



## CURRICULUM VITAE OF SVETLANA MARKOVIĆ

First name: Svetlana  
Family name: Marković  
Maiden name: Petrović  
Date of birth: April 18, 1959  
Country and place of birth: Serbia, Kruševac  
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### Education

1966 - 1978: Primary and secondary schooling in Kruševac, Serbia

1978 - 1983: Study of chemistry at the Faculty of Science, University of Kragujevac, Serbia

1983: B. Sc. degree in chemistry

1988: M. Sc. degree in chemistry (Faculty of Science, University of Kragujevac  
Supervisor - Prof. Dr. Ivan Gutman)

1992: Ph. D. degree in chemistry (Faculty of Science, University of Kragujevac  
Supervisor - Prof. Dr. Ivan Gutman)

Field of research: Mathematical and computational chemistry

Post-doctoral studies:

1999 – 2001: Technikon Pretoria, Department of Chemistry and Physics

Supervisor: Dr. Johan P. Engelbrecht

Field of research: Chemistry under supercritical conditions

Lecturing: Physical Chemistry

## Employment

1986 - 1993: Teaching assistant at the Faculty of Science, Kragujevac  
1993 – 2003: Docent at the Faculty of Science, Kragujevac  
2003 – 2009: Associate professor at the Faculty of Science, Kragujevac  
2009 – present: Full professor at the Faculty of Science, Kragujevac

**Lecturing:** Computers in Chemistry  
Programming in Chemistry  
Physical Chemistry  
Molecular modeling  
Methodology of scientific work in Chemistry

## List of scientific papers

99. Jelena Tošović, **Svetlana Marković**  
*Reactivity of chlorogenic acid towards hydroxyl and methyl peroxy radicals relative to trolox in nonpolar media*  
Theor. Chem. Acc. **137** (2018) 76. DOI: 10.1007/s00214-018-2251-y.  
ISSN: 1432-881X, **M22**, IF(2016)=**1,890**
98. Adrijana Burmudžija, **Svetlana Marković**, Jovana Muškinja, Anka Pejović, Jelena Tošović  
*Influence of counterion on the methylation of some ambident nucleophiles: DFT study*  
React. Kinet. Cat. **123** (2018) 201-214. DOI: 10.1007/s11144-017-1263-2.  
ISSN: 1878-5190, **M23**, IF(2016)=**1,264**
97. Izudin Redžepović, **Svetlana Marković**, Jelena Tošović  
*ANTIOXIDATIVE ACTIVITY OF CAFFEIC ACID – MECHANISTIC DFT STUDY*  
Kragujevac J. Sci. **39** (2017) 109-122. DOI: 10.5937/KgJSci1739109R.  
ISSN: 1450-9636, UDC: 541.127:547.587.52, **M51**
96. Jelena Tošović, **Svetlana Marković**, Jasmina M. Dimitrić Marković, Miloš Mojović, Dejan Milenković  
*Antioxidative mechanisms in chlorogenic acid*  
Food Chem. **237** (2017) 390-398. DOI:  
<http://dx.doi.org/10.1016/j.foodchem.2017.05.080>.  
ISSN: 0308-8146, **M21a**, IF(2016)=**4,529**
95. Jelena Tošović, **Svetlana Marković**  
*Structural and Antioxidative Features of Chlorogenic Acid*  
Croat. Chem. Acta **89(4)** 535-541 (2016). DOI: <http://dx.doi.org/10.5562/cca3026>.  
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94. Jelena Tošović, **Svetlana Marković**, Dejan Milenković, Zoran Marković  
*Solvation Enthalpies and Gibbs Energies of the Proton and Electron – Influence of Solvation Models*  
J. Serb. Soc. Comp. Mech. **10(2)** (2016) 66-76. UDC: 539.125.4:66.093.1, 539.124:66.093.1
93. Jelena Tošović, **Svetlana Marković**  
*Reproduction and interpretation of the UV-vis spectra of some flavonoids*  
Chem. Pap. **71** (2017) 543-552. DOI: 10.1007/s11696-016-0002-x.  
ISSN: 0366-6352, **M22**, IF(2015)=**1,326**
92. Ana Amić, Bono Lučić, Višnja Stepanić, Zoran Marković, **Svetlana Marković**, Jasmina M. Dimitrić Marković, Dragan Amić  
*Free radical scavenging potency of quercetin catecholic colonic metabolites: Thermodynamics of  $2H^+/2e^-$  processes*  
Food Chem. **218** (2017) 144-151. DOI: 10.1016/j.foodchem.2016.09.018.  
ISSN: 0308-8146, **M21a**, IF(2016)=**4,529**
91. **Svetlana Marković**, Jelena Tošović  
*Comparative study of the antioxidative activities of caffeoylquinic and caffeic acids*  
Food Chem. **210** (2016) 585-592. DOI: 10.1016/j.foodchem.2016.05.019.
90. **Svetlana Marković**, Jelena Tošović, Jasmina M. Dimitrić Marković  
*Synergic application of spectroscopic and theoretical methods to the chlorogenic acid structure elucidation*  
Spectrochim. Acta A **164** (2016) 67-75. DOI:  
<http://dx.doi.org/10.1016/j.saa.2016.03.044>.
89. Zoran Marković, Jelena Tošović, Dejan Milenković, **Svetlana Marković**  
*Revisiting the solvation enthalpies and free energies of the proton and electron in various solvents*  
Comput. Theor. Chem. **1077** (2016) 11-17. DOI: 10.1016/j.comptc.2015.09.007.
88. **Svetlana Marković**, Jelena Tošović  
*Application of Time-Dependent Density Functional and Natural Bond Orbital Theories to the UV-vis Absorption Spectra of Some Phenolic Compounds*  
J. Phys. Chem. A **119** (2015) 9352-9362. DOI: 10.1021/acs.jpca.5b05129.
87. Vladimir P. Petrović, Dušica Simijonović, Slađana B. Novaković, Goran A. Bogdanović, **Svetlana Marković**, Zorica D. Petrović  
*Structural characterisation of some vanillic Mannich bases: Experimental and theoretical study*  
J. Mol. Struct. **1098** (2015) 34-40. DOI: 10.1016/j.molstruc.2015.05.040.
86. Vladimir P. Petrović, Dušica Simijonović, Zorica D. Petrović, **Svetlana Marković**

*Formation of a vanillic Mannich base – theoretical study*  
Chem. Pap. **69(9)** (2015) 1244-1252. DOI: 10.1515/chempap-2015-0123.

85. **Svetlana Marković**, Ljubiša Mitrović, Jelena Đurđević, Jelena Tošović, Zorica Petrović

*Alkylation of potassium ethyl acetoacetate: HSAB versus Marcus theory*  
Comput. Theor. Chem. **1066** (2015) 14-19. DOI: 10.1016/j.comptc.2015.05.005.

84. **Svetlana Marković**, Igor Đurović, Zoran Marković

*Revisiting the Kolbe–Schmitt reaction of sodium 2-naphthoxide*  
Theor. Chem. Acc. **134** (2015) 45. DOI: 10.1007/s00214-015-1648-0.

83. Nenad Janković, Zorica Bugarčić, **Svetlana Marković**

*Double catalytic effect of  $(PhNH_3)_2CuCl_4$  in a novel, highly efficient synthesis of 2-oxo and thioxo-1,2,3,4-tetrahydropyrimidines*  
J. Serb. Chem. Soc. **80(5)** (2015) 595-604. DOI: 10.2298/JSC141028011J.

82. **Svetlana Marković**, Nenad Janković, Zorica Bugarčić

*Influence of the counteranion on the phenylselenoetherification reaction of nerolidol*  
Monatsh. Chem. **146(2)** (2015) 275-282. DOI: 10.1007/s00706-014-1361-z.

81. Igor Đurović, **Svetlana Marković**, Zoran Marković

*Karboksilacija natrijum-2-naftoksida. Preispitivanje mehanizma pomoću meta-hibridnog funkcionala gustine*  
*Carboxylation of sodium 2-naphthoxide. Reinvestigation of the mechanism by means of a hybrid meta density functional theory method*  
Hem. Ind. **69(5)** (2015) 485-492. DOI:10.2298/HEMIND140625066D.

80. Vladimir P. Petrović, Dušica Simijonović, Marko N. Živanović, Jelena V. Košarić, Zorica D. Petrović, **Svetlana Marković**, Snežana D. Marković

*Vanillic Mannich Bases: Synthesis and Screening of Biological Activity. Mechanistic Insight into the Reaction with 4-Chloroaniline*  
RSC Advances **4** (2014) 24635-24644. DOI: 10.1039/c4ra03909b.

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*DFT study of the mechanism of the phenylselenoetherification reaction of linalool*  
Monatsh. Chem. **145** (2014) 1287-1296. DOI: 10.1007/s00706-014-1226-5.

78. **Svetlana Marković**, Ivan Gutman, Nataša Simić

*Local Aromaticity in Benzo- and Benzocyclobutadieno-annelated Perylenes*  
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*Debromination of endo-(+)-3-Bromocamphor with Primary Amines*

J. Braz. Chem. Soc. **24(7)** (2013) 1099-1108. DOI: 10.5935/0103-5053.20130144.

75. Zoran Marković, Dragan Amić, Dejan Milenković, Jasmina M. Dimitrić-Marković, **Svetlana Marković**

*Examination of the chemical behavior of the quercetin radical cation towards some bases*

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*DFT study of free radical scavenging activity of erodiol*

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*Mechanistic investigation and DFT calculation of the new reaction between S-methylisothiosemicarbazide and methyl acetoacetate*

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71. Slavko Radenković, **Svetlana Marković**, Vladimir Milenković

*Electronic structure study of the triplet azulene-like molecules*

Chem. Phys. Lett. **545** (2012) 132-137.

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*Mechanistic insight into the formation of cinnamates in phosphine-free Heck reaction*

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69. Ivan Gutman, Jelena Tošović, Slavko Radenković, **Svetlana Marković**

*On atom-bond connectivity index and its chemical applicability*

Indian J. Chem. **51A** (2012) 690-694.

68. Zorica D. Petrović, Vladimir P. Petrović, Dušica Simijonović, **Svetlana Marković**  
*Stereoselective homogeneous catalytic arylation of methyl methacrylate: Experimental and computational study*

J. Mol. Cat. A: Chemical, **356** (2012) 144-151.

67. Slavko Radenković, **Svetlana Marković**, Ratko Kuč, Nevena Stanković  
*The diradical character of polyacenequinododimethides*  
Monatsh. Chem., **142** (2011) 1013-1019.
66. Alexandru T. Balaban, Ivan Gutman, **Svetlana Marković**, Dušica Simijonović,  
Jelena Đurđević  
*Local aromaticity in benzo- and benzocyclobutadieno-annelated phenanthrenes*  
Polycyc. Arom. Comp., **31** (2011) 339-349.
65. Zorica D. Petrović, Vladimir P. Petrović, Dušica Simijonović, **Svetlana Marković**  
*Insight into hydrolytic reaction of N-acetylated L-histidylglycine dipeptide with novel  
mechlorethamine platinum(II) complex. NMR and DFT study of the hydrolytic reaction*  
Dalton Trans., **40** (2011) 9284-9288.
64. Zoran S. Marković, **Svetlana Marković**, Jasmina M. Dimitrić-Marković, Dejan  
Milenković  
*Structure and Reactivity of Baicalein Radical Cation*  
Int. J. Quant. Chem., **112(8)** (2012) 2009-2017.
63. Alexandru T. Balaban, Ivan Gutman, **Svetlana Marković**, Dušica Simijonović  
*Local aromaticity in benzo- and benzocyclobutadieno-annelated anthracenes*  
Monatsh. Chem. **142** (2011) 797-800.
62. **Svetlana Marković**, Slavko Radenković, Zoran Marković, Ivan Gutman  
*DFT Study on Singlet Diradical Character of Zethrenes*  
Russ. J. Phys. Chem. **85(13)** (2011) 2368-2372.
61. Zorica D. Petrović, **Svetlana Marković**, Vladimir P. Petrović, Dušica Simijonović  
*Triethanolammonium acetate as multifunctional ionic liquid in palladium-catalyzed  
green Heck reaction*  
J. Mol. Mod. **18** (2012) 433-440.
60. Vladimir P. Petrović, **Svetlana Marković**, Zorica D. Petrović  
*A new aspect of Heck catalyst formation*  
Monatsh. Chem. **142** (2011) 141-144.
59. **Svetlana Marković**, Jelena Đurđević, Svetlana Jeremić, Ivan Gutman  
*Triplet fluoranthenes: aromaticity versus unpaired electrons*  
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58. **Svetlana Marković**, Milan D. Joksović, Petra Bombicz, Vukadin M. Leovac, Violeta  
Marković, Ljubinka Joksović

*Theoretical study on structural and mechanistic aspects of synthesis of a 3-aminopyrazole derivative*

Tetrahedron, **66** (2010) 6205-6211.

57. **Svetlana Marković**, Jelena Đurđević, Svetlana Jeremić, Ivan Gutman

*Diradical character of some fluoranthenes*

J. Serb. Chem. Soc., **75(9)** (2010) 1241-1249.

56. Ivan Gutman, **Svetlana Marković**, Svetlana Jeremić

*A case of breakdown of the Kekulé-structure model*

Polycyc. Arom. Comp., **30(4)** (2010) 240-246.

55. Zorica D. Petrović, Dušica Simijonović, Vladimir P. Petrović, **Svetlana Marković**

*Diethanolamine and N,N-diethylethanolamine ionic liquids as precatalyst-precursors and reaction media in green Heck reaction protocol*

J. Mol. Cat. A, **327(1-2)** (2010) 45-50.

54. Sonja Stanković, **Svetlana Marković**, Ivan Gutman, Silva Sretenović

*Hydrogen-mediated Stone-Wales isomerization of dicyclopenta[de,mn]anthracene*

J. Mol. Model. **16** (2010) 1519-1527, DOI 10.1007/s00894-010-0669-9.

53. Zorica D. Petrović, Vladimir P. Petrović, Dušica Simijonović, **Svetlana Marković**

*Mechanistic Pathways for Oxidative Addition of Aryl Iodides to the Low-Ligated Diethanolamine Palladium(0) Complex in Phosphine-Free Heck Reactions*

J. Organomet. Chem. **694(24)** (2009) 3852-3858.

52. Jelena Đurđević, Slavko Radenković, Ivan Gutman, **Svetlana Marković**

*Testing the PCP-rule*

Monatsh. Chem. **140(11)** (2009) 1305-1309.

51. **Svetlana Marković**, Ana Despotović, Dejan Jovanović, Igor Đurović

*Enthalpy of Formation of Acyclic Saturated Ketones*

Russ. J. Phys. Chem. **83(9)** (2009) 1430-1435.

50. Sonja Stanković, **Svetlana Marković**, Slavko Radenković, Ivan Gutman

*Formation and Isomerization of Dicyclopenta[de,mn]anthracene. Electronic Structure Study*

J. Mol. Model. **15(8)** (2009) 953-958.

49. **S. Marković**, Z. D. Petrović, V. Petrović

*DFT study on the preactivation reaction of a palladium catalyst precursor in phosphine-free Heck reactions*

Monatsh. Chem. **140(2)** (2009) 171-175.

48. **S. Marković**, S. Stanković, S. Radenković, I. Gutman

*Thermal isomerization in cyclopenta[fg]aceanthrylene*

Monatsh. Chem. **140**(2) (2009) 153-156.

47. **S. Marković**, S. Stanković, S. Radenković, I. Gutman  
*Electronic Structure Study of Thermal Intraconversions of Some Dicyclopenta-Fused Polycyclic Aromatic Compounds*

J. Chem. Inf. Model. **48** (2008) 1984-1989.

46. V. M. Leovac, **S. Marković**, V. Divjaković, K. M. Szécsényi, M. D. Joksović, I. Leban

*Structural and DFT studies on molecular structure of Ni(II) chloride complex with pyridoxal semicarbazone (PLSC). Unusual coordination mode of PLSC*

Acta Chim. Slov. **55** (2008) 850-860.

45. Z. D. Petrović, **S. Marković**, D. Simijonović, V. Petrović

*Mechanistic Insight into Preactivation of a Modern Palladium Catalyst Precursor in Phosphine-free Heck Reactions*

Monatsh. Chem. **140**(4) (2009) 371-374.

44. **S. Marković**, I. Đurović, Z. Marković

*Formation of Sodium 6-Hydroxy-2-Naphthoate in the Kolbe-Schmitt Reaction*

Monatsh. Chem. **139** (2008) 1169-1174.

43. Z. Marković, **S. Marković**

*Last Step of the Para Route of the Kolbe-Schmitt Reaction*

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42. Z. Marković, **S. Marković**, I. Đurović

*Kolbe-Schmitt Reaction of Sodium 2-Naphthoxide*

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41. Z. Marković, **S. Marković**, N. Manojlović, J. Predojević-Simović

*Mechanism of the Kolbe-Schmitt Reaction. Structure of the Intermediate Potassium Phenoxide - CO<sub>2</sub> Complex*

J. Chem. Inf. Model. **47**(4) (2007) 1520-1525.

40. **S. Marković**, Z. Marković, N. Begović, N. Manojlović

*Mechanism of the Kolbe-Schmitt Reaction with Lithium and Sodium Phenoxides*

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*Kinetic Determination of Morphine by means of Bray-Liebhaufsky Oscillatory Reaction System Using Analyte Pulse Perturbation Technique*

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*Influence of Alkali Metal Cations upon the Kolbe-Schmitt Reaction Mechanism*  
*J. Chem. Inf. Model.* **46** (2006) 1957-1964.
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*Kinetics of Extraction of Coal-Tar Pitch Components with Supercritical Carbon Dioxide*  
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35. **S. Marković**  
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34. **S. Marković**, Z. Marković, J.P. Engelbrecht, R.I. McCrindle  
*Spectral moments of polycyclic aromatic hydrocarbons. Solution of a kinetic problem*  
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*Theoretical study of the Kolbe-Schmitt reaction mechanism*  
*Z. Naturforsch.* **57 a** (2002) 812-818.
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*Spectral moments of phenylenes*  
*J. Chem. Inf. Comput. Sci.* **41(1)** (2001) 112-119.
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*S. Afr. J. Chem.* **53(3)** (2000) 179-190.
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*Spectral moments of the edge adjacency matrix in molecular graphs. Benzenoid hydrocarbons*  
*J. Chem. Inf. Comput. Sci.* **39(2)** (1999) 289-293.
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*Approximating total  $\pi$ -electron energy in terms of spectral moments. A quantitative*

*approach*

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27. **S. Marković**, A. Stajković

*The evaluation of spectral moments for molecular graphs of phenylenes*

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26. I. Gutman, **S. Marković**, Lj. Popović, Z. Spalević, Lj. Pavlović

*The relation between the Wiener indices of phenylenes and their hexagonal squeezes*

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25. I. Gutman, **S. Marković**, A. Stajković, S. Kamidžorac

*Correlations between  $\pi$ -electron properties of phenylenes and their hexagonal squeezes*

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*The dependence of the total  $\pi$ -electron energy of isomeric unbranched cata-condensed benzenoid hydrocarbons with a fixed number of bay regions on the number of Kekulé structures*

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*The dependence of total  $\pi$ -electron energy of large benzenoid hydrocarbons on the number of Kekulé structures is non-linear*

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*Revisiting a simple regularity for benzenoid hydrocarbons. Total  $\pi$ -electron energy versus the number of Kekulé structures*

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*Dependence of total  $\pi$ -electron energy of phenylenes on Kekulé structure count*

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*Almost-isospectral benzenoid systems*

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16. I. Gutman, **S. Marković**, V. Grbović

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*Proof of an equality for benzenoid systems*

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14. **S. Marković**

*The evaluation of the eighth moment for benzenoid graphs*

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*Effect of bay regions on the total  $\pi$ -electron energy of benzenoid hydrocarbons*

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*Dependence of spectral moments of benzenoid hydrocarbons on molecular structure*

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*Topological properties of benzenoid systems. XLVIIIb. A further empirical study of Hall's and Cioslowski's formulae*

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*Some more isomer-undistinguishing approximate formulas for the total  $\pi$ -electron energy of benzenoid hydrocarbons*

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