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ANTIMIKROBNI POTENCIJAL BENZALDOKSIMA: SINTEZA, BIOLOŠKA AKTIVNOST I *IN SILICO* STUDIJE

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Oksimi su jedinjenja zastupljena u biljnom i životinjskom svetu, gde čine deo odbrambenog sistema i učestvuju u olfaktornoj komunikaciji. Predstavljaju intermedijere u biosintezi velikog broja metabolita i jedan su od proizvoda enzimske oksidacije i dekarboksilacije aminokiselina. Važna su klasa jedinjenja sa širokom primenom u sintetskoj hemiji. Oksimska grupa poseduje ulogu i donora i akceptora vodonične veze što omogućava dobru interakciju sa biološkim targetima i ispoljavanje širokog spektra bioloških aktivnosti, kao što su antimikrobna, antiinflamatorna, antioksidativna i antikancerska aktivnost (1). Usled sve veće ekspanzije multirezistentnih patogenih sojeva i činjenice da brojna istraživanja potvrđuju antibakterijsko, antivirusno i antifungalno delovanje raličitih derivata oksima, ova jedinjenja predstavljaju pogodne kandidate za razvoj novih antimikrobnih lekova. Sprovedeno istraživanje obuhvatalo je sintezu benzaldoksima standardnim postupkom kondenzacije benzaldehida i soli hidroksilamina (2), ispitivanje antimikrobne aktivnosti sintetisanih jedinjenja mikrodilucionom metodom (3) na laboratorijski kontrolisanim sojevima bakterija *Bacillus subtilis* i *Staphylococcus aureus*, plesni *Aspergillus niger* i gljivice *Candida albicans*, kao i *in silico* studije korišćenjem SwissADME i DataWarrior softvera. Ispitana jedinjenja ne utiču na rast bakterijskih sojeva u ispitanim koncentracijama, dok inhibiraju rast gljivice *Candida albicans* i plesni *Aspergillus niger* u rasponu koncentracija 62,5-500 μg ml^{-1} i 125-500 μg ml^{-1}. Na osnovu dobijenih rezultata uočava se fungistatski potencijal benzaldoksima supstituisanih elektronegativnim polarnim grupama, dok *in silico* studije uglavnom predviđaju pogodne fizičkohemijske, farmakokinetičke i toksikološke karakteristike sintetisanih benzaldoksima.

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ANTIMICROBIAL POTENTIAL OF BENZALDOXIMES: SYNTHESIS, BIOLOGICAL ACTIVITY AND *IN SILICO* STUDY

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Oximes are found in plants and animals where are either part of the defense system or participate in olfactory communication. Oximes are intermediates in the biosynthesis of a large number of metabolites and are among the products of enzymatic oxidation and decarboxylation of amino acids. With many applications in synthetic chemistry they stand as an important class of organic compounds. Being a H-bond donor and an acceptor, oxime funcionality enables interaction with biological targets, exibiting a wide range of biological activities: antimicrobial, anti-inflammatory, antioxidant and anticancer (1). As oxime derivatives represent suitable candidates for development of new antimicrobial drugs, we synthesized several benzaldoximes by condensation of benzaldehyde and hydroxylamine salt (2). Antimicrobial activity of compounds was tested in a micro-dilution assay (3) on laboratory-controlled strains of microorganisms: *Bacillus subtilis*, *Staphylococcus aureus*, *Aspergillus niger* and *Candida albicans*. With a purpose of estimating physicochemical, pharmacokinetic and toxicological profile, *in silico* predictions using SwissADME and DataWarrior were made. Compounds didn't affect the growth of bacterial strains, however inhibited the growth of *C. albicans* and *A. niger* (tested range 62.5-500 μg ml^{-1} and 125-500 μg ml^{-1}). From the obtained results, the fungistatic potential of benzaldoximes substituted with electronegative polar groups can be observed, while *in silico* studies indicate mostly favorable characteristics of benzaldoximes we synthesized.

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