

ARTIGOS 2003

- 1) GAMBARDELLA, M.T. do P., GUILARDI, S., BARBOSA, L.C. de A., DEMUNER, A.J., VELOSO, D.P., RESENDE, J.A.L.C. 21 alfa-fluoro-7-nor-12, 13, 15 16-tetrahydrovouacapan-17beta, 21alfa-lactone. **Acta Crystallogr E.**, v 59, p.1935-1937, 2003.
- 2) VIEIRA FILHO, S. A., DUARTE, L. P., SILVA, G. D. F., HOWARTH, O., LULA, I. S. 3beta-(Stearyloxy)olean-12-ene from *Austroplenckia populnea*: Structure Elucidation by 2D-NMR and Quantitative ¹³C-NMR Spectroscopy. **Helvetica Chimica Acta**, v.86, p.3445-3449, 2003.
- 3) MENEZES, I. R. A., LOPES, J. C. D., MONTANARI, C. A. 3D QSAR studies on binds affinities of coumann natural products for glycosomal gapdh of *T. Cruzi*. **Journal of Computer Aided Molecular Design**, v.17, p.277-290, 2003.
- 4) DORIGUETTO, A. C., DUARTE, L. P., JAVIER, E. A., SILVA, G. D. F., MASCARENHAS, Y. P., COTA, A. B. 3-Oxoolean-12-en-20yl alpha-methylcarboxylate. **Acta Crystallographica Section E Structure Reports Online.**, v.E59, p.164-166, 2003.
- 5) DUARTE, H. A., DUANI, H., ALMEIDA, W. B. Ab initio correlated comparative study of the torsional potentials for 2,2'-bipyrrole and 2,2'-bifuran five membered heterocyclic dimers. **Chemical Physics Letters**, v.369, p.114-124, 2003.
- 6) NASCIMENTO, F. C., BOAVENTURA, M. A. D., ASSUNCAO, A. C. S., PIMENTA, L. P. S. Acetogeninas de Anonáceas isoladas de folhas de *ROLLINIA LAURIFOLIA*. **Química Nova**, v.26, n.3, p.319-322, 2003.
- 7) TEMBA, E. S. C., OLIVEIRA, I. M. F., DONNICI, C. L. Álcoois quirais: métodos químicos e catalíticos de obtenção por redução assimétrica. **Química Nova**, v.26, n.1, p.112-122, 2003
- 8) PARREIRA, F. V., CARVALHO, C. R., CARDEAL, Z. L. Analysis of Airborne Volatile Organic Compounds of a Steel Industry by Solid Phase Microextraction and Gas Chromatography/Mass Spectrometry. **Bulletin of Environmental Contamination and Toxicology**, v.70, p.957-963, 2003.
- 9) MATENCIO, T., PERNAUT, J. M., VIEIL, E. Analysis of hysteresis phenomenon as observed from voltammetric data of conducting polymers. Part I. **Journal Brazilian Chemical Society.**, v.14, n.1, p.90-96, 2003.
- 10) LUNA, H. G. S., CANUTO, M. H., SILVA, J. B. B., LIMA, G. M. Antimony and chromium determination in Brazilian sugar cane spirit, cachaça, by electrothermal atomic absorption spectrometry using matrix matching calibration and ruthenium as permanent modifier, **J. Anal. Atom. Spectrom.**, v.18, n.11, p.1404-1406, 2003.

- 11) TOLEDO, L. C., SILVA, A. C. B., AUGUSTI, R., LAGO, R. M. Application of Fenton's reagent to regenerate activated carbon saturated with organochloro compounds. **Chemosphere**, v.50, n.8, p.1049-1054, 2003.
- 12) LAGO, R. M., SILVA, A. C. B., TEIXEIRA, A. C. M., AUGUSTI, R. Application of membrane introduction mass spectrometry to the study of adsorption of organic compounds on activated carbon and solid phase extraction experiments. **Analyst**, v.128, p.884-888, 2003
- 13) CASTELLANOS, A. E. B., MILLAN, R. D. S., AUGUSTI, R., LAGO, R. M. Application of the MIMS technique to study the stability constants of small organic guest molecules into cyclodextrin hosts in aqueous medium. **Journal of Inclusion Phenomena and Macrocyclic Chemistry**, v.45, p.149-154, 2003.
- 14) SEBASTIÃO, R.C.O, BRAGA, J.P, YOSHIDA, M.I. Artificial neural network applied to solid state thermal decomposition. **Journal of Thermal Analysis and Calorimetry**, v.74, p. 811-818, 2003.
- 15) LOMBARDI, J.A., VALADARES, Y.M., BRAGA, F.C., OLIVEIRA, A.B. de, Atividade vasodilatadora in vitro de espécies de Ouratea(Ochnaceae) e de frações de Ouratea (Mart.) Engl.. **Rev. Bras. Ciênc. Farm.**, v. 39, p. 83-91, 2003.
- 16) PIMENTA, L. P. S., PINTO, G. V., TAKAHASHI, J. A., SILVA, L. G. F., BOAVENTURA, M. A. D. Biological screening of Annonaceous Brazilian Medicinal Plants using Artemia salina (Brine Shrimp Test). **Phytomedicine**, v.10, p.209-212, 2003.
- 17) DUARTE, H. A. Carga nuclear efetiva e sua consequência para a compreensão da estrutura eletrônica dos átomos. **Química Nova Na Escola**, v.17, p.22-26, 2003.
- 18) LAGO, R. M., NAGEM, N. F., DALMAZIO, I., AUGUSTI, R. Catalytic hydrodehalogenation of aromatic halides monitored by membrane introduction mass spectrometry. **Rapid communications in mass Spectrometry**, v.17, p.1507-1510, 2003.
- 19) LANA, S. L. B., MAGALHÃES, W. F., MOHALLEM, N. D. S. Characterisation of ormosil composites obtained by the sol-gel process using positron annihilation lifetime spectroscopy. **Physics and Chemistry of Glasses**, v.44, n.1, p.36-38, 2003.
- 20) ROBLES-DUTENHEFNER, P.A., NUNES, D.L., MOHALLEM, N.D.S., GOUSEVSKAIA, E.V., DE SOUSA, E.M.B. Characterization and catalytic studies of sol-gel Co-SiO₂ nanocomposites. **Materials Characterization**, v50, p. 95-99, 2003.

- 21) DORIGUETTO, A. C., FERNANDES, N. G., PERSIANO, A. I. C., FILHO NUNES, E., 'GRENÉCHE', J. M., FABRIS, J. D. Characterization of a Natural Magnetite. **Physics and Chemistry of Minerals**, v.30, n.5, p.249-255, 2003.
- 22) HARAS, A., WITKO, M., SALAHUB, D. R., DUARTE, H. A. Chemical nature of point defects at the (VO)2P2O7(100) surface. **Surface Science**, v.538, p.160-170, . 2003.
- 23) DONNICI, C. L., GUIMARAES, S., MELO, A. C. Chemical Oxidation Studies of beta-hydroxysulfides with tris(4-bromophenyl)aminium hexachloroantimonate: Diastereoselective sulfoxide obtaining and pinacol-type rearrangement. **Synthetic Communications**, v.33, n.9, p.1489-1497, 2003.
- 24) OLIVEIRA, L. C. A., RIOS, R. V. R. A., FABRIS, J. D, SAPAG, K., VIJAYENDRA, LAGO, R. M. Clay-iron oxide magnetic composites for the adsorption of contaminants in water. **Applied Clay Science**, v.22, n.4, p.169-177, 2003.
- 25) PEREIRA, C. L. M., PEDROSO, E. F., NOVAK, M. A., BRANDL, A. L., KNOBEL, M., STUMPF, H. O. Cluster glass-like behavior in a 2D bimetallic molecule-based magnet. **Polyhedron**, v.22, n.14-17, p.2387-2390, 2003.
- 26) SILVA, M. J., DUTENHEFNER, P. A. R., MENINI, L., GOUSSEVSKAIA, E. V. Cobalt catalyzed autoxidation of monoterpenes in acetic acid and acetonitrile solutions. **Journal of Molecular Catalysis A: Chemical**, v.201, p.71-77, 2003.
- 27) MELO, B.N., PASA, V.M.D. Composites base on eucalyptus tar pitch/castor oil polyurethane and short sisal fibers. **Journal of Applied Polymer Science**, v 14, p. 3797-3802, 2003.
- 28) FARIA, L. E., DONNICI, C. L., LOPES, J. C. D. Conformational analysis and electronic interactions of 2-thiosubstituted cyclohexanones by semiempirical method PM3. **International Journal of Quantum Chemistry**, v.95, n.3, p.313-321, 2003.
- 29) JERRY, P. J., HEIDI, E. E., CASTINEIRAS, A., BERMEJO, E., BERALDO, H. O., WEST, D. X. Copper(II) complexes 1-phenylpropane-1,2-dione- and benzil bis(3-piperidylthiosemicarbazone): A structural study. **Journal of Chemical Crystallography**, v.33, n.1, p.11-18, 2003.
- 30) SOUSA, E. M. B., SOUSA, A. P. G., MOHALLEM, N. D. S., LAGO, R. M. Copper-Silica Sol-Gel catalysts: structural changes of Cu species upon thermal treatment.. **Journal of Sol-Gel Science and Technology**, v.26, p.873-877, 2003.
- 31) CRUZ, A. T., SILVA, G. G., SOUZA, P. P., MATENCIO, T., PERNAUT, J. M., DE PAOLI, M. A. Cross-linking effect on thermal, conducting and electrochemical

- properties of an elastomeric polymer electrolyte. **Solid State Ionics**, v.159, p.301-311, 2003.
- 32) OLIVEIRA, J. A., ALMEIDA, W. B., DUARTE, H. A. Density functional study of the MoxO_y and $\text{MoxO}+\text{y}$ ($x = 1-3$; $y = 1-9$) oxide clusters. **Chemical Physics Letters**, v.372, p.650-658, 2003.
- 33) SILVA, J. B. B., BORGES, D. L. G., VEIGA, M. A. M. S., CURTIUS, A. J., WELZ, B. Determination of cadmium in biological samples solubilized with tetramethylammonium hydroxide by electrothermal atomic absorption spectrometry, using ruthenium as permanent modifier. **Talanta**, v.60, p.977-982, 2003.
- 34) MACIEL, C. J. C., SILVA, J. B. B., MIRANDA, G. M., OLIVEIRA, D. P., SIQUEIRA, M. E. P., LEITE, E. M. A., SILVEIRA, J. N. Determination of cadmium in human urine by electrothermal atomic absorption spectrometry. **Analytica Chimica Acta**, v.491, p.231-237, 2003.
- 35) LORDEIRO, R. A., GUIMARAES, F. F., BELCHIOR, J. C., JOHSTON, R. L. Determination of main structural compositions of nanoalloy clusters of Cu_nAu_y ($x \text{ e } y < \sim 30$) using a genetic algorithm approach. **International Journal of Quantum Chemistry**, v.95, n.3, p.112-125, 2003.
- 36) MAGALHAES, C. G., NUNES, B. R., GIACOMELLI, M. B. O., SILVA, J. B. B. Direct determination of bismuth in urine samples by electrothermal atomic absorption spectrometry: study of chemical modifiers. **Journal of Analytical Atomic Spectrometry**, v.18, n.7, p.787-789, 2003.
- 37) MELO, M. N., FREZARD, F. J. G., DEMICHELI, C. P., BICALHO, A. P. C. V., MICHALICK, M. S. M. Distribution of liposome-encapsulated antimony in dogs. **Brazilian Journal of Medical and Biological Research**, v.36, n.2, p.269-272, 2003.
- 38) SPASOJEVIC, I., BATINIÉ-HABERLE, I., REBOUCAS, J. S., IDEMORI, Y. M., FRIDOVICH, I. Electrostatic Contribution in the Catalysis of O_2 Dismutation by Superoxide Dismutase Mimics. **The Journal of Biological Chemistry**, v.278, p.6831-6837, 2003.
- 39) GOUSSEVSKAIA, E. V., SILVA, M. J. Elucidation of the Stereochemistry of Diterpene Derivatives Obtained by Palladium Catalyzed Oxidative Coupling-Oxidation of Camphene. **Brazilian Chemical Society. Journal**, v.14, p.83-89, 2003.
- 40) SOBRINHO, S. I., SEGURA, M. E. C., MOHALLEM, N. D. S. Emprego de forças magnéticas em ortodontia e ortopedia facial. Uma revisão. **Revista Dental Press de Ortodontia e Ortopedia Facial**, v.8, n.4, p.63-72, 2003.

- 41) MELO, A. L., SILVA-BARCELLOS, N. M. S., DEMICHELI, C. P., FREZARD, F. J. G. Enhanced schistosomicidal efficacy of tartar emetic encapsulated in pegylated liposomes. **International Journal of Pharmaceutics**, v.255, p.227-230, 2003.
- 42) BRAGA, F. C., VALADARES, Y. M., LOMBARDI, J. A., OLIVEIRA, A. B. Estudo fitoquímico de *Erythraea centaurium*, *Jacaranda caroba*, *Remijia ferruginea* e *Solanum paniculatum* visando identificar marcadores químicos para o fitoterápico lerobina. **Revista Brasileira de Farmacognosia**, v.13, n.2, p.28-31, 2003.
- 43) FREITAS, C. S., DINIZ, H. F. O., GOMES, J. B., MILLAN, R. D. S., SEGURA, M. E. C. Evaluation of the substantivity of chlorhexidine in association with sodium fluoride in vitro. **Pesquisa Odontológica Brasileira**, v.17, p.78-81, 2003.
- 44) OLIVEIRA, L. C. A., FABRIS, J. D., RIOS, R. V. R. A., MUSSEL, W. N., LAGO, R. M. Fe₃-xMnxO₄ catalysts: Phase transformations and carbon/ monoxide oxidation. **Applied Catalysis A: General**, v.1, p.2104-2114, 2003.
- 45) SANTOS, C. M. P., FARIA, R. B., DE ALMEIDA, W. B., MACHUCA-HERRERA, J. O., MACHADO, S. P. Geometrical and vibrational DFT studies of HOBr center dot(H₂O)(n) clusters (n = 1-4). **Canadian Journal of Chemistry-Revue Canadienne de Chimie**, v.81, n.9, p.961-970, 2003.
- 46) SALES, J. A., CARDEAL, Z. L. Headspace solid-phase micro-extraction gas chromatography method for the determination of methanol in aspartame sweeteners. **Food Additives and Contaminants**, v.20, n.6, p.519-523, 2003.
- 47) SILVA, K. A., GOUSSEVSKAIA, E. V., KOZHEVNIKOV, I. V. Hydration and acetoxylation of camphene catalyzed by heteropoly acid. **Journal of Molecular Catalysis A: Chemical**, v.192, p.129-134, 2003.
- 48) FOCA, C. M., BARROS, H. J. V., SANTOS, E. N., GOUSSEVSKAIA, E. V., BAYÓN, J. C. Hydroformylation of myrcene: metal and ligand effects in the hydroformylation of conjugated dienes. **New Journal of Chemistry**, v.27, p.533-539, 2003.
- 49) RIBEIRO, F. R., MUSSEL, W. N., FABRIS, J. D., NOVAIS, R., GARG, V. K. Identification of Iron-Bearing Minerals in Solid Residues from Industrial Kaolin Processing. **Hyperfine Interactions**, v.148-149, p.47-52, 2003.
- 50) MAIA, E. C. P., GARNIER-SUILLEROT, A. Impaired hydrolysis of cisplatin derivatives to aquated species prevents energy-dependent uptake in GLC4 cells resistant to cisplatin. **Journal of Biological Inorganic Chemistry**, v.8, n.6, p.626-634, 2003.
- 51) FRANCO, C. F., PATARO, A. L., RIBEIRO E SOUZA, L. C., SANTOS, V. R., SEGURA, M. E. C., MILLAN, R. D. S. In Vitro Effects of a Chlorhexidine Controlled Delivery System. **Artificial Organs**, v.27, n.5, p.474-479, 2003.

- 52) OLIVEIRA, R. B., PASSOS, A.P.F., ALVES, R.O., ROMANHA, A.J., PRADO, M. A. F, R. J., SOUZA FILHO, J. D., In vitro evaluation of activity of aromatic nitocompounds against *Tripanosoma cruzi*. **Memórias do Instituto Oswaldo Cruz**, v.98, n.1, p.141-144, 2003.
- 53) TEIXEIRA, L. R., SINISTERRA, R.D., VIEIRA, R.P., DORETTO, M.C., BERALDO, H. Inclusion of benzaldehyde semicarbazone into beta-cyclodextrin produces a very effective anticonvulsant formulation, **Journal of Inclusion Phenomena and Macrocyclic Chemistry**, v.47, p.77-82, 2003.
- 54) PIZARRO, C., ESCUDEY, M., FABRIS, J. D. Influence of Organic Matter on the Iron Oxide Mineralogy of Volcanic Soils. **Hyperfine Interactions**, v.148-149, p.53-59, 2003.
- 55) XAVIER, E. S., DUARTE, H. A. Interaction of M-Sn (M=Ru, Rh, Pd) Dimers with CH₂ and CF₂: A density functional study. **International Journal of Quantum Chemistry**, v.95, p.164-176, 2003.
- 56) VITERBO, V. C., NEVES, J. L., BRAGA, J. P., MONTEIRO, R. P. G., MAGALHÃES, W. F. Inversion of simulated positron annihilation lifetime spectra by moving boundary subspaces. **International Journal of Quantum Chemistry**, v.95, n.3, p.97-102, 2003.
- 57) DUANI, H., DUARTE, H. A., ALMEIDA, W. B. Investigation of the quality of standard sulfur basis sets for molecules using a new generator coordinate method approach: application to 2,2'-bithiophene. **International Journal of Quantum Chemistry**, v.95, p.194-204, 2003
- 58) AUGUSTI, R., ZHENG, X., TUROWSKI, M., COOKS, R. G. Kinetic isotope and collision energy effects in the dissociation of chloride and bromide adducts of aliphatic alcohols, benzaldehyde, and 2,4-pentanedione. **Australian Journal of Chemistry**, v.56, n.5, p.415-421, 2003.
- 59) MOHALLEM, N. D. S., SEARA, L. M. Magnetic nanocomposite thin films of NiFe₂O₄/SiO₂ prepared by sol-gel process. **Applied Surface Science**, v.214, n.1-4, p.143-150, 2003.
- 60) NOVAK, M. A., VAZ, M. G. F., SPEZIALI, N. L., COSTA, W. V., STUMPF, H. O. Magnetic Properties of an Interlocked Molecular Magnet. **Polyhedron**, v.22, n.14-17, p.2391-2394, 2003.
- 61) ARAÚJO, R.C. e S., PASA, V.M.D, Mechanical and thermal properties of polyurethane elastomers based on hydroxyl-terminated polybutadienes and biopitch, **Journal of Applied Polymer Science**, v.88, 759-766, 2003.

- 62) ESPINOSA, L. A., LAGO, R. M., PENA, M. A., FIERRO, J. L. G. Mechanistic aspects of hydrogen production by partial oxidation of methanol over Cu/ZnO catalysts. **Topics in Catalysis**, v.22, n.3-4, p.245-251, 2003.
- 63) AUGUSTI, R., TUROWSKI, M., COOKS, R. G. Membrane introduction mass spectrometry for monitoring complexation equilibria of B-Cyclodextrin with substituted benzenes.. **Analyst**, v.128, p.61-64, 2003.
- 64) OLIVEIRA, M. R. L., DINIZ, R., BELLIS, V. M., FERNANDES, N. G. Nickel(II) complexes of dithiocarbimates from sulfonamides: syntheses and crystal structures. **Polyhedron**, v.22, n.14-17, p.1561-1566, 2003.
- 65) SEBASTIAO, R. C. O., LEMES, N. H. T., VIRTUOSO, L. S., BRAGA, J. P. Nonlinear global inversion of potential energy surfaces from the experimentally determined second virial coefficients. **Chemical Physics Letters**, v.378, n.3-4, p.406-409, 2003
- 66) ALVES, T. M. A., ROMANHA, A. J., RIBEIRO, A., SOUZA FILHO, J. D. Novel diterpenes from *Alomia myriadenia* (Asteraceae) with cytotoxic and trypanocidal activity. **Phytochemistry**, v.64, n.6, p.1125-1131, 2003.
- 67) GOUSSEVSKAIA, E. V. Organometallic catalysis: some contributions to organic synthesis. **Química Nova**, São Paulo, v.26, n.2, p.242-248, abr. 2003.
GOUSSEVSKAIA, E. V. Organometallic catalysis: some contributions to organic synthesis. **Química Nova**, São Paulo, v.26, n.2, p.242-248, 2003.
- 68) FERREIRA, B. A., FABRIS, J. D., SANTANA, D. P., CURI, N. Óxidos de ferro das frações areia e silte de um nitossolo desenvolvido de basalto. **Revista Brasileira de Ciência do Solo**, v.27, p.404-413, 2003.
- 69) DEMICHELI, C. P., BEJARANO, R. O., LULA, I. S., GOZZO, F. C., EBERLIN, M. N., FREZARD, F. J. G. Pentavalent organoantimonial derivatives: two simple and efficient synthetic methods for meglumine antimonate. **Applied Organometallic Chemistry**, n.17, p.226-231, 2003
- 70) SANTIAGO, M.O., DONNICI, C. L., MOREIRA, Í. S., CARLOS, R.M., QUEIROZ, S.L., BATISTA, A.A., Photochemical isomerization of trans- to cis-[RuCl₂(dppb) (4,4'-X₂-2,2'-bipy)] (X = -H, -NO₂, -Me, -COOH, -SMe, -O=SMe, -Cl, -OMe) complexes. **Polyhedron**, v.22, n.14-17, p.3205-3211, 2003
- 71) RIBEIRO E SILVA, M. E. S., MACHADO, J. C., MANO, V., SILVA, G. G. Positron Annihilation and Differential Scanning Calorimetry Studies of Polyacrylamide and Poly(dimethylacrylamide)/Poly(ethylene glycol) Blends. **Journal of Polymer Science. Part B: Polymer Physics**, v.41, p.1493-1500, 2003.
- 72) SANTOS, J. M. S., CARVALHO, S., PANIAGO, E. B., DUARTE, H. A. Potentiometric, spectrophotometric and density functional study of the interaction of

- N-hydroxyacetamide with oxovanadium(IV): the influence of ligand to the V(IV)/V(V) oxi-reduction reaction. **Journal of Inorganic Biochemistry**, v.95, p.14-24, 2003.
- 73) LELIS, M. F. F., FABRIS, J. D., MUSSEL, W. N., TAKEUCHI, A. Y. Preparation and Characterization of Nickel- and Cobalt-doped Magnetites. **Materials Research**, v.6, n.2, p.145-150, 2003
- 74) SILVA, A. C. B., SOUSA, A. P. G., ARDISSON, J. D., LUNA, H. G. S., MOURA, E. M., SANTOS, E. N., MOHALLEM, N. D. S., LAGO, R. M. Preparation of highly dispersed Ru-Sn Bimetallic Supported Catalysts from the single source precursors $\text{Cp}(\text{PPh}_3)_2\text{Ru-SnX}_3$ ($\text{X} = \text{Cl}$ or Br). **Materials Research**, v.6, n.2, p.137-144, 2003.
- 75) OLIVEIRA, M. R. L., RUBINGER, M. M. M., BELLIS, V. M. Preparation of novel palladium(II) complexes with dithiocarbimates from sulfonamides. **Transition Metal Chemistry**, v.28, p.455-459, 2003.
- 76) OLIVEIRA, A. B., BRAGA, F. C. Produtos naturais bioativos de plantas brasileiras e sua contribuição para o desenvolvimento da química medicinal. **Arquivos Brasileiros de Fitomedicina Científica**, v.1, n.1, p.49-58, 2003.
- 77) OLIVEIRA, A. M., CUSTODIO, F. B., DONNICI, C. L., MONTANARI, C. A. QSAR and molecular modelling studies on B-DNA recognition of minor groove binders. **European Journal of Medicinal Chemistry**, v.38, p.141-155, 2003.
- 78) LIMA, L. C. G., LIMA, M. B. G., MENEZES, M. R., MATOS, R. M. Reactions of bis(diphenylphosphine)acetylene with metal carbonyl complexes. **Journal of Coordination Chemistry**, v.56, n.4, p.321-327, 2003.
- 79) AUGUSTI, D. V., CARAZZA, F., OKUMA, A. A., AUGUSTI, R. Reactivity of some novel multifunctional benzoyl esters towards nucleophiles investigated by electrospray ionization tandem mass spectrometry. **Rapid communications in mass Spectrometry**, v.17, p.1084-1088, 2003
- 80) ROCHA, W. R., ALMEIDA, W. B. Regioselectivity in the interaction of rhodium hidridotricarbonyl with propene: a theoretical. **Journal of Molecular Structure: Theochem**, v.634, p.95-106, 2003.
- 81) COSTA, R. C. C., LELIS, M. F. F., OLIVEIRA, L. C. A., FABRIS, J. D., ARDISSON, J. D., RIOS, R. V. R. A., SILVA, C. N., LAGO, R. M. Remarkable effect of Co and Mn on the activity of $\text{Fe}_3\text{-XMxO}_4$ promoted oxidation of organic contaminants in aqueous medium with H_2O_2 . **Catalysis Communications**, v.4, p.525-529, 2003.
- 82) BARROS, H. J. V., OSPINA, M. L., ARGUELLO, E., ROCHA, W. R., GOUSSEVSKAIA, E. V., SANTOS, E. N. Rhodium catalyzed hydroformylation

of beta-pinene and camphene: effect of phosphorous ligands and reaction conditions on diastereoselectivity. **Journal of Organometallic Chemistry**, v.671, p.150-157, 2003.

- 83) PEREIRA, A. G., PORTO, A. O., LIMA, G. M., LUNA, H. G. S., ARDISSON, J. D. Sn-119 Mössbauer spectroscopic study of nanometric tin dioxide powders prepared by pyrolysis of organotin oxides. **Solid State Communications**, v.127, n.3, p.223-227, 2003.
- 84) MOURA, E. M., TERRA, V. R., LUNA, H. G. S., LIMA, G. M., PAIM, L. A., DIAS, F. M. Sn-Mössbauer spectroscopic studies on organoheterobimetallic half sandwich ruthenium-tin containing derivatives. **Transition Metal Chemistry**, v.28, p.437-442, 2003
- 85) OLIVEIRA, R. B., ALVES, R. J., SOUZA FILHO, J. D., PRADO, M. A. F. Stereoselective synthesis of carbohydrate-based fused bicyclic delta-lactones. **Journal of the Brazilian Chemical Society**, v.14, n.3, p.442-448, 2003.
- 86) BERALDO, H. O., BASTOS, A. M. B., VIEIRA, R. P., REBOLLEDO, A. P., SPEZIALI, N. L., PINHEIRO, C.B., CHAPUIS, G. Structural Studies and Spectral Characteristics of 4-benzoylpyridine Thiosemicarbazone and N (4')-Phenyl-4-Benzoylpyridine Thiosemicarbazone. **Journal of Molecular Structure**, v.645, n.2-3, p.213-220, 2003
- 87) PATARO, A. L., SANTOS, V. R., FRANCO, C. F., SEGURA, M. E. C., MILLAN, R. D. S. Surface effects and desorption of tetracycline supramolecular complex on bovine dentine. **Biomaterials**, v.24, n.6, p.1075-1080, 2003.
- 88) PERPÉTUO, G.J., OLIVEIRA, M.R.L., JANCZAK, J., VIEIRA, H.P., AMARAL, F.F. DE BELLIS, V.M. Syntheses, crystal structure and spectroscopic characterization of novel N-R-sulfonyldithiocarbamate zinc(II) complexes. **Polyhedron**, v.22, p. 3355-3362, 2003.
- 89) MATOS, R. M., VERKADE, J. G. Synthesis and Characterization of [(CO)₄FeL-L] and [(CO)₄FeL-LFe(CO)₄] wherein L-L is N(CH₂CH₂)₃N and also P(NMeNMe)₃P in the Latter Complex. Single Crystal X-ray Molecular Structure of [Fe(CO)₄DABCO]. **Journal of Brazilian Chemical Society**, v.14, n.1, p.77-75, 2003
- 90) ARAÚJO, M.H., HITCHCOCK, P.B., NIXON, J.F., KUEHNER, U., STELZER, O., Synthesis of a eta(2)-2,3-diphosphabutadiene complex of zerovalent platinum from the corresponding eta(2)-phosphaalkyne complex, **Chemical Communication**, v. 9, p.1092-1093, 2003.
- 91) FARACO, A.A.G., PRADO, M.A.F., ALVES, R.J., SOUZA, J.D., ALVES, R.B., FARACO, R.F.P., Synthesis of benzomacrolactam by 12-endo selective aryl radical

cyclization of N-(4-allyloxybutyl)-2-iodobenzene, **Synthetic Communications**, v.33, p.463-474, 2003.

- 92) PEDROSA, M. T. C., ALVES, R. B., PRADO, M. A. F., SOUZA FILHO, J. D. , ALVES, R. J. Synthesis of nitrogen heterocycles from methyl - α and - β -D-glucopyranosides. **Journal of Carbohydrate Chemistry**, v.22, n.6, p.433-442, 2003
- 93) MELO, J. O. F., DONNICI, C. L., AUGUSTI, R., LOPES, M. T. P., MIKHAILOVSKII, A. G. Synthesis of novel and hardly-obtainable 1,2,3-triazoles with potential antitumoral activity by a diazo-transfer reaction from 5,7-dinitro-3-diazo-1,3-dihydro-2H-indol-2-one to enaminones. **Heterocyclic Communications**, v.9, n.3, p.235-238, 2003.
- 94) CESAR, E. T., ALMEIDA, M. V., FONTES, A. P. S., MAIA, E. C. P., GARNIER-SUILLEROT, A., COURI, M. R. C., FELÍCIO, E. C. A. Synthesis, characterization, cytotoxic activity, and cellular accumulation of dinuclear platinum complexes derived from N,N'-di-(2-aminoethyl)-1,3-diamino-2-propanol, aryl substituted N-benzyl-1,4-butanediamines, and N-benzyl-1,6-hexanediamines. **Journal of Inorganic Biochemistry**, v.95, p.297-305, fev. 2003
- 95) JANCZAK, J., IDEMORI, Y. M. Synthesis, crystal structure and characterisation of aquamagnesium phthalocyanine - MgPc(H₂O). The origin of an intense near-IR absorption of magnesium phthalocyanine known as 'X-phase'. **Polyhedron**, v.22, n.14-17, p.1167-1181, 2003.
- 96) RIOS, R. V. R. A., ALVES, D.E., DALMAZIO, I., BENTO, S. F. V., DONNICI, C. L., LAGO, R. M. Tailoring Activated Carbon by Surface Chemical Modification with O,S, N Containing Molecules. **Materials Research**, v.6, n.2, p.129-135, 2003
- 97) SANTOS, H. F., DE ALMEIDA, W. B. The conformational and tautomeric equilibrium of 5a,6-anhydrotetracycline in aqueous solution at pH7. **Journal of Molecular Structure: Theochem**, v.626, p.305-319, 2003.
- 98) SILVA, R. A., SILVA, G. G., MOREIRA, R. L., PIMENTA, M. A. The Effects of Salt Concentration on Cation Complexation in Triblock-polyether Electrolyte. **Physical Chemistry Chemical Physics**, v.5, n.11, p.2424-2428, 2003.
- 99) COSTA, L. A. S., ROCHA, W. R., DE ALMEIDA, W. B., SANTOS, H. F. The hydrolysis process of the cis-dichloro(ethylenediamine)platinum(II): A theoretical study. **Journal of Chemical Physics**, v.118, n.23, p.10584-10592, 2003.
- 100) MEURER, E. C., GOZZO, F. C., AUGUSTI, R., EBERLIN, M. N. The kinetic method as a structural diagnostic tool: ionized α -diketones as loosely one -electron bonded diacylium ion dimers. **European Journal of Mass Spectrometry**, v.9, n.4, p.295-304, 2003.

- 101) MOURA, E. M., LUNA, H. G. S., LIMA, G. M., PORTO, A. O., MOURA, C. V. R., HORNER, M. The synthesis and structural characterisation of Ru-Sn based derivatives bearing asymmetric X₂ClSn- (X = Br and F) anions. **Journal of Molecular Structure**, v.658, n.1-2, p.71-78, 2003.
- 102) JUNQUEIRA, G. M. A., ROCHA, W. R., ALMEIDA, W. B., SANTOS, H. F. Theoretical analysis of the oxocarbons: The solvent and counter-ion effects on the structure and spectroscopy properties of the squarate ion. **Physical Chemistry Chemical Physics**, v.5, n.3, p.437-445, 2003.
- 103) FERREIRA, C. S., MARTINS, P. S., DEMICHELI, C. P., BROCHU, C., OUELLETE, M., FREZARD, F. J. G. Thiol-induced reduction of antimony(V) into antimony(III): A comparative study with trypanothione, cysteinyl-glycine, cysteine and glutathione. **BioMetals**, n.16, p.441-446, 2003.
- 104) REBOLLEDO, A.P., DE LIMA, G.M., GAMBI, L.N., SPEZIALI, N.L. MAIA, D.F., PINHEIRO, C.B., ARDISSON, J.D., CORTES, M.E., BERALDO, H. Tin(IV) complexes of 2-benzoylpyridine N(4)-phenyl-thiosemicarbazone: spectral characterization, structural studies and antifungal activity. **Applied Organometallic Chemistry**, v. 17, p.945-951, 2003.
- 105) OLIVEIRA, L. C. A., LAGO, R. M., FABRIS, J. D., SOLAR, C., SAPAG, Transition metals supported on Al-PILCs as catalysts for C₆H₅Cl oxidation. **Brazilian Journal Of Chemical Engineering**, v.20, n.1, p.45-50, 2003.
- 106) FABIANO, R. L., MONTANARI, C. A. Um novo modelo para os sítios de interação dos antagonistas H₂, baseado na caracterização química dos sítios primário e secundário por QSAR - 3D. **Química Nova**, v.26, n.4, p.499-506, 2003.
- 107) GOULART, M. O., CIOLETTI, A. G., FILHO, J. D. S., SIMONE, C. A., CASTELLANO, E. E., EMERY, F. S., MOURA, K. C., C.F.R.PINTO, M., PINTO, A. V. Unexpected oxidation of a substituted benzo[a]phenazine: oxidative cleavage of a double bond and formation of a macrolactone. **Tetrahedron Letters**, v.44, p.3581-3585, 2003.

PATENTES:

BELCHIOR, J.C., PEREIRA, G.V., Process of molecular analysis and sequencing for the classification and identification of RNA, DNA and/or proteins utilizing techniques of artificial intelligence. PI 0205900-2.

BERALDO, H. O., MILLAN, R.D.S., VIEIRA, R.P., COELHO, M.G., TEIXEIRA, L.R.S., Process to prepare semicarbazones and/or thiosemicarbazones formulations using

cyclodextrins and their derivatives and products obtained by this process. No. WO03066038.

VELOSO, D.P., Processo para isolamento e purificação da lignina do “Eucalyptus grandis” (LIPE) e emprego desta lignina como indicador em ensaio de digestibilidade aparente em diferentes espécies animais. PI 0304736-9.

LAGO, R.M., RIOS, R.V.R.A., MACHADO, L.C. de R., BERALDO, H.O. Processo de Preparação de Adsorventes Magnéticos para Aplicações Ambientais e Industriais.

FREZARD, F.J.G., MILLÁN, R.D.S., BEJARANO, R.O., DEMICHELI, C.P., Processo de preparação de compostos entre as ciclodextrinas ou seus derivados e o antimônio ou seus derivados, de formulações contendo esses compostos e produtos associados, para o tratamento das leishmanioses e da esquistossomose. PI 03044952-3.

CAPÍTULO DE LIVROS:

BELCHIOR, J.C., Novas fronteiras: aplicações de inteligência artificial em ciências em ênfase em químicas: redes neurais, algoritmos genéticos e lógica fuzzy In: Escola Brasileira de Estrutura Eletrônica, 2003.