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2nd EAI International Conference on Future Access Enablers of Ubiquitous and Intelligent Infrastructures

OCTOBER 24–25, 2016 | BELGRADE, SERBIA

FABULOUS 2016 PROGRAM

Monday, 24 Oct 2016

09:30-10:00	Conference opening	**Prof. Nenad Filipovic** - Faculty of Engineering, University of Kragujevac - FABULOUS 2016 General Chair
10:00-10:45	Keynote speech	**Prof. Liljana Gavrilovska**, Faculty of Electrical Engineering and Information Technologies, Ss. Cyril and Methodius University in Skopje, Macedonia "5G: the Dawn of the new Era"
10:45-11:30	Keynote speech	**Dr. Prof. Onur Mutlu**, ETH Zurich, Switzerland "Rethinking Memory System Design for Data-Intensive Computing"
11:30-11:45	Sponsor presentation	**Dusan Vukasinovic**, **Andjelko Cajkovic**, National Instruments
11:45-12:15	Coffee break	
12:15-13:45	**FAN 2016** Chair: Prof. Onur Mutlu, ETH Zurich, Switzerland	• Milos Radovic, Milos Jordanski and Nenad Filipovic, "T-Relief: Feature Selection for Temporal High-Dimensional Gene Expression Data" • Bojan Marinkovic, Paola Glavan and Zoran Ognjanovic, "Correctness of the Chord Protocol Using the Frame of the Logic of Time and Knowledge" • Fadi Alturjman, "Identification Framework for Smart Environments in the Era of Cloud-IoT" • Radu Alexandru Badea, Octaviana Datcu and Robert Dobre, "A Multi-Level Protocol Stack for Flexible and Secure Client-App to Cloud Communication" • Tijana Sustercic, Aleksandra Vulovic, Nenad Filipovic and Aleksandar Peulic, "FPGA Implementation of Face Recognition Algorithm" • Tijana Djukic and Nenad Filipovic, "Parallelization of the numerical simulation of motion of deformable objects within fluid domain on a GPU device" • Alexandru Stancu, Stefan Arseni, Alexandru Vulpe, Octavian Fratu and Simona Halunga, "Intrusion Prevention System Evaluation for SDN-enabled IoT Networks" • Ivan Petrov, Prof. Toni Janevski "5G-TCP: Enhanced transport protocol for Future Mobile Networks" • Ioana Marcu, Carmen Voicu, Simona Halunga and Radu Preda, "LDPC encoding performances for fading suppression in MIMO-CDMA wireless networks"
13:45-14:45	Lunch	
14:45-15:30	Keynote speech	**Prof.** Dimitrios I. Fotiadis, University of Ioannina, Greece "Fighting for a healthcare environment based on mobile solutions"

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15:30-16:00	Coffee break	
16:00-18:20	**HeBiEn 2016** Chair: Prof. Dimitrios I. Fotiadis, University of Ioannina, Greece	• Nikola Mijailovic, Radivoje Radakovic, Aleksandar Peulic, Neda Vidanovic, Djordje Dimitrijevic and Nenad Filipovic, "Assessment of mechanical stiffness of jumping using force plate" • Bojana Andjelkovic Cirkovic, Aleksandar Cvetkovic, Danijela Cvetkovic, Srdjan Ninkovic and Nenad Filipovic, "Prediction of the Five Years Survival Rate for Breast Cancer Patients within the Ensemble Feature Ranking Framework" • Lejla Gurbeta, Almir Badnjevic, Zijad Dzemic, Elvira Ruiz Jimenez and Alma Jakupovic, "Testing of Therapeutic Ultrasound Equipment in Healthcare Institutions in Bosnia and Herzegovina" • Valentine Nwachukwu, Emil Jovanov and Aleksandar Milenkovic, "An Implementation of an IoT Server for Home Health Monitoring Applications" • Krasimir Tonchev, Georgi Tsenov, Valeri Mladenov, Agata Manolova and Vladimir Poulkov, "Personalized and intelligent sleep lifestyle reasoner with web application for improving quality of sleep part of AAL architecture" • Zarko Milosevic, Dalibor Nikolic, Nebojsa Zdravkovic, Neda Vidanovic and Nenad Filipovic, "Three-Dimensional Computer Model of Benign Paroxysmal Positional Vertigo in The Semi-Circular Canal" • Aleksandra Vulovic, Tijana Sustercic, Vesna Rankovic, Aleksandar Peulic and Nenad Filipovic, "Comparison of Different Neural Network Training Algorithms with Application to Face Recognition Problem" • Marko Zivanovic, Danijela Cvetkovic and Nenad Filipovic, "uSense Cancer Procedure for Detection of microRNAs as Cancer Biomarkers – From Science to Patients" • Strahinja Starcevic, Smiljana Djorovic and Nenad Filipovic, "Fractional Flow Reserve: Comparison between Invasive and Non-invasive Methods for Calculation of FFR" • Igor Saveljic, Velibor Isailovic, Lazar Velicki, Dalibor Nikolic and Nenad Filipovic "Numerical modeling and simulations of type B aortic dissection" • Smiljana Djorovic, Igor Koncar, Lazar Davidovic, Strahinja Starcevic and Nenad Filipovic, "Computational Analysis of Blood Flow Characteristics in an Aortic System with Abdominal and Left Common Iliac Aneurysm Pre- and Post-Stent Grafting" • Arso M. Vukicevic, Gordana Jovicic, Nebojsa Jovicic and Nenad Filipovic, "Estimating Cortical Bone Fracture Resistance by using Artificial Neural Networks and Linear Regression" • Velibor Isailovic, Milica Nikolic, Thanos Bibas, Antonis Sakellarios, Nikolaos Tachos, Miljan Milosevic and Nenad Filipovic, "Numerical simulation of human hearing system" • Miljan Milosevic, Vladimir Simic and Milos Kojic "Numerical modeling of drug delivery in organs: from CT scans to FE model" • Dalibor Nikolic, Igor Saveljic, Milos Radovic and Nenad Filipovic, "Shear stress in the arteries with myocardial bridge "solved" by neural networks"
20:00-	Gala dinner	

Tuesday, 25 Oct 2016

10:00-10:45	Keynote speech	**Dr. Emil Jovanov**, University of Alabama in Huntsville,

		USA "Smart Stuff and Wearable Monitoring"
10:45-12:15	**EnFuSI 2016** Chair: Dr. Emil Jovanov, University of Alabama in Huntsville, USA	• George Suciu, Iulia Rotaru, Ana-Maria Coman and Octavian Fratu, "Tele-Monitoring the Battery of an Electric Vehicle" • Radu Mihnea Udrea, Claudia Cristina Oprea and Cristian Stanciu, "Multi-microphone Noise Reduction System Integrating Nonlinear Multi-Band Spectral Subtraction" • Krasimir Tonchev, Yuliyan Velchev, Pavlina Koleva, Agata Manolova, Georgi Balabanov and Vladimir Poulkov, "Implementation of Daily Functioning and Habits Building Reasoner part of AAL Architecture" • Ana-Maria Claudia Dragulinescu, Ioana M. Marcu, Simona V. Halunga and Octavian Fratu, "Persons Counting and Monitoring System based on Passive Infrared Sensors and Ultrasonic Sensors (PIRUS)" • Robert Alexandru Dobre, Alexandru Vulpe, Octaviana Datcu, Radu Badea and Octavian Fratu, "Novel Method for Determining the Position of Speakers in a Room Using Beamforming" • George Suciu, Octavian Fratu, Victor Suciu and Iulian Grigore, "Monitoring the Black Sea Region using Satellite Earth Observation and Ground Telemetry" • Milorad Tosic, Valentina Nejkovic, Filip Jelenkovic and Ivan Seskar, "An Ontological Framework for Wireless Experimentation" • Elena-Madalina Oproiu, Alexandru Razvan Vulpe, Ion Marghescu and Octavian Fratu, "High Capacity Ethernet Radio Relay Networks in Mobile Communications" • Konstantin Chomu, Vladimir Atanasovski, Liljana Gavrilovska and Michele Magno, "Practical Implementation Aspects of the Data Timed Sending (DTS) Protocol Using Wake-up Radio (WuR)"
12:15-12:45	Coffee break	
12:45-14:15	Keynote speech	**Prof. Veljko Milutinovic**, School of Electrical Engineering, University of Belgrade, Serbia "DataFlow SuperComputing for DataAnalytics"
14:15-15:15	Lunch	
15:15-15:35	**DaMBiC 2016** Chair: Prof. Veljko Milutinovic, University of Belgrade, Serbia	• Emre Goynugur, Geeth de Mel and Murat Sensoy, "Tractable Policy Management Framework for Cognitive IoT" • Velislava Stoykova, "Extracting Academic Subject Semantic Relations Using Collocations"
15:35-16:05	**Computational Chemistry** Chair: Prof. Zeljko Cupic, Institute of Chemistry, Technology and Metallurgy, Belgrade	• Dejan Milenkovic, Srecko Trifunovic, Edina Avdovic, Nenad Vukovic, Milena Vukic, Jasmin Dimitric-Markovic and Zoran Markovic, "Experimental and theoretical study of the UV-Vis spectrum of a new coumarine-derived ligand" • Jelena Djorovic, Zoran Markovic, Svetlana Jeremic and Dejan Milenkovc, "Investigation of the antioxidative and radical scavenging activities of 2,4-, 2,5-, 3,5-dihydroxybenzoic acids" • Svetlana Jeremic, Dejan Milenkovic, Jelena Djorovic, Milos Filipovic, Slavko Radenkovic, Marija Antc, Zoran Markovic, "Importance of Some Conceptual DFT Reactivity Indices in QSAR Modelling of the Antioxidative Capacity of Simply Phenolic Antioxidants"

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Investigation of the antioxidative and radical scavenging activities of 2,4-, 2,5-, 3,5-dihydroxybenzoic acids

Jelena Đorović[1*], Zoran Marković[1,2], Svetlana Jeremić[2] and Dejan Milenković[1]

[1]*Bioengineering Research and Development Center, Prvoslava Stojanovića 6,34000 Kragujevac, Serbia.*
[2]*Department of Chemical-Technological Sciences, State University of Novi Pazar, Vuka Karadžića bb, 36300 Novi Pazar, Serbia.*

Abstract. For evaluation of scavenging potency of 2,4-, 2,5-, and 3,5-dihydroxybenzoic acids (DHBAs) the M05-2X/6-311++G(d,p) model was applied. Three potential antioxidant mechanisms were examined. For all of these scavenging mechanisms reaction enthalpies were calculated in two solvent, water and benzene, which simulated polar and non polar enviroment. Hydrogen atom transfer is a possible reaction pathway in benzene, while sequential proton loss electron transfer is a predominant reaction pathway in polar solvent, water, for all three examined dihydroxybenzoic acids.

Keywords: dihydroxybenozic acids, DFT, antioxidant activity

1 Introduction

Phenolic compounds are plant secondary metabolites commonly found in herbs and fruits. The term phenolics encompasses more than several thousands of naturally occurring compounds. The common structural feature of all phenolics is an aromatic ring bearing one or more hydroxyl substituent. Phenolic acids are phenols posessing one carboxylic acid functionality. Naturally occurring phenolic acids, with common basic skeleton, are devided in hydroxycinnamic and hydroxybenzoic structures [1, 2]. Phenolic acids exist in almost all vegetables, fruits, and grains. They are sometimes found in free state but most commonly they occur in plant materials as linked through ester, ether, or acetal bonds or as structural components of the cellulose, proteins and lignin [3-5].

The in vivo role of phenolic acids is still unknown but there is some evidence indicating their multiple roles and functions including protein

* Bioengineering Research and Development Center, Prvoslava Stojanovića 6,34000 Kragujevac, Serbia (jelena.djorovic@kg.ac.rs)

synthesis, nutrient uptake, enzyme activity, photosynthesis, structural components, and allelopathy [6-8]. As everyday part of a human diet they are involved in appreciation of good food quality, sensory qualities, color, nutritional and antioxidant properties of foods. The consumption of fruits and vegetables have a preventive role, due to a variety of constituents, including minerals, vitamins, fiber and numerous phytochemicals among phenolics (flavonoids and phenolic acids) [9]. The possible association between the consumption of foods containing phenolics and a reduced risk of developing several disorders, including cancer and cardiovascular diseases, has been evaluated in several epidemiological investigations [10-13].

The human body constantly generates free radicals and other reactive species. The imbalance between the production of reactive oxygen and a biological system's ability to readily detoxify reactive intermediates or easily repair the resulting damage results in oxidative stress. It is considered that this oxidative stress plays an crucial role in the pathogenesis of many diseases such as: inflammation, cancer, hypertension, diabetes mellitus, atherosclerosis, ischemia/reperfusion injury, neurodegenerative disorders, rheumatoid arthritis, and ageing [14-18]. To counteract the damaging effect of free radicals, the organisms have developed a variety of the internal defense mechanisms that include endogenous enzymes (such as superoxide dismutase and catalase), copper and iron transport proteins, water-soluble and lipid-soluble antioxidants. There are also some external factors including dietary substances, such as flavonoids, phenolic acids, vitamins C and E, hydroquinones and various sulfhydryl compounds which help in preventing free radical damage. All these substances constitute complex antioxidant defense systems.

Scavenging properties of phenolic acids are related to their ability to transfer a hydrogen atom to a free radical species. There is an assuredness that antioxidant ability of phenolic acids is greatly influenced by the number and relative position of the OH groups in the ring. In the radical scavenging mechanisms reactive radical species are inactivated by accepting a hydrogen atom from a hydroxyl group of the phenolic acid. This transfer can be visualized through at least three mechanisms characteristic to all phenolic compounds generally: hydrogen atom transfer (HAT, Eq. 1), sequential proton loss electron transfer (SPLET, Eq. 2), and single electron transfer followed by proton transfer (SET-PT, Eq. 3) [19].

$$PhOH + R^{\bullet} \rightarrow PhO^{\bullet} + RH \quad (1)$$

$$PhOH \rightarrow PhO^{-} + H^{+} \quad (2.1)$$

$$PhO^{-} + R^{\bullet} \rightarrow PhO^{\bullet} + R^{-} \quad (2.2)$$

$$PhOH + R^{\bullet} \rightarrow PhOH^{+\bullet} + R^{-} \quad (3.1)$$

$$PhOH^{+\bullet} + R^{-} \rightarrow PhO^{\bullet} + RH \quad (3.2)$$

These mechanisms are described by thermodynamic parameters: bond dissociation enthalpy (BDE) related to Eq. (1), proton affinity (PA) related to Eq. (2.1), electron transfer enthalpy (ETE), ionization potential (IP) related to Eq. (3.1), proton dissociation enthalpy (PDE) related to Eq. (3.2), and these can be determined from the total enthalpies of the individual species:

$$BDE = H(Ph{-}O^{\bullet}) + H(H^{\bullet}) - H(Ph{-}OH) \quad (4)$$
$$IP = H(Ph{-}OH^{\bullet+}) + H(e^{-}) - H(Ph{-}OH) \quad (5.1)$$
$$PDE = H(Ph{-}O^{\bullet}) + H(H^{+}) - H(Ph{-}OH^{\bullet+}) \quad (5.2)$$
$$PA = H(Ph{-}O^{-}) + H(H^{+}) - H(Ph{-}OH) \quad (6.1)$$
$$ETE = H(Ph{-}O^{\bullet}) + H(e^{-}) - H(Ph{-}O^{-}) \quad (6.2)$$

Preferred mechanism of antioxidant activity of phenols can be estimated from the BDE, IP, and PA values. The lowest of these three values shows which mechanism is thermodynamically more favorable and which antioxidant mechanism is the most probable patway for scavenging of free radicals.

In the present paper are given some results from which can be estimated the antioxidant capacity of folowing dihydroxybenzoic acids (DHBA): 2,4-, 2,5- and 3,5- DHBAs (Fig. 1).

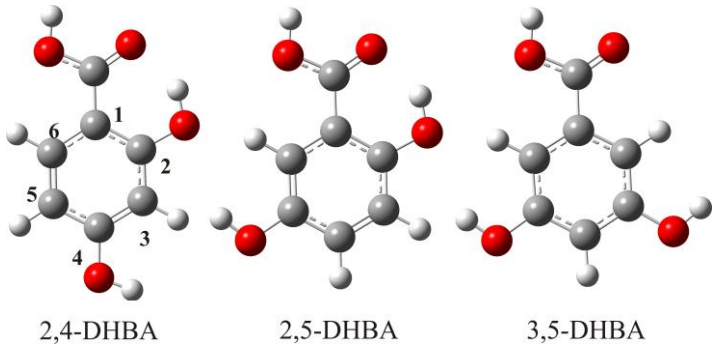

Fig. 1. The most stable structures of investigated dihydroxybenzoic acids

2 Methodology section

The equilibrium geometries of investigated DHBAs and corresponding radicals, radical cations, and anions were fully optimized. For this, the hybrid density functional method (M05-2X) was used, developed by the Truhlar group [20] and 6-311++G(d,p) basis set, which are implemented in the Gaussian 09 package. Vibrational frequencies were computed: no imaginary frequencies were obtained. The influence of water and benzene as solvents, which mimic polar and nonpolar

solutions was estimated using the SMD solvation model. The SMD is continuum solvation model based on the quantum mechanical charge density of a solute molecule interacting with a continuum description of the solvent. “D” in the model name stands for “density” and denotes that full solute electron density is used without defining partial atomic charges.

3 Results and discussion

All of three examined DHBAs are planar molecules. Two of three investigated compounds form internal hydrogen bonds with oxygen from carboxyl group (2,4-, 2,5- DHBA). It is notable from Fig.1 that molecule of 3,5-DHBA is symmetrical. In Table 1 are presented the thermodynamic data for all three DHBAs in two solvents, water and benzene.

Table 1: M052X/6-311++G(d,p) calculated parameters of antioxidant mechanisms for DHBAs in kJ mol^{-1} in water and benzene

		WATER					BENZENE				
		HAT	***SET-PT***		***SPLET***		***HAT***	***SET-PT***		***SPLET***	
		BDE	***IP***	***PDE***	***PA***	***ETE***	***BDE***	***IP***	***PDE***	***PA***	***ETE***
DHBAs			551					694			
	$2O^{-}$	408		39	146	443	420		135	455	374
	$4O^{-}$	401		31	129	453	392		107	404	397
			505					649			
	$2O^{-}$	373		49	153	401	389		149	464	334
	$5O^{-}$	358		34	153	386	350		110	447	312
			537					688			
	$3O^{-}$	383		27	144	420	375		96	431	353
	$5O^{-}$	382		26	143	420	374		95	430	353

On the basis of the thermodynamic data (Table 1), it is clear that the IP values are high for all DHBAs in both solvents. It means that SET-PT is not a believable mechanism under these conditions. On the other hand, in water the PAs of the OH groups of DHBAs are significantly lower than the corresponding BDE values. This fact indicates that SPLET mechanism represents the most probable reaction pathway in polar solvent. In benzene, the provided BDE values of DHBAs are lower than the corresponding PA values. That indicates that HAT mechanism is a probable reaction path in nonpolar solvent.

Further analysis of thermodynamic values in Table 1 imply that, based on the values of BDE and PA, 2,4-DHBA is stronger antioxidant in comparison with other two DHBAs in water, but in benzene we can say that for 2,5-DHBA.

4 CONCLUSION

Antioxidant activity of 2,4-, 2,5- and 3,5- dihydroxybenzoic acids was examined by analysing the thermodynamic properties of the parent molecules, the corresponding radicals, radical cations and anions. From the obtained results it can be concluded that HAT mechanism is favorable in non-polar solvent while SPLET mechanism is suitable reaction pathway in polar solvent. It should be pointed out that according to the obtained results 2,4–DHBA and 2,5-DHBA shows better radical scavenging activities and that they are probably better antioxidants than 3,5- DHBA.

Acknowledgments. This work was partially supported by the Ministry of Science and Technological Development of the Republic of Serbia (Grant no. 172015 and 174028).

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