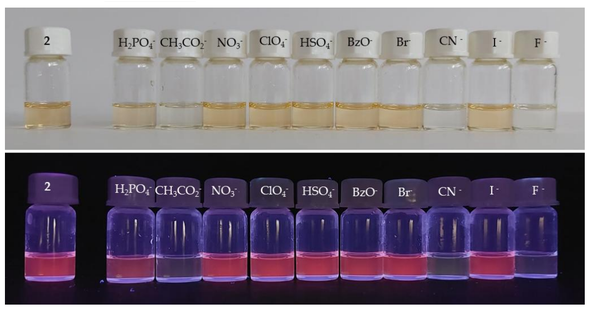
RESULTS & DISCUSSION

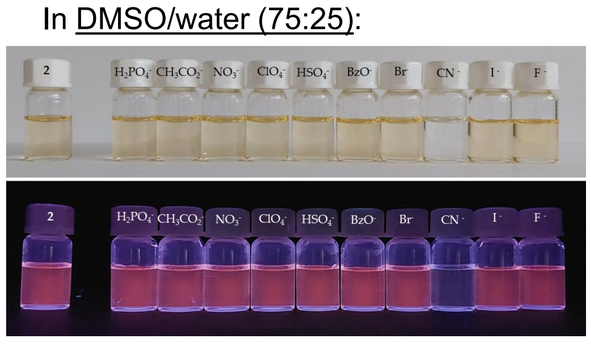
Chemosensory studies of benzothiadiazole **2**

- **Preliminary studies:**

In DMSO:



In DMSO/water (75:25):



- **Spectrophotometric and spectrofluorimetric titrations with CN^-:**
  - In DMSO: 5 equivalents → total decrease of absorbance at 465 nm and of fluorescence intensity at 657 nm (**Figure 2a**)
  - In DMSO/water (75:25): 50 equivalents → fluorescence intensity decreased (**Figure 2b**)

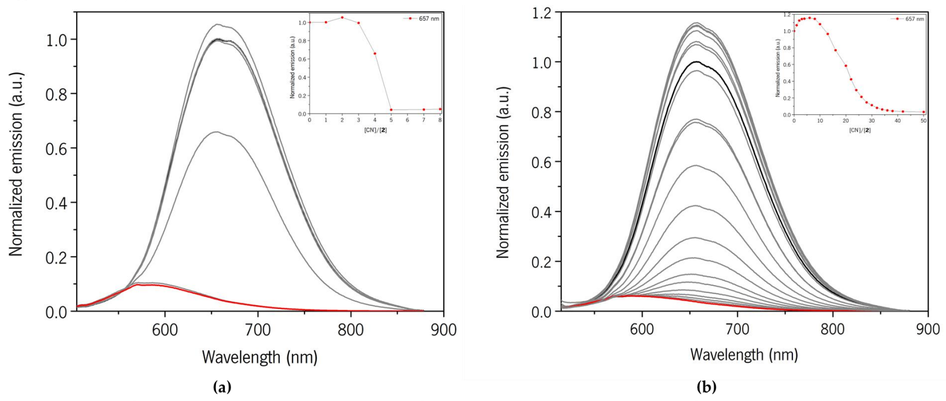
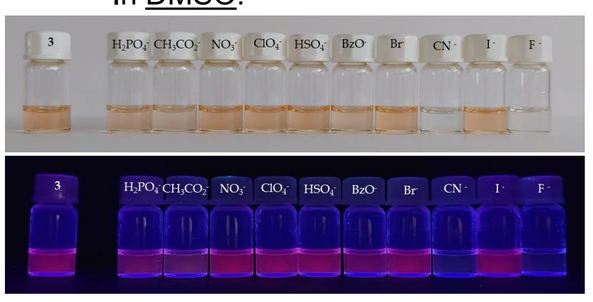


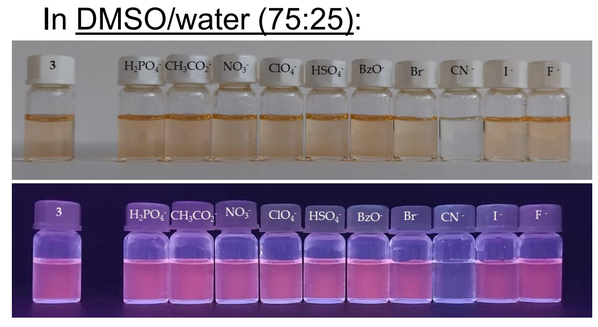
Figure 2. Spectrofluorimetric titration of compound **2** with CN^- in (**a**) DMSO and in (**b**) DMSO/water (75:25). Insets show normalized emission at 657 nm as a function of [CN^-]/[**2**]. (Conditions: (**a**) [**2**] = 1 × 10^{-5} M, (**b**) [**2**] = 7.5 × 10^{-6} M, [CN^-] = 1 × 10^{-2} M, λ_{exc} = 465 nm, T = 293 K).

Chemosensory studies of benzothiadiazole **3**

- **Preliminary studies:**
  - In DMSO:



In DMSO/water (75:25):



- **Spectrophotometric and spectrofluorimetric titrations with CN^-:**
  - In DMSO: 7 equivalents → total decrease of absorbance at 480 nm and of fluorescence intensity at 666 nm (**Figure 3**)
  - In DMSO/water (75:25): 76 equivalents → fluorescence intensity decreased

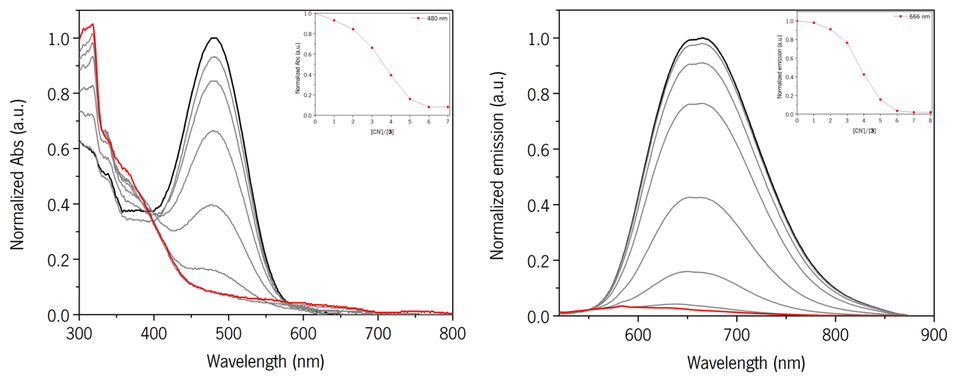


Figure 3. Spectrophotometric (**a**) and spectrofluorimetric (**b**) titrations for compound **3** with CN^- in DMSO. The insets represent the normalized absorbance and emission at 480 nm and 666 nm, respectively as a function of [CN^-]/[**3**]. ([**3**] = 1 × 10^{-5} M, [CN^-] = 1 × 10^{-2} M, λ_{abs} = λ_{exc} = 480 nm, T = 293 K).

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