

Functionalized heteroacetonitriles as analytical reagents for spectrophotometric determination of zinc

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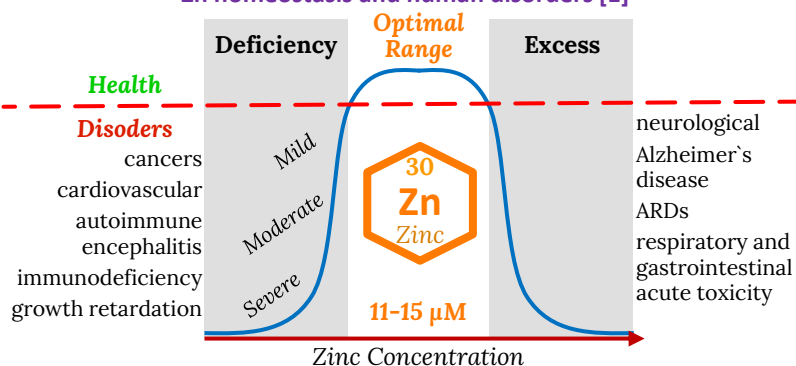
Functions of Zinc

- ❖ Structural, catalytic cofactor
- ❖ Replication of DNA and RNA
- ❖ Metabolism and apoptosis
- ❖ Growth and development
- ❖ Signal mediator and neurotransmitter

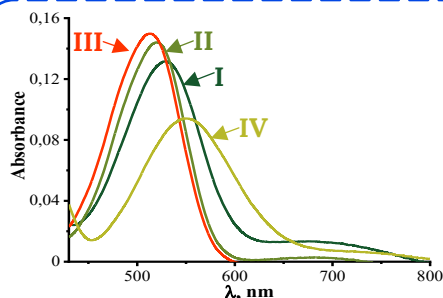
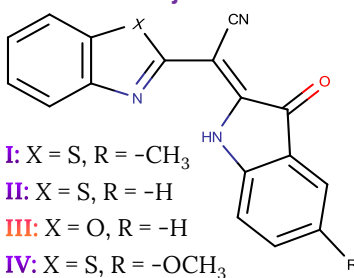
Derivatives properties

- ❖ Anticancer activity
- ❖ Antimicrobial activity
- ❖ Antiviral effect
- ❖ Antiinflammatory activity
- ❖ Chromophore and fluorescent

Zn homeostasis and human disorders [1]



Objects



Optical characteristics

R	λ_{\max} , nm	ϵ^{λ} , l·mol ⁻¹ ·cm ⁻¹ , 10 ⁴
I	530	1,38±0,05
II	520	1,48±0,05
III	514	1,66±0,10
IV	550	1,03±0,05

Protolytic properties

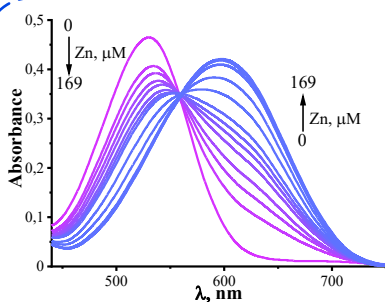
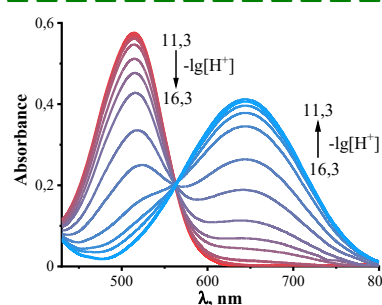
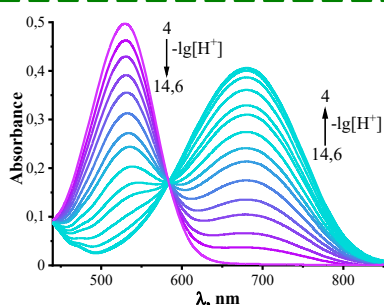


pK_a^f

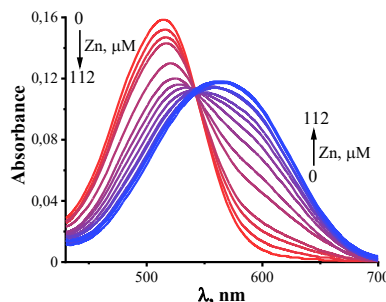
13,7±0,1 15,2±0,2

Red shift ($\Delta\lambda$)

150 nm 130 nm



$\varphi(\text{DMSO}) = 83\%$, $C_I = 38 \mu\text{M}$, $\text{pH} = 7,2$



$\varphi(\text{DMSO}) = 70\%$, $C_{III} = 10 \mu\text{M}$, $\text{pH} = 7,2$

Complexation with Zn



C_{Zn}

Zn:I = 1:1 Zn:III = 1:1

$\lg K = 7,88 \pm 0,02$ $\lg K = 9,4 \pm 0,2$

LOD = 0,4 µM LOD = 1,0 µM

Conclusions

- Reagents interact with Zinc(II) at the acidity of biological fluids. The absorption spectra has a broaden band in the range of 550–650 nm.
- The limits of Zinc(II) detection with benzothiazole and benzoxazole derivatives is 0,4 µM and 1,0 µM consequently.
- The formal associate stability constants of complexes with Zinc(II) are calculated, which are in the range 10⁷–10⁹.