

**Radu Silaghi-Dumitrescu, list of publications (numbering maintained from the original publication list, thus showing the chronological order of publications):**

a) 10 papers cf. OM 5691:

**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 .

**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.

**72. Silaghi-Dumitrescu, Radu. Superoxide interaction with nickel and iron superoxide dismutases,** *Journal of Molecular Graphics and Modelling* 2009, 28(2), 156-61.

**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.

**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.

**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.

**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.

## b) PhD theses

Non-heme iron proteins involved in oxidative and nitrosative stress defense – University of Georgia, Athens, GA, 2004 – prof. Donald M. Kurtz, Jr.

Activarea unor molecule mici de către hemoproteine și sisteme înrudite – Universitatea “Babeș-Bolyai”, Cluj-Napoca 2005 – prof. Ionel Haiduc

## c) Patents

-

## d) 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

## e) In the “main scientific flux” (defined here by the author in a subjective manner)

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

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

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)
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
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
106. **Silaghi-Dumitrescu, Radu**; Makarov, Sergei V.; Uta, Matei-Maria Dereven'kov, Iliia 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.
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.

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.

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.

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.

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.

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.

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.

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.

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.

60. Reeder, Brandon J.; Grey, Marie; **Silaghi-Dumitrescu, Radu**; Svistunenko, 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.

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.

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.

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.

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.

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.

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.

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

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.

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.

f) In conferences

-

g) others

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.

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.

119. **Silaghi-Dumitrescu, Radu. DFT vibrational analysis of metal-hydroperoxo bleomycin complexes.** Studia Universitatis Babes-Bolyai, Chemia 2012, in press

116. Lupan, Alexandru; Matyas, Csongor; Moț, 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.

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.

107. Prejmerean, Cristina; Moldovan, Marioara; Silaghi-Dumitrescu, Laura; Prodan, Doina; Furtos, Gabriel; Trif, Marcela; Popescu, Violeta; Pascalau, Violeta; Petrea, Celina-Maria; **Silaghi-Dumitrescu, Radu. Composition Versus Physico-mechanical**

**Properties of Some Dental Experimental Polymers.** Materiale Plastice, 2011, 48(1), 27-32.

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.

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.

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.

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.

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.

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.

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

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.

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.

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

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.

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.

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.

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 Babeş-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*.
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**; Paizs, 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.