

This event is endorsed
and organized by



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

OCTOBER 24–25, 2016 | BELGRADE, SERBIA

[Home](#) [Committees](#) [Calls](#) [Author Instructions](#) [Program](#) [Workshops](#) [Registration](#) [Practical Information](#) [Sponsorship](#) [Contact Us](#)

[Home](#) > [Preliminary Program in Full](#) >

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	<ul style="list-style-type: none"> 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 Daciu 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"



Important dates

Workshops proposal deadline
3 June 2016

Full Paper Submission deadline
31 July 2016

Notification deadline
15 September 2016

Camera-ready deadline
17 October 2016

Start of Conference
24 October 2016

End of Conference
25 October 2016

[Previous Fabulous Conferences](#)
[2015](#) - Ohrid, Republic of Macedonia

Sponsors



15:30-16:00	Coffee break	
16:00-18:20	HeBiEn 2016	<ul style="list-style-type: none"> • 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	

Chair:
[Prof. Dimitrios I. Fotiadis](#), University of Ioannina, Greece



[Tweets by @EAIchannel](#)

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	<ul style="list-style-type: none"> • 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, Yuliyana 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	<ul style="list-style-type: none"> • 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	<ul style="list-style-type: none"> • 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 Milenkovic, "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"

This event is endorsed
and organized by



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

OCTOBER 24–25, 2016 | BELGRADE, SERBIA

[Home](#) [Committees](#) [Calls](#) [Author Instructions](#) [Program](#) [Workshops](#) [Registration](#) [Practical Information](#) [Sponsorship](#) [Contact Us](#)

[Home](#) > [Organizing Committee](#) >

General Chair

Nenad Filipovic

Nenad Filipovic, Professor of Faculty of Engineering, University of Kragujevac, Serbia

General Co-Chairs

Ljiljana Gavrilovska

Ljiljana Gavrilovska, Ss. Cyril and Methodius University in Skopje, Macedonia

Veljko Milutinovic

Veljko Milutinovic, School of Electrical Engineering, University of Belgrade, Serbia

Technical Program Committee Chair

Dalibor Nikolic

Dalibor Nikolic, University of Kragujevac, Serbia

Web Chair



Important dates

Workshops proposal deadline
3 June 2016

Full Paper Submission deadline
31 July 2016

Notification deadline
15 September 2016

Camera-ready deadline
17 October 2016

Start of Conference
24 October 2016

End of Conference
25 October 2016

Previous Fabulous Conferences

[2015](#) - Ohrid, Republic of Macedonia

Sponsors



Djordje Dimitrijevic



[Tweets by @EAIchannel](#)

[Djordje Dimitrijevic](#), University of Kragujevac, Serbia

Publicity and Social Media Chair

Milena Djordjevic

[Milena Djordjevic](#), University of Kragujevac, Serbia

Workshops Chair

Aleksandar Peulic

[Aleksandar Peulic](#), University of Kragujevac, Serbia

• **Workshop #1: Future access networks**

Workshop Chair: Prof. Veljko Milutinovic, Serbia

Workshop Co-Chair: Vladisav Jelisavcic

• **Workshop #2: Enablers of future smart infrastructures**

Workshop Chair: Prof. Emil Jovanov, USA

• **Workshop #3: Data Mining, Big Data and Cloud Computing**

Workshop Chair: Onur Mutlu, Carnegie Mellon University

• **Workshop #4: eHealth and Biomedical engineering**

Workshop Chair: Prof. Dimitrios Fotiadis, Greece

Sponsorship & Exhibits Chair

Neda Vidanovic

[Neda Vidanovic](#), University of Kragujevac, Serbia

Publications Chair

Velibor Isailovic

Velibor Isailovic, University of Kragujevac, Serbia

Local Chair

Milica Kaplarevic

Milica Kaplarevic, University of Kragujevac, Serbia

Conference Manager

Anna Horvathova, EAI - European Alliance for Innovation

EAI Institutional Members



This event is endorsed
and organized by



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

OCTOBER 24–25, 2016 | BELGRADE, SERBIA

[Home](#) [Committees](#) [Calls](#) [Author Instructions](#) [Program](#) [Workshops](#) [Registration](#) [Practical Information](#) [Sponsorship](#) [Contact Us](#)

[Home](#) > [Technical Program Committee](#) >

Last name	First name	Affiliation
Akyildiz	Ian	Georgia Institute of Technology, Atlanta, GA, USA
Andjelkovic Cirkovic	Bojana	Faculty of Engineering, University of Kragujevac
Atanasovski	Vladimir	Ss. Cyril and Methodius University in Skopje, Faculty of Electrical Engineering and Information Technologies
Babovic	Zoran	University of Belgrade
Bourbakis	Nikolaos	Wright State University
Delic	Hakan	Bogaziçi University
De Nardis	Luca	Sapienza University of Rome
Denkovski	Daniel	Faculty of Electrical Engineering and Information Technologies
Exarchos	Themis	FORTH
Filipovic	Nenad	University of Kragujevac
Fotiadis	Dimitris	University of Ioannina
Fratu	Octavian	University POLITEHNICA of Bucharest
Gavrilovska	Ada	Georgia Tech
Gavrilovska	Liljana	Faculty of Electrical Engineering and Information Technologies
Ghalwash	Mohamed	SERC
Giorgetti	Andrea	Univ of Bologna
Isailovic	Velibor	University of Kragujevac, Serbia
Ivanovic	Milos	Faculty of Science, University of Kragujevac
Jelisavcic	Vladisav	Mathematical Institute of the Serbia Academy of Sciences and Arts
Jovanov	Emil	Associate Professor
Kos	Anton	Ljubljana University
Kyriazakos	Sofoklis	Aalborg University
Manic	Miodrag	University of Nis, Mechanical Engineering Faculty, Nis, Serbia
Mihaljevic	Miodrag	Mathematical Institute SANU
Milosevic	Zarko	University of Kragujevac



Important dates

Workshops proposal deadline
3 June 2016

Full Paper Submission deadline
31 July 2016

Notification deadline
15 September 2016

Camera-ready deadline
17 October 2016

Start of Conference
24 October 2016

End of Conference
25 October 2016

[Previous Fabulous Conferences](#)
[2015](#) - Ohrid, Republic of Macedonia

Sponsors



Milosevic	Miljan	University of Kragujevac
Milutinovic	Veljko	School of Electrical Engineering
Mutlu	Onur	Carnegie Mellon University
Nikolic	Dalibor	University of Kragujevac, Serbia
Obradovic	Zoran	Temple University
Peulic	Aleksandar	University of Kragujevac, Serbia
Popovski	Petar	Aalborg University
Poulkov	Vladimir	TU Sofia
Radovic	Milos	University of Kragujevac
Rakovic	Valentin	Faculty of Electrical Engineering and Information Technologies
Rankovic	Vesna	Faculty of Engineering, University of Kragujevac, Serbia
Saveljic	Igor	University of Kragujevac
Schwefel	Hans-Peter	FTW
Seker	Huseyin	Northumbria University
Stojanovic	Boban	University of Kragujevac
Trajanov	Dimitar	Ss. Cyril and Methodius University in Skopje, Macedonia
Trajanovic	Miroslav	Department of Technical Mechanics
van de Beek	Jaap	Luleå University of Technology
Vukicevic	Arso	University of Kragujevac
Yurdakul	Arda	Bogazici University
Zlokolica	Vladimir	University of Novi Sad



[Tweets by @EAIchannel](#)

EAI Institutional Members



This event is endorsed
and organized by



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

OCTOBER 24–25, 2016 | BELGRADE, SERBIA

[Home](#) [Committees](#) [Calls](#) [Author Instructions](#) [Program](#) [Workshops](#) [Registration](#) [Practical Information](#) [Sponsorship](#) [Contact Us](#)

[Home](#) > [Steering Committee](#) >

Steering Committee

Imrich Chlamtac, Create-Net and University of Trento, Italy

Liljana Gavrilovska, Ss. Cyril and Methodius University in Skopje, Macedonia

Alberto Leon-Garcia, University of Toronto, Canada



Important dates

Workshops proposal deadline
3 June 2016

Full Paper Submission deadline
31 July 2016

Notification deadline
15 September 2016

Camera-ready deadline
17 October 2016

Start of Conference
24 October 2016

End of Conference
25 October 2016

[Previous Fabulous Conferences](#)
[2015](#) - Ohrid, Republic of Macedonia

Sponsors



Experimental and theoretical study of the UV-Vis spectrum of a new coumarine-derived ligand

Dejan Milenković^{1*}, Srećko Trifunović², Edina Avdović², Nenad Vuković², Milena Vukić², Jasmina Dimitrić-Marković³, and Zoran Marković^{1,4}

¹Bioengineering Research and Development Center, Prvoslava Stojanovića 6, 34000 Kragujevac, Serbia

²Faculty of Science, University of Kragujevac, 12 Radoja Domanovića, P.O. Box 60, 34000 Kragujevac, Serbia

³Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12-16, 11000 Belgrade, Republic of Serbia

⁴Department of Chemical-Technological Sciences, State University of Novi Pazar, Vuka Karadžića bb, 36300 Novi Pazar, Serbia

Abstract. The UV-Vis properties of new coumarine-derived ligand (3-(1-(3-hydroxypropylamino)propylidene)-chroman-2,4-dione) were investigated. The time-dependent density functional theory (TDDFT) approach in combination with the B3LYP functional was used for simulation of UV-Vis spectra of examined compound. The agreement between the observed wavelengths and intensities in the UV spectrum of ligand **1** and those predicted with B3LYP functional, is satisfactory.

Keywords: UV-Vis spectra, TDDFT, B3LYP, coumarine-derived ligand (ligand **1**), oscillator strengths

1 Introduction

Coumarins (2*H*-1-benzopyran-2-one) consist of a large class of phenolic substances found in plants and are made of fused benzene and α -pyrone rings [1]. Coumarine and its derivatives are natural compounds with high and significant biological activities like spasmolytic, antiarrhythmic, cardiogenic and photodynamic properties [2]. Also, coumarine and its derivatives were tested against several tumor cell lines [3]. These compounds can be found in different food sources such as fruits, herbs and vegetables [4]. Coumarin and its derivatives have important role in the fields of biology, medicine, industry, botany and chemistry. Some metal complexes with coumarine derivatives showed significant anticoagulant [5] and antitumor activity [2,6].

* Dejan Milenković, Bioengineering Research and Development Center, Prvoslava Stojanovića 6, 34000 Kragujevac, Serbia (deki82@kg.ac.rs)

2 Methodology section

The equilibrium geometry of coumarine-derived ligand (**1**) was optimized by density functional theory (DFT) using B3LYP exchange correlation functional first proposed by Becke [7], in combination with the 6-311+G(d,p) basis set. The optimization was carried out using Gaussian 09 package [8]. The structure was optimized at 298 K without any geometrical restrictions. The nature of the stationary points was determined by performing frequency analysis: equilibrium geometries have no imaginary vibrations. The effect of methanol as solvent was taken into account in geometry optimization and energy calculation by using the SMD model [9].

To simulate the UV spectrum of investigated compound TDDFT (Time Dependent Density Functional Theory) approach [10] was employed for predicting the electronic transitions. TD calculation was performed in methanol. All transitions were considered. All parameters important for the simulation of UV-VIS spectra such as excited state energies, oscillator strengths (f), and a list of the transitions that gave rise to each excited state were calculated. Natural Bond orbital (NBO) analysis [11] was performed for the explanation of the interactions inside of molecule and visualization of orbitals involved in electronic transitions. The B3LYP ground state geometry was used to perform the NBO.

3 Results and discussion

3.1 Structural analysis

The structure of most stable conformation of ligand **1** defined by using B3LYP local density functional method in conjunction with 6-311+G(d,p) basis set, in methanol as solvent. From the optimized molecular structure of the ligand **1** (Fig. 1), it is found that torsion angle, τ , defined by the C4-C3-C1'-N1 atoms is 172° , which indicated nonplanarity of molecule. The investigated molecule has one internal hydrogen bond (IHB) which additionally stabilize corresponding compound. For this IHB the NBO analysis revealed that electron density is donated from the p and sp^2 orbitals of the oxygen atoms into the proximate σ^* antibonding H-N1 bond. These donor-acceptor interactions are responsible for hydrogen bond formation.

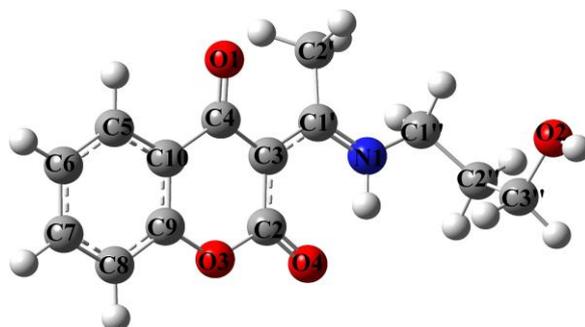


Figure 1. Optimized geometry of the ligand **1** obtained at the B3LYP/6-311+G(d,p) level of theory in methanol.

3.2 UV spectrum

The experimental and computed UV spectra are presented in Fig. 2, whereas calculated electronic transitions, absorption wavelengths, and oscillator strength, as well as experimental absorption wavelengths are presented in Table 1.

Table 1. UV spectral data for compound **1**.

Expt	B3LYP/6-311+G(d,p)		
λ_{max} (nm)	λ_{max}	f	Orbital description
319	294	0.52	H \rightarrow L (66%)
243	248	0.18	H \rightarrow L+1 (48%)
234	238	0.28	H-1 \rightarrow L+1 (58%)

The experimental spectrum of **1** in of methanol shows two wide peaks at 319 and 243 nm. The theoretical investigation of electronic transition was also performed in methanol. The UV spectrum of the compound **1** was simulated using the TDDFT approach. In Table 1 are given data for the UV spectrum. The two absorption peaks are prominent, i.e., at 294 nm which is absorption maximum and the second peak has been observed at 248 nm which are in good agreement with the experimental evidences (Table 1, Fig. 2). As mentioned above, electronic transitions have been investigated. The first transition state at 294 nm dominated with maximum absorption which is caused by HOMO \rightarrow LUMO with 66% contribution. The second transition state caused by HOMO \rightarrow LUMO+1 at 248 nm with 48% contribution. The third state has 58% contribution from HOMO-1 \rightarrow LUMO+1. The orbitals cooresponding for these electronic transitions were presented in Fig. 3.

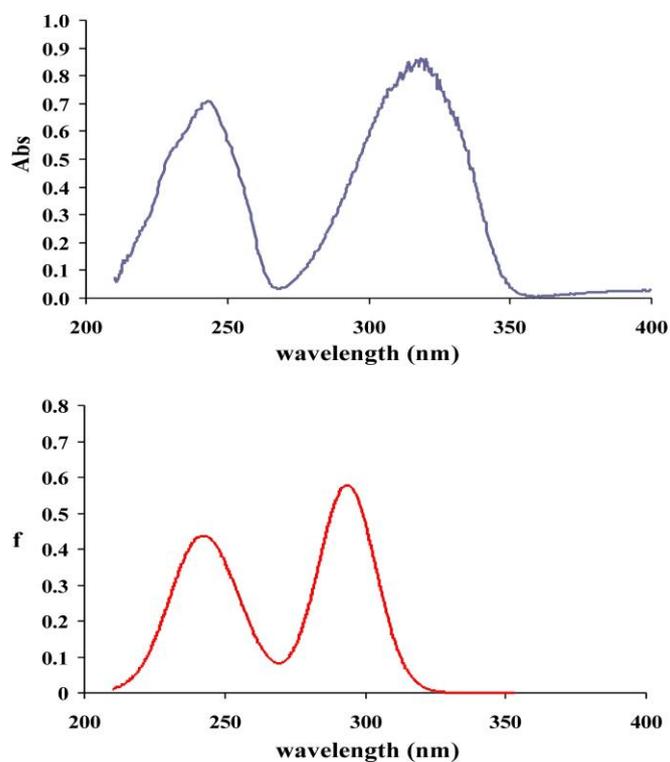


Figure 2. Experimental (blue line) and simulated (red line) UV spectrum of ligand **1** in methanol. The calculation of the spectrum was carried out at the B3LYP-D3/6-311+G(d,p) level of theory in combination with the SMD solvation model.

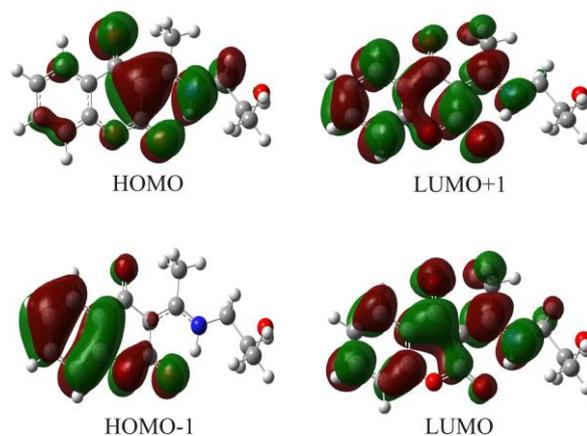


Figure 3. The occupied and virtual orbitals responsible for the UV spectrum of ligand **1**.

The shapes of the corresponding orbitals confirm that these transitions were associated with significant charge transfer between the coumarine moiety and side alkyl chain.

4 Conclusion

All results were obtained using the B3LYP/6-311+G(d,p) level of theory. On the basis of conformational analysis, it was found that **1** is the most stable structure. Re-optimized structure of **1** in methanol was used to simulate the UV-vis spectra. Both methods, experimental and theoretical showed as two major peaks. The results showed that there is good agreement between experimental and calculated values for λ_{max} . On the basis of new facts, it is clear that this functional (B3LYP) can be used successfully in the study of this class of compounds. According to the analysis of frontier orbitals it was found that for these transitions was responsible charge transfer between the coumarine moiety and side alkyl chain.

Acknowledgments. This work was supported by the Ministry of Science of the Republic of Serbia (Projects Nos. 172015, 174028 and 172016).

References

1. Aoyama, Y., Katayama, T., Yamamoto, M., Tanaka, H., Kon, K.: A new antitumor antibiotic product, demethylchartreusin. Isolation and biological activities. *J. Antibiot.* 45, 875-888 (1992)
2. Manolov, I., Kostova, I., Netzeva, T., Konstantinov, S., Karaivanova, M.: Cytotoxic activity of cerium complexes with coumarin derivatives. Molecular modeling of the ligands. *Arch. Pharm. (Weinheim)* 333, 93-98 (2000).
3. Weber, U.S., Steffen, B., Siegers, C.: Antitumor-activities of coumarin, 7- hydroxy-coumarin and its glucuronide in several human tumor cell lines. *Res. Commun. Mol. Pathol. Pharmacol.* 99, 193-206 (1998)
4. Kleiner, H.E., Vulimiri, S.V., Miller, L., Johnson, W.H. Whitman, C.P., DiGiovanni, J.: Oral administration of naturally occurring coumarins leads to altered phase I and II enzyme activities and reduced DNA adduct formation by polycyclic aromatic hydrocarbons in various tissues of SENCAR mice. *Carcinogenesis.* 22, 73-82 (2001).
5. Jiang, D., Deng, R., Wu, J.: Synthesis and properties of lanthanide compounds of 3-sulfo-4-hydroxycoumarin. *Wuji Huaxue.* 5, 21-28 (1989)
6. Kostova, I., Manolov, I., Konstantinov, S., Karaivanova, M.: Synthesis, physicochemical characterisation and cytotoxic screening of new complexes of cerium, lanthanum and neodymium with Warfarin and Coumachlor sodium salts. *Eur. J. Med. Chem.* 34, 63-68 (1999)
7. Becke, A.D.: Density-functional exchange-energy approximation with correct asymptotic behavior. *Phys. Rev. A Gen. Phys.* 38, 3098-3100 (1988)
8. Frisch, M. J., Trucks, G. W., Schlegel, H. B., et al. Gaussian 09, revision A.1-SMP. Wallingford, CT: Gaussian, Inc. (2009).

9. Marenich, A.V., Cramer, C.J. Truhlar, D.G.: Universal solvation model based on solute electron density and on a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions. *J. Phys. Chem. B* 113, 6378-6396 (2009)
10. Bauernschmitt, R., Ahlrichs, R.: Treatment of electronic excitations within the adiabatic approximation of time dependent density functional theory. *Chem. Phys. Lett.* 256, 454-464 (1996)
11. Foster, J.P., Weinhold, F.: Natural hybrid orbitals. *J. Am. Chem. Soc.* 102, 7211-7218 (1980)