



**Curriculum vitae  
Europass**



**Personal information**

Name **Silaghi-Dumitrescu, Radu**

Address 11, Arany Janos str, 400028 Cluj-Napoca, Romania

Telephone 0264593833

Mobil:

Fax 0264590818

E-mail rsilaghi@chem.ubbcluj.ro

Nationality Romanian

Date of birth 1974

Sex male

**Professional experience**

Time **1. 2011-present**

**2. 2007-present**

**3. 2000- 2007**

**4. 1998-2000**

**5. 2000-2004**

**6. 2004-2006**

Position 1. Co-director of the Institute for Technologies of the Babes-Bolyai University

2. associate professor

3. teaching assistant

4. junior teaching assistant

5. graduate student,

6. Senior Research Officer

Activities, responsibilities	<ol style="list-style-type: none"> <li>1. Director, in charge of the chemical direction: research, scale-up, pilot production</li> <li>2. research, teaching – bioinorganic chemistry, biochemistry</li> <li>3. research, teaching – biochemistry, enzymatic technology (laboratory sections only)</li> <li>4. research, teaching organic chemistry (laboratory section onby)</li> </ol>
Name and address of employer	<ol style="list-style-type: none"> <li>1-3. Universitatea “Babes-Bolyai”, Cluj-Napoca, Romania – Facultatea de Chimie si Inginerie Chimica, str Arany Janos 11, Cluj-Napoca, Romania</li> <li>4. Department of Chemistry, University of Georgia, Athens, Georgia, USA</li> <li>5. Department of Biological Sciences, University of Essex, Colchester CO43SQ, UK</li> </ol>
<b>Education</b>	
Time	<ol style="list-style-type: none"> <li>1. <b>2000-2004</b></li> <li>2. <b>1998-2005</b></li> <li>3. <b>july 2001</b></li> <li>4. <b>1997-1998</b></li> <li>5. <b>1993-1997</b></li> </ol>
Degree	<ol style="list-style-type: none"> <li>1. <b>PhD in chemistry</b> (bio-inorganic)</li> <li>2. <b>PhD in chemistry</b> (inorganic)</li> <li>3. <b>Summer Course in Crystallography</b></li> <li>4. <b>M.Sc. in Chemistry</b></li> <li>5. <b>B.Sc. in Chemistry</b></li> </ol>
Institution awarding the degree	<ol style="list-style-type: none"> <li>1. University of Georgia, Athens, Georgia , USA.</li> <li>2. Universitatea “Babes-Bolyai”, Cluj-Napoca, Romania</li> <li>3. American Crystallography Association, University of Georgia, Athens, Georgia, 2001</li> <li>4. Universitatea “Babes-Bolyai”, Cluj-Napoca, Romania</li> <li>5. Universitatea “Babes-Bolyai”, Cluj-Napoca, Romania</li> </ol>

## Competences

- Protein expression and purification (soluble proteins, inclusion bodies).
- Protein crystallization, protein crystallography
- Enzymatic assays, enzyme kinetics: including steady state, transient kinetic stopped-flow/rapid-scanning
- Cryo-enzymology
- Enzymatic product determination and isolation; chemical (enzyme-free) synthesis of compounds, characterization with UV-visible, FTIR, NMR spectroscopies, (GC/LC)-MS, HPLC
- Preparative bio-transformation of chemicals, using whole cells or purified enzymes; method development
- DNA manipulation including cloning and mutagenesis techniques
- Bacterial cell cultures, including anaerobic nitrosative/oxidative stress experiments
- Anaerobic protein/chemical manipulation
- Record and interpret UV-visible, electron paramagnetic resonance, circular dichroism, and infrared spectra
- Sample (protein) preparation (and interpretation, where applicable) for EPR, Mössbauer, (VTVH)MCD, ENDOR, resonance Raman, NMR spectroscopies, (GC/LC)-MS
- Proficient in the use of the following equipment: microplate spectrophotometer, UV-visible recording spectrophotometer, infrared spectrophotometer, biological oxygen monitor, nitric oxide monitor, fast-pressure liquid chromatography apparatus, thermocyclers, centrifuge, electrophoresis apparatus, anaerobic chamber.
- Electronic structure calculation (ab initio, semiempirical, DFT, molecular mechanics) and protein modelling (sequence homology, docking) programs (e.g., Gaussian, Spartan, Titan, Hyperchem, Cache, Sybyl, Insight), including UNIX and Linux applications
- Word processing programs, spreadsheet applications, presentation applications, scientific plotting programs, chemical structure drawing programs, DNA and protein sequence manipulation programs.
- Teaching/mentoring: Directly supervised and mentored ~20 undergraduate students and 3 graduate students in designing/successfully completing chemical/biochemical research projects and writing dissertations. Devised, written, and supervised general biochemistry and bioinorganic chemistry laboratory experiments.

Native language **Romanian**

Foreign languages **A1, A2 – basic knowledge**  
**B1, B2 – Independent user**  
**C1 și C2 – experienced user**

Autoevaluare  
*Nivel european (\*)*

**English**  
**French**

Comprehension		Spoken		written
Listening	Reading	conversation	Oral speech	Written language
C1	C1	C1	C1	C1
B1	B1	B1	B1	B1

Leading/organizer abilities

Supervised ~20 diploma works for undergraduate students, 3 MSc dissertations, won and completed several research grants from national funding bodies.  
Member of the Biochemistry and Molecular Biology Commissions of the Romanian National Council for Scientific Research and of the National Council for Accreditation of University Degrees and Titles.

**Appendix**

**List of publications**

124. Prejmerean, Cristina , Moldovan, Marioara, Petrea, C.M., Prodan, Doina, Silaghi-Dumitrescu, Laura, Vasile, E., Furtos, Gabriel, Boboia, Stanca, **Silaghi-Dumitrescu, Radu. Physico-chemical and mechanical characterization of some experimental dental nanocomposites.** Materiale Plastice, 2011, 48, 279-284.

123. Imre, Anamaria; Moț, Augustin C; **Silaghi-Dumitrescu, Radu. Exploring the possibility of high-valent copper in models of copper proteins with a three-histidine copper-binding motif.** Central European Journal of Chemistry, 2012, in press.

122. **Silaghi-Dumitrescu, Radu. Redox activation of small molecules at biological metal centers.** Structure & Bonding, 2012, accepted.

121. Salnikov, Denis S.; Dereven'kov, Ilya A.; Makarov, Sergei V.; Ageeva, Elena S.; Lupan, Alexandru; Surducun, Mihai; **Silaghi-Dumitrescu, Radu. Kinetics Of Reduction Of Cobalamin By Sulfoxylate In Aqueous Solutions.** Revue Roumaine de Chimie, 2012, accepted.

120. Moț, Augustin C.; Pârvu, Marcel; Damian, Grigore; Darula, Irimie, Florin D.; Zsuzsanna; Medzihradsky, Katalin F.; Brem, Balazs; **Silaghi-Dumitrescu, Radu. A “yellow” laccase with “blue” spectroscopic features, from Sclerotinia sclerotiorum.** Process Biochemistry, 2012, 47(6), 968–975.

119. **Silaghi-Dumitrescu, Radu. DFT vibrational analysis of metal-hydroperoxo bleomycin complexes.** Studia Universitatis Babes-Bolyai, Chemia 2012, in press
118. Cioloboc, Daniela; Tomsa, Adrian-Raul; Damian, Grigore; **Silaghi-Dumitrescu, Radu. High spin to low spin change induced by reductive chemistry with iron-substituted Dawson polyoxometalate.** Inorganic Chemistry Communications 2012, 20(1), 70-72. DOI: 10.1016/j.inoche.2012.02.019
117. Kozma, Ágnes; Ibáñez, Susana; **Silaghi-Dumitrescu, Radu**; Sanz Miguel, Pablo J.; Gupta, Deepali; Lippert, Bernhard. **7-Methylguanine: protonation, formation of linkage isomers with trans-(NH<sub>3</sub>)<sub>2</sub>Pt<sup>II</sup>, and base pairing properties.** Dalton Transactions, 2012, 41 (20), 6094 – 6103. (assigned as „hot article” by the journal)
116. Lupan, Alexandru; Matyas, Csongor; Mot, Augustin; **Silaghi-Dumitrescu, Radu. Can geometrical distortions make a laccase change color from blue to yellow?** Studia Universitatis Babes-Bolyai, Chemia 2011, 56(3), 201-206.
115. Prodan, Doina; Silaghi-Dumitrescu, Laura; Prejmerean, Cristina; **Silaghi-Dumitrescu, Radu**; Bolojan, Laura; Damian, Grigore. **Evaluation of free radical concentration in some new dental composite materials by ESR spectroscopy.** Studia Universitatis Babes-Bolyai, Chemia 2011, 56(3), 231-238.
114. Mot, Augustin C.; Syrbu, Sergei A.; Makarov, Sergei V.; Damian, Grigore; **Silaghi-Dumitrescu, Radu. Axial ligation in water-soluble copper porphyrinates: contrasts between EPR and UV-vis.** Inorganic Chemistry Communications 2012, 18(4), 1-3.
113. Iacob, Bianca; Deac, Florina; Cioloboc, Daniela; Damian, Grigore; **Silaghi-Dumitrescu, Radu. Hemoglobin-albumin Crosslinked Copolymers: Reduced Prooxidant Reactivity.** Artificial Cells Blood Substitutes And Biotechnology 2011, 39(5), 293-297.
112. **Silaghi-Dumitrescu, Radu**; Mich, Mihaela; Matyas, Csongor; Cooper, Chris E. **Nitrite and nitrate reduction by molybdenum centers of the nitrate reductase type: Computational predictions on the catalytic mechanism.** Nitric Oxide 2012, 26(1):27-31
111. **Silaghi-Dumitrescu, Radu**; Ghinga, Radu. **A computational investigation of the decay mechanism of the reaction product of anthranilate dioxygenase (anthranilic acid diol).** Studia Universitatis Babes-Bolyai, Chemia 2011, in press.
110. Bischin, Cristina; Taciuc, Vicentiu; **Silaghi-Dumitrescu, Radu. Cisplatin**

**effect on hemoglobin and myoglobin autooxidation.** Studia Universitatis Babes-Bolyai, *Chemia* 2010, 55(4), 313-318.

109. Irsai, Izabella ; Majdik, Cornelia; Lupan, Alexandru; **Silaghi-Dumitrescu, Radu. Secondary structure elements in polylactic acid models,** *J. Math Chem*, 2011, 50(4), 703-733.

108. Salnikov, Denis S.; **Silaghi-Dumitrescu, Radu;** Makarov, Sergei V.; van Eldik R, Boss GR **Cobalamin reduction by dithionite. Evidence for the formation of a six-coordinate cobalamin(II) complex.** *Dalton Trans.* 2011 40(38), 9831-4

107. Prejmerean, Cristina; Moldovan, Marioara; Silaghi-Dumitrescu, Laura; Prodan, Doina; Furtos, Gabriel; Trif, Marcela; Popescu, Violeta; Pascallau, Violeta; Petrea, Celina-Maria; **Silaghi-Dumitrescu, Radu. Composition Versus Physico-mechanical Properties of Some Dental Experimental Polymers.** *Materiale Plastice*, 2011, 48(1), 27-32.

106. **Silaghi-Dumitrescu, Radu;** Makarov, Sergei V.; Uta, Matei-Maria Dereven'kov, Ilia A.; Stuzhin Pavel A. **Redox non-innocence of a nitrido bridge in a methane-activating dimer of iron phthalocyanine,** *New Journal of Chemistry*, 2011, 35(5), 1140-1145.

105. **Silaghi-Dumitrescu, Radu. What causes iron-sulphur bonds in active sites of one-iron superoxide reductase and two-iron superoxide reductase to differ?.** *Chemical Papers*, 2011, 65 (4), 559–565.

104. Bischin, Cristina; Lupan, Alexandru; Taciuc, Vicentiu; **Silaghi-Dumitrescu, Radu. Interactions between proteins and platinum-containing anti-cancer drugs.** *Mini-Reviews in Medicinal Chemistry*, 2011, 11, 214-224.

103. Fischer-Fodor, Eva; Mot, Augustin; Deac, Florina; Arkosi, Mariann; **Silaghi-Dumitrescu, Radu. Towards hemerythrin-based blood substitutes: comparative performance to hemoglobin on human leukocytes and umbilical vein endothelial cells.** *Journal of Biosciences*, 2011, 36(2), 215-221.

102. **Silaghi-Dumitrescu, Radu;** Makarov, Sergei. **Siroheme-containing sulfite reductase: a density functional investigation of the mechanism,** *International Journal of Quantum Chemistry* 2012, 112(3), 900-908.

101. **Silaghi-Dumitrescu, Radu. Assays for peroxidase activity: the HRP case,** *Studia Universitatis Babes-Bolyai, Chemia* 2010, 55(3), 207-222.

100. Kun, Attila; Lupan, Alexandru; **Silaghi-Dumitrescu, Radu. PM6 modeling of alpha helical polypeptide structures,** *Studia Universitatis Babes-Bolyai, Chemia* 2010, 55(1), 31-36.

99. Zolog, Oana; Mot, Augustin; Deac, Florina; Roman, Alina; Fischer-Fodor, Eva; **Silaghi-Dumitrescu, Radu. A new polyethyleneglycol-derivatized hemoglobin derivative with decreased oxygen affinity and limited toxicity** The Protein Journal, 2010, 30(1), 27–31.

98. Deac, Florina-Violeta; Bolfa, Ana Maria; Magdas, Cristian; Sevastre, Bogdan; Turc, Silvia; **Silaghi-Dumitrescu, Radu. Hemoglobin-based blood substitutes: which hemoglobin to use?**, Romanian Journal of Biochemistry, 2010, 47(2), 135–141.

97. Mot, Augustin; **Silaghi-Dumitrescu, Radu**; Sarbu, Costel. **Rapid and effective evaluation of antioxidant capacity of propolis extracts using DPPH bleaching kinetic profiles, FT-IR and UV-vis spectral data** Journal of Food Composition and Analysis, 2011, 516–522.

96. Deac, Florina; Cotolan, Nicoleta; Kis, Zoltan; **Silaghi-Dumitrescu, Radu. A dithionite-induced six-coordinated species at the heme in deoxy-hemoglobin**, Metal Elements in Environment, Medicine and Biology Tome X, Radu Silaghi-Dumitrescu, Gabriela Garban, Eds., 2010, Eurobit Publishing House, Timisoara, Romania, pp 121-126.

95. Lupan, Alexandru; Kun, Attila; **Silaghi-Dumitrescu, Radu. Computational modeling metal-protein interactions: cisplatin**, Metal Elements in Environment, Medicine and Biology Tome X, Radu Silaghi-Dumitrescu, Gabriela Garban, Eds., 2010, Eurobit Publishing House, Timisoara, Romania, pp 199-204.

94. Bischin, Cristina; Taciuc, Vicentiu; **Silaghi-Dumitrescu, Radu. Effects of antioxidants in cisplatin toxicology**, Metal Elements in Environment, Medicine and Biology Tome X, Radu Silaghi-Dumitrescu, Gabriela Garban, Eds., 2010, Eurobit Publishing House, Timisoara, Romania, pp 265-270.

93. **Silaghi-Dumitrescu, Radu**; Seff, Amalia-Laura. **Superoxide reductase: a debated mechanism, comparison with superoxide dismutases**, Metal Elements in Environment, Medicine and Biology Tome X, Radu Silaghi-Dumitrescu, Gabriela Garban, Eds., 2010, Eurobit Publishing House, Timisoara, Romania, pp 21-26.

92. Bischin, Cristina; Deac, Florina; Deac, Florina; **Silaghi-Dumitrescu, Radu**; Worrall, Jonathan A. R.; Rajagopal, Badri S.; Damian, Grigore; Cooper, Chris E. **Ascorbate peroxidase activity of cytochrome c** Free Radical Research, 2010, 45(4), 439-444.

91. Deac, Florina; Iacob, Bianca; Fischer-Fodor, Eva; Damian, Grigore; **Silaghi-Dumitrescu, Radu. Derivatization of hemoglobin with periodate-generated reticulation agents: evaluation of oxidative reactivity for potential blood**

**substitutes** Journal of Biochemistry, 2010, 149(1), 75-82 .

90. Mot, Augustin C.; Roman, Alina; Lupan, Iulia; Kurtz, Jr. Donald M.; **Silaghi-Dumitrescu, Radu. Towards the development of hemerythrin-based blood substitutes** The Protein Journal, 2010, 29(6), 387-393.

89. **Silaghi-Dumitrescu, Radu. High-valent metalloporphyrins in hydrocarbon activation: metal(V)-oxo or metal(V)-hydroxo?** New Journal of Chemistry, 2010, 34(9), 1830-1833 .

88. **Silaghi-Dumitrescu, Radu, Uta, Matei-Maria; Makarov, Sergei V. Nitrite linkage isomerism in hemes and related complexes: modulation by metal, oxidation state, macrocycle, and medium polarity** Revue Roumaine de Chimie, 2010, 55(11-12), 897-903.

87. **Silaghi-Dumitrescu, Radu. Computational analysis of bonding in PhIO and related 'hypervalent' iodine complexes** Studia Universitatis Babes-Bolyai, Chemia 2010, 55(2), 63-67.

86. **Silaghi-Dumitrescu, Radu; Makarov, Sergei V. A computational analysis of electromerism in hemoprotein Fe(I) models**, Journal of Biological Inorganic Chemistry, 2010, 15(6), 977-986.

85. **Tomşa, Adrian-Raul; Cioloboc, Daniela; Todea, Ana Maria; Silaghi-Dumitrescu, Radu; Damian, Grigore; Rusu, Mariana. Synthesis, spectroscopic and electrochemical characterization of a new chromium (III) substituted Dawson polyoxometalate** Studia Universitatis Babes-Bolyai, Chemia 2009, 54 (4), 95-105.

84. **Silaghi-Dumitrescu, Radu. A density functional investigation of hydrogen peroxide activation by high-valent heme centers: implications for the catalase catalytic cycle** Journal of Porphyrins and Phthalocyanines, 2010, 14(5), 371-374.

83. **Silaghi-Dumitrescu, Radu. Computational description of peptide architectures based on hydrogen bonds** Studia Universitatis Babes-Bolyai, Chemia 2010, LV(1), 31-36.

82. Kis, Zoltan; Makarov, Sergei V; **Silaghi-Dumitrescu, Radu. Computational investigations on the electronic structure and reactivity of thiourea dioxide: sulfoxylate formation, tautomerism, dioxygen liberation**, Journal of Sulphur Chemistry, 2010, 31(1), 27-39.

81. **Silaghi-Dumitrescu, Radu; Makarov, Sergei V. Hydrocarbon oxygenation by metal-nitrite adducts: a theoretical comparison with ferryl-based oxygenation agents**, European Journal of Inorganic Chemistry, 2010,



39(6):1464-6.

80. Mot, Augustin; Kis, Zoltan; Svistunenko, Dimitri A.; Damian, Grigore; Makarov, Sergei V.; **Silaghi-Dumitrescu, Radu. 'Super-reduced' iron under physiologically-relevant conditions**, Dalton Transactions, 2010, 39(6):1464-6.

79. Deac, Florina-Violeta; Todea, Anamaria; Bolfa, Ana Maria; Podea, Paula; Petrar, Petronela; **Silaghi-Dumitrescu, Radu. Ascorbate binding to globins**, Romanian Journal of Biochemistry, 2009, 46(2), 115–121.

78. Mot, Augustin Catalin; Damian, Grigore; Sarbu, Costel; **Silaghi-Dumitrescu, Radu. Redox reactivity in propolis: direct detection of free radicals in basic medium and interaction with hemoglobin**, Redox Report, 2009, 14(6), 267-74.

77. Arkosi, Mariann-Kinga; Deac, Florina; **Silaghi-Dumitrescu, Radu. Hemoglobin peroxidase activity: interaction with hydroquinone and anthracene**, Metal Elements in Environment, Medicine and Biology Tome IX, Radu Silaghi-Dumitrescu, Gabriela Garban, Eds., 2009, Cluj University Press, Cluj-Napoca, Romania, pp 99-110.

76. Mot, Augustin; Roman, Alina; **Silaghi-Dumitrescu, Radu. Blood substitutes: can we do without hemoglobin?**, Metal Elements in Environment, Medicine and Biology Tome IX, Radu Silaghi-Dumitrescu, Gabriela Garban, Eds., 2009, Cluj University Press, Cluj-Napoca, Romania, pp 122-125.

75. Taciuc, Vicentiu; Bischin, Cristina; **Silaghi-Dumitrescu, Radu. A novel mechanism for platinum-based drugs: cisplatin and related compounds as pro-oxidants in blood**, Metal Elements in Environment, Medicine and Biology Tome IX, Radu Silaghi-Dumitrescu, Gabriela Garban, Eds., 2009, Cluj University Press, Cluj-Napoca, Romania, pp 130-134.

74. Deac, Florina; Todea, Anamaria; **Silaghi-Dumitrescu, Radu. Glutaraldehyde derivatization of hemoglobin: a potential blood substitute**, Metal Elements in Environment, Medicine and Biology Tome IX, Radu Silaghi-Dumitrescu, Gabriela Garban, Eds., 2009, Cluj University Press, Cluj-Napoca, Romania, pp 165-173.

73. **Silaghi-Dumitrescu, Radu**; Bischin, Cristina; Deac, Florina; Kis, Zoltan; Mot, Augustin; Makarov, Sergei V. **Unusual metal oxidation states in metalloproteins and related complexes: from degenerate orbitals to apoptosis**, Metal Elements in Environment, Medicine and Biology Tome IX, Radu Silaghi-Dumitrescu, Gabriela Garban, Eds., 2009, Cluj University Press, Cluj-Napoca, Romania, pp 174-182.

72. **Silaghi-Dumitrescu, Radu. Superoxide interaction with nickel and iron superoxide dismutases**, Journal of Molecular Graphics and Modelling 2009,

28(2), 156-61.

71. Haiduc, Ionel; Silaghi-Dumitrescu, Ioan; Garban, Zeno; Fischer-Fodor, Eva; **Silaghi-Dumitrescu, Radu. Metallomics**, Metal Elements in Environment, Medicine and Biology Tome VIII, Corneliu Davidescu, Gabriela Garban, Iosif Gergen, Simona Dragan, Nicolae Vaszilcsin, Adina Avacovici, Eds., 2008, Eurobit Publishing House, Timisoara, Romania, pp 5-14.

70. **Silaghi-Dumitrescu, Radu**; Deac, Florina. **The redox reactivity of globins: the chicken and egg paradox**, Metal Elements in Environment, Medicine and Biology Tome VIII, Corneliu Davidescu, Gabriela Garban, Iosif Gergen, Simona Dragan, Nicolae Vaszilcsin, Adina Avacovici, Eds., 2008, Eurobit Publishing House, Timosara, Romania, pp 271-276.

69. Kis, Zoltan; **Silaghi-Dumitrescu, Radu. The Electronic Structure of Biologically Relevant Fe(0) Systems**, International Journal of Quantum Chemistry 2010, 110(10), 1848-1856.

68. Pogorelova, Anna S.; Makarov, Sergei V.; Ageeva, Tatiana; **Silaghi-Dumitrescu, Radu. Cobalt tetrasulfophthalocyaninate – a catalyst for nitrite reduction by thiourea dioxide**, Russian Journal of Physical Chemistry 2009, 83(12), 2250-2254.

67. Makarov, Sergei V.; Salnikov Denis S.; Pogorelova, Anna S.; Kis, Zoltan; Silaghi-Dumitrescu, Radu. **A new route to carbon monoxide adducts of heme proteins**, Journal of Porphyrins and Phthalocyanines 2008, 12, 1096-1099.

66. **Silaghi-Dumitrescu, Radu**; Kallay, Andras. **Carbon dioxide hydration: mechanistic lessons from enzymatic systems** Studia Universitatis Babes-Bolyai, Chemia 2008, (3), 47-50.

65. **Silaghi-Dumitrescu, Radu. Halide activation by heme peroxidases: theoretical predictions on putative adducts of halides with Compound I** European Journal of Inorganic Chemistry, 2008, 5404-5407.

64. **Silaghi-Dumitrescu, Radu. Carbon dioxide activation: hydration by carbonic anhydrase and related systems - what makes a good catalyst?** Journal of Molecular Structure THEOCHEM 2010, 942(1-3), 15-18.

63. **Silaghi-Dumitrescu, Radu. An alternative mechanism for catalase activity** Studia Universitatis Babes-Bolyai, Chemia 2007, (4), 127-130.

62. **Silaghi-Dumitrescu, Radu. Bonding in biologically-relevant high-valent iron centers** International Journal of Chemical Modeling 2008, 1 (4).

61. **Silaghi-Dumitrescu, Radu. Nitric oxide and nitrite reduction by**

**metalloenzymes** *Revue Roumaine de Chimie*, 2009, 54(6), 513–522.

60. Reeder, Brandon J.; Grey, Marie; **Silaghi-Dumitrescu, Radu**; Svistunenکو, Dimitri A.; Bülow, L; Cooper, Chris E.; Wilson, Michael T. **Tyrosine residues as redox cofactors in human hemoglobin: implications for engineering non toxic blood substitutes** *Journal of Biological Chemistry*, 2008, 283, (45), 30780-30787.

59. **Silaghi-Dumitrescu, Radu**. **The ferric-oxo moiety in porphyrin complexes – a ferryl in disguise?** *Macroheterocycles*, 2008, 1, 79-81.

58. **Silaghi-Dumitrescu, Radu; Uta, Matei-Maria**. **Nitrite linkage isomerism in bioinorganic chemistry – a case for mechanistic promiscuity** *Studia Universitatis Babes-Bolyai, Chemia* 2008, (2), 61-65.

57. Cooper, Chris E.; **Silaghi-Dumitrescu, Radu**; Rukengwa, Martine; Alayash, Abdu I.; Buehler, Paul W.. **Peroxidase-activity of hemoglobin towards ascorbate and urate: a synergistic protective strategy against toxicity of hemoglobin-based oxygen carriers (HBOC)** *Biochimica Biophysica Acta*, 2008, 1784, 1415–1420.

56. **Silaghi-Dumitrescu, Radu**. **Halide activation by heme peroxidases: theoretical predictions on putative adducts of halides with Compound I**. *Journal of Biological Inorganic Chemistry*, 2007, 12(S1), S229.

55. **Silaghi-Dumitrescu, Radu**. **The “push” effect of the thiolate axial ligand in superoxide reductase: a density functional study** *Revue Roumaine de Chimie*, 2008, 53(12), 1149–1156.

54. **Silaghi-Dumitrescu, Radu**. **A density functional study of aromatic ring oxygenation by Rieske dioxygenase active sites. 2. Energetics of the proposed reaction mechanisms.** *Studia Universitatis Babes-Bolyai, Chemia* 2007, (2), 127-139.

53. **Silaghi-Dumitrescu, Radu**. **Dioxygen activation by Rieske dioxygenases – computational studies. 1. Possible catalytic intermediates.** *Studia Universitatis Babes-Bolyai, Chemia* 2007, (2), 103-126.

52. **Silaghi-Dumitrescu, Radu**. **A paradigm for O-O bond cleavage in ferric-hydroperoxo complexes.** *Studia Universitatis Babes-Bolyai, Chemia* 2007, 52, 47-54.

51. **Silaghi-Dumitrescu, Radu**. **Electronic structures of Fe(IV) and Fe(V) systems with oxo, sulfido and nitrido ligands in octahedral environments.** *Revista de Chimie*, 2007, 58(5), 461-464.

50. Svistunenko, Dimitri A.; Reeder, Brandon J.; Wankasi, Meebi M.; **Silaghi-Dumitrescu, Radu**; Cooper, Chris E. Rinaldo, Serena; Cutruzzolà, Francesca; Wilson, Michael T. **Interaction of *Aplysia limacina* metmyoglobin with hydrogen peroxide.** Dalton Transactions 2007, 840-50.
49. **Silaghi-Dumitrescu, Radu**; Reeder, Brandon; Nicholls, Peter; Cooper, Chris E.; Wilson, Michael T. **Ferryl haem protonation gates peroxidatic reactivity in globins.** Biochemical Journal 2007, 403, 391–395.
48. Schwartz, Jennifer K.; Liu XF; Albetel Angela Nadia; **Silaghi-Dumitrescu, Radu**, Kurtz, Donald M, Jr.; Theil, Elizabeth C; Solomon, Edward I; **Structure/function correlations in binuclear non-heme ferrous sites: Specific characterization of the active sites in m-Ferritin and nitric oxide reductases** Abstracts of Papers, 231st ACS National Meeting, United States, March 26, 2006 (2006), INOR-89
47. **Silaghi-Dumitrescu, Radu. Hemes Revisited by Density Functional Approaches. 2. A Paradigm for Axial Ligation In Hemoproteins.** Studia Universitatis Babes-Bolyai, Chemia 2006, 51, 167-174.
46. **Silaghi-Dumitrescu, Radu. Fe(IV)-Fe(II) electromerism in hemoprotein complexes: implications for ferryl chemistry.** Proceedings of the Romanian Academy Series B 2006, 2-3, 95-101.
45. **Silaghi-Dumitrescu, Radu**; Silaghi-Dumitrescu, Ioan; **Editorial – special issue on Computational Inorganic Chemistry.** Chemtracts – Inorganic Chemistry 2005, 50, 11-16.
44. **Silaghi-Dumitrescu, Radu**; Silaghi-Dumitrescu, Ioan; **Computational Inorganic Chemistry – a useful tool, and more.** Chemtracts – Inorganic Chemistry 2005, 684-708.
43. Isaza, Clara E.; **Silaghi-Dumitrescu, Radu**; Iyer, Ramesh B.; Kurtz, Donald M. Jr.; Chan, Michael K. **Structural Basis for O<sub>2</sub> Sensing by the Hemerythrin-like Domain of a Bacterial Chemotaxis Protein: Substrate Tunnel and Fluxional N Terminus.** Biochemistry 2006, 45(30), 9023-9031.
42. Dunne, Jacqueline; Caron, Alexis; Menu, Patrick; Alayash, Abdu I.; Buehler, Paul W.; Wilson, Michael T.; **Silaghi-Dumitrescu, Radu**; Faivre, Beatrice; Cooper, Chris E. **Ascorbate removes key precursors to oxidative damage by cell free hemoglobin in vitro and in vivo.** Biochemical Journal 2006, **399(3)**, 513-24.
41. **Silaghi-Dumitrescu, Radu**; **Copper-containing nitrite reductase: a DFT study of nitrite and nitric oxide adducts.** Journal of Inorganic Biochemistry 2006, 100(3), 396-402.

40. **Silaghi-Dumitrescu, Radu; Silaghi-Dumitrescu, Ioan; DFT and the electromerism in complexes of iron with diatomic ligands.** Journal of Inorganic Biochemistry 2006, 100(1), 161-166.
39. **Silaghi-Dumitrescu, Radu; Cooper, Chris E., Transient species involved in catalytic dioxygen/peroxide activation by hemoproteins: possible involvement of protonated compound I species.** Dalton Transactions 2005, 3477-3482.
38. Iyer, Ramesh B.; **Silaghi-Dumitrescu, Radu; Lanzilotta, William N.; Kurtz, Donald M. Novel non-heme diiron bacterial peroxidases.** Abstracts of Papers, 229th ACS National Meeting, San Diego, CA, United States, March 13-17, 2005 (2005), INOR-556
37. Iyer, Ramesh,\* **Silaghi-Dumitrescu, Radu,\* Lanzilotta, William N. Kurtz, Donald M. Jr. High-resolution crystal structures of *Desulfovibrio vulgaris* (Hildenborough) nigerythrin: facile, redox-dependent iron movement, domain interface variability, and peroxidase activity in the rubrerythrin** Journal of Biological Inorganic Chemistry 2005, 10, 407-416. (\*authors marked "contributed equally to this work")
36. **Silaghi-Dumitrescu, Radu, Kurtz, Donald M. Jr., Ljungdahl, Lars G., Lanzilotta, William N. X-ray Crystal Structures of *Moorella thermoacetica* FprA. Novel Diiron Site Structure and Mechanistic Insights into a Scavenging Nitric Oxide Reductase.** Biochemistry 2005, 44(17), 6492-6501.
35. **Silaghi-Dumitrescu, Radu. A density functional study of heme-peroxynitrite adducts.** Journal of Molecular Structure THEOCHEM, (2005), 722, 233-237.
34. **Silaghi-Dumitrescu, Radu. "High-valent" ferryl-oxo complexes: how "high" are they really?** Studia Universitatis Babes-Bolyai, Chemia 2005, 50, 17-21.
33. **Silaghi-Dumitrescu, Radu. Discontinuum between ferrous-superoxo and ferric-peroxo in heme [FeO<sub>2</sub>]<sup>9</sup> complexes?** Studia Universitatis Babes-Bolyai, Chemia 2005, 11-16.
32. **Silaghi-Dumitrescu, Radu. Nitrile hydration by the cobalt-containing nitrile hydratase. DFT investigation of the mechanism** Revista de Chimie 2005, 56(4), 359-362.
31. **Silaghi-Dumitrescu, Radu; Ng, Kim Yong; Viswanathan, Rathinam, Kurtz, Donald M. Jr. A Flavo-diiron protein from *Desulfovibrio vulgaris* with oxidase and nitric oxide reductase activities. Evidence for an *In vivo* nitric**

**oxide scavenging function.** Biochemistry 2005, 44(9), 3572-9.

30. Das, Amaresh; **Silaghi-Dumitrescu, Radu**; Ljungdahl, Lars G.; Kurtz, Donald M., Jr., **Cytochrome bd oxidase, oxidative stress and dioxygen tolerance of the strictly anaerobic bacterium, *Moorella thermoacetica*.** Journal of Bacteriology 2005, 187(6), 2020-2029.

29. Kurtz, Donald M.; Lanzilotta, William N.; **Silaghi-Dumitrescu, Radu.** **How microbes detoxify superoxide, hydrogen peroxide, and nitric oxide: The non-heme iron reductive paradigm.** Abstracts of Papers, 227th ACS National Meeting, Anaheim, CA, United States, March 28-April 1, 2004 (2004), INOR-418

28. **Silaghi-Dumitrescu, Radu.** **Factors controlling O-O bond cleavage in ferric-hydroperoxo complexes.** Proceedings of the Romanian Academy Series B 2004, 3, 155-163.

27. **Silaghi-Dumitrescu, Radu.** **Bioorganometallic complexes relevant to the “push effect” in hemoproteins.** Proceedings of the Romanian Academy Series B 2004, 3, 149-154.

26. **Silaghi-Dumitrescu, Radu.** **Bonding in ferric-oxo complexes.** Studia Universitatis Babes-Bolyai, Chemia 2004, 49(2), 235-240.

25. **Silaghi-Dumitrescu, Radu;** **Linkage isomerism in nitrite reduction by cytochrome cd<sub>1</sub> nitrite reductase.** Inorganic Chemistry 2004, 43(12), 3715-3718.

24. **Silaghi-Dumitrescu, Radu;** **The nature of the “high-valent” complexes in the catalytic cycles of hemoproteins.** Journal of Biological Inorganic Chemistry 2004, 9, 471-476.

23. **Silaghi-Dumitrescu, Radu;** **The nitric oxide adducts of cytochrome cd<sub>1</sub> nitrite reductase.** Revista de Chimie 2004, 55, 496-498.

22. **Silaghi-Dumitrescu, Radu;** **On the performance of the PM3 semiempirical method with heme complexes relevant to dioxygen and peroxide activation.** Revista de Chimie 2004, 55, 304-307.

21. **Silaghi-Dumitrescu, Radu;** **Heme ferrous-hydroperoxo complexes: some theoretical considerations.** Archives of Biochemistry and Biophysics 2004, 424, 137-140.

20. **Silaghi-Dumitrescu, Radu; Silaghi-Dumitrescu, Ioan. Hemes revisited by density functional approaches. 1. The axial ligand and the dioxygen-peroxo chemistry.** *Revue Roumaine de Chimie* 2004, 3-4, 257-268.
19. **Silaghi-Dumitrescu, Radu; Amthor, Stephan; Paizs, Csaba; Majdik, Cornelia; Tosa, Monica; Moldovan, Paula; Sas, Angela; Tamas, Liana; Irimie, Florin-Dan. Horseradish peroxidase - catalyzed oxidation of water - insoluble phenothiazines.** *Studia Universitatis Babes-Bolyai, Chemia* 2003, 48, 165.
18. Kurtz, Donald M., Jr.; Emerson, Joseph P; **Silaghi-Dumitrescu, Radu; Kung, Irene; Das, Amaresh; Ljungdahl, Lars; How microbes detoxify superoxide, hydrogen peroxide and nitric oxide. The non-heme iron reductive paradigm** *Journal of Inorganic Biochemistry* 2003, 96, 69.
17. Kurtz, Donald M., Jr.; **Silaghi-Dumitrescu, Radu; Das, Amaresh; Jameson, Guy; Ljungdahl, Lars; Huynh, Boi Hanh A non-heme iron nitric oxide reductase that protects against nitrosative stress in acetogenic bacteria** *Journal of Inorganic Biochemistry* 2003, 96, 174.
16. **Silaghi-Dumitrescu, Radu; Kurtz, Donald M., Jr. High-resolution crystal structures and spectroscopy of native and Compound I Cytochrome c Peroxidase** *Chemtracts – Inorganic Chemistry* 2003, 16, 722-728 – *Commentary*.
15. **Silaghi-Dumitrescu, Radu; Irimie, Florin-Dan; Paizs, Csaba; Majdik, Cornelia; Tosa, Monica; Moldovan, Paula; Sas, Angela; Tamas, Liana. Horseradish peroxidase catalyzed oxidation of some benzyl-type alcohols.** *Studia Universitatis Babes-Bolyai, Chemia* 2003, 48, 177-182.
14. **Silaghi-Dumitrescu, Radu; Kurtz, Donald M., Jr. Tuning the electronic structure of octahedral iron complexes {FeL(X)} (L = 1-alkyl-4,7-bis(4-tert-butyl-2-mercaptobenzyl)-1,4,7-triazacyclononane, X = Cl, CH<sub>3</sub>O, CN, NO): the S = 1/2 - S = 3/2 spin equilibrium of {FeLPr(NO)}.** *Chemtracts – Inorganic Chemistry* 2003, 16(8), 468-473 – *Commentary*.
13. **Silaghi-Dumitrescu, Radu. Nitric oxide reduction by heme-thiolate enzymes (P450<sub>nor</sub>): A reevaluation of the mechanism.** *European Journal of Inorganic Chemistry* 2003, (6), 1048-1052.
12. **Silaghi-Dumitrescu, Radu; Coulter, Eric D.; Das, Amaresh; Ljungdahl, Lars G.; Jameson, Guy N. L.; Huynh, Boi Hanh; Kurtz, Donald M., Jr. A flavodiiron protein and high molecular weight rubredoxin from *Moorella thermoacetica* with nitric oxide reductase activity.** *Biochemistry* 2003, 42(10), 2806-2815.

11. **Silaghi-Dumitrescu, Radu**; Silaghi-Dumitrescu, Ioan; Coulter, Eric D.; Kurtz, Donald M., Jr. **Computational study of the non-heme iron active site in superoxide reductase and its reaction with superoxide.** Inorganic Chemistry 2003, 42(2), 446-456.

10. Silaghi-Dumitrescu, Luminita; **Silaghi-Dumitrescu, Radu**; Blake, Alexander J; Cooke, Paul A.; Sowerby, D. Bryan, **Chlorination of (AsPh<sub>2</sub>)<sub>2</sub>O: Supramolecular structure of dihydroxodiphenylarsonium hydrogensulfate [AsPh<sub>2</sub>(OH)<sub>2</sub>] [HOSO<sub>3</sub>],** Revue Roumaine de Chimie 2002, 47(10-11), 1063-1068.

9. Irimie, Florin-Dan; Paizs, Csaba; Majdik, Cornelia; Tosa, Monica; Misca, Radu; **Silaghi-Dumitrescu, Radu.** **Bioorganic synthesis of some (5-benzothiazol-2-yl-furan-2-yl)-methanols in cell catalysis using Saccharomyces cerevisiae.** Heterocyclic Communications 2002, 8(5), 489-492.

8. **Silaghi-Dumitrescu, Radu**; Silaghi-Dumitrescu, Ioan; Coulter, Eric D.; Emerson, Joseph P; Kurtz, Donald M., Jr. **Computational study of the non-heme iron active site in superoxide reductase and its reaction with superoxide.** Journal of Inorganic Biochemistry 2001, 86(1), 432.

7. Silaghi-Dumitrescu, Luminita; Silaghi-Dumitrescu, Ioan; **Silaghi-Dumitrescu, Radu**; Haiduc, Ionel; Blake, Alexander J.; Sowerby, D. Bryan. **Bromination of (AsPh<sub>2</sub>)<sub>2</sub>O: the structure of tribromo-diphenylarsenic(V).** Revista de la Sociedad Quimica de Mexico 2000, 44(2), 134-138.

6. Irimie, Florin-Dan; Paisz, Csaba; Joo, Francisc; **Silaghi-Dumitrescu, Radu**; Tosa, Monica; Majdik, Cornelia. **Biocatalytical reduction of some 5-(carboxyethyl-phenyl)-furyl-2-carboxaldehydes mediated by baker's yeast.** Progress in Catalysis 1999, 8(2), 70-73.

5. Irimie, Florin-Dan; Paizs, Csaba; Joo, Francisc; **Silaghi-Dumitrescu, Radu**; Tosa, Monica; Majdik, Cornelia. **Bioorganic reduction of some 5-phenyl-furyl-2-carboxaldehydes mediated by bakers' yeast.** Roumanian Biotechnological Letters 1999, 4(1), 71-74.

4. Irimie, Florin-Dan; Paizs, Csaba; **Silaghi-Dumitrescu, Radu**; Damian, G.; Majdik, Cornelia; Tosa, Monica. **Mass spectrometry of some new 2-hydroxymethyl-5-phenyl-furans obtained through cell catalysis.** Studia Universitatis Babes-Bolyai, Chemia 1998, 43(1-2), 173-177.

3. Majdik, Cornelia; Irimie, Florin-Dan; Paizs, Csaba; **Silaghi-Dumitrescu, Radu**; Joo, Francisc; Tosa, Monica. **Synthesis and reduction of some nitro-benzofurans.** Studia Universitatis Babes-Bolyai, Chemia 1998, 43(1-2), 115-120.



2. Irimie, Florin-Dan; Paizs, Csaba; Chender, C.; Joo, Francisc; **Silaghi-Dumitrescu, Radu**; Majdik, Cornelia; Tosa, Monica. **Furyl-benzothiazoles. Synthesis and reactivity.** Studia Universitatis Babes-Bolyai, Chemia 1998, 43(1-2), 109-114.

1. **Silaghi-Dumitrescu, Radu**; Paisz, Csaba; Irimie, Florin-Dan; Joo, Francisc; Majdik, Cornelia; Tosa, Monica. **Biotransformation of nitroso naphthols bioassisted by Baker's yeast.** Studia Universitatis Babes-Bolyai, Chemia 1998, 43(1-2), 83-90.

### **Books, chapters:**

1. Radu Silaghi-Dumitrescu, **Horseradish peroxidase – a versatile catalyst** 2006, Research Signpost, India

2. Radu Silaghi-Dumitrescu, **Bonding in biologically-relevant high-valent iron centers**, in „Quantum Frontiers of Atoms and Molecules”, Ed. Mihai V. Putz, NOVA Publishing Inc. (New York), 22pp

3. Radu Silaghi-Dumitrescu, **Metalele in sistemele vii**, 2011, Presa Universitara Clujeana, Cluj-Napoca.

4. Radu Ghinga, Iulia Ghinga, Radu Silaghi-Dumitrescu, **Notiuni de baza in chimia organica**, 2012, Presa Universitara Clujeana, Cluj-Napoca.

5. Radu Silaghi-Dumitrescu, Luminita Silaghi-Dumitrescu, **On binary logic in Chemistry and beyond**, in “On psychology and beyond”, Ed. Enikö Batiz, 2012, Presa Universitara Clujeana, Cluj-Napoca

### **Oral communications and posters:**

#### **Oral communications:**

21. **Superoxide reductase: a debated mechanism, comparison with superoxide dismutases**  
Radu Silaghi-Dumitrescu  
**Metal Elements in Environment, Medicine and Biology 2010, Timisoara, Romania**

20. Walking the plank in small molecule activation by metalloenzymes and related centers  
Radu Silaghi-Dumitrescu  
**Molecular modeling in chemistry and biochemistry MOLMOD 2010, Cluj-Napoca, May 2010**

19. Unusual metal oxidation states in metalloproteins and related complexes:

from degenerate orbitals to blood substitutes

Radu Silaghi-Dumitrescu

**7th International Conference of the Chemical Societies of the South-Eastern European Countries – Bucharest, Spetember 2010**

18. Walking the plank in small molecule activation by metalloenzymes and related centers

Radu Silaghi-Dumitrescu

**Humboldt Conference on non-covalent interactions, Vrsac, Serbia, 2009**

17. Fe(I) and Fe(0) states in biologically-relevant systems

Radu Silaghi-Dumitrescu, Zoltan Kis, Sergei V. Makarov

**Molecular modeling in chemistry and biochemistry MOLMOD 2009, Cluj-Napoca, May 2009**

16. Fe(I) states in biologically-relevant systems

Radu Silaghi-Dumitrescu, Zoltan Kis, Sergei V. Makarov

**The 30<sup>th</sup> National Chemistry Conference, Calimanesti-Caciulata, Romania, October 2008**

15. Bioinorganic spectroscopy

Radu Silaghi-Dumitrescu

**SOE Workshop “From Molecules to Functionalised Materials” – Cluj-Napoca, October 2009**

14. The redox reactivity of globins: the chicken and egg paradox

Radu Silaghi-Dumitrescu

**Metal Elements in Environment, Medicine and Biology, 8th edn., Timisoara, Romania, 2008**

13. Unusual metal oxidation states in metalloproteins and related complexes: from degenerate orbitals to apoptosis

Radu Silaghi-Dumitrescu

**Metal Elements in Environment, Medicine and Biology, 9th edn., Cluj-Napoca, Romania, 2009**

12. Sang et orbitales

Radu Silaghi-Dumitrescu

**Le Cinquième Colloque Franco – Roumain De Chimie Appliquée (COFrRoCA), Bacau, Romania, 2008**

11. The Sarajevo train: stress and unusual valence

Radu Silaghi-Dumitrescu

**Exploratory workshop in Chemistry with the Scientific Romanian Diaspora, Bucharest, Romania, 2008**

10. The reactivity of myoglobin towards sulfoxylate  
Radu Silaghi-Dumitrescu, Sergei Makarov  
**The Fifth International Conference on Porphyrins and Phthalocyanines (ICPP5), Moscow, 2008**
  
9. Drawing blood over computational arguments: the ferryl case  
Radu Silaghi-Dumitrescu  
**From Molecular Informatics to Bioinformatics – an International Symposium, Budapest, Hungary, 2008**
  
8. Nitrite linkage isomerism in hemoproteins and related complexes: experimental and theoretical evidence  
Radu Silaghi-Dumitrescu, Sergei Makarov  
**37th Inorganic Reaction Mechanisms Group Meeting, 37IRMGM, Barcelona, Spain, 2008**
  
7. Nitrite linkage isomerism in hemoproteins and related complexes: experimental and theoretical evidence  
Radu Silaghi-Dumitrescu  
**Molecular and supramolecular chemistry of multimetallic systems, Bucharest, Romania, 2007**
  
6. Artificial blood: how and why do we make it?  
Radu Silaghi-Dumitrescu  
**Workshop in Material Science and Engineering, Cluj-Napoca, Romania, 2007**
  
5. Nitrite linkage isomerism in hemoproteins and related complexes – a case for mechanistic promiscuity  
Radu Silaghi-Dumitrescu  
**From Molecular Informatics to Bioinformatics – an International Symposium, Budapest, Hungary, 2007**
  
4. Nitrite linkage isomerism in hemoproteins and related complexes: experimental and theoretical evidence  
Radu Silaghi-Dumitrescu  
**Molecular Modelling in Chemistry and Biochemistry – MolMod, Aralia, Romania, 2007**
  
3. Ferryl heme protonation gates reactivity in hemoproteins  
Radu Silaghi-Dumitrescu, Brandon J. Reeder, Peter Nicholls, Chris E. Cooper, Michael T. Wilson  
**The 29<sup>th</sup> National Chemistry Conference, Calimanesti-Caciulata, Romania, October 2006**
  
2. Transient species involved in catalytic dioxygen/peroxide activation by

hemoproteins: possible involvement of protonated Compound I species

Radu Silaghi-Dumitrescu, Chris E. Cooper

**Dalton Discussions 8, Metals: Centers of Biological Activity, Nottingham, UK, 2005**

1. Ferryl heme protonation gates reactivity in hemoproteins

Radu Silaghi-Dumitrescu, Brandon J. Reeder, Peter Nicholls, Chris E. Cooper, Michael T. Wilson

**Young Researchers Forum, 8th European Biological Chemistry Conference, EUROBIC 8, Aveiro, Portugal, 2006**

### **Posters:**

44. Computational modeling metal-protein interactions: cisplatin

Alexandru Lupan, Attila Kun, Radu Silaghi-Dumitrescu

Metal Elements in Environment, Medicine and Biology 2010, Timisoara, Romania

43. Effects of antioxidants in cisplatin toxicology

Cristina Bischin, Vicentiu Taciuc, Radu Silaghi-Dumitrescu,

Metal Elements in Environment, Medicine and Biology 2010, Timisoara, Romania

42. Ab initio modelling of secondary structure elements in proteins. Interaction with cisplatin and related compounds

Alexandru Lupan, Attila Kun, Radu Silaghi-Dumitrescu

**The 32<sup>nd</sup> National Chemistry Conference, Ramnicu-Valcea, Romania, October 2010**

41. Cisplatin modulates dioxygen binding and peroxide reactivity in globins and cytochrome c

Cristina Bischin, Vicentiu Taciuc, Violeta-Florina Deac, Grigore Damian, Turc Silvia, Magdas Cristian, Eva Fischer-Fodor, Radu Silaghi-Dumitrescu

**The 32<sup>nd</sup> National Chemistry Conference, Ramnicu-Valcea, Romania, October 2010**

40. A new protocol for derivatization of hemoglobin with polyethylene glycol: evaluation for potential blood substitutes

Deac Florina, Oana Zolog, Eva Fischer-Fodor, Augustin Mot, Alina Roman, Radu Silaghi-Dumitrescu

**The 32<sup>nd</sup> National Chemistry Conference, Ramnicu-Valcea, Romania, October 2010**

39. Isolation and characterisation of *Sclerotinia sclerotiorum* laccase: a "yellow" laccase with "blue" spectroscopic features

Augustin Cătălin Moț, Radu Silaghi-Dumitrescu, Marcel Pârvu, Florin Dan Irimie

**3rd EuCheMS Chemistry Congress, Nurnberg, Germany, 2010**

38. Derivatization of hemoglobin with periodate-generated reticulation agent: evaluation of oxidative reactivity for potential blood substitutes  
Florina Deac, Bianca Iacob, Eva Fischer-Fodor, Grigore Damian, Vasile Miclăuș, Radu Silaghi-Dumitrescu

**3rd EuCheMS Chemistry Congress, Nurnberg, Germany, 2010**

37. Isolation and characterisation of *Sclerotinia sclerotiorum* laccase: a “yellow” laccase with “blue” spectroscopic features and iron content

Augustin Cătălin Moț, Radu Silaghi-Dumitrescu, Marcel Pârvu, Florin Dan Irimie

**The 32<sup>nd</sup> National Chemistry Conference, Ramnicu-Valcea, Romania, October 2010**

36. Derivatization of hemoglobin with periodate-generated reticulation agent: evaluation of oxidative reactivity for potential blood substitutes

Florina Deac, Bianca Iacob, Eva Fischer-Fodor, Grigore Damian, Vasile Miclăuș, Radu Silaghi-Dumitrescu

**The 32<sup>nd</sup> National Chemistry Conference, Ramnicu-Valcea, Romania, October 2010**

35. Derivatization of hemoglobin with periodate-generated reticulation agent: evaluation of oxidative reactivity for potential blood substitutes

Florina Deac, Bianca Iacob, Eva Fischer-Fodor, Grigore Damian, Vasile Miclăuș, Radu Silaghi-Dumitrescu

**7th International Conference of the Chemical Societies of the South-Eastern European Countries – Bucharest, September 2010**

35. Derivatization of hemoglobin with periodate-generated reticulation agent: evaluation of oxidative reactivity for potential blood substitutes

Florina Deac, Bianca Iacob, Eva Fischer-Fodor, Grigore Damian, Vasile Miclăuș, Radu Silaghi-Dumitrescu

**7th International Conference of the Chemical Societies of the South-Eastern European Countries – Bucharest, September 2010**

34. Ascorbate peroxidase activity with cytochrome *c*

Cristina Bischin, Violeta-Florina Deac, Radu Silaghi-Dumitrescu

**7th International Conference of the Chemical Societies of the South-Eastern European Countries – Bucharest, September 2010**

33. Ascorbate peroxidase activity with cytochrome *c*

Cristina Bischin, Violeta-Florina Deac, Radu Silaghi-Dumitrescu

**7th International Conference of the Chemical Societies of the South-Eastern European Countries – Bucharest, September 2010**

32. Strategies for combatting autooxidation in blood, relevant for blood substitute

preparation and chemotherapy

Bianca Iacob, Florina Deac, Augustin Mot, Vicentiu Taciuc, Denisa Hathazi,  
Radu Silaghi-Dumitrescu

**7th International Conference of the Chemical Societies of the South-Eastern European Countries – Bucharest, September 2010**

31. Ab initio modelling of secondary structure elements in proteins

Alexandru Lupan, Radu Silaghi-Dumitrescu

**7th International Conference of the Chemical Societies of the South-Eastern European Countries – Bucharest, September 2010**

30. Towards 'super-reduced' iron in biological systems – experimental and theoretical evidence

Radu Silaghi-Dumitrescu, Sergei Makarov, Augustin Mot, Zoltan Kis, Denis Salnikov, Anna Pogorelova, Grigore Damian, Dmitri Svistunenkob

**10th European Biological Chemistry Conference EUROBIC 2010, Thessaloniki, 2010**

29. Hemoglobin is an ascorbate-binding protein with high affinity for ascorbate: implications for blood substitutes

Anamaria Todea, Florina Deac, Paula Podea, Radu Silaghi-Dumitrescu

**Students for students conference 2009, Cluj-Napoca, 2009**

28. Investigations on the electronic structure and reactivity of thiourea dioxide and its decomposition product, sulfoxylate

Zoltan Kis, Radu Silaghi-Dumitrescu, Sergei V. Makarov

**Molecular modeling in chemistry and biochemistry MOLMOD 2009, Cluj-Napoca, May 2009**

27. 'Super-reduced' iron under physiologically-relevant conditions

Anamaria Todea, Deac Florina, Paula Podea, Radu Silaghi-Dumitrescu

**11<sup>th</sup> Central and Eastern European NMR Symposium, Cluj-Napoca, Romania, October 2009**

26. Hemoglobin is an ascorbate peroxidase with a remarkably high affinity for ascorbate

Anamaria Todea, Deac Florina, Paula Podea, Radu Silaghi-Dumitrescu

**11<sup>th</sup> Central and Eastern European NMR Symposium, Cluj-Napoca, Romania, October 2009**

25. Hemoglobin is an ascorbate peroxidase with a remarkably high affinity for ascorbate

Florina Deac, Radu Silaghi-Dumitrescu

**The 30<sup>th</sup> National Chemistry Conference, Calimanesti-Caciulata, Romania, October 2006**

24. Computational investigations on the electronic structure and reactivity of thiourea dioxide and its decomposition product, sulfoxylate  
Zoltan Kis, Sergei V. Makarov, Radu Silaghi-Dumitrescu  
**The 30<sup>th</sup> National Chemistry Conference, Calimanesti-Caciulata, Romania, October 2008**

23. Carbon dioxide hydration by carbonic anhydrase – a computational investigation  
Andras Kallay, Radu Silaghi-Dumitrescu  
**International Conference on Biochemistry and Molecular Biology, Timisoara, Romania, 2007**

22. Halide activation by heme peroxidases: theoretical predictions on putative adducts of halides with Compound I  
Radu Silaghi-Dumitrescu  
**13th International Conference on Biological Inorganic Chemistry, Vienna, Austria, 2007**

21. Nitrite linkage isomerism in hemoproteins and related complexes: experimental and theoretical evidence  
Matei-Maria Uta, Radu Silaghi-Dumitrescu  
**13th International Conference on Biological Inorganic Chemistry, Vienna, Austria, 2007**

21. Nitrite linkage isomerism in hemoproteins and related complexes: experimental and theoretical evidence  
Matei-Maria Uta, Radu Silaghi-Dumitrescu  
**Humboldt Conference on non-covalent interactions, Vrsac, Serbia, 2007**

20. Nitrite linkage isomerism in hemoproteins and related complexes: experimental and theoretical evidence  
Matei-Maria Uta, Radu Silaghi-Dumitrescu  
**Molecular Modelling in Chemistry and Biochemistry – MolMod, Arcalia, Romania, 2007**

19. Computational investigation of architectures based on hydrogen bonds  
Radu Silaghi-Dumitrescu  
**Humboldt Conference on non-covalent interactions, Vrsac, Serbia, 2007**

18. Computational investigation of architectures based on hydrogen bonds  
Radu Silaghi-Dumitrescu  
**Supramolecular Chemistry from design to applications - SUPCHEM, Cluj-Napoca, Romania, 2007**

17. Carbon dioxide hydration by carbonic anhydrase – a computational investigation

Radu Silaghi-Dumitrescu, Andras Kallay

**Techniques of Chemical and Biochemical Remediation - BIOREMEDIATION, Cluj-Napoca, Romania, 2007**

16. Ferryl heme protonation gates reactivity in hemoproteins

Radu Silaghi-Dumitrescu, Brandon J. Reeder, Peter Nicholls, Chris E. Cooper, Michael T. Wilson

**8th European Biological Chemistry Conference, EUROBIC 8, Aveiro, Portugal, 2006**

15. Ferryl heme protonation gates reactivity in hemoproteins

Radu Silaghi-Dumitrescu, Brandon J. Reeder, Peter Nicholls, Chris E. Cooper, Michael T. Wilson

**PEROXIDASE 2006, Aveiro, Portugal, 2006**

14. Copper-containing nitrite reductase: a dft study of nitrite and nitric oxide adducts

Radu Silaghi-Dumitrescu

**Inorganic Biochemistry Discussion Group and ESR Group of the Royal Society of Chemistry, London, UK, 2006**

13. Nitrite and nitric oxide adducts of copper-containing nitrite reductases. Theoretical insight into the catalytic cycle

Radu Silaghi-Dumitrescu

**Nitric oxide - a radical in control; Harden(Biochemical Society)/EMBO workshop, 2006 Cirencester, UK, 2006**

12. Tuning biological diiron site reactivity: lessons learned from a novel class of nitric oxide reductases

Radu Silaghi-Dumitrescu, William N. Lanzilotta, Ricardo Garcia, Boi Hanh Huynh, Donald M. Kurtz, Jr.

**Inorganic Biochemistry Discussion Group of the Royal Society of Chemistry, UK, 2005**

11. Novel Non-Heme Diiron Peroxidases from Air-Sensitive Bacteria

Kurtz, Donald; Iyer, Ramesh Chemistry, Silaghi-Dumitrescu, Radu, Lanzilotta, William

**12th International Conference on Biological Inorganic Chemistry, Ann Arbor, USA, 2005**

10. Spectroscopic Characterization and Comparison of the Binuclear Non-Heme Ferrous sites in m- Ferritin and S-Nitric Oxide Reductase

Schwartz, Jennifer Liu, Xiaofeng, Theil, Elizabeth C., Silaghi-Dumitrescu, Radu, Kurtz, Donald M., Solomon, Edward I.



**12th International Conference on Biological Inorganic Chemistry, Ann Arbor, USA, 2005**

9. Tuning biological diiron site reactivity: a novel class of nitric oxide reductases  
Radu Silaghi-Dumitrescu, William N. Lanzilotta, Ricardo Garcia, Boi Hanh Huynh, Donald M. Kurtz, Jr.

**Procter & Gamble Poster Competition, University of Georgia, USA 2004**

8. A Non-Heme Iron Nitric Oxide Reductase that Protects Against Nitrosative Stress in Acetogenic Bacteria

Radu Silaghi-Dumitrescu, Amaresh Das, Lars G. Ljungdahl, Guy N. L. Jameson, Ricardo Garcia, Boi Hanh Huynh, William N. Lanzilotta, and Donald M. Kurtz, Jr.

**Gordon Graduate Research Seminar: Bioinorganic Chemistry, Ventura, CA, USA 2003**

7. Nitric oxide reductase activity of a bacterial flavo-diiron protein (FprA)

Radu Silaghi-Dumitrescu, Eric D. Coulter, Amaresh Das, Lars G. Ljungdahl, Donald M. Kurtz, Jr.

**Procter & Gamble Poster Competition, University of Georgia, USA 2003**

6. Nitric oxide reduction by P450nor: computational investigation of a bioinorganic mechanism

Radu Silaghi-Dumitrescu

**2003 Procter & Gamble Poster Competition, University of Georgia, USA 2003**

5. A Non-Heme Iron Nitric Oxide Reductase that Protects Against Nitrosative Stress in Acetogenic Bacteria

Radu Silaghi-Dumitrescu, Eric D. Coulter, Amaresh Das, Lars G. Ljungdahl, Donald M. Kurtz, Jr.

**11th International Conference on Biological Inorganic Chemistry, Cairns, Australia, 2003**

4. A computational study of the non-heme iron site in superoxide reductase and its reaction with superoxide

Radu Silaghi-Dumitrescu, Ioan Silaghi-Dumitrescu, Eric D. Coulter, Joseph P. Emerson, Donald M. Kurtz, Jr.

**2002 Procter & Gamble Poster Competition, University of Georgia, USA 2002**

3. Why thiolate as a ligand in SORs? In silico site-directed mutagenesis studies

Radu Silaghi-Dumitrescu, Donald M. Kurtz, Jr

**2002 Procter & Gamble Poster Competition, University of Georgia, USA 2002**

2. Superoxide reactivity of rubredoxin oxidoreductase (desulfoferrodoxin) from *D. vulgaris*: a computational study.

Radu Silaghi-Dumitrescu, Ioan Silaghi-Dumitrescu, Eric D. Coulter, Joseph P. Emerson, Donald M. Kurtz, Jr

**10th International Conference on Biological Inorganic Chemistry, Florence, Italy, 2001**

1. Novel Non-Heme Iron Proteins Involved in Aerotolerance in the Anaerobe *Moorella (Clostridium) thermoacetica*

Eric D. Coulter, Amaresh Das, Radu Silaghi-Dumitrescu, Donald M. Kurtz, Jr., and Lars G. Ljungdahl

**10th International Conference on Biological Inorganic Chemistry, Florence, Italy 2001**