OH P 3

Sinteza i biološka aktivnost Pd(II)-kompleksa salicilaldehidno-anilinskih Šifovih baza

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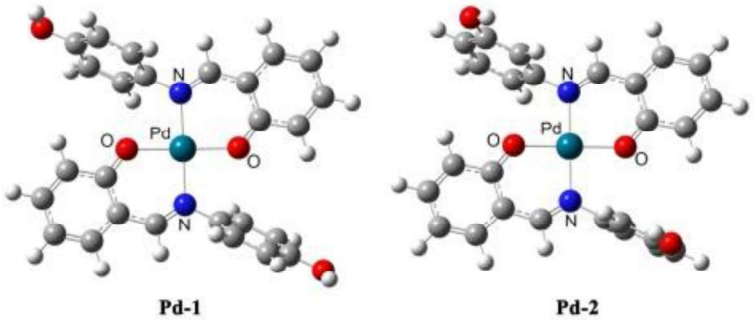
Sintetizovane su salicilaldehidne Šifove baze, 2-(((4-hidroksifenil)imino)metil)fenol (**1**) i 2-(((3-hidroksifenil)imino)metil)fenol (**2**) i njihovi odgovarajući Pd(II)-kompleksi (**Pd-1** i **Pd-2**), slika 1. Za razliku od liganada, oba kompleksa ispoljavaju veliku citotoksičnost prema ispitivanim ćelijskim linijama raka debelog creva (HCT-116) i raka dojke (MDA-MB-231).



Slika 1. *Strukture kompleksa*
Figure 1. *Structures of the complexes*

Tabela 1. *Citotoksični efekti ispitivanih uzoraka*
Table 1. *Cytotoxic effects of examined compound*

	HCT-116		MDA-MB-231	
IC_{50}, μM	24 h	72 h	24 h	72 h
1	142.3	368.0	440.2	133.6
Pd-1	11. 8	17.1	276.9	7.2
2	>500	277.6	>500	>500
Pd-2	5.8	0.6	55.6	40.7

Synthesis and biolgical activity of Pd(II)-complexes derived from salicylaldehyde-aniline Schiff bases

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Salicylaldehyde Schiff bases, 2-(((4-hydroxylphenyl)imino)methyl)phenol (**1**) and 2-(((3-hydroxylphenyl)imino)methyl)phenol (**2**) and their corresponding Pd(II)-complexes (**Pd-1** and **Pd-2**) were synthesized, Fig. 1. Both complexes exert outstanding cytotoxic character, while ligands are much less cytotoxic on the human colon cancer cell line, HCT-116 and breast cancer cell line, MDA-MB-231.

KRATKI IZVODI
ABSTRACTS

Plenarna predavanja / Plenary Lectures

PP 1

Mechanisms of electron-transfer reactions between dynamic metalloproteins

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Oxidoreduction reactions of metalloproteins are important because they occur in photosynthesis and respiration. Cytochrome c_6 and cytochrome *f* react by three different electron-transfer mechanisms under similar conditions. Protein docking and kinetics of the photoinduced electron-transfer reaction ^{3}Zncyt c_6 + cyt *f*(III) $\rightarrow$ Zncyt c_6^+ + cyt *f*(II) were studied by laser photolysis. This net reaction occurs between associated proteins with the rate constant k^{pr} and between colliding proteins with the rate constant k^{tr}. The viscosity independence of k^{pr}, the heme-heme electronic coupling, and reorganizational energy show that the reaction between associated proteins is *true* electron transfer. The viscosity dependence of k^{tr} and a remarkable break at 30 °C in the Eyring plot for the reaction between colliding proteins reveal mechanisms that are reversibly switched as temperature changes. Protein friction parameters below and above 30 °C differ. Colliding proteins undergo *coupled* electron transfer below 30 °C and *gated* electron transfer above 30 °C. Brownian dynamics simulations reveal two dynamic ensembles of protein-protein configurations "bridged" by relatively few configurations through which the dynamic ensembles interconvert.

Mehanizmi reakcija prenosa elektrona između dinamičnih metaloproteina

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Oksidoredukcione reakcije metaloproteina važne su jer učestvuju u fotosintezi i respiraciji. Citohrom c_6 i citohrom *f* reaguju trima različitim mehanizmima prenosa elektrona pod sličnim uslovima. Uzajamno "uklapanje" proteina i kinetika fotoindukovanog prenosa elektrona ^{3}Zncyt c_6 + cyt *f*(III) $\rightarrow$ Zncyt c_6^+ + cyt *f*(II) proučavani su laserskom fotolizom. Ova ista ukupna reakcija ima konstantu brzine k^{pr} kad se događa među asosovanim proteinima, ali konstanu brzine k^{tr} kad se događa među sudarenim proteinima. Nezavisnost k^{pr} od viskoznosti rastvora, hem-hem elektronsko kuplovanje i energija reorganizacije ukazuju da je reakcija među asosovanim proteinima *pravi* prenos elektrona. Zavisnost k^{tr} od viskoznosti rastvora i značajan prelom na 30 °C u Ajringovom grafiku za reakciju među sudarenim proteinima otkrivaju mehanizme koji se reverzibilno smenjuju sa promenom temperature. Parametri trenja proteina ispod i iznad 30 °C razlikuju se. Sudareni proteini učestvuju u *kuplovanom* prenosu elektrona ispod 30 °C i prenosu elektrona "*sa zadrškom*" iznad 30 °C. Simulacije Braunove dinamike ukazuju na dva dinamična ansambla protein-protein konfiguracija "premošćena" relativno malobrojnim konfiguracijama kroz koje se ona dva dinamična ansambla pretvaraju jedan u drugi.