PIRYDOBENZOTHIAZOLEDICARBONITRILES-BASED FLUORESCENT PROBES FOR pH

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Motivation

In live cells pH is stabilized within certain limits

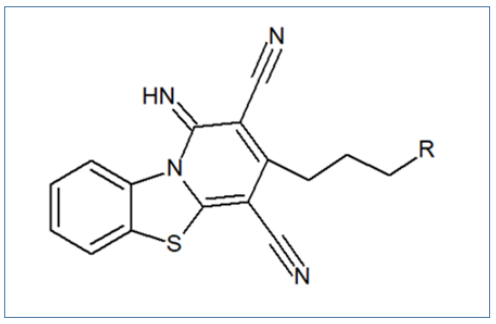
Slight changes in pH could lead to disease development

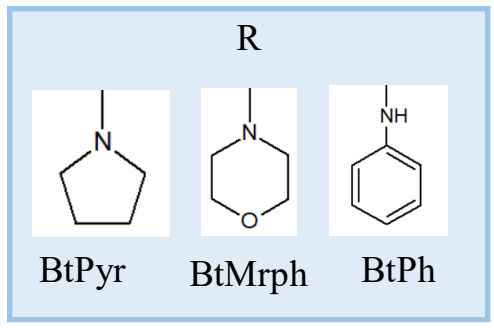
Fluorescent probes based on heterocyclic compounds:

Noninvasiveness

High sensitivity

Selectivity

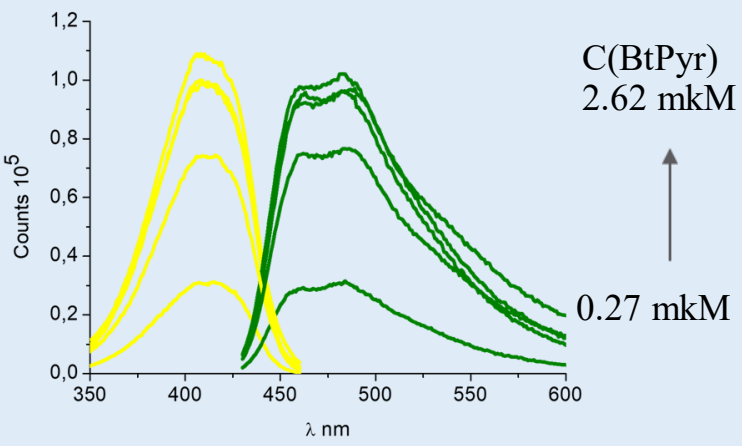




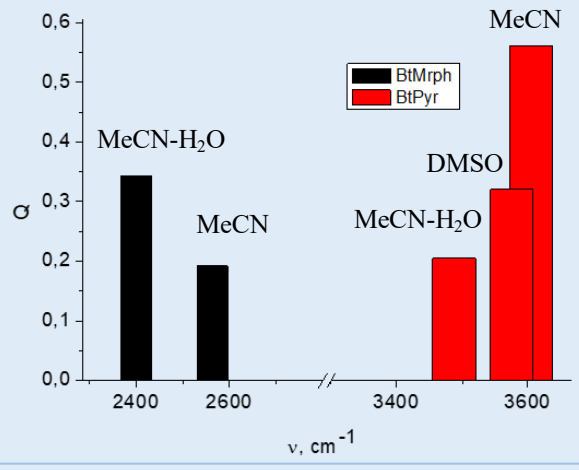
Main objectives

- To investigate spectroscopic properties and study the link between substituent and pH response
- To determine quantum yields

Fluorescence



1. Fluorescence spectra in aqua-organic mixture (3.2% ACN)

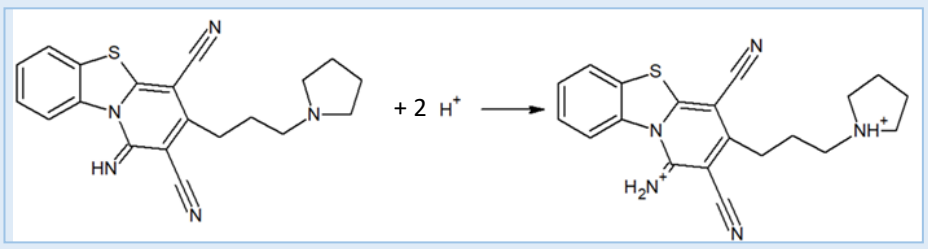


2. Quantum yield as the function of Stokes shift

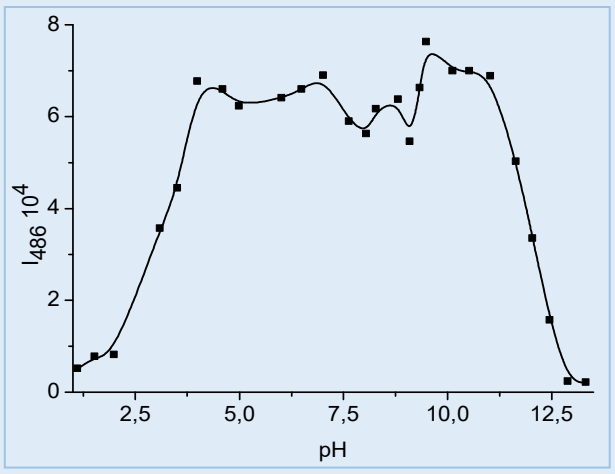
Aqua-organic mixture (3.2% ACN):

Probe	λ_{abs}, nm	λ_{em}, nm	ε_{max}, 10^4	QY
BtPyr	415	486	0.36 ± 0.04	20
BtMrph	428	480	0.54 ± 0.07	34
BtPh	413	490	0.55 ± 0.23	-

Protonation



3. Fluorescent probe protonation



4. Fluorescence intensity of BtPyr (0.27 mkM) in phosphate buffers (0.17% ACN) under different pH

Aqua-organic mixture (0.17% ACN):

Probe	pKa_1	pKa_2
BtPyr	12.10	3.17
BtMrph	8.05	4.12
BtPh	4.17	2.49

Conclusions

1. Probes are characterized by the presence of a broad absorption band in the region of 350-450 nm and emission band between 450-550 nm
2. Reagents are insensitive to the polar environment (except pyrrolidine derivative);
3. Amino derivatives are characterized by high quantum yields from 19% to 56% depending on the polarity of the solvent and water content;
4. Fluorescence intensity increases with increasing acidity within certain limits; at pH <4, the fluorescence intensity decreases, which indicates the protonation of the imino group
5.Probes are characterized by intense fluorescence in buffers imitating biological fluids, the ratio of the aqueous phase to the organic phase is 600:1.