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Organizers

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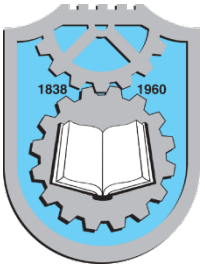

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10:30 - 11:00	Keynote speaker: **"Computational Modeling of Long Bone Microstructure and Ultrasonic Evaluation of the Fracture Healing Process"** **Prof. Dimitrios Fotiadis** *University of Ioannina, Greece*

11:00 - 11:30	Coffee Break

11:30 - 12:00	Keynote speaker: **"Theoretical Study of Primary Antioxidant Action Thermodynamics"** **Prof. Erik Klein** *Slovak Technical University, Slovakia*

some compounds found in a certain anticancer herbs. Results derived from this analysis show that some of them like curcumin and artemisinin have poor water solubility, thus limiting their use, at least in their native form. At the same time, we found that computer driven molecular conformation between these compounds may help to show the way of increasing their bioavailability, thus enhancing their anticancer activity.

T.1.4 - *Modification of Polysaccharides with Phenols for Hydrogels fFormation and Electrospinnig* - Nikolina Popović, Olga Prodanović, Ivana Gađanski, Danijela Cvetković, Marko Živanović, Vladimir Pavlović, Nenad Filipović, Radivoje Prodanović

Carboxymethylcellulose (CMC) and alginate (ALG) are water-soluble polysaccharides used in food and cosmetics industry. They have big potential for use in pharmaceutical products due to their high biocompatibility, biodegradibility, low immunogenicity and low price. When crosslinked they can absorb large amounts of water and swell to form hydrogels with great physical properties. The need for new biomaterials and hydrogels is growing daily, due to their use in tissue engineering, drug delivery and cell and enzyme immobilization studies. In this study we modified ALG and CMC, in order to get a cross-linkable polymer that can make hydrogels by chemical and enzymatic means. After periodate oxidation we obtained polysaccharides with different degrees of oxidation: 2.5, 5, 10, 15 and 20 mol%. Further modification using reductive amination in the presence of different phenolic compounds like tyramine, was done. This modification was confirmed by UV–VIS and FT-IR spectroscopy, while concentration of phenol and ionizable groups was determined using absorbance at 275 nm and acid–base titration. All CMC and AlG tyramines were able to form hydrogels after cross-linking with horse radish peroxidase (HRP) and hydrogen peroxide. Both derivatives have been successfully electrospun and crosslinked afterwards. Due to the introduction of amino groups and decrease in molecular weight, they were significantly more soluble in water up to 30 % (w/w) compared to native polysaccharides and their electrospinability also improved. We aim to make nanofibers using tyramine-polysaccharides that will be more stable in cell culture media after cross-linking covalently and with calcium/barium ions. Diameter of nanofibers was determined by scanning electron microscopy (SEM). Cross-linked nanofibers that we obtained will be used for tissue engineering of blood vessels.

Session T.2 - 09:40-10:30
Coputational Chemistry (part I)

Chair: Dejan Milenković

T.2.1 - *Theoretical Investigation of Antioxidative Activity of Caffeic Acid* - Izudin Redžepović, Svetlana Marković, Jelena Tošović

Caffeic acid (CA) is one of the most abundant dietary polyphenols, which exhibits significant antioxidative activity. However, its antioxidative mechanisms are not fully elucidated. This work reports the results of mechanistic research of the hydrogen atom transfer (HAT), radical adduct formation (RAF), sequential proton loss electron transfer (SPLET), and single electron transfer – proton transfer (SET-PT) mechanisms of CA in benzene and water solutions. Our results revealed that HAT and RAF are competitive antioxidative mechanisms of CA, because HAT pathways lead to more stable radical products, and RAF pathways require smaller activation barriers. In polar basic media SPLET is a probable antioxidative mechanism of CA, and extremely fast, while SET-PT is not a favorable antioxidative pathway of CA in any medium.

T.2.2 - *QSAR Analysis of Antioxidant Properties of Polyphenols by OH-Related Molecular Descriptors* - Nenad Raos, Ante Miličević

For the theoretical modeling of radical scavenging activity (RSA) and the first oxidation potential (Epa) of the three sets of polyphenolic compounds we used two models based on the number of OH groups in molecules. The first model distinguishes vicinal (Nv) and non-vicinal (Nnv) OH groups. The second model is based on two variables, the number of OH-bearing moieties (Nm) and the total number of OH groups (NOH). All models gave fairly good agreement with the experiment (r = 0.91- 0.98).

T.2.3 - *Antioxidant Activity of the Carboxylate Anions of the Selected Dihydroxybenzoic Acids* - Jelena Đorović, Svetlana Jeremić, Edina Avdović, Ana Amić, Jasmina M. Dimitrić Marković

In the present study the M05-2X/6-311++G(d,p) theoretical model was used to evaluate scavenging potency of the carboxylate anions of 2,3-, 2,6-, and 3,4-dihydroxybenzoic acids. Reaction enthalpies related to the antioxidant mechanisms of the investigated species were calculated in water and benzene. The single electron transfer followed by proton transfer is not favorable reaction pathway under any conditions. Hydrogen atom transfer is the preferred reaction pathway in benzene, while sequential proton loss electron transfer is the predominant reaction pathway in polar solvent, water, for all examined compounds. The approach, based on the reactions enthalpies related to the examined radical scavenging mechanisms, shows that thermodynamically favoured mechanism depends on the polarity of the reaction media and properties of free radical reactive species.

T.2.4 - *Thermodynamics of 2H+/2e- Free Radical Scavenging Mechanisms of 3-(4-Hydroxy-3-*