



## 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  
Marital status: Married (two children)  
Mother tongue: Serbian  
Other languages: English

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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:** Physical Chemistry  
Molecular modeling  
Computers in Chemistry

## List of scientific papers

### List of scientific papers of Svetlana Marković (maiden name Petrović)

103. Izudin Redžepović, **Svetlana Marković**  
*Theoretical study on the heat of formation of some polycyclic aromatic hydrocarbons*  
Chem. Pap. DOI: 10.1007/s11696-019-00914-7
102. Izudin Redžepović, **Svetlana Marković**, Boris Furtula  
*On Structural Dependence of Enthalpy of Formation of Catacondensed Benzenoid Hydrocarbons*  
MATCH Commun. Math. Comput. Chem. **82(3)** (2019) 663-678.  
ISSN: 0340-6253, **M21**, IF(2017)=**2,580**
101. Jelena Tošović, **Svetlana Marković**  
*Antioxidative activity of chlorogenic acid relative to trolox in aqueous solution – DFT study*  
Food Chem. **278** (2019) 469-475. DOI: <https://doi.org/10.1016/j.foodchem.2018.11.070>  
ISSN: 0308-8146, **M21a**, IF(2018)=**5,399**
100. Ana Gligorijević, **Svetlana Marković**, Izudin Redžepović, Boris Furtula  
*Application of spectral graph theory on the enthalpy change of formation of acyclic saturated ketones*  
J. Serb. Chem. Soc. **83** (2018) 1339-1349. <https://doi.org/10.2298/JSC180906086G>  
ISSN: 0352-5139, **M23**, IF(2018)=**0,828**
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(2018)=**1,428**
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(2017)=**4,946**
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>.  
ISSN: 0011-1643, **M23**, IF(2016)=**0,586**
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*  
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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(2017)=**4,946**
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*  
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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<sub>3</sub>)<sub>2</sub>CuCl<sub>4</sub> in a novel, highly efficient synthesis of 2-oxo and thioxo-1,2,3,4-tetrahydropyrimidines*  
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*Influence of the counteranion on the phenylselenoetherification reaction of nerolidol*  
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81. Igor Đurović, **Svetlana Marković**, Zoran Marković  
*Karboksilacija natrijum-2-naftoksida. Preispitivanje mehanizma pomoću meta-hibridnog funkcionala gustine*  
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*Vanillic Mannich Bases: Synthesis and Screening of Biological Activity. Mechanistic Insight into the Reaction with 4-Chloroaniline*  
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*DFT study of the mechanism of the phenylselenoetherification reaction of linalool*  
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*Influence of anthraquinone scaffold on E/Z isomer distribution of two thiosemicarbazone derivatives. 2D NMR and DFT studies*  
J. Mol. Struct. **1058** (2014) 291-297. DOI: 10.1016/j.molstruc.2013.11.025.

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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*  
Phys. Chem. Chem. Phys. **15(19)** (2013) 7370-7378. DOI: 10.1039/c3cp44605k.

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*DFT study of free radical scavenging activity of erodiol*  
Chem. Pap. **67(11)** (2013) 1453-1461. DOI: 10.2478/s11696-013-0402-0.

73. Violeta Marković, **Svetlana Marković**, Ana Janićijević, Marko V. Rodić, Vukadin M. Leovac, Nina Todorović, Snežana Trifunović, Milan D. Joksović  
*Mechanistic investigation and DFT calculation of the new reaction between S-methylisothiosemicarbazide and methyl acetoacetate*  
Struct. Chem. **24(6)** (2013) 2127-2136. DOI: 10.1007/s11224-013-0223-3.
72. **Svetlana Marković**, Jelena Đurđević, Milica Vukosavljević, Zorica Petrović  
*Mechanistic insight into alkylation of the ethyl acetoacetate anion with different ethyl halides*  
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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.
70. Vladimir P. Petrović, **Svetlana Marković**, Zorica D. Petrović  
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Monatsh. Chem. **143** (2012) 1497-1502.
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*  
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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*  
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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*

J. Mol. Mod. **17** (2011) 805-810.

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*

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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*  
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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*  
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*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*  
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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*  
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40. **S. Marković**, Z. Marković, N. Begović, N. Manojlović  
*Mechanism of the Kolbe-Schmitt Reaction with Lithium and Sodium Phenoxides*  
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39. N. Pejić, S. Blagojević, S. Anić, V. Vukojević, M. Mijatović, J. Ćirić, Z. Marković, **S. Marković**, Lj. Kolar-Anić  
*Kinetic Determination of Morphine by means of Bray–Liebhafsky Oscillatory Reaction System Using Analyte Pulse Perturbation Technique*  
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*Gas Chromatographic Determination of the Degree of Substitution of CMC*  
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37. Z. Marković, **S. Marković**, N. Begović  
*Influence of Alkali Metal Cations upon the Kolbe-Schmitt Reaction Mechanism*  
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*Kinetics of Extraction of Coal-Tar Pitch Components with Supercritical Carbon Dioxide*  
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*Approximating total  $\pi$ -electron energy of phenylenes in terms of spectral moments*  
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*Spectral moments of phenylenes*  
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J. Serb. Chem. Soc. **61(10)** (1996) 873-879.
24. **S. Marković**, I. Gutman, J. Šuković  
*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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J. Serb. Chem. Soc. **60(7)** (1995) 633-636.
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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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*Benzenoid graph with equal maximum eigenvalues*  
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*The smallest pair of isospectral benzenoid systems*  
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