

*1st Brazilian Symposium on Medicinal Chemistry*  
*New Approaches in Drug Design*  
*1º Simpósio Brasileiro em Química Medicinal*  
*Novas Estratégias em Planejamento Racional de Fármacos*

# *Program*

*November, 11-16, 2001*  
*Caxambu, Minas Gerais – Brazil*

Dear Sirs,

Brazil has entered an era where public health has also to deal with the discovery and production of medicines. Dipped in the spirit of collaboration to the public causes, Brazilian scientists are accomplishing several projects of scientific research with the objective of contributing for the development of the Brazilian natural products as source of new potential drugs. Synthetic chemistry efforts are widespread in the Country with many efforts to produce generic drugs and also modifying chemical structures of known drugs.

With the aim of bringing renown Research Scientists to discuss the possibilities Brazil may have in the area of drug design, the First Brazilian Symposium on Medicinal Chemistry is intended to show the world wide state-of-art in the field. Several Brazilian and foreign researchers both from the academy and of the pharmaceutical industry shall be present.

We welcome all of you with the wishes that we be successful in pursuing this.

Thank you very much for coming.

Carlos Montanari

On behalf of the Brazmedchem Committee

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*Co-chairman*

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## Sunday, 11<sup>th</sup> November

14h:00-18h:00 Registration

18h:00-19h:30 Dinner

19h:30-20h:00 Opening sessions  
Antonio Salustiano Machado, BR  
Secretary of Minas Gerais State for Science and Technology

20h:00-21h:00 Christophe L. M. J. Verlinde, USA  
Protein structure-based design of antiprotozoal drugs

21h:00-23h:00 Get-together party

## Monday, 12<sup>th</sup> November

8h:45 Perspectives in drug discovery and design of antiprotozoal drugs  
Chair: Elizabeth Igne Ferreira, BR

9h. Plenary lecture by: David W. Boykin, USA  
DNA minor groove binders as antiprotozoal agents

10h:00-10h:30 Coffee break

10h:30 Plenary lecture by: Glaucius Oliva, BR  
Target-directed drug discovery in tropical diseases

11h:30 Short Lecture by: Richard Garratt, BR  
Drug and Vaccine Targets from *Schistosoma mansoni*

12h:30-13h:45 Lunch

14h:00-15h:00 Plenary lecture by: John Dearden, UK  
QSAR modelling of toxicity of drugs

15h:00-15h:30 Short Lecture (PDD5) by: Yuji Takahata; BR

15h:30-16h:00 Short Lecture (APM13) by: Osman F. Güner; USA

16h:00-16h:30 Short Lecture (MPN16) by: Fabio S. Menezes; BR

16h:30-18h:00 Free group meeting (Open discussions)

18h:00-19h:30 Dinner

19h:30-21h:30 Poster session  
Perspectives in drug discovery                      PDD1- PDD20  
Synthesis and Bioassays                                SYB1 - SYB16

## Tuesday, 13<sup>th</sup> November

08h:45 Structure-based drug design  
Chair: José Daniel Figueroa-Villar, BR

9h Plenary lecture by: Tudor Oprea, SW  
Integrating DMPK and binding affinity predictions: a paradigm shift in lead discovery

10h:00-10h:30 Coffee break

10h:30 Plenary lecture by: Ferran Sanz, ES  
Comparison of biomolecules on the basis of molecular interaction potentials

11h:30 Plenary lecture by: Luiz Juliano, BR



## Friday, 16<sup>th</sup> November

**08h:45-12h:30 Medicinal Chemistry of Natural Products**

**Chair: Maria Fátima das Graças Fernandes da Silva, BR**

**9h:00 Plenary lecture by: Otto Richard Gottlieb and Maria Renata de M. B. Borin, BR**

**Quantitative chemobiology: a guide into the understanding of plant bioactivity**

**10h:00 Plenary lecture by: Benjamin Gilbert, BR**

**The Application of Medicinal Plants in Public Health**

**11h:00-11h:30 Coffee break**

**11h:30 Plenary lecture by: João B. Calixto, BR**

**The role of natural products in the process of drug discovery and development**

**12h:30 Naftale Katz, BR**

**FAPEMIG: Desenvolvimento Científico Tecnológico em Minas Gerais**

**Closing of Symposium**

**12h:45-14:30 Lunch (optional)**

## *Short Lectures*

**Monday 12<sup>th</sup>, 15h:00 - PDD5 - SAR ANALYSIS AND MODELING OF NEOLIGNANS WHICH ARE ANTI-LEISHMANIASIS USING PATTERN RECOGNITION METHODS**

Costa, M. C. A.; Barata, L. E. S.; Rossi-Bergmann, B.; Santos, L.S.; and Takahata, Y.

**Monday 12<sup>th</sup>, 16h:00 - APM13 - SEEKING NOVEL DRUG CANDIDATES THROUGH DE NOVO PHARMACOPHORE DESIGN**

Güner, O.F.; Fisher, L.S.

**Monday 12<sup>th</sup>, 16h:30 - MPN16 - ACTION OF AÇAÍ (*EUTERPE OLERACEA*) ON THE NITRIC OXIDE PRODUCTION IN THE CELLS RAW264.7**

Frazão, F.L.; Mantovani, I.S.B.; Santos, G.B.; Matheus, M.E.; Menezes, F.S.; Fernandes, P.D.

**Tuesday 13<sup>th</sup>, 15h:00 - APM1 - GETTING PAST DIVERSITY IN ASSESSING VIRTUAL LIBRARY DESIGNS**

Clark, R.D.

**Tuesday 13<sup>th</sup>, 15h:30 - APM10 - UNIVERSAL MOLECULAR QUANTUM DESCRIPTORS: A NEW SAR METHODOLOGY**

Coluci, V.R.; Braga, S.F.; Vendrame, R.; Barone, P.M.V.B. and Galvão, D.S.

**Tuesday 13<sup>th</sup>, 16h:00 - APM20 - A COMBINED CHEMOMETRIC, STRUCTURAL, MOLECULAR GRAPHICS AND MODELING STUDY OF PROGESTOGENS**

Ferreira, M.M.C.; Kiralj, R.

**Thursday 15<sup>th</sup>, 15h:00 - MSC12 - REDEFINING FRONTIERS IN NUCLEOSIDE PROCESS TECHNOLOGY. A NEW GENERATION OF HIGHLY SELECTIVE ANTIMIRAL AGENTS**

Rabi, J.A.

**Thursday 15<sup>th</sup>, 15h:30 - APM30 - 3D-QSAR: MULTIPLE BINDING MODES**

Balaz, S.

**Thursday 15<sup>th</sup>, 16h:00 - MSC2 - ENANTIOSELECTIVE ASSAY FOR MONITORING THE ALDO-KETO REDUCTASE-MEDIATED REDUCTION OF METYRAPONE IN PLASMA BY MULTIDIMENSIONAL HPLC**

Cass, Q.B.; Cassiano, N.M.; Degani, A.L.G. and Wainer, I.W.

# Posters

## 1. Perspectives in drug discovery and design of antiprotozoal drugs:

**PDD1)** EVALUATION OF TRYPANOCIDAL AND MOLLUSCICIDAL ACTIVITIES OF AROMATIC ARYLAZOXY COMPOUNDS. CORRELATION BETWEEN ELECTROCHEMICAL PARAMETERS AND BIOLOGICAL ACTIVITIES

Paula, F.S.; Cioletti, A. G.; Romanha, A.; Fruttero, R.; Gasco, A.; Filho, J.F.S.; Santos, A.F; Santana, A.E.G.; Goulart, M.O.F.

**PDD2)** COUMARINS AS POTENTIAL INHIBITORS OF THE GLYCOLYTIC ENZYME GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE (GGAPDH) FROM TRYPANOSOMA CRUZI

Marchi, A.A.; Jacoveto, D.C. M.; Archanjo, F.C.; Del Ponte, G.; Pupo, M.T.; Castilho, M.S.; Oliva, G.

**PDD3)** SOLID-PHASE PREPARATION AND EVALUATION OF A SITE-DIRECTED COMBINATORIAL LIBRARY OF COUMARIN DERIVATIVES

Dias, R.L.A.; Corrêa, A.G.; Wentworth Jr, P.; Janda, K.D., Oliva, G.

**PDD4)** SYNTHESIS AND IN VITRO EVALUATION OF AROMATIC NITRO COMPOUNDS ACTIVITY AGAINST TRYPANOSOMA CRUZI

Oliveira, R.B.; Alves, R.J.; Prado, M.A.F.; Souza Filho, J.D.; Passos, A.P.F.; Romanha, A.J.; Alves, R.O.

**PDD5)** SAR ANALYSIS AND MODELING OF NEOLIGNANS WHICH ARE ANTI-LEISHMANIASIS USING PATTERN RECOGNITION METHODS

Costa, M. C. A.; Barata, L. E. S.; Rossi-Bergmann, B.; Santos, L.S.; Takahata, Y.

**PDD6)** GENERATION AND TOPOLOGICAL MOLECULAR MODELING STUDY OF WILD-TYPE AND MUTANTS PLASMODIUM FALCIPARUM DHFR

Delfino, R. T., Figueroa-Villar, J. D.; Santos Filho, O. A.

**PDD7)** TRYPANOCIDAL ACTIVITY OF QUESNELIA QUESNELIANA (BRONGNIART) L. B. SMITH (BROMELIACEAE)

Gibaldi, D.; Chedier, L.M.; Bozza, M.T.; Henriques, M.G.M.O.; Figueiredo, M.R.; Kaplan, M.A.C.

**PDD8)** PRÓ-FÁRMACOS DO OROTATO: SÍNTESE E ATIVIDADE BIOLÓGICA CONTRA A MALÁRIA E TOXOPLASMOSE

Alves, I. C.; Cardoso, R.P.A; Andrade Jr, H.F.; Felli, V.M.A.

**PDD9)** THE RESPONSE OF SCHISTOSOMA MANSONI MAINTAINED IN VITRO TO IMIDAZOLIDINONE COMPOUNDS

Oliveira, S. M.; Albuquerque, M.C.P.A.; Luna1, S.J.S.; Silva, P.G.; Pitta, M.G.R., Malagueño, E.; Santana, J.V.; Lima, M.C.A.; Pitta, I.R., Galdino, S.

**PDD10)** ON THE IMPORTANCE OF QUANTUM AND CLASSICAL VARIABLE ON PCA STUDIES OF ANTIMICROBIAL  $\beta$ -CARBOLINES AND THEIR ANALOGUES

Carvalho, M.A.; Silva, J.B.P.; Montanari, C.A.

**PDD11)** SYNTHESIS AND STRUCTURE-ACTIVITY RELATIONSHIP OF TRYPANOCIDAL LIGNANS ANALOGS

Bernandes, L.S.C.; Carvalho, I.; Kato, M.J.; Pupo, M.T.; Lopes, N.P.; Albuquerque, S.

**PDD12)** MOLECULAR RECOGNITION OF B-DNA DRUG BINDERS.

Silva, V.A.; Leitão, A.; Almeida, V.L.; Oliveira, A.M.; Rocha, R. K.; Menezes, I.R.A.; Menezes, F.A.S.; Donnici, C.L.; Montanari, C.A.; Lopes, J.C.D.

**PDD13)** A POSSIBLE EXPLANATION OF THE ACTIVE ENANTIOMER OF NEOLIGNANS THAT WERE TESTED AGAINST LEISHMANIASIS

Costa, M.C.A; Barata, L.E.S.; Takahata, Y.

**PDD14)** HOMOLOGY MODELING OF DIHYDROFOLATE REDUCTASE-TYMIDILATE SYNTHASE OF PLASMODIUM FALCIPARUM. A POTENTIAL MODEL TO DESIGN NEW ANTIMALARIALS.

Medeiros, A.L.R.; Figueroa-Villar, J.D.; Santos Filho, O.A.

**PDD15)** HYDROXYNAPHTHOQUINONES: EFFECTS OF STRUCTURE ON THEIR MOLLUSCIDAL ACTIVITY. SEARCH FOR A USEFUL SUBSTRATE FOR CHEMOPROPHYLAXIS OF SCHISTOSOMIASIS

Lima, N. M. F.; Santos, A. F.; Correia, C. S.; Silva, L. A.; Pinto, A.V.; Pinto, M.C.R.F.; Santana, A. E. G.; Goulart, M. O. F.

**PDD16)** SYNTHESIS OF NOVEL N, N'-DIALKYL BERENIL DERIVATIVES

Rocha, R.K.; Donnici, C.L.; Montanari, C.A.; Lopes, J.C.D.; Boykin, D.W.

**PDD17)** NEW TRIPANOTIONE REDUCTASE INHIBITORS

Athouguia, D. R.; Souza, C. P.; Zani, C. L. and Montanari, C. A.

**PDD18)** A CRITICAL ANALYSIS OF PUBLISHED QSAR STUDIES ON ANTIMALARIAL ARTEMISININ DERIVATIVES

Taranto, A.G.; Carneiro, J. W. de M.; Araújo, M. T.

**PDD19)** ANTILEISHMANIAL DRUGS: SPECIATION OF ANTIMONY AND IDENTIFICATION OF TOXIC CONTAMINANTS

Kepler, A.F.; Imbrunito, T.R.; Jesús, M.N.; Trivelin, L.A.; Barone, J.S.; Bueno, M.I.M.S.; Tempone, A.G.; Andrade Jr., H.F.; Rath, S.

**PDD20)** FERROCENYL CHALCONES: A NEW CLASS OF INHIBITORS OF THE GLYCOLYTIC ENZYME GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE (GGAPDH) FROM TRYPANOSOMA CRUZI.

Afonso, M.M.F.; Federman Neto, .A.; Pupo, M.T.; Castilho, M.S.; Oliva, G.

**PDD21)** DESIGN, SYNTHESIS AND EVALUATION OF A COMBINATORIAL LIBRARY OF FLAVONOID DERIVATIVES

Nogueira, C.M.; Alvim Jr., J.; Dias, R.L.A.; Corrêa, A.G.; Oliva, G.

## ***2. Receptor-based Prediction of Binding Affinities:***

**RPA1)** A MOLECULAR MODELING STUDY ON THE ISONIAZID-KATG INTERACTION

Cunha, E.F.F.; Maia, E.R. and Alencastro, R.B.

**RPA2)** EXPLORING THE SUB-SITE SPECIFICITY OF SCHISTOSOMA MANSONI CATHEPSIN D-LIKE PROTEASE

Silva-Jr, F.P.; Ribeiro, F.; Katz, N. and Giovanni-De-Simone, S.

**RPA3)** INHIBITION OF MUTALYSIN II, A METALLOPROTEINASE FROM BUSHMASTER SNAKE VENOM BY HUMAN  $\alpha$ 2-MACROGLOBULIN AND RABBIT IMMUNOGLOBULIN

Souza, C.T.; Moura, M.B.; Magalhaes, A.; Heneine, L.G.D.; Olortegui, C.C.; Diniz, C.R. and Sanchez, E.F.

**RPA4)** MOLECULAR ANALYSIS OF PUTATIVE SCH28080 BINDING SITES OF H<sup>+</sup>,K<sup>(+)</sup>-ATPase AND H<sup>+</sup>,Na<sup>(+)</sup>-ATPase

Borges, E.G. and Takahata, Y.

**RPA5)** MOLECULAR MODELING FOR INHIBITORS OF TAT/TAR COMPLEX OF HIV-1

Gomes, L.P.; Figueiredo, L.J.O.; Antunes, O.A.C.

**RPA6)** A MOLECULAR MODELLING STUDY ON NOVEL HIV-1 PROTEASE INHIBITORS

Figueiredo, L.J.O.; Peçanha, E.P.; Bongertz, V.; Brindeiro, R.M.; Tanuri, A.; Antunes, O.A.C.; Sanches, M. Polikarpov, I.

**RPA7)** RELATIVE BINDING AFFINITIES OF ENZYME INHIBITORS: MOLECULAR MODELING OF *T. CRUZI* CYSTEINE PROTEASES INHIBITON

Carvalho, M.L., Vieira, F.M.C.; Pascutti, P.G.; Bisch, P.M.



### **3. Applications of Multivariate QSAR:**

**APM1) GETTING PAST DIVERSITY IN ASSESSING VIRTUAL LIBRARY DESIGNS**

Clark, R.D.

**APM2) ANALYSIS OF ANTIGENIC PEPTIDES PRESENTATION THROUGH COMPUTER COMBINATORIAL LIBRARIES**

Dametto, M.; Jacchieri, S.G.

**APM3) MOLECULAR MODELLING STUDIES ON THE REACTIVATION OF ACETYLCHOLINESTERASE INHIBITED BY ORGANOPHOSPHATES: A SUGGESTED MODIFICATION OF THE GENERALLY ACCEPTED MECHANISM**

Figuroa-Villar, J.D.; Castro, A.T.

**APM4) RANDOM CONFORMATIONAL SEARCH OF A C16 FATTY ACYL MODEL AND MINIMIZATION OF THE ACTIVE SITE MODEL OF INHA, THE ENOYL-ACP REDUCTASE FROM *MYCOBACTERIUM TUBERCULOSIS***

Pasqualoto, K.F.M.; Ferreira, E.I.

**APM5) STUDY OF SODIUM CHANNEL BLOCKING ANTIEPILEPTIC DRUGS**

Tasso, S.M.; Bruno-Blanch, L.E.; Estiu, G.L.

**APM6) COMPARATIVE QSAR OF ANTIMICROBIAL HYDRAZIDES.**

Montanari, M.L.C.; Montanari, C.A.; Gaudio, A.C.

**APM7) HANSCH ANALYSIS OF 5-NITRO-2-FURFURILIDENE DERIVATIVES WITH ANTIMICROBIAL ACTIVITY**

Tavares, L.C.; Vessoni-Penna, T.C.; Amaral, A.T.

**APM8) QUANTITATIVE STRUCTURE-ACTIVITY RELATIONSHIP FOR A SET OF [2-(4-X-BENZAMIDO)ETHYL]BENZYL DIMETHYLAMMONIUM BROMIDE WITH NEUROMUSCULAR BLOCKAGE**

Siqueira, L. J. A.; Lapa, A. J.; Souccar, C.; do Amaral, A. T.

**APM9) 3D-QSAR MODELS: LOCAL INTERSECTION VOLUME (LIV)**

Martins, R.C.A.; Albuquerque, M.G.; Alencastro, R.B.

**APM10) UNIVERSAL MOLECULAR QUANTUM DESCRIPTORS: A NEW SAR METHODOLOGY**

Coluci, V.R.; Braga, S.F.; Vendrame, R.; Barone, P.M.V.B.; Galvão, D.S.

**APM11) QSAR MODEL OF THE PHOTOTOXICITY OF POLYCYCLIC AROMATIC HYDROCARBONS**

Ribeiro, F. A. L.; Ferreira, M. M. C.

**APM12) QSAR STUDY OF OMEPRAZOLE AND ANALOGUE COMPOUNDS AS ANTI *HELICOBACTER PYLORI* AGENTS**

Bruni, A.T.; Ferreira, M.M.C.

**APM13) SEEKING NOVEL DRUG CANDIDATES THROUGH DE NOVO PHARMACOPHORE DESIGN.**

Güner, O.F.; Fisher, L.S.

**APM14) RATIONAL DRUG DESIGN OF NOVEL ORGANOSULFUR COMPOUNDS WITH ANTICANCER ACTIVITY AND STUDY OF THE MECHANISM DRUG-RECEPTOR**

Reina, L.C.B.; Donnici, C.L.; Montanari, C.A.; Oliveira, I.M.F.; Idemori, Y.; Augusti, R.

**APM15) A STUDY OF HIV-1 PROTEASE ? INHIBITOR INTERMOLECULAR INTERACTIONS BY USING QUANTITATIVE MOLECULAR GRAPHICS AND A PRIORI QSAR**

Kiralj, R.; Ferreira, M.M.C.

**APM16) RATIONAL DRUG DESIGN BY QSAR OF NOVEL BENZAMIDINES WITH POTENTIAL ACTIVITY AGAINST PNEUMOCYSTIS CARINII (PCP)**

Almeida, V. L. ; Montanari, C. A.; Donnici, C. L.

- APM17)** QSPR MODELS TO PREDICT THE ORGANIC CARBON-WATER PARTITION COEFFICIENT (KOC) AND BIOCONCENTRATION FACTOR (BCF) FOR POLYCYCLIC AROMATIC HYDROCARBONS (PAH)  
Ribeiro, F. A. L.; Sabino, L. C. ; Ferreira, M. M. C.
- APM18)** MOLECULAR RECOGNITION OF B-DNA DRUG BINDERS.  
Silva, V.A.; Leitão, A.; Almeida, V.L.; Oliveira, A.M.; Rocha, R. K.; Menezes, I.R.A.; Menezes, F.A.S.; Donnici, C.L.; Montanari, C.A.; Lopes, J.C.D.
- APM19)** ESTUDO TEÓRICO DA RELAÇÃO ESTRUTURA-ATIVIDADE (SAR) DE COMPOSTOS DERIVADOS DO MEGAZOL COM ATIVIDADE TRIPANOSOMICIDA  
Rosselli, P. R.; Silva, A. B. F.
- APM20)** A COMBINED CHEMOMETRIC, STRUCTURAL, MOLECULAR GRAPHICS AND MODELING STUDY OF PROGESTOGENS  
Ferreira, M.M.C.; Kiralj, R.
- APM21)** 3D-QSAR STUDIES OF NON-STEROID ESTROGEN RECEPTOR LIGANDS.  
Menezes, I.R.A.; Montanari, C.A.; Lopes, J. C. D.
- APM22)** QUANTITATIVE STRUCTURE-ANTIVIRAL ACTIVITY RELATIONSHIPS OF DEOXY ANALOGS OF 1-[(2-HYDROXYETHOXY)METHYL]-6-(PHENYLTHIO)THYMINE (HEPT) AS POTENT AND SELECTIVE ANTI-HIV AGENTS  
Souza, A.M.A.; Lima, M.C.A.; Galdino, S.L.; Pitta, I.R.
- APM23)** ON THE IMPORTANCE OF QUANTUM AND CLASSICAL VARIABLE ON PCA STUDIES OF ANTIMICROBIAL BETA-CARBOLINES AND THEIR ANALOGUES  
Carvalho, A.M.A.; Silva, J.B.P.; Montanari, C.A.
- APM24)** RATIONAL PROCEDURES FOR SELECTION OF SEAL PARAMETERS  
Ishiki, H.M.; Bruns, R.E.; Brandão, L.O.; Galembeck, S.E.; Amaral, A.T.
- APM25)** 3D- AND 4D-QSAR STUDIES AIMING AT THE DISCRIMINATION BETWEEN THE CATALYTIC AND THE HIGH AFFINITY ROLIPRAM BINDING SITES OF PDE-4  
Romeiro, N.C.; Hopfinger, A.J.; Albuquerque, M.G.; Alencastro, R.B.
- APM26)** WINCLUS: ADVANCES IN AUTOMATED SEARCH FOR POTENTIALLY COMPOUNDS BY USING CLUSTER ANALYSIS.  
Menezes, I.R.A.; Araújo, A.A.S.; Alves, A.J.
- APM27)** QUANTITATIVE STRUCTURE-ATIVITY CYTOTOXIC RELATIONSHIPS STUDY OF TWO SETS OF MANNICH BASES DERIVATIVES  
Raminelli, C.; Rogero, S. O.; do Amaral, A. T.
- APM28)** DISTINGUISHING THE IONIZED FROM THE UNIONIZED SPECIES AS THE ACTIVE FORM.  
Malvezzi A.; do Amaral, A. T.
- APM29)** MOLECULAR RECOGNITION OF SPECIFIC SEQUENCES OF B-DNA  
Silva, V.A.S.; Montanari, C.A.; Menezes, I.R.A.; Leitão, A.
- APM30)** 3D-QSAR: MULTIPLE BINDING MODES  
Balaz, S.
- APM31)** QSAR OF COMBILEXINS DERIVATIVES  
Leitao, A.; Montanari, C. A.
- APM32)** PATTERN RECOGNITION STUDIES ON ANTIMALARIAL 3-SUBSTITUTED TRIOXANES  
Júnior, A. H.; Machado, C.; Montanari, C. A.
- APM33)** A QSAR STUDY OF THE ACUTE TOXICITY OF A SERIES OF HYDROCHLORIDES OF N,N-[(DIMETHYL AMINO)ETHYL] 3-SUBSTITUTED BENZOATES  
Sousa, W.A.; Gallacci, M.; Amaral, A.T.
- APM34)** CONFORMATIONAL ANALYSES AND SAR STUDIES OF ANTISPERMATOGENIC HEXAHIDROINDENOPIRIDINES.

Segala, M.; Takahata, Y.

**APM35) CHEMOMETRIC DESCRIPTION OF 4,9-DIAZAPYRENENIUM-NUCLEOTIDE BINDING**

Kiralj, R.; Ferreira, M.M.C.

**4. Medicinal Chemistry of Natural Products:**

**MPN1) SYNTHESIS OF NITROGENATED DERIVATIVES OF 6-ALPHA,7-BETA-DI-HYDROXYVOUACAPAN-17-BETA-OIC ACID.**

Berinel, V.J.; Veloso, D.P.; Stefani, G.M.; Reis, G.T.; Alves, D.L.F.

**MPN2) METAL COMPOUNDS OF QUININE AND RELATED ALKALOIDS**

Rey, N. A.; dos Santos, K. C.; Pereira-Maia, E. C.

**MPN3) ROLLINIA SYLVATICA DEVELOP ANTINOCICEPTIVE ACTIVITY**

Herdy, S.A.; Marinho, B.G.; Leite, A.V.C.; Matheus, M.E.; Leitão, G.G.; Leitão, S.G.; Fernandes, P.D.

**MPN4) NUTANIN, A NEW ADJACENT BIS-TETRAHYDROFURAN ANNONACEOUS ACETOGENIN FROM ANNONA NUTANS SEEDS**

Santos, L.A.R.; Pimenta, L.P.S.; Boaventura, M.A.D.

**MPN5) ANTINOCICEPTIVE AND ANTIINFLAMMATORY ACTIVITY OF *HYPTIS FASCICULATA***

Monteiro, G. C; Gomes, N.M.; Marinho, B.G.; Falcão, D.Q.; Menezes, F.S. Fernandes, P. D.

**MPN6) SEDATIVE AND ANTINOCICEPTIVE ACTIVITY FROM EXTRACTS OF *LANTANA TRIFOLIA***

Martins, F.R.; Marinho, B.G.; Matheus, M.E.; Leitão, S.G.; Fernandes, P.D.

**MPN7) ANTIOXIDANT ACTIVITY OF *EUTERPE PALM* EXTRACTS**

Arruda, D.C.; Felippi, R.; Mantovani, I.S.B.; Santos, G.B.; Gabriel, F.T.; Ribeiro-do-Valle, R.M.; Ckless, K and Menezes, F. S.

**MPN8) CYTOTOXIC ACTIVITIES OF ALKALOIDS AND FLAVONOID FROM *SOLANUM CRINITUM LAM.***

Esteves-Souza, A.; Silva, T. M. S.; Alves, C. C. F.; de Carvalho, M. G; Braz-Filho, R.; and Echevarria, A.

**MPN9) ANTIINFLAMMATORY AND ANTINOCICEPTIVE ACTIVITY FROM LEAVES OF *VYTEX CYMOSA***

Marinho, B.G.; Santos, T.; Matheus, M.E.; Leitão, S.G.; Fernandes, P.D.

**MPN10) ANTIMICROBIAL ACTIVITY OF BARKS OF *CROTON LANJOUWENSIS JABL.***

Ohana, D.T.; Amaral, A.C.F.; Kuster, R.M.; Santos, K.R.N.; Machado, T.B.; Leal, I.C.R.

**MPN11) ANTIMICROBIAL AND ANTI DIABETES ACTIVITY OF *CISSUS SICYOIDES***

Cavalcante, C. V. G.; de Souza, G. M. L.; Machado, L. P.; de Albuquerque, J. F. C.; Chiappeta, A. A.; de Sena, K. X. F. R.; Catanho, M. T. J. A.

**MPN12) SYNTHESIS AND PRELIMINARY PHARMACOLOGICAL EVALUATION OF COUMESTANS WITH DIFFERENT PATTERNS OF OXYGENATION**

Costa, P. R. R.; da Silva, A. J. M.; Melo, P. A.; Silva, N. M. V.; Brito, F. V.; Buarque, C. D.; de Souza, D. V.; Rodrigues, V. P.; Poças, E. S. C.; Noel, F.; Castro, N. G.; Caruso, R. R. B.; Albuquerque, E. X.

**MPN13) SYNTHESIS AND PRELIMINARY PHARMACOLOGICAL EVALUATION OF NEW 1,4-NAPHTHOQUINONES STRUCTURALLY RELATED TO LAPACHOL**

Costa, P. R. R.; Silva, A. J. M.; Melo, P. A.; Silva, N. M. V.; Brito, F. V.; Buarque, C. D.; Souza, D. V.; Poças, E. S. C.; Noel, F.; Castro, N. G.; Caruso, R. R. B. Murakami, Y. L. B.; Aurelian, L.; Macedo, L.F.; Malkas, L.; Hickey, R.

**MPN14) ANALGESIC AND ANTI-INFLAMMATORY EFFECTS OF BRAZILIAN COPAÍBA OIL-RESIN**

Pennaforte, R.J.; Tappin, M.R.R.; Siani, A.C.; Henriques, M.G.M.O.

**MPN15) MARINE NATURAL COMPOUNDS WITH POTENTIAL MEDICINAL USE IN BRAZILIAN COAST**

Freitas, J.C.

**MPN16)** ACTION OF AÇAÍ (*EUTERPE OLERACEA*) ON THE NITRIC OXIDE PRODUCTION IN THE CELLS RAW264.7

Frazão, F.L.; Mantovani, I.S.B.; Santos, G.B.; Matheus, M.E.; Menezes, F.S.; Fernandes, P.D.

**MPN17)** SEPARATION OF MULTI-MILLIGRAMS QUANTITIES OF GOSSYPOL ENANTIOMERS ON POLYSACCHARIDE-BASED STATIONARY PHASES

Cass, Q. B.; Oliveira, R. V.

**MPN18)** *ARRABIDAEA SAMYDOIDES*: A POTENTIAL SOURCE OF ANTIMALARIAL LEAD COMPOUND

Pauletti, P. M.; Young, M. C. M.; Benedetti, C. E.; Bolzani, V. S.

**MPN19)** BIOLOGICAL ACTIVITY OF 2,5-DISUBSTITUTED TETRAHYDROFURAN DERIVATIVES OBTAINED FROM ALFA-(-)-BISABOLOL

Aleixo, A.M.; Baptistella, L.H.B; Nogueira, R.T.; Imamura, P.M.; Limberger, R.P.; Ferreira, L.; Castilhos, T.; Zen, R.P.; Aleixo, A.M.; Germani, J.C.; Henriques, A.T.; Baptistella, L.H.B.

**MPN20)** FORMATION OF 2,5-DISUBSTITUTED TETRAHYDROFURAN DERIVATIVES FROM BISABOLOL BY CELL CULTURE OF *BIPOLARIS SOROKINIANA*

Limberger, R.P.; Ferreira, L.; Castilhos, T.; Zen, R.P.; Aleixo, A.M.; Germani, J.C.; Henriques, A.T.; Baptistella, L.H.B.

**MPN21)** SEDATIVE PROPERTIES OF ETHANOLIC EXTRATS FROM *LIPPIA ALBA MILL. N. E. BROWN*: COMPARISON OF THE ACTIVITIES OF THREE DIFFERENT CHEMOTYPES

Dip, E.C.; Tavares, E.S.; Julião, L.S.; Matheus, M.E.; Leitão, S.G.; Lage, C.L.S.; Fernandes, P.D.

**MPN22)** FLAVONOIDS FROM RUTACEAE AND LEGUMINOSAE AND THEIR *TRYPANOSOMA CRUZI* GLYCOSOMAL GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE-INHIBITORY ACTIVITIES

Tomazela, D. M.; Moraes, V. R. S.; Ruiz, A. L. T. G.; Maia, B. H. L. N. S.; Fermino, C. A.; Nogueira, M. A.; Sannomiya, M.; Castilho, M. S.; da Silva, M. F. G. F.; Vieira, P. C.; Fernandes, J. B.; Magalhães, E. G.; Magalhães, A. F.; Oliva, G.

**MNP23)** LUPANE AND URSANE-DERIVED TRITERPENES FROM *ASPIDOSPERMA OLIVACEUM* (APOCYNACEAE).

Carneiro, F. J. C.; Bolzani, V. S.; Young, M. C. M.; Silva, D. H. S.

**MPN24)** ACTION OF *PHYLLANTHUS NIRURI* ON THE HORMONES OF PREGNANT FEMALE RATS

Souza, G.M.L.; Cavalcante, C.V.G.; Paiva, A.L.A.; Bezerra, A.L.; Carvalho, E.F.N.B.; Machado, L.P.; Albuquerque, J.F.C.; Catanho, M.T.J.A.

## **5. Synthesis and Bioassays**

**SYB1)** DESIGN, SYNTHESIS AND BIOASSAYS OF ANTIBIOTIC GUANYL HYDRAZONES

Martins, L.C.; Ramasine, C.A.M.; Figueroa-Villar, J.D.

**SYB2)** METAL COMPLEXES OF N(4')-PHENYL-2-BENZOYLPYRIDINE THIOSEMICARBAZONE CAN INHIBIT IN VITRO GROWTH OF *CANDIDA ALBICANS* AND *STAPHYLOCOCCUS AUREUS*

Beraldo, H.; Cortés, M.E.; Costa, R.F.F.; Nacif, W.; Gariano, G.X.; Vieira, R.P.

**SYB3)** NEW OXADIAZOLO-PHTHALIMIDES AS POSSIBLE COX-2 INHIBITORS: INTERACTION MECHANISM

Antunes, R.; Batista, H.; Srivastava, R. M. ; Thomas, G.; Araújo, C. C.; Longo, R.; Leão, M.B.C.; Pavão, A. C.

**SYB4)** TOTAL ENANTIOSELECTIVE SYNTHESIS OF THE NATURAL IMINOCYCLITOL (2R, 3R, 4R, 5R)-2,5-DIHYDROXYMETHYL-3,4-DIHYDROXYPYRROLIDINE

Garcia, A.L.L.; Correia, C.R.D.

**SYB5)** BIOLOGICAL ACTIVITY OF SOME PODOCARPIC ACID DERIVATIVES

Soriano, M.P.C.; Imamura, P.M.

- SYB6)** ESTUDO DE ATIVIDADE BIOLÓGICA DE ALGUNS PERIDROBENZ[E]INDANOS SINTETIZADOS A PARTIR DO ÁCIDO ABIÉTICO  
Santos, C.; Imamura, P. M.
- SYB7)** HYDROPHOBIC EFFECT OF 1,3-DITHIOLIUM-4-THIOLATE ALKYL-SUBSTITUTED ON ARTEMIA SALINA LEACH TOXICITY  
Mello, H.; Almeida, P.A.; Silva, T.M.S.; Echevarria, A.
- SYB8)** SYNTHESIS AND CHARACTERIZATION OF BUTYLALLYLSTARCH  
Zeni, M.; Riveros, R.; Gower, A.E.; Rasesa, K.
- SYB9)** SYNTHESIS AND ANTICANCER ACTIVITY OF ACRIDINYLDENE-THIAZOLIDINE DERIVATIVE  
Silva, T.G.; Silva, F. S.V.C.B.; Souza, I.A.; Lima, M.C.A.; Galdino, S.L.; Barbe, J.; Pitta, I.R.
- SYB10)** ANTI-HIV ACTIVITY OF NEW PEPTIDEMIMETIC TARTARIC ACID DERIVATIVES.  
Peçanha, E.P.; Figueiredo, L.J.O.; Calazans, A.; Brindeiro, R.M.; Tanuri, A.; Antunes, O.A.C.
- SYB11)** SYNTHESIS, ANTI-INFLAMATORY AND ANTIMICROBIAL ACTIVITIES OF NEW 1,2,4-OXADIAZOLES PEPTIDOMIMETICS  
Leite, A.C.L., Vieira, R.F.F.; Srivastava, R.M.; Doboszewski, B.; Afitpour, P.; Ximenes, E.C.P.A.; Wanderley, A.G.; Oliveira, C.F.; Medeiros, M.V.; Antunes, E.; Brondani, D.
- SYB12)** SYNTHESIS AND ANTITUMOR ACTIVITY OF PEPTIDYL DEIVATIVES FROM NATURAL SAFROLE  
Leite, A.C.L.; Silva, K.P.; Souza, I.A.; Doboszewski, B.; Brondani, D.
- SYB13)** SYNTHESIS OF STARCH-CI AND DERIVATES  
Zeni, M. , Paloschi, R., Riveros, R.; Gower, A
- SYB14)** ON THE SYNTHESIS OF NEW ANTI-HIV COMPOUNDS  
Antunes, O.A.C; Bastos, M.L.; Sabino, S.J.; Peçanha, E.P., Costa, J.S., Arcuri, M.B.; Machado, G.D.C.; Almeida, R.M., Cotrim, B.A.; Lobo, V.S.; Rangel, L.P.; Paredes, B.A.; Gomes Jr., M.; Gomes, L.P.; Hernandez-Valdez, R.; Figueiredo, J.O.; Gonçalves, L.P.B.; Pinto,G.F.; Oestreicher, E.G.
- SYB15)** THE CYTOTOXIC/MUTAGENIC EFFECT OF A NEWLY SYNTHESIZED DENDRITIC MEDICINE MOLECULES  
Andrade, C.H.; Salas, C.E.; Lopes, M.T.P; Donnici, C.L.; Montanari, C.A., Bento, S.F.V., Assis, M.M.
- SYB16)** SÍNTESE DE FURANOQUINOLINAS, PRECURSORES DE NOVOS ANTIMALÁRICOS  
Solis, M.M.P.; Brandt, C.A.; Cardoso, R.P.A.; Andrade Jr, H.F.; Silveira, M.A.B.
- SYB17)** INVESTIGATION OF ANTICANCER ACTIVITY OF 1,3,4-THIADIAZOLIUM-2-AMINIDE MESOIONIC COMPOUNDS  
Britto, M. M.; Donnici, C. L.; Montanari, C. A; Lopes, M.T.P.
- SYB18)** SYNTHESIS AND EVALUATION OF ANTICANCER ACTIVITY OF SOME SUBSTITUTED 1,2,3-TRIAZOLES  
Melo, J. O. F.; Augusti, R. Donnici, C. L.; Lopes, M. T. P
- SYB19)** SYNTHESIS AND ANTIDERMOPHYTE ACTIVITY OF ALKYLAMINOALKANETHIOSULFURIC ACIDS  
Nelson, D.L.; Penido, M.L.O.; Almada, M.L. Piló-Veloso, D.
- SYB20)** SÍNTESE DE FURANOQUINOLINAS, PRECURSORES DE NOVOS ANTIMALÁRICOS  
Solis, M.M.P.; Brandt, C.A.; Cardoso, R.P.A.; Andrade Jr, H.F.; Silveira, M.A.B.
- SYB21)** IN VITRO ANTIFUNGAL ACTIVITY OF TIN(IV) COMPLEXES OF 3- AND 4-FORMYL AND 3- AND 4-ACETIL SEMICARBAZONES DERIVED FROM PYRIDINE.  
Beraldo, H.; Cortés, M.E.; Costa, R.F.F.; Nacif, W.; Gariano, G.X.; Vieira, R.P.
- SYB22)** SYNTHESIS OF NOVEL N,N-DIALKYL ANALOGUES OF BERENIL, PLANNED BY RATIONAL DRUG DESIGN, VIA AMIDOXIME ROUTE.  
Andrade, A.F.D.; Rocha, R.K.; Donnici, C.D.

**SYB23)** SYNTHESIS OF PRECURSORS OF NOVEL BENZAMIDINES WITH POTENTIAL ACTIVITY AGAINST PNEUMOCYSTIS CARINII (PCP) PLANNED THROUGH RATIONAL DRUG DESIGN BY QSAR.

Almeida, V. L. ; Donnici, C. L. ;Montanari, C. A.

**SYB24)** ANTIPROLIFERATIVE EFFECTS ON EHRlich TUMOR CELLS BY NEW LAPACHOL DERIVATIVES

Esteves-Souza, A.; Echevarria, A.; Vargas, M.; Pinto, A.C.; Celso, A.C.

## **6. Miscellaneous:**

**MSC1)** ESTRATÉGIAS PARA INIBIDORES DE HIV1 PROTEASES DE CEPAS MUTANTES: CLONAGEM E EXPRESSÃO DE HIV-1 PROTEASES

Sanches, M.; Antunes, O. A. C.; Peçanha, E.P.; Tanuri, A.; Polikarpov, I.

**MSC2)** ENANTIOSELECTIVE ASSAY FOR MONITORING THE ALDO-KETO REDUCTASE-MEDIATED REDUCTION OF METYRAPONE IN PLASMA BY MULTIDIMENSIONAL HPLC

Cass, Q.B.; Cassiano, N.M.; Degani, A.L.G.; Wainer, I.W.

**MSC3)** LIPOPHILICITY OF MESOIONIC COMPOUNDS EVALUATED BY HIGH PERFORMANCE LIQUID CHROMATOGRAPHY

Britto, M.M.; Montanari, C.A.; Donnici, C.L.; Jardim, I.C.S.F.

**MSC4)** INFLUENCE OF DIFFERENT THIOLS AND OF THE STATE OF COMPLEXATION OF SB(V) ON THE RATE OF REDUCTION OF SB(V) INTO SB(III)

Ferreirab, C.S.; Frézarda, F.; Demichelib, C.

**MSC5)** INTERACTION OF SB(V) WITH ADENINE AND URIDINE RIBONUCLEOSIDE

Demichelia, C.; Caetanoa, M.L.; Bejaranoa, R.O.; Frézardb, F.; Lecouveyc, M.; Garnier-Suillerotd, A.

**MSC6)** ISOLATION OF SECONDARY METABOLITES OF PLUMBAGO AURICULATA LAM. BY COUNTERCURRENT CHROMATOGRAPHY

Paiva, S.R.; Figueiredo, M.R.; Kaplan, M.A.C.

**MSC7)** pH INFLUENCE OF log D VALUES, BY RP-HPLC

Almeida, T.M.G.; Montanari, C.A.; Jardim, I.C.S.F.

**MSC8)** FRACIONAMENTO E AFERIÇÃO DA PUREZA DA APITOXINA

Maia, A.B.R.A.; Rocha, M.P.S.; Nelson, D.L.

**MSC9)** THE USE OF THE BLACK BONE (BLACK STONE) AS AN ATTENUANT OF HEMORRHAGIC LESIONS INDUCED BY THE BOTHROPS ATROX SNAKE VENOM.

Silva, L.P.; Oliveira, J.R.S.; Silva, H.A.; Neto, R.C.L.; Filho, W.E.M.; Costa, M.C.P.

**MSC10)** THE MIOTOXIC ACTION INDUCED BY BOTHROPS ATROX SNAKE VENOM

Vale, V.; Silva, L.P.; Oliveira, J.R.S.; Oliveira, E.G.; Neto, R.C.L.; Borges, A.C.R.; Costa, M.C.P.

**MSC11)** THE POTENTIALITY OF THE BLACK BONE (BLACK-STONE) IN THE ADSORPTION OF BOTHROPS ATROX VENOM.

Santos, M.N.R.; Moreira, I.; Oliveira, E.G.; Silva, F.C.;Bezerra, C.W.B.; Costa, M.C.P.

**MSC12)** REDEFINING FRONTIERS IN NUCLEOSIDE PROCESS TECHNOLOGY. A NEW GENERATION OF HIGHLY SELECTIVE ANTIVIRAL AGENTS

Rabi, J.A.

**MSC13)** THE STUDY OF THE RADIOPROTECTIVE ACTIVITY OF 1-PHENYL-2-(BUTYLAMINO)ETHANE-1-THIOSSULFURIC ACID

Moreira, L.S.A.; Nelson, D.L.; Camelo, R.M.; Lopes, M.T.P.; Piló-Veloso, D.

**MSC14)** CRYSTALLIZATION OF PHARMACEUTICALS.

Ojinnako, I.; Chibundu, Y.; Onwudiwe, M.C