INCT OF DRUGS AND MEDICINES

2011

ANNUAL ACTIVITIES REPORT

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2011

ANNUAL ACTIVITIES REPORT

Drugs and Medicines INCT

ABOUT THE COVER

The expression used of the allegory of Don Quixote in the previous versions has attempted to show the investigative nature of the human being searching for knowledge and truth. The current character, Don Quixote himself, sets the tone for the current stage, where contemplation is given up for the reality of research in full, in the scientist who uncovers the universe and the truths it contains.

Dr. Angelo da Cunha Pinto

DRUGS AND MEDICINES INCT

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SUMMARY

EDITORIAL

This is the third edition of the Annual Activities Report of the National Institute of Science and Technology in Drugs and Medicines (INCT-INOFAR), describing the activities conducted during 2011. We have chosen the same format as the one used in the previous years, including the results of the research subprojects in radical innovation in drugs as well as of those relating to incremental innovation, in accordance with our mission and vocation.

In the field of radical innovation, design, planning, synthesis and evaluation of substances candidate for new drugs, we act in six areas, compatible with the expertise of the teams associated with the INCT-INOFAR network, which include inflammation, pulmonary disease, especially chronic obstructive pulmonary disease, pain, central nervous system, cardiovascular system, as well as chemotherapy for cancer and antiparasitary, especially leishmaniasis. In this radical innovation environment, we have achieved significant results, especially in the subprojects classified as advanced in the chain of drug innovation. Nevertheless, all the other subprojects have seen significant progress that has led us to conclude, in our V Follow-Up and Evaluation Meeting, in November 2011, that we need to reorganize the INCT-INOFAR portfolio for the following two years, according to the previously established timeline.

INCT-INOFAR established, on November 18, 2011, a cooperation agreement with the Interdisciplinary Center of Pharmacogenomics and Pharmaceutical Research (ICEPHA) of the University of Tübingen, Germany. Through this deal, we broaden the international scope of INCT-INOFAR and the bases for scientific exchange and the development of innovative research projects in new drugs. On the other hand, the agreement establishes the organization of scientific and academic activities, like courses, conferences, seminars, symposiums, or lectures, and the exchange of researchers and/or students, as well as the exchange of materials and publications of mutual interest.

In the field of incremental innovation, we have achieved very valuable results that have crowned the efforts of the research groups led by Professors Angelo da Cunha Pinto of the Institute of Chemistry at UFRJ and Luiz Carlos Dias, of the Institute of Chemistry at UNICAMP, who by supervising the work of Doctors Barbara Vasconcelos Silva and Adriano Siqueira Vieira, at UFRJ and UNICAMP, respectively, have concluded the synthesis of two important drugs, sunitinib and fluoxetine, respectively. The first is an important tyrosine-kinase inhibitor, still under patent, indicated for the control of stomach cancer, with countless judicial sentences that force the national health care system (SUS) to spend a significant amount of money to carry out. The route developed, at a bench scale (2g), represents a significant

contribution to the full verticalization of the chain of generic medications, representing a synthesis technology capable of being scaled and transferred to the business sector, public or otherwise, in case the Ministry of Health decides to support it. We understand that the synthesis of this important anticancer drug supports, in a significant manner, a future political decision by the Brazilian government on the issue. The second drug, fluoxetine, which does not have an effective patent, represents another contribution by the research group to led by Professor Dias (UNICAMP) to our technological qualification in generic drugs, because it is an important resource in the treatment of central illnesses. Still in the environment of incremental innovation, we also achieved, in 2011, a patent request for the synthesis route developed by the same group for atorvastatin (see page 55), described in our AAR-2010. Considering that atorvastatin is the most valuable drug in the market, a member of the HMGCoA-reductase inhibitors, which made Pfizer worldwide, during the patent monopoly (1991-2001), a total of US$ 120 billion. Considering this is the biggest best seller in the history of drugs, and that its patent was voided in November 2011 in its main world market and a few months before that in Brazil, it then became the most promising and coveted generic drug, since the branded drug (Lipitor™), sold, worldwide, US$ 13 billion just on the last year the patent was effective. The synthetic route developed by INCT-INOFAR greatly surpasses the efficiency and yield of the original one described by Pfizer, so this patent request represents an important technological property created by INCT-INOFAR, deserving future scaling and transfer to the drug industry sector.

There were countless activities carried out by INCT-INOFAR during this time referring to education, promotion, and increasing awareness of pharmaceutical sciences, and they are listed in a bilingual booklet, which is available in our portal (www.inct-inofar.ccs.ufrj.br/revista). We highlight the booklet on the correct and rational use of medications in general (http://www.portaldosfarmacos.ccs.ufrj.br/) and most of all, the second booklet, on antibiotics (http://www.portaldosfarmacos.ccs.ufrj.br/). This second booklet was made available at the site for the Brazilian regulatory agency (ANVISA), and it will have an animated version produced by INCT-INOFAR, currently under production. O INCT-INOFAR keeps the Pharmaceuticals Portal updated (http://www.portaldosfarmacos.ccs.ufrj.br), a web page where it publicizes its activities and publishes articles on topics related to drugs and medications (http://www.portaldosfarmacos.ccs.ufrj.br/).

I wish that this volume of the Annual Activities Report of the National Institute of Science and Technology in Drugs and Medicines (INCT-INOFAR), describing the activities developed in 2011, is a pleasant and easy read, as well as a perpetual reference source.

Rio de Janeiro, June 2012.

Eliezer J. Barreiro
INCT-INOFAR Coordinator


1º Seminário de Acompanhamento e Avaliação
INSTITUTOS NACIONAIS DE CIÊNCIA E TECNOLOGIA

NATIONAL INSTITUTES OF SCIENCE AND TECHNOLOGY

The National Institutes of Science and Technology (INCTs) were created by the Brazilian government with the goal of promoting the creation of research networks in areas strategic for sustainable development.

The INCTs connect laboratories or associated research groups in different parts of Brazil to act in a defined area or theme, each of them coordinated by a hosting institution renowned for its scientific and technological excellence.

With 122 Institutes created since the end of 2008, the INCT Program (publication number MCT/CNPQ no014/2008) is the largest program to promote Science and Technology in Brazil.

The INCTs are an initiative of the Ministry of Science and Technology (MCT), through the National Council for Scientific and Technological Development (CNPq), with the financial support of the state Foundations for Research Support (FAPERJ, FAPESP, FAPEAM, FAPESC, FAPESPA, and FAPEMIG), of the Ministry of Health through its Department of Science and Technology (DECIT/MS), of the Ministry of Education, through the Coordination for the Improvement of Higher Education Personnel (CAPES), and of the National Bank for Social and Economic Development (BNDES).

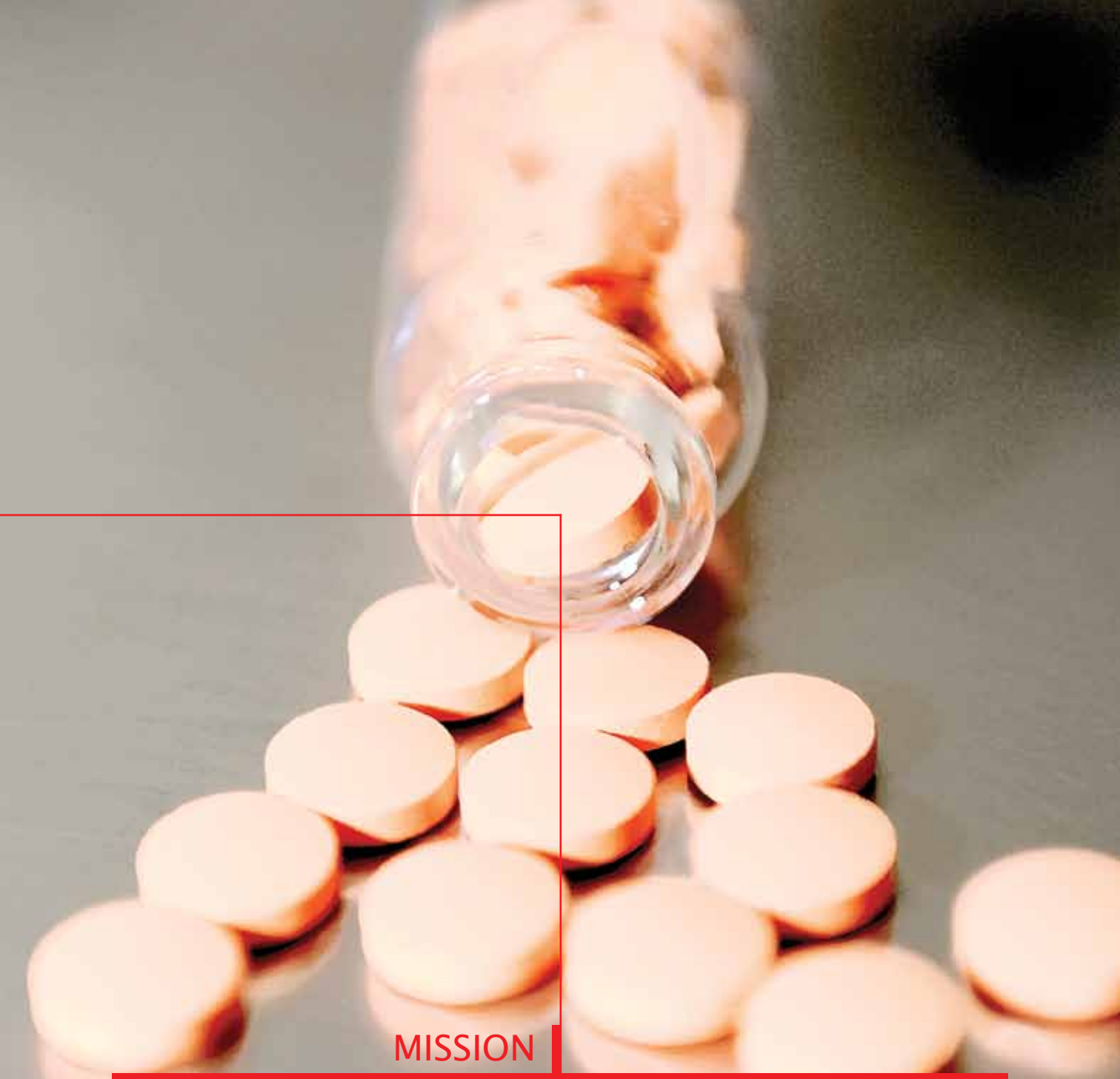
DRUGS AND MEDICINES INCT (INCT–INOFAR)

The National Institute of Science and Technology of Drugs and Medicines (INCT-INOFAR) brings together nationwide scientific expertise in pharmaceutical innovation (radical innovation) and generic pharmaceuticals (incremental innovation), building active bridges between its scientists and industry, both private and public, that is capable of adopting the technology developed by the Institute.

INCT-INOFAR has as its main goal to coordinate different research subprojects in the theme of the complex chain of innovation in pharmaceuticals and medications. The network of scientific expertises that comprises INCT-INOFAR is made up of 31 research groups located in 15 teaching and research institutions in 8 Brazilian states.

INCT-INOFAR has the task of training human resources making them qualified in technical-scientific areas of expertise in all the distinct stages of the process of discovery and invention of new pharmaceuticals – from the election of the most adequate therapeutic target for the treatment of the chosen physiopathology to the completion of bioassays in the preclinical stage.

Parallel to laboratory research, INCT-INOFAR coordinates activities in Scientific Awareness and Health Education that aim to create critical conscience in the use of medications. For this, INCT-INOFAR has created the Pharmaceuticals Portal www.portaldosfarmacos.ccs.ufrj.br, a website where the Institute publicizes its research activities and where its Health Education materials are made available.



MISSION

- To organize national scientific expertises into an effective and productive network of research in pharmaceuticals and medications;

- To support scientific research subprojects on the chain of innovation in pharmaceuticals and medications;

- To act in both incremental and radical innovation, in generic drugs and new pharmaceutical candidates, respectively;

- To study and develop total synthesis routes for generic pharmaceuticals, advanced intermediaries and raw materials strategic for the sector;

- To contribute to the qualified scientific training of personnel in Medicinal Chemistry & Pharmacology;

- To promote awareness in the sciences related to pharmaceuticals and medications, as well as effectively promoting their rational and safe use.

PHARMACEUTICAL INNOVATION

With the help of its entire research network, INCT-INOFAR studies and develops several subprojects classified as radical innovation. It is also a part, in a more minor role, in incremental innovation subprojects, studying new routes for the total synthesis of generic pharmaceuticals.

In the field of radical innovation, the Institute aims to discover/invent original substances, active in *in vivo* pharmacological models, widely validated, that are capable of originating new pharmaceutical candidates in several therapeutic classes.

In the field of incremental innovation, INCT-INOFAR leads projects that focus on the search of new, efficient, and accessible synthetic routes, for generic drugs already available in the market – and that represent important tools in public health policies and in the pharmaceutical care of the population – as well as for those medications that are about to have their patents expire, and that represent new business opportunities from a marketing point of view.

INCT-INOFAR Research Areas

- INFLAMMATION
- PULMONARY DISEASE
- PAIN
- CENTRAL NERVOUS SYSTEM
- CARDIOVASCULAR SYSTEM
- CHEMOTHERAPY: ANTICANCER AND ANTIPARASITIC
- GENERIC DRUGS

CURRENT INCT–INOFAR SUBPROJECTS

INCREMENTAL INNOVATION

1] ***Sunitinib synthesis.***
Prof. Eliezer J. Barreiro (UFRJ) – CV Lattes
Prof. Angelo da Cunha Pinto (UFRJ) – CV Lattes
Profa. Bárbara Vasconcelos (UFRJ) – CV Lattes

2] ***Fluoxetin synthesis.***
Prof. Eliezer J. Barreiro (UFRJ) – CV Lattes
Prof. Luiz Carlos Dias (UNICAMP) – CV Lattes
Dr. Adriano V. Siqueira (UNICAMP) – CV Lattes

3] ***Atorvastatin synthesis (patent).***
Prof. Eliezer J. Barreiro (UFRJ) – CV Lattes
Prof. Luiz Carlos Dias (UNICAMP) – CV Lattes
Dr. Adriano V. Siqueira (UNICAMP) – CV Lattes

RADICAL INNOVATION

ADVANCED STAGE

4] ***Development of new antiasthma pharmaceutical prototypes (LASSBio-596).***
Prof. Patricia Rieken Macedo Rocco (UFRJ) – CV-Lattes
Prof. Lidia Moreira Lima (UFRJ) – CV-Lattes

5] ***Study of N-phenylpiperazine derivates functionalized as prototypes for the development of new atypical antipsychotics.***
Prof. Stela Maris Kuze Rates (UFRGS) – CV-Lattes
Prof. Carlos Alberto Manssour Fraga (UFRJ) – CV-Lattes

SEMI-ADVANCED STAGE

6] ***Study of the potential anti-inflammatory effect of compound LASSBio 897, in models of silicosis and asthma.***
Prof. Patricia Machado Rodrigues e Silva (FIOCRUZ – RJ) – CV-Lattes
Prof. Marco Aurelio Martins (FIOCRUZ – RJ) – CV-Lattes

INTERMEDIATE STAGES

7] ***Semicarbazone benzaldehyde (BS).***
Prof. Heloisa de Oliveira Beraldo (UFMG) – CV-Lattes

8] ***Therapeutic potential of new vasodilator (LASSBio 1289) in arterial and pulmonary hypertension.***
Prof. Gisele Zapata Sudo (UFRJ) – CV-Lattes

9] ***Pharmacological evaluation of new neuroactive derivates of Zolpidem***
Prof. Roberto Takashi Sudo (UFRJ) – CV-Lattes

10] ***"In silico" prediction and "in vitro" production by bioconversion of human metabolites of pharmaceutical prototype candidates.***
Prof. Valeria de Oliveira (UFG) – CV-Lattes

11] ***Planning, synthesis, and pharmacological evaluation of vectorized and self-organized neuroactive pharmaceutical.***
Prof. Ricardo Menegatti (UFG) – CV-Lattes

12] ***Planning, synthesis, structural characterization and pharmacological evaluation of new candidates for anti-inflammatory and neuroactive pharmaceuticals.***
Prof. Claudio Viegas Junior (UNIFAL) – CV-Lattes

13.] ***Evaluation of the leishmanicide activity of a series of semicarbazone and hydrazine-N-acylhydrazone derivates.***
Prof. Magna Suzana Alexandre Moreira (UFAL) – CV-Lattes

EARLY STAGES

14] ***Theoretical investigation of the action mechanism of dialkylphosphorylidrazones as inhibitors of the ribose 5-phosphate isomerase enzyme of the Trypanosoma cruzi and plasmodium falciparum.***
Prof. Carlos Mauricio R. de Sant'Anna (UFRRJ) – CV-Lattes

15] ***Triage of new inhibitors of the replication of the human immunodeficiency virus type 1 (HIV-1) from LASSBio chemical library.***
Prof. Luciana Jesus da Costa (UFRJ) – CV-Lattes

16] ***Evaluation of antitumor activity of new molecules structurally planned from imatinib prototype.***
Prof. Patricia Dias Fernandes (UFRJ) – CV-Lattes

17] ***Prospection of opportunities in new generics and innovative generics.***
Prof. Adelaide Mª de Souza Antunes (UFRJ) – CV-Lattes

NEW APPROVED SUBMISSIONS

18] ***Pharmacological and toxicological evaluation of new pharmaceutical candidates for the prevention and treatment of myocardiopathy and neuropathy caused by diabetes mellitus.***
Prof. Gisele Zapata Sudo (UFRJ) – CV-Lattes

19] ***Planning of structural changes for the optimization of the affinity of the IKK2, LASSBio-1524 enzyme selective inhibitor.***
Prof. Laurent Emmanuel Dardenne (LNCC) – CV-Lattes

20] ***New 5-aril-2-furfuril-N-acylhydrazone derivates functionalized with Power anti-inflammatory and analgesic activity: LASSBio-1609 and LASSBio-1636.***
Prof. Carlos Alberto Manssour Fraga (UFRJ) – CV-Lattes

21] ***Technological prospection of new generics in Brazil.***
Prof. Adelaide Maria de Souza Antunes (UFRJ) – CV-Lattes

22] ***Synthesis and theoretical study of the action mechanism of new dialkylphosphorylhydrazones as inhibitors of the ribose 5-phosphate isomerase enzyme.***
Prof. Carlos Mauricio R. de Sant'Anna (UFRRJ) – CV-Lattes

23] ***Impact of nanoparticle therapy on the thymuline gene in chronic allergic asthma model.***
Prof. Patricia Rieken Macedo Rocco (UFRJ) – CV-Lattes

24] ***Development of new antiarthritis pharmaceutical candidates, MAPK p-38 modulators.***
Prof. Lidia Moreira Lima (UFRJ) – CV-Lattes

25] ***Discovery of new antitumor pharmaceutical candidates analog to combrestatin A4.***
Prof. Lidia Moreira Lima (UFRJ) – CV-Lattes

26] ***Development of new anti-inflammatory and analgesic pharmaceutical candidates from safrole.***
Prof. Lidia Moreira Lima (UFRJ) – CV-Lattes

27] ***Study for the identification of new sulfonamide compounds effective in the control of pulmonary inflammation caused by silica in mice.***
Prof. Patricia Machado Rodrigues e Silva Martins (FIOCRUZ-RJ) – CV-Lattes

28] ***Implementation and validation of pre-clinical trial model for the evaluation of the teratogenic effect of bioactive substances: evaluation of the LASSBio 468 and LASSBio 596 prototypes.***
Prof. Aloa Machado de Souza – CV-Lattes

MULTIDISCIPLINARY RESEARCH NETWORK

The pharmaceutical innovation process has clear interdisciplinary and multidisciplinary characteristics that demand competences in distinct areas of health sciences. INCT-INOFAR is aware of this, and therefore coordinates a network of research groups that excel scientifically and academically in different areas, and that have a history of previous results that makes them qualified to carry out successfully the several stages of the process of rational invention of new pharmaceuticals.

INCT-INOFAR has a multidisciplinary staff of experts in several areas such as Medicinal Chemistry, Pharmacology, Organic Chemistry, Toxicology, Organic Synthesis, Biochemistry, Computational Chemistry, Spectroscopy, and Natural Products Chemistry, among others.

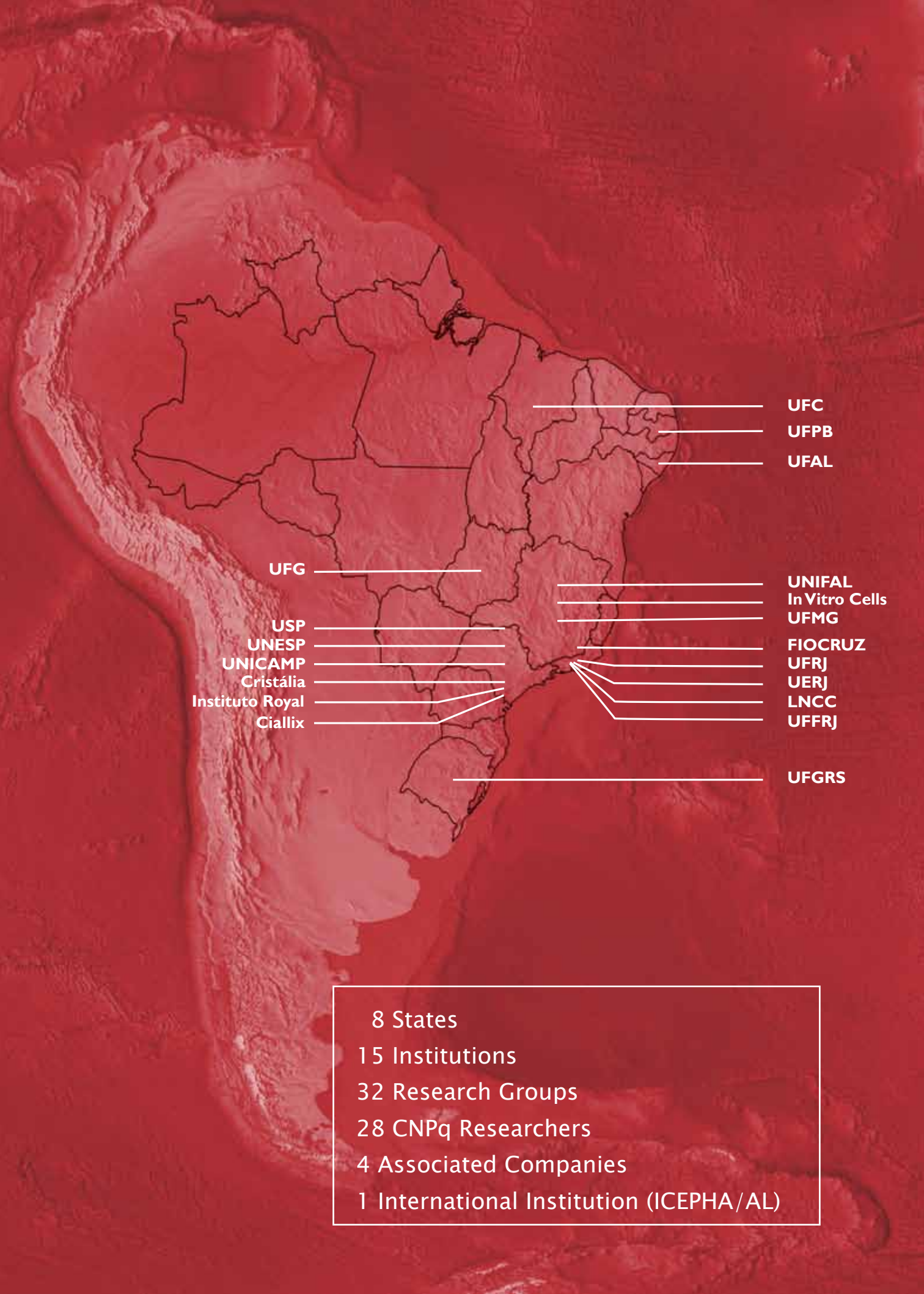
SCIENTIFIC EXCHANGE

By allowing researchers from several different institutions and geographical regions to work together, INCT-INOFAR enables the exchange between large research centers and emerging research groups. Through cooperative action, INCT-INOFAR contributes for the increase of scientific and technological production in emerging centers, especially in the Midwest and Northeast regions, which in turn benefits the professional qualification of undergraduate and graduate students.

Through the past three years, INCT-INOFAR has seen remarkable benefits in the advancement of these emerging science groups. So INCT-INOFAR actively contributes to reduce the regional scientific imbalance in Brazil, as well as strengthens the expertise in a sector that is strategic for Brazil.

INCT-INOFAR has been laying the groundwork for more international cooperation, and it signed a cooperation agreement in November 2011 with the Interdisciplinary Center of Pharmacogenomics and Pharmaceutical Research of the University (ICEPHA) of Tübingen, in Germany. The agreement was signed (see page 30) to enhance the scientific exchange in the development of new research between both Institutions.

Among the main goals of the agreement are the development of joint projects, the organizing of academic and scientific activities like courses, conferences, seminars, symposiums or lectures, the exchange of researchers and/or students and also the exchange of materials and publications of mutual interest.



8 States
15 Institutions
32 Research Groups
28 CNPq Researchers
4 Associated Companies
1 International Institution (ICEPHA/AL)

INCT-INOFAR RESEARCH GROUPS: LABORATORIES AND SUPERVISORS

RIO DE JANEIRO

1] FIOCRUZ

Laboratory of Inflammation
Marco Aurelio Martins - CV-Lattes

National School of Public Health
Francisco Jose Roma Paumgartten - CV-Lattes

2] UERJ

Department of Pharmacology
Theresa Christina Barja-Fidalgo - CV-Lattes

3] UFRJ

Laboratory of Evaluation and Synthesis of Bioactive Substances – LASSBio
Carlos Alberto Manssour Fraga - CV-Lattes
Lidia Moreira Lima - CV-Lattes

Chemical Industry Information System – SIQUIM
Adelaide Maria de Souza Antunes - CV-Lattes

Pulmonary Investigation Laboratory
Patricia Rieken Macedo Rocco - CV-Lattes

Biochemical and Molecular Pharmacology Laboratory
François Germain Noel - CV-Lattes

Cardiovascular Pharmacology Laboratory
Gisele Zapata Sudo - CV-Lattes

Muscular Excitement-Contraction Coupling Laboratory
Roberto Takashi Sudo - CV-Lattes

Molecular Virology I Laboratory
Jose Nelson dos Santos Silva Couceiro - CV-Lattes

Natural Products and Chemical Transformations Laboratory
Angelo da Cunha Pinto - CV-Lattes

Technological Development Support Laboratory
Francisco Radler de Aquino Neto - CV-Lattes

Pharmacology of Inflammation and Nitric Oxide Laboratory
Patricia Dias Fernandes - CV-Lattes

Genetic and Immunology of Viral Infections Laboratory
Luciana de Jesus da Costa - CV-Lattes

4] UFRRJ

Exact Sciences Institute
Carlos Mauricio Rabello de Sant'Anna - CV-Lattes

5] LNCC

Molecular Modeling of Biological Systems Group
Laurent Emmanuel Dardenne - CV-Lattes

SAO PAULO

6] USP-RP
Pain and Inflammation Laboratory
Fernando de Queiroz Cunha - CV-Lattes

7] UNESP ARARAQUARA
Bioassays, Biosynthesis, and Ecophysiology of Natural Products Nucleus (NUBBe)
Vanderlan da Silva Bolzani - CV-Lattes

8] UNICAMP
Synthetic Organic Chemistry Laboratory
Luiz Carlos Dias - CV-Lattes

MINAS GERAIS

9] UFMG
Innovation in Organic and Inorganic Compounds with Pharmacological Activity Group
Heloisa de Oliveira Beraldo - CV-Lattes

10] UNIFAL
Phytochemistry and Medicinal Chemistry Laboratory
Claudio Viegas Junior - CV-Lattes
Marcia Paranho Veloso - CV-Lattes

RIO GRANDE DE SUL

11] UFRGS
Genotox-Royal Unit
Joao Antonio Pegas Henriques - CV-Lattes

Experimental Psychopharmacology Laboratory
Stela Maris Kuze Rates - CV-Lattes

GOIAS

12] UFG
Bioconversion Laboratory
Valeria de Oliveira - CV-Lattes

Pharmacology and Cellular Toxicology Laboratory (contributor)
Marize Campos Valadares Bozinis - CV-Lattes

Medicinal Pharmaceutical Chemistry Laboratory
Ricardo Menegatti - CV-Lattes

Cardiovascular Pharmacology Laboratory (contributor)
Matheus Lavorenti Rocha - CV-Lattes

ALAGOAS

13] UFAL
Pharmacology and Immunity Laboratory
Magna Suzana Alexandre Moreira - CV-Lattes

CEARA

14] UFC
Clinical Pharmacology Unit
Manoel Odorico de Moraes - CV-Lattes

Inflammation and Cancer Pharmacology Laboratory
Ronaldo de Albuquerque Ribeiro - CV-Lattes

PARAIBA

15] UFPB
Toxicological Assays Laboratory (LABETOX)
Margareth de Fatima Formiga Melo Diniz - CV-Lattes

QUALIFICATION OF HUMAN RESOURCES

So that a truly innovative medication is discovered, diverse and highly qualified personnel is required to successfully carry out all the stages in the chain of innovation.

By contributing to enhance Brazilian expertise in the discovery/invention of new pharmaceuticals and medications, INCT-INOFAR strongly acts in the qualification of human resources in the several research centers that are associated with it.

INCT-INOFAR promotes scientific qualification on all academic levels: undergraduate, master, doctorate, and post-doctorate. As part of this qualification, graduate students connected to the subprojects studied are encouraged to take part in scientific exchange with laboratories with scientific expertise, so that the established goals can be achieved in the correct deadlines.

Through the scientific exchange promoted and encouraged by INCT-INOFAR, the Institute contributes not only for the qualification of new researchers, but also for the updating of the skills of senior researchers. Keeping renowned talented researchers in the country is also one of the INCT-INOFAR goals.

INCT-INOFAR researchers are an active part of qualification and training activities through their connection to 17 renowned Graduate Programs throughout Brazil. Over half of the Graduate Programs that are connected to INCT-INOFAR researchers are qualified as 6 or 7 in excellence out of a possible maximum of 7. Under the guidance of professors and researchers associated with INCT-INOFAR, during the three years of the Institute, 39 doctoral theses and 39 master theses have been completed.

Graduate Programs with INCT-INOFAR researchers:

- (USP/RP) GRADUATE PROGRAM IN BIOLOGICAL SCIENCES (PHARMACOLOGY) M / D – CAPES – 7
- (UNICAMP) GRADUATE PROGRAM IN CHEMISTRY – M / D – CAPES 7
- (UFRJ) GRADUATE PROGRAM IN CHEMISTRY M/D – CAPES 7
- (UNESP/ARAR) GRADUATE PROGRAM IN CHEMISTRY M / D– CAPES 6
- (UERJ) GRADUATE PROGRAM IN BIOSCIENCES – CAPES 6
- (UFC) GRADUATE PROGRAM IN PHARMACOLOGY – CAPES 6
- (FIOCRUZ) GRADUATE PROGRAM IN CELLULAR AND MOLECULAR BIOLOGY M / D – CAPES 6
- (UFMG) GRADUATE PROGRAM IN CHEMISTRY – M/D – CAPES 6
- (UFRGS) GRADUATE PROGRAM IN PHARMACEUTICAL SCIENCES M / D – CAPES 6
- (UFPB) GRADUATE PROGRAM IN BIOACTIVE NATURAL AND SYNTHETIC PRODUCTS – M / D – CAPES 5
- (UFRJ) GRADUATE PROGRAM IN BIOLOGICAL SCIENCES (PHARMACOLOGY AND MEDICINAL CHEMISTRY) M/D – CAPES 4
- (UNIFAL) GRADUATE PROGRAM IN CHEMISTRY M – CAPES 4
- (UFRRJ) GRADUATE PROGRAM IN CHE ISTRY AND BIOTECHNOLOGY M / D – CAPES 4
- (UFAL) GRADUATE PROGRAM IN HEALTH SCIENCES M – CAPES 3
- (UNIFAL) GRADUATE PROGRAM IN PHARMACEUTICAL SCIENCES M – CAPES 3
- (UFG) GRADUATE PROGRAM IN PHARMACEUTICAL SCIENCES M – CAPES 3

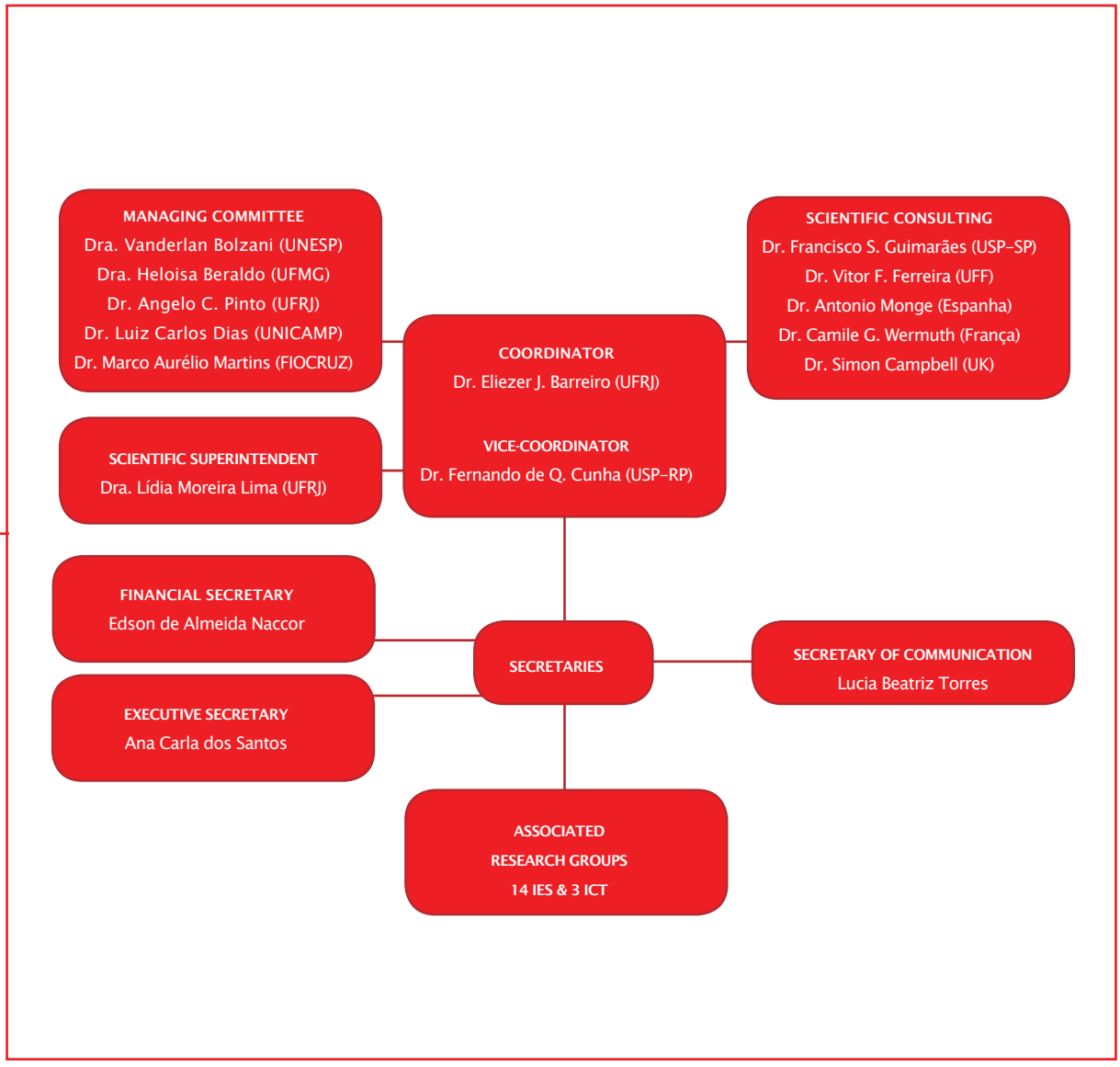
ORGANIZATIONAL STRUCTURE

The organizational structure of INCT-INOFAR is made up of a Coordinator, a Vice-Coordinator, and the Management and Follow-Up Committee (CGA). The CGA is a consulting and decision-making body that is responsible for the strategic planning of INCT-INOFAR activities.

The Scientific Superintendence supports the Coordination, acting in the technical-scientific evaluation of projects, as well as on making sure previously established deadlines are met. INCT-INOFAR also has, under confidentiality terms, specialist consultants acting on the evaluation of projects, so that research activities may be optimized. In a few of the projects, the consultants suggest changes necessary to meeting the Institute goal of discovering new Brazilian pharmaceuticals.

The INCT-INOFAR network of scientific competencies is made up of 32 research groups located in 15 institutions distributed in 8 Brazilian states. Each research group associated with INCT-INOFAR is led by a specialist responsible for the scientific interaction of his or her team among themselves and with other research groups.

The Financial, Executive, and Media Secretaries provide the support needed for the full development of the research and publicizing activities carried out by INCT-INOFAR. They are physically located in the Health Sciences Center of UFRJ, where the Institute headquarters is located.


MANAGING COMMITTEE
Dra. Vanderlan Bolzani (UNESP)
Dra. Heloisa Beraldo (UFMG)
Dr. Angelo C. Pinto (UFRJ)
Dr. Luiz Carlos Dias (UNICAMP)
Dr. Marco Aurélio Martins (FIOCRUZ)
SCIENTIFIC CONSULTING
Dr. Francisco S. Guimarães (USP-SP)
Dr. Vitor F. Ferreira (UFF)
Dr. Antonio Monge (Espanha)
Dr. Camile G. Wermuth (França)
Dr. Simon Campbell (UK)
COORDINATOR
Dr. Eliezer J. Barreiro (UFRJ)
VICE-COORDINATOR
Dr. Fernando de Q. Cunha (USP-RP)
SCIENTIFIC SUPERINTENDENT
Dra. Lídia Moreira Lima (UFRJ)
FINANCIAL SECRETARY
Edson de Almeida Naccor
EXECUTIVE SECRETARY
Ana Carla dos Santos
SECRETARIES
SECRETARY OF COMMUNICATION
Lucia Beatriz Torres
ASSOCIATED
RESEARCH GROUPS
14 IES & 3 ICT

INCT-INOFAR has the support, albeit informal, of pharmaceutical companies like Cristalia Chemical Pharmaceutical Products Ltd., Royal Institute, In Vitro Cells Toxicological Research S.A. and Ciallyx Laboratories & Consultants.

ASSOCIATED COMPANIES

IN VITRO CELLS

www.invitrocells.com.br

In Vitro Cells – Toxicological Research S.A. is a technology based company located at Biominas Foundation (Belo Horizonte, MG). Its founders are professors of the Federal University of Minas Gerais (UFMG) in the fields of Toxicology and Biochemistry. The company is an INCT-INOFAR partner to conduct in vitro bioassays to test the safety and efficacy of new pharmaceutical candidates developed by the Institute.

CRISTALIA LABORATORIES CHEMICAL AND PHARMACEUTICAL PRODUCTS

www.2cristalia.com.br

Cristalia is a pharmaceutical company associated with INCT-INOFAR, capable of supporting the stages of pharmacotechnical developing of new prototype compounds that reach this advanced stage of the chain of innovation in pharmaceuticals and medications. Under confidentiality and non-disclosure terms, Cristalia will benefit, if it wishes, from information on the current projects, by expressing an interest in absorbing the technology developed at INCT-INOFAR. So that the technology may be transferred, the Innovation Agency of UFRJ and its peer at another INCT-INOFAR research institution will negotiate directly with the interested parties, including financial backers.

ROYAL INSTITUTE (INSTITUTO ROYAL)

www.institutoroyal.org.br

Toxicology is a very delicate stage that might absolve or condemn forever a pharmaceutical candidate prototype. INCT-INOFAR prioritizes the studies of cytotoxicity, mutatoxicity, and genotoxicity, as well as acute toxicology, with the molecules that have proven attractive in terms of pharmacological activities as early as possible in the chain of pharmaceutical innovation. To ensure that all the preclinical toxicology stages are accredited in good laboratory practices (BPL/GLP), INCT-INOFAR has a partnership with the Royal Institute, which is a result of the merger of two toxicology laboratories housed in two different universities. The Genotox-Royal Institute, located at UFRGS, is responsible for the genetic toxicity studies, while Unitox-Royal, located at the University of Santo Amaro (UNISA-SP) is responsible for animal toxicity tests.

CIALLYX LABORATORIES & CONSULTANTS

www.ciallyx.com.br

Ciallyx Laboratories & Consultants is a company housed at CIETEC (Incubator Center for Technological Companies) that carries out efficacy studies (concept tests) and safety studies (studies and toxicological assays) for new molecules, medications, and formulations. Ciallyx achieves results by following national and international protocols under strict quality parameters, guided by the international guidelines of the Good Laboratory Practices – GLP. The company is an INCT-INOFAR partner to conduct in vivo bioassays to evaluate the safety and efficacy of new pharmaceutical candidates developed by the Institute.

INTERNATIONAL ACTIVITIES

INCT-INOFAR established, on November 18, 2011, a cooperation agreement with the Interdisciplinary Center of Pharmacogenomics and Pharmaceutical Research (ICEPHA) of the University of Tübingen, Germany. Through this deal, we broaden the international scope of INCT-INOFAR and the bases for scientific exchange and the development of innovative research projects in new pharmaceuticals. On the other hand, the agreement establishes the organization of scientific and academic activities, like courses, conferences, seminars, symposiums, or lectures, and the exchange of researchers and/or students, as well as the exchange of materials and publications of mutual interest.

SYNTHESIS OF SUNITINIB

Eliezer J. Barreiro[a], Angelo C. Pinto[b], Bárbara V. Silva[b]
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INTRODUCTION

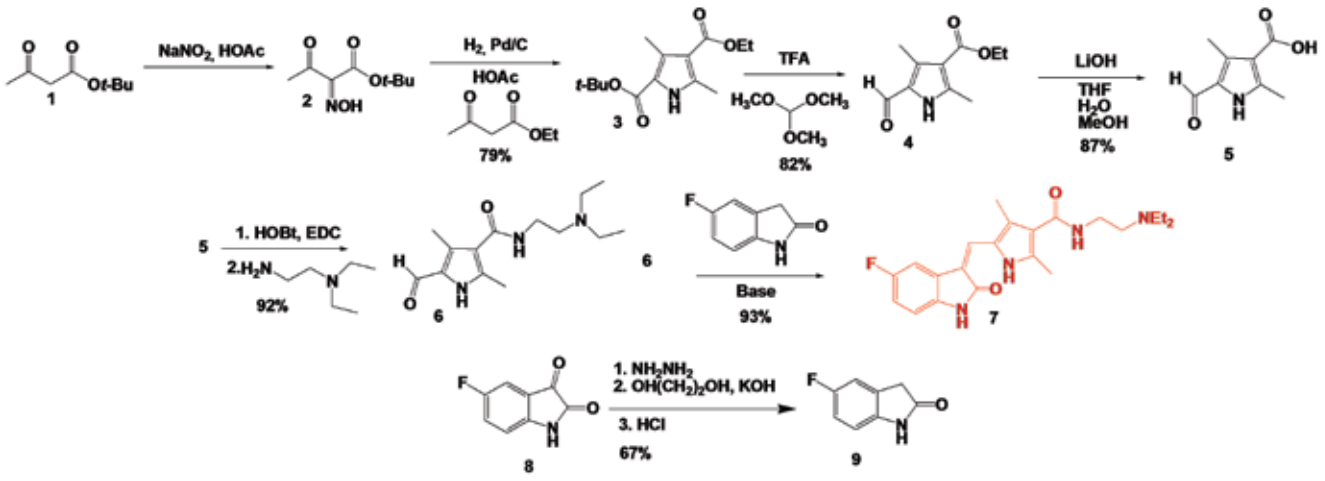
The INCT-INOFAR leads projects that aim to develop new and innovative synthetic routes to generic drugs already available in the market, as well as to those whose patents are about to expire. These projects are in the area of incremental and radical innovation, one of the important focus of the INCT-INOFAR. In this project, the selected drug was sunitinib. Sunitinib, marketed as Sutent by Pfizer, is an oral multi-targeted receptor tyrosine kinase, employed in the treatment of gastrointestinal stromal tumor, pancreatic neuroendocrine tumors and renal cell carcinoma.

RESULTS AND DISCUSSION

Our initial efforts were focused on the preparation of the 5-formyl 2,4-dimethyl 1H- pirrole 3-carboxylic acid [5], according to the route reported in the literature. Aldehyde [5] was prepared in 4 steps (55% overall yield), according to the synthetic route in Scheme 1. Activation of the carboxylic acid with HOBt, EDC, followed by reaction with diethylethylenediamine, furnished amide [6] in 92% yield. Oxindole [9] was prepared from 5-fluorisatin by two methods: Wolff-Kishner reduction and hydrogenation under 62 psi (4.3 bar) using Pd/C as catalyst. Knoevenagel condensation between aldehyde [6] and oxindole [9] using KOH or piperidine afforded 7 in 93% yield.

Synthesis of Sunitinib and Synthesis of Fluoxetine

SCHEME 1



CONCLUSIONS

Sunitinib was synthesized with an overall yield of ~35% in 6 steps from 5-fluorisatin.

SYNTHESIS OF FLUOXETINE HYDROCLORIDE

Eliezer J. Barreiro[a], Luiz C. Dias[b], Adriano S. Vieira[b]

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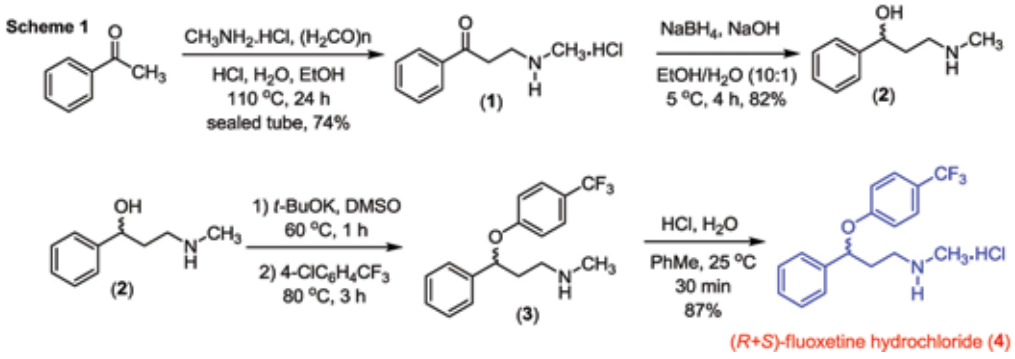
[b]Universidade Estadual de Campinas, Instituto de Química, Departamento de Química Orgânica, Campinas-SP.



INTRODUCTION

The INCT-INOFAR leads projects that aim to develop new and innovative synthetic routes of generic drugs already available in the market as well as for those that have patents about to expire. These projects are in the area of incremental and radical innovation, one of the important focus of the INCT-INOFAR. In this part of the project ,the selected drug was fluoxetine hydrochloride.

Fluoxetine hydrochloride is an antidepressant of the class of selective inhibitors of serotonin reuptake. Its main indications are for use in moderate to severe depression, obsessive compulsive disorder (OCD) and nervous bulimia. It is marketed and used as a racemic mixture.

RESULTS AND DISCUSSION

Initially, we carried out a literature search on the synthetic routes of fluoxetine hydrochloride described in patents and papers. We have developed a very efficient synthetic strategy to prepare 2g of fluoxetin hydrochloride.

The synthetic route developed is short, efficient and uses inputs readily available commercially available in the national market (only two inputs are imported) at a relatively low cost. Moreover, the process generates a lower environmental impact since some of the employed solvents are from renewable sources. This fact has a very positive impact on reducing the cost of production of the active ingredient.

CONCLUSIONS

In summary, fluoxetine hydrochloride was obtained in four steps in an overall yield of 51.5% after recrystallization from acetonitrile at -20 °C.

In this process, we used incremental innovation to propose an efficient synthetic route, not described in prior patents of Fluoxetine, in which the drug can be prepared in a practical way.

HIGHLIGHTS

THE METHYLATION EFFECT IN MEDICINAL CHEMISTRY

Eliezer J. Barreiro* Arthur E. Kümmerle and Carlos A. M. Fraga. Chemical Reviews 111 (2011) 5215-5246. DOI: 10.1021/cr200060g

In this review, we aimed to highlight the importance of the simple methyl group as a very useful structural modification in the rational design of bioactive compounds and drugs. The methyl effect, alter both biological phases of a drug, represented by its pharmacodynamics and pharmacokinetics profile, due to the modifications introduced in the stereoelectronic properties. The methyl group is very important in the molecular recognition of endogenous and exogenous organic compounds by bioreceptors. Although it only participates in London dispersion interactions, which are the weakest of all intermolecular interactions,[1] methyl groups have stereoelectronic effects[2] on micromolecules and biomacromolecules, thereby leading to diverse biological effects, including selectivity among bioreceptors, increased potency, and protection against enzyme metabolism.[3] Cognizant of the methyl group's importance in molecular recognition, Wermuth wrote:[3] "The methyl group, so often considered as chemically inert, is able to alter deeply the pharmacological properties of a molecule."

The stereoelectronic changes promoted by methyl groups are directly involved in many biological process.[4] For example, in pyrimidine bases described in Figure 1, one difference between DNA and RNA is the exchange of a thymine for a uracil, two pyrimidine bases that are differentiated by a methyl group at position 5 of the pyrimidine ring of thymine (Figure 1A).

Many of the non-polar aliphatic amino acids, such as glycine, alanine, valine, isoleucine, leucine and methionine, differ solely through homologation or inversion of the positions of methyl groups (Figure 1B). For example, isoleucine has one homologated methyl in comparison to valine. Moreover, alanine is the methyl-homologue of glycine.

Morphine was first described in 1805 by the German pharmacist Sertürner,[5,6] although it was originally isolated by Seguin and Courtois in 1804.[7] Sertürner described the isolation of a white alkaline solid with hypnotic properties, which he called morphine after the Greek god of sleep Morpheus.[5,6] The complex chemical structure of morphine was fully elucidated by Sir Robert Robinson in 1925,[8] who was awarded a Nobel Prize in Chemistry in 1947. Morphine provides a good illustration of the importance of methyl groups and how their simple introduction or removal may significantly alter the pharmacological activity of a bioactive compound, leading to different pharmacokinetic and pharmacodynamic profiles.

Studies of the structure-activity relationships of morphine revealed that removal of the methyl group attached to the sp^3 nitrogen of its benzylisoquinoline ring to generate normorphine causes ca. 6-fold reduction in in vivo analgesic activity (morphine ED_{50} = 4.8 mg/kg and normorphine ED_{50} = 31.5 mg/kg in mice).[9] On the other hand, the simple *O*-methylation of morphine's phenolic hydroxyl group at C-3 generate codeine (Figure 1C)[10] reduces its receptor affinity by 200-fold,[11] demonstrating that methyl groups may also have a negative influence on activity. In this case, the presence of an additional methyl group of codeine reduces its interaction with opioid receptors because the phenolic hydroxyl group of morphine is responsible for the hydrogen bond interactions with the target receptor site (Figure 1C).[12,13] Despite being 200-fold less potent *in vitro*, codeine is only 3-fold less potent than morphine *in vivo* (codeine ED_{50} = 14.5 mg/kg in mice),[9] enabling this drug could be used for the treatment of moderate pain, cough, and diarrhea.[14]

The importance of naturally methylated products as prototype substances for the development of new drugs can be observed in the history of the discovery of compactin.[15] This hexahydronaphthalene derivative is the source for antilipemic agents known as statins; in fact, the statin atorvastatin (Lipitor®) is currently the best-selling drug worldwide (Figure 1D).[16] All of the statins structures contain two methyl groups in an isopropyl group connected to the central heterocyclic system. These methyl groups are important for activity due to their involvement in hydrophobic interactions with Leu562, Cys561 and His752, which create an entropic gain in the interaction with the target receptor. The removal of the methyl groups leads to an 18-fold reduction in potency, as shown in initial structure-activity relationship studies with certain pyrrole derivatives.[17]

Omeprazole (Losec®), is a pyrimidinyl-benzoimidazol derivative with important antiulcer properties, was the first selective gastric H^+-K^+-ATPase inhibitor, which are also referred to as proton pump inhibitors (PPIs) (Figure 1E).[18] Structure-activity relationship studies of omeprazole showed that the introduction of methyl groups into the pyridine ring, due to their electron-donating effects, is beneficial for activity and increases its potency against H^+-K^+-ATPase. The introduction of methyl groups into these inhibitors allows fine tuning

of their pKa and increases the nucleophilicity of the pyridine nitrogen atom, which is a lipophilic weak base (pKa 4.0).[19] By remaining in their non-ionized form at physiological pH, these molecules can diffuse through plasma membranes to the target tissue.

Evaluation of the pharmacologic mechanism of action of these two *N*-acylhydrazones compounds (NAH) showed that the vasodilator activity of LASSBio-294 is totally dependent on the vascular endothelium, whereas LASSBio-785 promotes vasodilatation in a manner that is independent of the endothelium.[20] These results indicate different mechanisms of action and reveal that methylation of LASSBio-294 led to more relevant structural differences than simply the loss of a hydrogen bond donor and increased lipophilicity. Studies using X-ray crystallography, molecular modeling and ultraviolet spectroscopy have elucidated the bioactive conformations of these *N*-acylhydrazone compounds, revealing that the methylation of the *N*-acylhydrazone moiety leads to a conformational change that might be responsible for the different bioactivities of these two derivatives (Figure 1F).[21]

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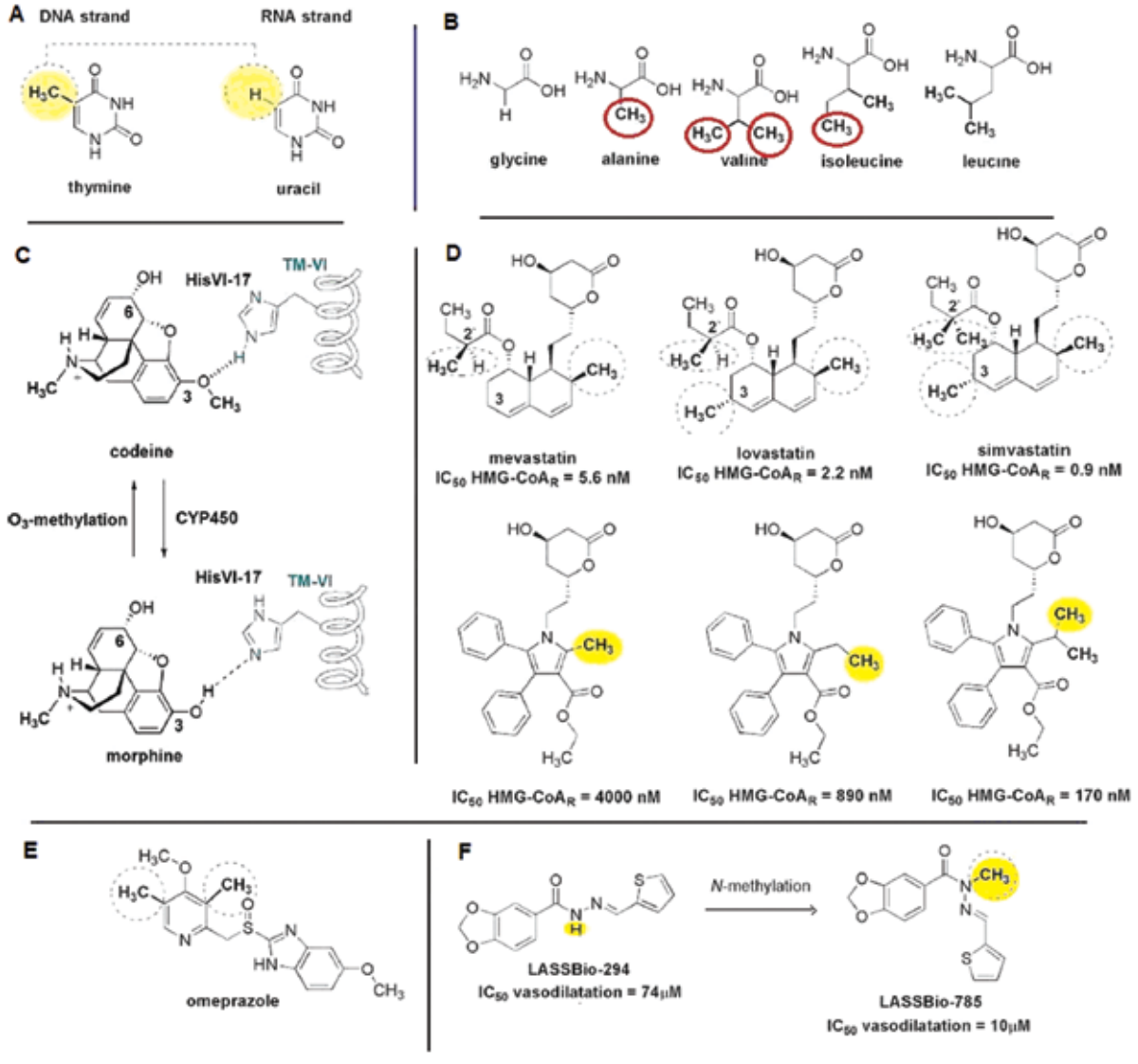
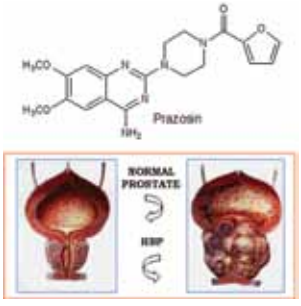


Figure 1 - Methyl effect in the biological activity and molecular recognition., 44, 4004.

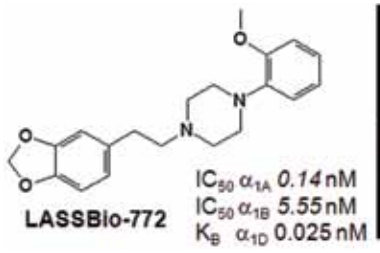
DISCOVERY OF LASSBIO-772, A 1,3-BENZODIOXOLE N-PHENYLPIPERAZINE DERIVATIVE WITH POTENT ALPHA 1A/D-ADRENERGIC RECEPTOR BLOCKING PROPERTIES

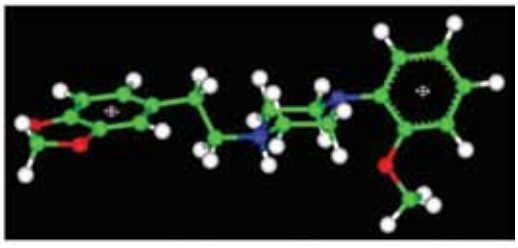
Romeiro, L. A. S.; Ferreira, M. S.; DaSilva, L. L.; Castro, H. C.; Miranda, A. L. P.; Silva, C. L. M.; Noel, F. G.; Nascimento, J. B.; Araujo, C. V.; Tibiriçá, E.; Barreiro, E. J.; Fraga, C. A. M. *Eur. J. Med. Chem.* 46 (**2011**) 3000-3012. **DOI:** 10.1016/j.ejmech.2011.04.032

The human adrenergic receptors are members of the G protein-coupled receptor superfamily that has been extensively exploited as targets for a great number of drugs useful in the treatment of many different diseases [1]. Alpha 1-AR subtypes, *i.e.* alpha 1A, alpha 1B, and alpha 1D have distinct pharmacology and tissue expression, a fact relevant for the treatment of several diseases, such as hypertension and the obstructive symptoms of the lower urinary tract, including the secondary urinary obstruction produced by benign prostatic hyperplasia (BPH). Alternatively to surgical procedures, alpha 1-AR antagonists are efficient to relief the obstructive symptoms of BPH by decreasing the prostatic muscular tonus, mainly through the blockage of alpha 1A-AR. The drugs used for BPH treatment include the some quinazoline derivatives, initially with prazosin and currently with terazosin, doxazosin and alfuzosin, which are nonselective alpha 1-AR antagonists, so that hypotension triggered by alpha 1B-AR blockade is their main adverse effect [2].

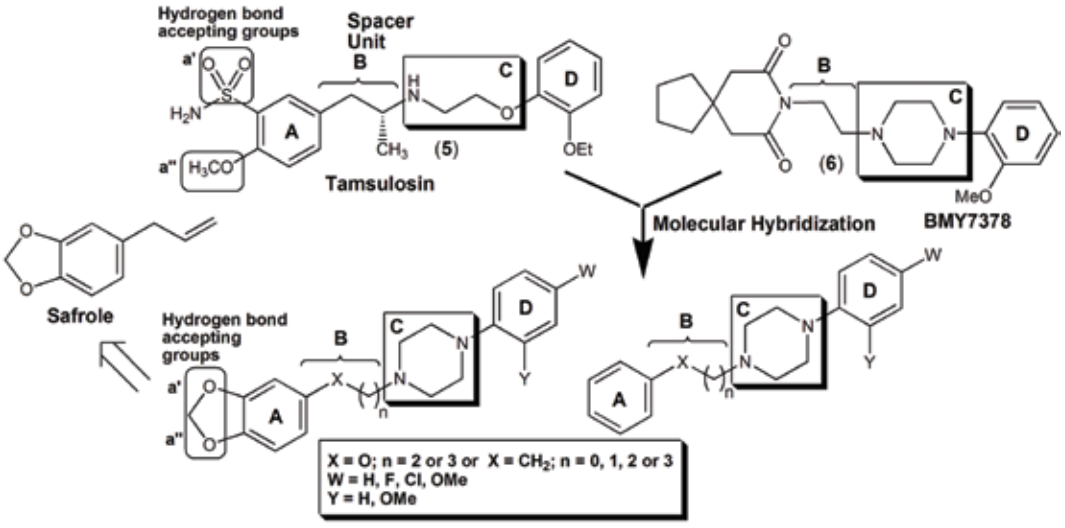


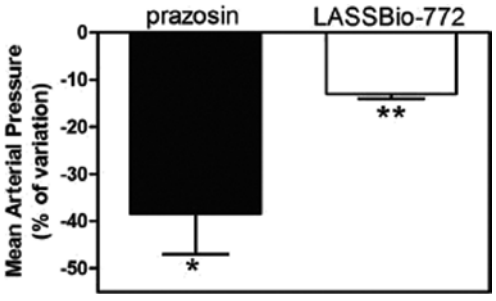
We described herein the discovery of 1-(2-(benzo[d][1,3]dioxol-6-yl)ethyl)-4-(2-methoxyphenyl) piperazine (LASSBio-772) as a novel potent and selective alpha 1A/1D adrenoceptor (AR) antagonist.





It was elected after screening of functionalized 1,3-benzodioxolyl-*N*-phenylpiperazine derivatives, synthesized from natural safrole, and unsubstituted-phenyl analogues in functional phenylephrine-induced vasoconstriction of rabbit aorta rings bioassays. The determination of LASSBio-772 affinity for alpha 1A (rat salivary gland) and alpha 1B (rat liver) subtypes, through displacement of [^{3}H]prazosin specific binding, led us to obtain IC_{50} values of 0.14 nM for the alpha 1A, similar to that displayed by tamsulosin (IC_{50} = 0.13 nM) [3], and 5.55 nM for the alpha 1B-AR, representing a 40-fold higher affinity for alpha 1A over alpha 1B, in contrast to 14.8-fold for tamsulosin. LASSBio-772 also presented high affinity (K_B = 0.025 nM) for the alpha 1D-AR subtype in functional rat aorta assays, showing to be equipotent to tamsulosin (K_B = 0.017 nM).





Considering that LASSBio-772 showed an alpha 1-AR antagonistic action *in vitro*, we decided to evaluate its effect *in vivo*. Analyzing the impact of LASSBio-772 upon arterial blood pressure as compared to a reference nonselective alpha 1-AR antagonist (prazosin), both at the same dose (100 µg/kg), we observed that the hypotensive effect of LASSBio-772 was significantly smaller than the one induced by prazosin.

LASSBio-772 is a novel alpha 1 adrenoceptor antagonist that presents higher affinity for the alpha 1A/1D than alpha 1B-AR, being therefore putatively useful for the treatment of the lower urinary tract symptoms, including the benign prostatic hyperplasia in mammals.

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QUERCETIN REDUCES NEUTROPHIL RECRUITMENT INDUCED BY CXCL8, LTB4, AND FMLP: INHIBITION OF ACTIN POLYMERIZATION

Souto, F.O.; Zarpelon, A. C.; Staurengo-Ferrari, L.; Fattori, V.; Casagrande, R.; Fonseca, M. J. V.; Cunha, T. M.; Ferreira, S. H.; Cunha, F. Q.; Verri Jr, W. A. *J. Nat. Prod*. 74 (2011) 113-118.
DOI:10.1021/ np1003017

Quercetin is known as a prototype antioxidant flavonoid, and most of its widely recognized biological effects are related to antioxidant properties. Recent *in vitro* data have suggested that the quercetin does not affect the functioning of neutrophils. These work aimed to investigate whether quercetin inhibits neutrophil recruitment *in vivo* and *in vitro* and if such activity depends on diminishing the expression of receptors for chemotatic inflammatory mediators and/or actin polymerization. Male Swiss mice were treated with quercetin (30, 100 and 300 mg/kg, s.c.) and 1 hour after, the cell migration was stimulated by intraperitoneal injections of chemotatic factors such as CXCL1, CXCL5, LTB4, and fMLP. Quercetin inhibited the recruitment of neutrophils to the peritoneal cavity (Fig 1).

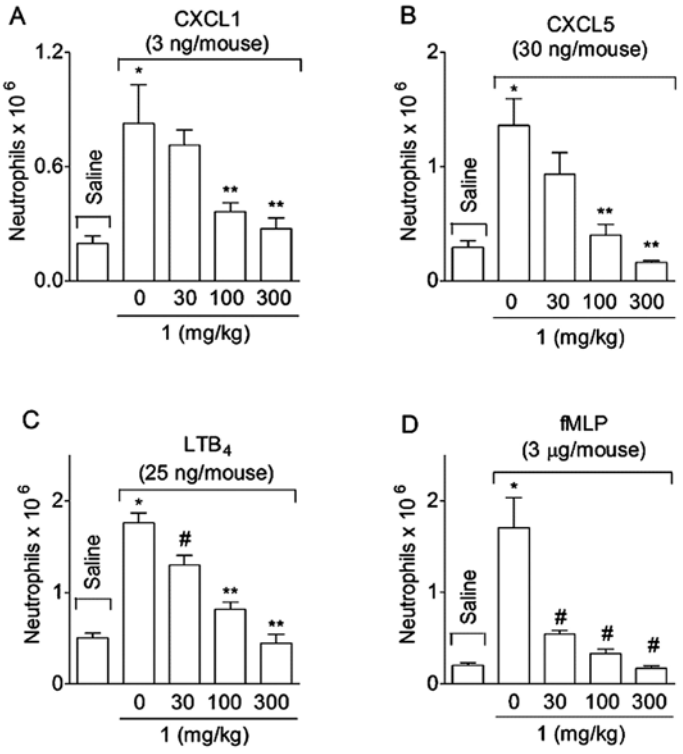


Figure 1: Treatment with quercetin (1) inhibits neutrophil recruitment *in vivo*, induced by different stimuli.

Furthermore, quercetin also inhibited the chemoattraction of human neutrophils induced by CXCL-8, LTB4 and fMLP in a Boyden chamber (Fig 2). In vitro treatment with quercetin did not affect human neutrophil surface expression of CXCR1, CXCR2, BLT1, or FLPR1, but rather reduced actin Polymerization (Fig.3).

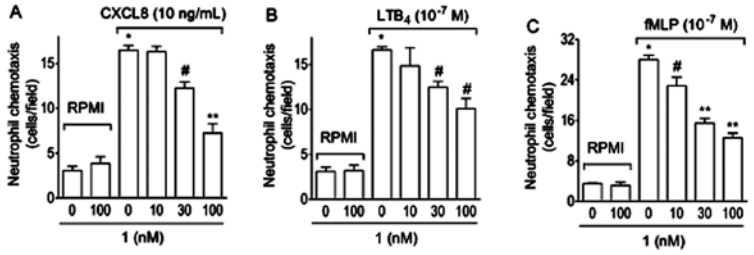


Figure 2: Quercetin (1) inhibits human neutrophil chemoattraction in the Boy den chamber.

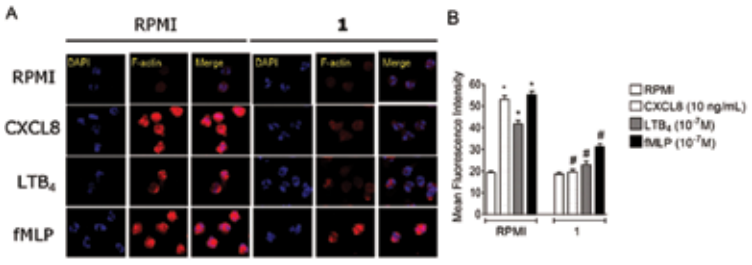


Figure 3: Quercetin (1) reduced human neutrophil F-actin polymerization induced by CXCL8, LTB4, and fMLP.

These results showed in this work suggest that quercetin inhibits neutrophil recruitment by inhibiting cellular signaling responsible for actin polymerization, indicating that treatment with this flavonoid is a conceivable approach to control excessive neutrophil recruitment during inflammation and to prevent neutrophil-mediated tissue lesions.

TADALAFIL ANALGESIA IN EXPERIMENTAL ARTHRITIS INVOLVES SUPPRESSION OF INTRA-ARTICULAR TNF RELEASE.

F.A.C., Rocha; F.S., Silva Jr; A.C.R.M., Leite; A.K.R.M., Leite; V.C.C., Girão; R.R., Castro;F.Q., Cunha. *Brit. J. Pharmacol.* 164 (2011) 828–835.
DOI: 10.1111/j.1476-5381.2011.01469.x

Modulation of pro-inflammatory and anti-inflammatory mediators by specific phosphodiesterase (PDE) inhibitors is a growing strategy for the treatment of inflammatory diseases. In the present study, we investigated the antinociceptive activity of tadalafil (a phosphodiesterase-5 inhibitor) in two models of arthritis, induced by zymosan or by transection of the anterior cruciate ligament, in rats. The treatment with tadalafil (0.5 mg/kg, p.o.) reduced the joint pain, that was measured and expressed as the paw elevation time (PET) on both models of arthritis (zymosan and transection of the anterior cruciate ligament) (Fig.1). Pretreatment with ODQ prevented the anti-inflammatory effects of tadalafil (Fig. 1 and Table 1).

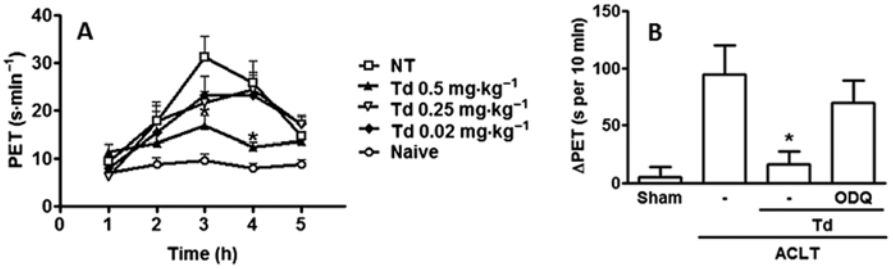


Figure 1: Antinociceptive effects of tadalafil in zymosan-induced arthritis (A) and experimental osteoarthritis, where was evaluated the effect of the guanylyl cyclase inhibitor (ODQ) on the anti-inflammatory activity of tadalafil (B).

Table 1: Effect of the guanylyl cyclase inhibitor (ODQ) on the anti-inflammatory activity of tadalafil in zymosan-induced arthritis.

Group	PET (s·min^{-1})	Cells mm^{-3}
Naïve	12.1 ± 1.2	133 ± 42.2
Saline	30.6 ± 3.7#	14 022 ± 2 429#
ODQ	30.1 ± 3.5	10 855 ± 1 226
Tadalafil	14.6 ± 1.1*	8 400 ± 2 728*
ODQ + tadalafil	37.2 ± 3.8	16 640 ± 1 141

In zymosan-induced arthritis, tadalafil significantly decreased the cell influx and TNF-α release to the articular cavity, but did not alter IL-1 or CINC-1 levels (Fig.3).

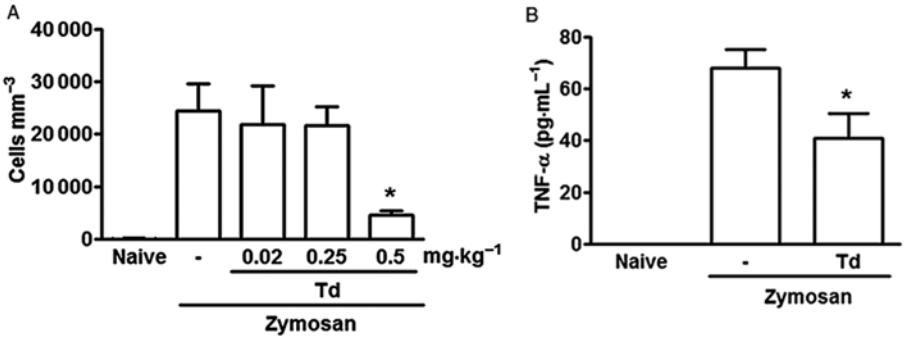


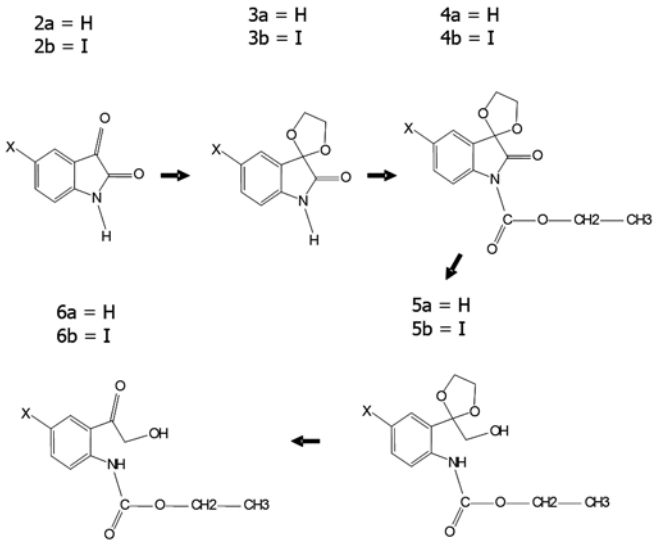
Figure 2: Effects of tadalafil on the acute cell influx and cytokine (TNF-α) release in zymosan arthritis.

The present data suggest that tadalafil has *in vivo*therapeutic anti-inflammatory effects by promoting antinociception and reducing the leukocyte influx into the synovial cavity in zymosan arthritis. Moreover, tadalafil was effective when given *per os*, indicating a therapeutic potential in humans. The analgesic effect is probably secondary to the activation of cGMP in nociceptive neurons and did not appear to depend on the release of endogenous opioids. In addition to the specific direct effect via cGMP modulation, we propose that the antinociceptive effect of tadalafil is also linked to a decreased release of TNF-a associated with the reduction of neutrophil migration into the joints. Usually, the patients prescribed PDE-5 inhibitors to treat erectile dysfunction are those also affected by osteoarthritis. The possibility of relief of joint pain provided by these compounds, as a side effect, could possibly increase patient compliance with the therapy.

PHARMACOLOGICAL ACTIVITY OF NOVEL 2-HYDROXYACETOPHENONE ISATIN DERIVATIVES ON CARDIAC AND VASCULAR SMOOTH MUSCLE IN RATS

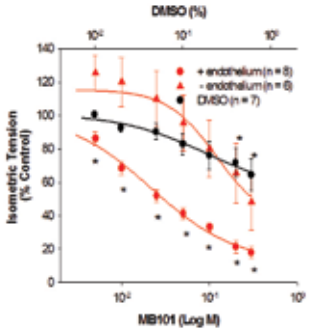
Daniele Gabriel; Luana Braga Pontes; Jaqueline Soares da Silva; Roberto Takashi Sudo; Marilza Baptista Corrêa; Ângelo da Cunha Pinto; Simon John Garden; Gisele Zapata-Sudo. *J. Cardiovasc. Pharmacol.* 57 (**2011**) 20-27.

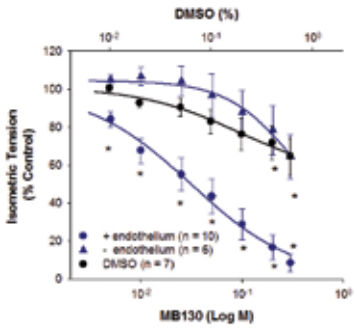
Isatin (1*H*-indole-2,3 dione) is an endogenous compound with biological activities. Many of its derivatives have pharmacological effects, including inhibition of cyclic guanosine monophosphate levels in cardiac tissue; sedative-hypnotic profiles; anticonvulsant, analgesic, antithermic and anti-inflammatory activities; and anxyolitic, antimicrobial and proapoptotic effects. This work investigated the effects on the cardiovascular system of two novel 2-hydroxyacetophenone derivatives of isatin. The MB101 and MB130 compounds were synthesized by introducing a carboethoxy group on isatin, resulting in novel molecules of unknown pharmacological profile.



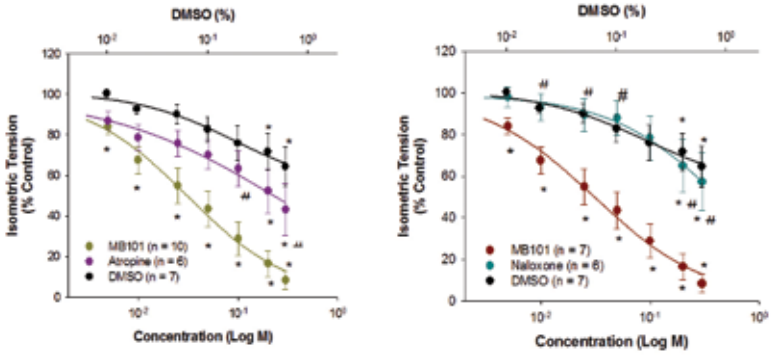
Synthesis of MB101(6a) and MB130 (6b) from isatin (2a and 2b).

The two novel 2-hydroxyacetophenones derived from isatin - MB101 and MB130 - produced vasodilatation and negative cardiac inotropism by stimulation of bradykinin, muscarinic and opioid receptors in smooth and cardiac muscles. MB101 was selective to vascular tissue, but less potent than MB130. This may be because iodine in the aromatic ring of MB101 possibly interfered with its affinity for different receptors.





Concentration-response curves for MB101 and MB130 on vascular smooth muscle. *P < 0.05 compared to control and # P < 0.05 compared to denuded tissue.



Concentration-response curves for MB101 in the presence of atropine or naloxone on vascular smooth muscle. *P < 0.05 compared to control and # P < 0.05 compared to denuded tissue.

Both compounds reduced systolic and diastolic pressures in a dose-dependent manner in anesthetized rats.

TABLE 1. Hemodynamic Parameters After Bolus Administration of Derivatives

	MB101				MB130			
Dose mg/kg	SAP	DAP	MAP	HR	SAP	DAP	MAP	HR
0.0	109.7 ± 15.3	80.7 ± 6.8	90.0 ± 11.2	285 ± 12	110.3 ± 9.5	85.3 ± 3.8	95.3 ± 5.7	267 ± 28
0.5	79.7 ± 6.0*	49.5 ± 3.4*	63.0 ± 8.8*	269 ± 8	111.7 ± 6.5	84.1 ± 5.7	94.7 ± 3.6	224 ± 23
1.0	77.7 ± 16.0*	35.1 ± 8.1*	48.5 ± 2.0*	271 ± 21	84.6 ± 8.9*	64.9 ± 6.6*	70.1 ± 4.9*	341 ± 30
5.0	69.7 ± 17.3*	30.5 ± 5.4*	35.9 ± 3.6*	346 ± 96	53.9 ± 7.1*	31.4 ± 3.2*	40.9 ± 6.0*	237 ± 17
10.0	44.9 ± 24.9*	31.9 ± 6.4*	37.8 ± 7.2*	276 ± 21	49.0 ± 3.2*	30.3 ± 4.1*	37.6 ± 2.7*	351 ± 32

Values are expressed as mean ± standard error of the mean in mm Hg of 10 rats.
*$P < 0.05$ compared with control.
DAP, diastolic arterial pressure; HR, heart rate; MAP, mean arterial pressure; SAP, systolic arterial pressure.

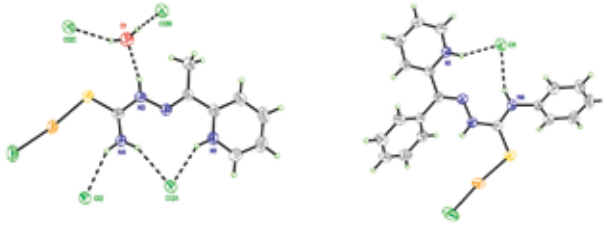
These findings provide information for designing new strategies for the treatment of cardiovascular disorders.

GOLD(I) COMPLEXES WITH THIOSEMICARBAZONES: CYTOTOXICITY AGAINST HUMAN TUMOR CELL LINES AND INHIBITION OF THIOREDOXIN REDUCTASE ACTIVITY

Josane A. Lessa[a], Juliana C. Guerra[b], Luana F. de Miranda[b], Carla F. D. Romeiro[b], Jeferson G. Da Silva[a], Isolda M. C. Mendes[c], Nivaldo L. Speziali[d], Elaine M. Souza-Fagundes[b] and Heloisa Beraldo[a]* J. Inorg. Biochem. 105 (2011) 1729-1739. **DOI:**10.1016/j.jinorgbio.2011.09.008

Platinum-based drugs belong to the blockbusters of anticancer drugs sold worldwide. However, many tumors are intrinsically resistant to these compounds and even the initially sensitive tumors can develop a resistance during treatment. In addition, the compounds cause severe side effects. Hence there is an increasing demand for novel metal-based-pharmaceuticals with a mode of action differing from that of the platinum anticancer drugs. Recently gold complexes have attracted major attention due to their tumor cell growth inhibiting effects, and their interactions with enzymes such as thioredoxine reductase (TRxR). The antitumor properties of thiosemicarbazones and their metal complexes have been extensively investigated. However to our knowledge studies on gold complexes with thiosemicarbazones have not involved investigation on their interaction with TrxR.

Complexes [Au(H2Ac4DH)Cl]·MeOH (**1**) [Au($H_2$2Ac4Me)Cl]Cl (**2**) [Au($H_2$2Ac4Ph)Cl]Cl·2H_2O (**3**) and [Au($H_2$2Bz4Ph)Cl]Cl (**4**) were obtained with 2-acetylpyridine thiosemicarbazone (H2Ac4DH), its *N*(4)-methyl (H2Ac4Me) and *N*(4)-phenyl (H2Ac4Ph) derivatives, as well as with *N*(4)-phenyl 2-benzoylpyridine thiosemicarbazone (H2Bz4Ph). The compounds were investigated for their cytotoxic activities against Jurkat (immortalized line of T lymphocyte), HL-60 (acute myeloid leukemia), MCF-7 (human breast adenocarcinoma) and HCT-116 (colorectal carcinoma) tumor cell lines. Since TrxR is considered as the most relevant molecular target for gold compounds, inhibition of TrxR's activity by the studied gold(I) complexes was investigated.

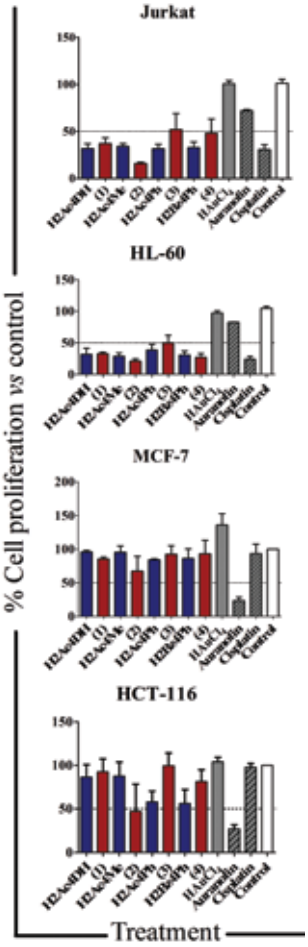


Molecular plot of [Au($H_2$2Ac4DH)Cl]Cl•H_2O (1a, left) and [Au($H_2$2Bz4Ph)Cl]Cl (4, right)

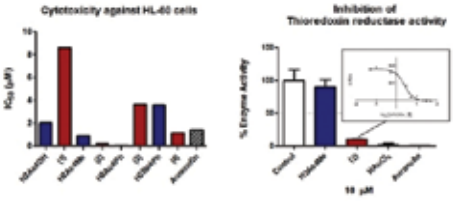
Jurkat and HL-60 leukemia cells were more sensitive to the compounds than MCF-7 and HCT-116 cells. The studied compounds were more cytotoxic than auranofin against Jurkat and HL-60 cells but were in general less active than auranofin against MCF-7 and HCT-116 cells. Many of the studied compounds

showed cytotoxicity similar to cisplatin against Jurkat and HL-60 cells. Among all compounds complex (**2**) was one of the most cytotoxic. Auranofin revealed to be less cytotoxic to the leukemia cells than to the MCF-7 and HCT-116 solid tumor cells. The opposite behavior was observed for cisplatin. $HAuCl_4$ showed no cytotoxic effect against all cell lineages.

Half maximal inhibitory concentrations (IC_{50}) were determined for the thiosemicarbazones and **1-4** against Jurkat and HL-60 cells and for **2** against MCF-7 and HCT-116 cells. To evaluate toxicity on normal cells, IC_{50} values were also determined against peripheral blood mononuclear cells (PBMC). The compounds were more cytotoxic against HL-60 than against Jurkat cells. H2Ac4Me and H2Ac4Ph were more cytotoxic than auranofin against both leukemia cell lineages. Activity improved on coordination in complexes (**2**) and (**4**) against HL-60 and Jurkat cells. **2** proved to be more than 4-fold more active against HL-60 cells than the H2Ac4Me ligand. **2** was the most active complex against both leukemia cell lines. **2** and **4** were more cytotoxic against HL-60 cells than auranofin. **2** was as active as auranofin against MCF-7 cells but less active than auranofin against HCT-116 cells. Most of the studied compounds were less toxic against PBMC cells than auranofin, except H2Ac4Me and **2**. Toxicity decreased on coordination in 3 and 4. H2Ac4DH and 4 showed a good therapeutic index in HL-60 cells.



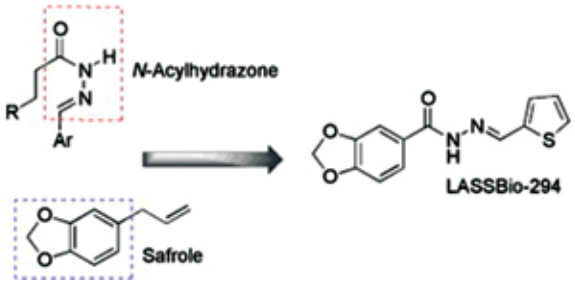
At 10 μM **2** inhibited 89 % of TrxR's activity, while $HAuCl_4$ and auranofin inhibited 97 % and 99% of TrxR's activity, respectively. H2Ac4Me was unable to inhibit TrxR's activity. Since not only complex (**2**) and auranofin but also $HAuCl_4$ strongly inhibited the enzyme's activity, the inhibitory effect on TrxR may be related to the presence of gold. However, although $HAuCl_4$ is an inhibitor of TrxR's activity, it exhibited no cytotoxic effect against all tumor cell lines. The hydrophilic character of $HAuCl_4$ probably hinders its passage through the cell membrane. Unlike $HAuCl_4$, 2 not only inhibited TrxR's activity but also presented cytotoxic effect, which suggests that the thiosemicarbazone H2Ac4Me, besides of its own cytotoxic activity, also probably acted as a carrier of the gold ion into the cells.



DETERMINATION OF THE CARDIOACTIVE PROTOTYPE LASSBIO–294 AND ITS METABOLITES IN DOG PLASMA BY LC–MS/MS: APPLICATION FOR A PHARMACOKINETIC STUDY

Rodolpho C. Braga, Andréa C.B. Tôrres, Camille B. Persiano, Rosângela O. Alves, Carlos A.M. Fraga, Eliezer J. Barreiro, Valéria de Oliveira. Journal of Pharmaceutical and Biomedical Analysis 55 (2011) 1024–1030. DOI:10.1016/j.jpba.2011.02.031

LASSBio-294 2-thienylidene-3,4-methylenedioxybenzoylhydrazine; L-294), was originally designed as phosphodiesterase (PDE) inhibitor candidate synthesized from natural safrole (**Fig. 1**), an abundant Brazilian natural product, obtained from Sassafras oil in high yield by classic distillation (*Ocotea pretiosa and Piper hispidinervum*). This *N*-acylhydrazone (NAH) derivative was characterized as a novel possible alternative for treatment of cardiac failure, once it was able to promote an effective positive inotropic and vasodilatory activity through a mechanism different from that displayed by cardiac glycosides and β-adrenergic agonists. L-294 increased the spontaneous contraction of isolated hearts of Wistar rats in a dose-dependent manner (maximum effect at 25 μM) and the Ca^{2+} uptake into sarcoplasmic reticulum (SR) without changing the sensitivity of the contractile proteins to Ca^{2+}. Moreover, this compound induced relaxation of isolated rat aorta with an IC_{50} of 74 μM by increasing intracellular cyclic GMP levels. These pharmacological evidences suggest a novel mechanism of action, circumventing the toxic effects resulted from calcium homeostasis alteration. More recently, L-294 was also described to prevent myocardial infarction induced cardiac dysfunction through improving intracellular Ca^{2+} regulation. Studies of drug absorption, distribution, metabolism, excretion and toxicity (ADMET) as well as drug metabolism and pharmacokinetic (DMPK) and studies are widely used in drug discovery and development to help obtain the optimal balance of properties necessary to convert lead compounds into drugs that are safe and effective for human use. Drug discovery efforts have been aimed at identifying and addressing metabolism issues at the earliest possible stage, by developing and applying innovative liquid chromatography mass spectrometry (LC–MS) based techniques and instrumentation, which are both faster and more accurate than prior techniques.



In this study we report for the first time the development and validation of a simple, rapid and sensitive high-performance liquid chromatography–tandem mass spectrometry (LC–MS/MS) method for the determination of the cardioactive prototype L-294 in dog plasma. The method was evaluated with regard to its accuracy, precision, selectivity, sensitivity, reproducibility, and stability. Furthermore, it was successfully used in a preliminary pharmacokinetic study of orally administered L-294.

No pharmacokinetic study of L-294 has been reported so far as we know. The developed method in this paper was successfully used for a pharmacokinetic study in which plasma concentration of L-294 up to 24 h after oral administration a dosage of 10 mg in 6 healthy beagles' dogs. Mean plasma concentration–time profiles are presented in Fig. 2.

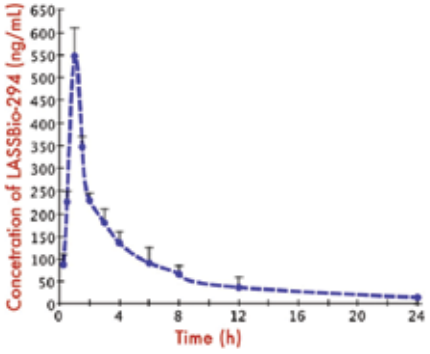


Fig. 2. Plasma concentration profile of L-294 in dogs after oral administration of a dose of 10 mg (mean ± S.D., *n* = 6)

The data analysis of pharmacokinetic parameters was performed by using The R Project for Statistical Computing (version R-2.11.1) package "PK" and the PK Solver (version 2.0). The non-compartmental pharmacokinetic parameters were calculated and are listed in Table 1. These results demonstrate that L-294 is rapidly absorbed and eliminated.

Table 1. The pharmacokinetic parameters of L-294 in beagles following an oral administration of 10 mg L-294 (*n* = 6).

Parameters	Mean	S.D.
AUC(0–24) (ng h/mL)	1621.77	41.66
AUC(0–∞) (ng h/mL)	2010.13	55.12
MRT (h)	7.06	0.47
$T_{1/2}$ (h)	5.74	0.55
T_{max} (h)	1.00	0.11
C_{max} (ng/mL)	547.66	35.12
$C_{l/F}$ (mg)/(ng/mL)/h	4.97	0.01
$V_{z/F}$ (ng)/(ng/mL)	41.25	0.04

A sensitive, specific and accurate method is first described for the quantification of the cardioactive prototype L-294 in dog plasma by LC–MS/MS in positive electrospray ionization mode using MRM and fully validated according to commonly accepted criteria. The method exhibited excellent performance in terms of high selectivity, low LLOQ (1.25 ng/mL), wide linear range (1.25–800 ng/mL), small organic solvent consumption (720 µL) and small plasma volume (200 µL). Moreover, the method has been successfully used for a pre-clinical pharmacokinetic study in dogs after oral administration of L-294. The pharmacokinetic parameters obtained from this study can give some useful information for further research of L-294.

ANTICHOLINESTERASIC, NEMATOSTATIC AND ANTHELMINTIC ACTIVITIES OF PYRIDINIC AND PYRAZINIC COMPOUNDS

Valli M.; DanuelloA.; Pivatto M.; Saldaña J.C.; Heinzen H.; Domínguez L.; Campos V.P.; Marqui S.R.; Young M.C.M.; Viegas Jr. C.; Silva D.H.S.; Bolzani V.S. *Current Medicinal Chemistry*. 18 (2011) 3423-3430. DOI:10.2174/092986711796504718

In the search for acetylcholinesterase inhibitors as a potential target for the discovery of anthelmintic drugs, a series of 27 pyridinic and pyrazinic compounds have been designed on the basis of molecular hybridization of two known AChE inhibitors, namely, tacrine and (–)-3-*O*-acetylspectaline, and on the concept of isosterism (Fig. 1).

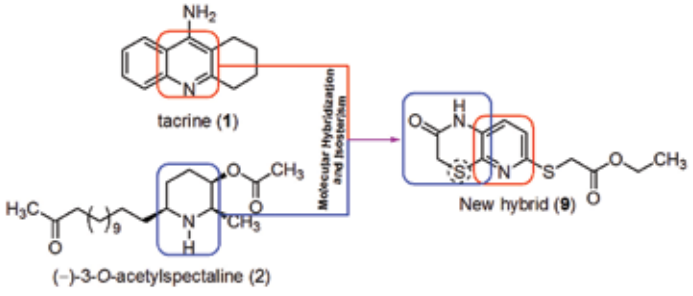
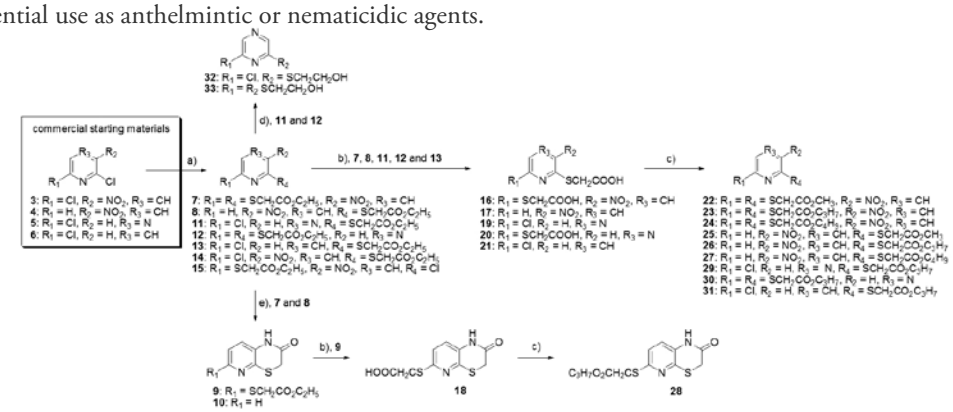


Fig. (1). Typical hybrid product (9) formed by molecular hybridization of tacrine (1) and (–)-3-*O*-acetylspectaline (2).

The synthesized compounds (Scheme 1) presented moderate anticholinesterasic activities when compared with the positive control physostigmine. One compound (ethyl 2-[(6-chloropyrazin-2-yl)sulfanyl] acetate, 11) exhibited an *in vitro* ability to immobilize the root-knot nematode *Meloidogyne incognita* that was

highly comparable to that of the positive control Temik. Moreover, in anthelmintic assays against the gastrointestinal parasitic nematode *Nippostrongylus brasiliensis* (L4), some of the compounds, such as (6-chloropyrazin-2-yl)sulfanyl ethanol (32, EC_{50} = 33 nM), presented activities that were considerably stronger than that of the positive control albendazole (EC_{50} = 340 nM).

In the light of the positive results obtained in the anthelmintic evaluations, the acute oral toxicity of the representative compound diethyl 2,2'-[(3-nitropyridine-2,6-diyl) bissulfanediyl] diacetate (7) was determined in rats, and the drug was shown to be non-toxic at a dose of 2000 mg/kg. These results, allied with the relatively simple structures of the active compounds and their facile synthesis, highlight their potential use as anthelmintic or nematicidic agents.



Scheme (1). Synthesis of compounds 7 - 33. Reagents and conditions: a) ethyl-2-mercaptoacetate, NaH, anhydrous THF, N_2 atmosphere, room temperature or ice bath, depending on the reaction, for 5 min to 12 h, depending on the starting material; b) NaOH, EtOH/H_2O (2:1), room temperature for 1 h; c) alcohol (MeOH, *n*-PrOH or *n*-BuOH), H_2SO_4, reflux for 12 h; d) $LiAlH_4$, anhydrous THF, N_2 atmosphere, ice bath for 12 h; e) Feo, NH_4Cl, EtOH/H_2O (2:1), reflux for 90 min.

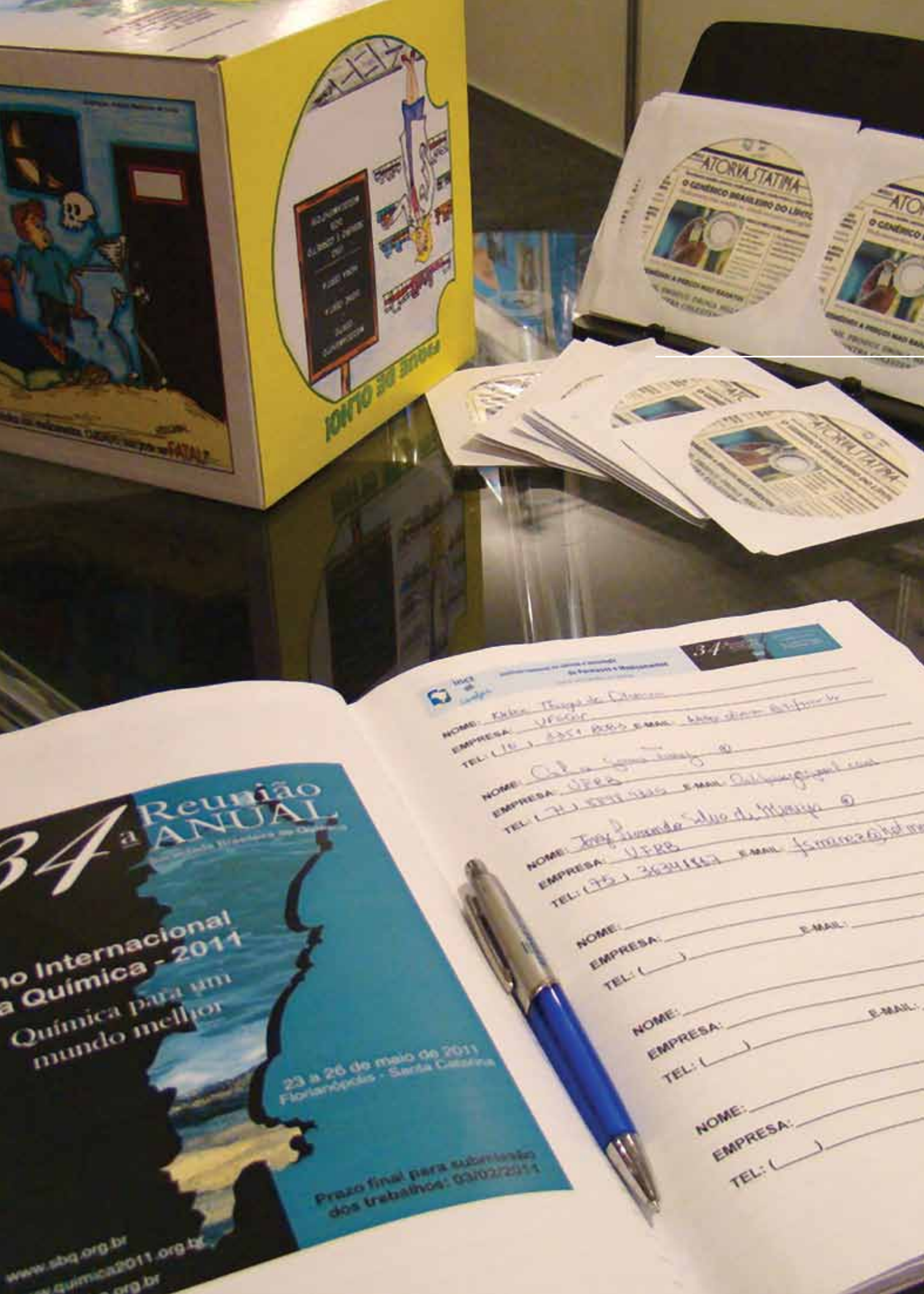
Table 1. *In vitro* AChE inhibitory, nematostatic and anthelmintic activities of the most active compounds.

Compound	AChE inhibition (LOD, nmol)	M. Incognita immobilization (%)	N. brasiliensis death (EC_{50}, nM)
7	8.6	12	56.0
10	-	19	34.0
11	13.0	98	-
17	-	-	230.0
18	-	-	-
21	-	-	60.0
26	12.0	-	69.0
32	130.0	-	33.0
Positive	0.2[a]	100[b]	50.0[c]

[a] physostigmine | [b] Temik | [c] albendazole

PATENT

LC Dias, AS Vieira, EJ Barreiro, Process for obtaining calcium atorvastatin using novel intermediates, PI 018110015039 (INPI, in 04/25/2011), PCT in december, 2011.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SCIENTIFIC AWARENESS AND PUBLICIZING AT INCT–INOFAR

Parallel to the research developed in the laboratory, INCT-INOFAR coordinates Scientific Awareness & Health Education initiatives, with a goal of contributing towards a critical conscience in the correct use of medications, and making basic scientific knowledge of Pharmaceutical Sciences available to the population.

INCT-INOFAR views the popularization and publicizing of Science, Technology, and Innovation as important factors in the construction of a critical view of the contemporary globalized world, allowing, especially among youth, for new vocations to be expressed even if they are not connected to their home environments.

INCT-INOFAR believes in the potential children have to multiply the knowledge they have acquired among their friends and family, and therefore it invests in Health Education initiatives aimed at making young people aware of the rational use of medications.

Since its creation, INCT-INOFAR has developed Scientific Awareness & Health Education materials. During these past three years, it has produced two booklets on the correct use of medications, 10 theme puzzles, and a video on the stages necessary to produce a medication, as well as an internet portal for publicizing Pharmaceutical Sciences – The Pharmaceuticals Portal www.portaldosfarmacos.ccs.ufrj.br.

"As relevant as the publicizing of knowledge in the knowhow of pharmaceuticals and medications is the building of critical knowledge among the population of Science as an effective tool of social promotion of citizenship. This awareness needs to start when they are children."

Prof. Eliezer J. Barreiro
INCT-INOFAR coordinator

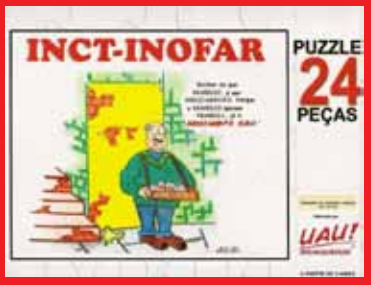
INCT–INOFAR ACTION PORTFOLIO

The complete portfolio of INCT-INOFAR actions developed to publicize and popularize science, including the production of events and the publicizing of its research in the media is in the "INCT-INOFAR Booklet 2009-2011: Scientific Awareness and Health Education". The booklet is available in a bilingual edition, in English and Portuguese, both in print and online at www.inct-inofar.ccs.ufrj.br/revista.

With colorful illustrations and a simple and dynamic language, the booklet "Commandments of the Correct Use of Medications" talks about the risks connected to using medications. In a didactical manner, the material offers guidance on the different medication categories, how to store medications at home, and how to critically understand pharmaceutical abusive advertisement.

In cartoon form, the booklet "Joey's crew in: The correct use of Antibiotics" talks about the risk of the incorrect use of medications, showing common practices that contribute to increasing bacterial resistance, like self-medication and purchasing medications on the advice of drugstore workers. The booklet has the approval of the National Agency of Sanitary Regulation (ANVISA).

The cartoons published on the Pharmaceuticals Portal have been turned into puzzles. Tem different versions of these theme toys have already been produced. The goal is that by assembling the puzzles, children will become aware of the risks involved in taking medications.



"LASSBIO 596: from molecule to medication" mixes fiction with science to tell the story of a substance developed by INCT-INOFAR to treat asthma. At 13 minutes long, the video presents the research stages necessary for the medication to reach drugstore shelves. At each stage, a different INCT-INOFAR researcher is shown explaining the process.

PHARMACEUTICALS PORTAL

The Pharmaceuticals Portal <www.portaldosfarmacos.ccs.ufrj.br> is the INCT-INOFAR website for the publicizing and popularization of Pharmaceutical Sciences. Through this portal, INCT-INOFAR publicizes its research activities, in language accessible to laypeople, and makes its Health Education materials available.

In sync with new trends in scientific journalism, the Pharmaceuticals Portal provides the schedule and also the media coverage of relevant scientific events. It also publishes new articles on current themes in pharmaceutical innovation and health sciences. It also produces cartoons that increase awareness of the irrational use of medications, proposing conscious alternatives for their use instead.

- Publicizing the research activities carried out by INCT-INOFAR, in language accessible to laypeople;
- Publishing new articles on current themes in pharmaceutical innovation and health sciences;
- Schedule and media coverage of the main scientific events in the field;
- *Download* of INCT-INOFAR educational booklets on the correct use of medications;
- Publishing cartoons to create awareness of the irrational use of medications.

In 2011, the International Year of Chemistry (AIQ) was celebrated, and the Pharmaceuticals Portal contributed by covering several events that were part of this celebration. Among them was the official launch of the AIQ in Brazil, the 34th RASBQ – Annual Meeting of the Brazilian Society of Chemistry, XVIII Regional Meeting of the Brazilian Society of Chemistry (SBQ-Rio) and the Nobel Prize in Chemistry 2008 Conference at UFRJ.

Some of the themes of the articles published in the Pharmaceuticals Portal in 2011 include advances in Medicinal Chemistry, vaccination, biodiversity as an inspiration, challenges of the Brazilian pharmaceutical industry, Pharmacy symbology, intellectual property, development of phytotherapeutics, history of Chemistry, government-private sector partnerships, pharmaceutical innovation, and new generic drugs. Over 100 never before published articles and interviews have been published so far in the Pharmaceuticals Portal since INCT-INOFAR was created in 2009.

Edmundo Lins Municipal School

INCT–INOFAR IN SCHOOLS

With the goal of teaching content that is not usually taught in schools – the importance of the correct use of medications – making children and teenagers multipliers of knowledge among their friends and families, the Drugs and Medicines INCT created the Project "INCT-INOFAR in schools".

Focused primarily on public schools in Rio de Janeiro, the city where the INCT-INOFAR headquarters are located, at UFRJ, the Institute has also encouraged its network of researchers in several parts of the country to carry out local educational initiatives.

INCT-INOFAR also helps increase awareness on the correct use of medications by providing their Health Education materials to institutions that wish to conduct educational campaigns in this area. Through visits and lectures in municipal and state schools in the state of Rio de Janeiro, the Institute deals with this subject.

INAUGURAL ACTION IN RIO DE JANEIRO

On June 17, 2011, INCT-INOFAR visited the Edmundo Lins Municipal School, located in the Ramos neighborhood, in Rio de Janeiro. The institution has students from grades 1 to 5, in two shifts (morning and afternoon). Approximately 260 students had the opportunity to attend the event promoted by INCT-INOFAR at the school.

In the dynamic with the children, a team of pharmacists from INCT-INOFAR connected to the Evaluation and Synthesis of Bioactive Substances Laboratory (LASSBio®/UFRJ) presented an animated booklet on the correct use of medications and interacted with the students, encouraging them to ask questions on the subject.

What is the difference between a doctor and a pharmacist?
What is the importance of taking medications at the right time?
Can I take a headache medication on an empty stomach?
How can we identify if a medication is fake?
If someone else goes to the doctor with the same symptoms I have, can I take the same medication?
Is drinking sugar water a placebo?

These were some of the questions that the INCT-INOFAR pharmacists answered didactically and humorously. The school visited received INCT-INOFAR kits with booklets and educational puzzles. In turn, the children recorded what they learned through drawings and essays.

INCT–INOFAR IN THE INTERNATIONAL YEAR OF CHEMISTRY

INCT-INOFAR was an active part of the celebrations of the International Year of Chemistry (AIQ), coordinating its researchers to develop actions in the publicizing and popularization of Chemistry in Brazil.

A special article for an important scientific publication in Brazil, interviews for the "365 Days of Chemistry" project, the production of an e-book on Chemistry and health, participation in the AIQ Cycle of Conferences and supporting the Nobel Prize in Chemistry 2008 conference in UFRJ were the main actions undertaken by INCT-INOFAR in the International Year of Chemistry.

SPECIAL ARTICLE ON "SCIENCE TODAY" MAGAZINE

At the request of the editors, INCT-INOFAR researchers Eliezer J. Barreiro, Lidia M. Lima, Carlos Manssour Fraga, and Rodolfo C. Maia, connected to the Evaluation and Synthesis of Bioactive Substances Laboratory (LASSBio®/ UFRJ) published a special article on Science Today magazine on the art of creating pharmaceuticals and medications of synthetic origin.

"The art of creating the artificial: the chemistry of pharmaceuticals and medications"

Science Today Magazine

Issue 286, volume 48, October 2011

INCT-INOFAR AT "365 DAYS OF CHEMISTRY"

INCT-INOFAR chemists were interviewed on their careers for the "365 Days of Chemistry" project, published daily at the AIQ blog <http://quimica2011.org.br >

The interview was made up of 6 questions that were the same for every interviewee. In a question and answer format, the interviewee described how and when it all began; why he or she had chosen Chemistry as a profession; summarized his or her current and past activities; provided tips to new professionals and students of Chemistry; and talked about which Chemical discovery he or she wishes he or she could have achieved. At the end of the interview, a small summary of the curriculum vitae of each interviewee was presented. After that, the molecule of the day was presented.

Among the INCT-INOFAR researchers honored by "365 Days of Chemistry" are Vanderlan da Silva Bolzani (member of the INCT-INOFAR Managing Committee); Vitor Francisco Ferreira (INCT-INOFAR consulting member and Vice-President of the Brazilian Chemistry Society); Lidia Moreira Lima (UFRJ) associate professor and in charge of INCT-INOFAR Scientific Superintendence), and Luiz Carlos Dias (member of the INCT-INOFAR Managing Committee and supervisor of the UNICAMP research group responsible for developing a new synthetic route for atorvastatin, the active principle of Lipitor®, the number one medication in sales worldwide).

INCT-INOFAR RESEARCHERS THAT WERE PART OF "365 DAYS OF CHEMISTRY"

01/08/2011 – INTERVIEW: FRANCISCO RADLER DE AQUINO NETO
MOLECULE OF THE DAY: PROPANE

01/09/2011 – INTERVIEW: LUIZ CARLOS DIAS
MOLECULE OF THE DAY: (–)-MENTOL

01/18/2011 – INTERVIEW: LIDIA MOREIRA LIMA
MOLECULE OF THE DAY: HELIUM

02/10//2011 – INTERVIEW: CARLOS SANT'ANNA
MOLECULE OF THE DAY: RADIUM

03/08/2011 – INTERVIEW: VITOR FRANCISCO FERREIRA
MOLECULE OF THE DAY: TAURINE

04/29/2011 – INTERVIEW: DULCE MARIA DE ARAUJO MELO
MOLECULE OF THE DAY: CAPTOPRIL

09/07/2011 – INTERVIEW: VANDERLAN DA SILVA BOLZANI
MOLECULE OF THE DAY: ESTRAGOLE

09/19/2011 – INTERVIEW: NELILMA CORREIA ROMEIRO
MOLECULE OF THE DAY: FENTANYL

11/17/2011 – INTERVIEW: HELOISA DE OLIVEIRA BERALDO
MOLECULE OF THE DAY: MICONAZOLE

E-BOOK "CHEMISTRY IN HEALTH"

INCT-INOFAR researchers Lidia Moreira Lima, Carlos Alberto Manssour Fraga, and Eliezer J. Barreiro, connected to the Evaluation and Synthesis of Bioactive Substances Laboratory (LASSBio®/ UFRJ), at the request of the Brazilian Chemistry Society (SBQ) have written an education e-book titled "Chemistry in Health" for the collection "Chemistry in Everyday Life", produced to celebrate the International Year of Chemistry.

The authors created the content of the e-book to highlight, in a dynamic and didactical fashion, the importance of Chemistry in health, dealing in a logical sequential manner from subjects that go from the fertilization of the ovum by the spermatozoa to the explanation of puberty through chemical reactions.

The first topic is fertilization and formation of the genome, which segues into chapter 2, focused on the chemical reactions in the umbilical cord and in breastfeeding. The following chapters are about the different kinds of molecules and the importance of each of them in different stages of the human life. Eating, energy, hygiene, sexuality, anxiety, wellness, happiness, sleep, and lastly, disease fighting are all subjects of these following chapters.

In the e-book, available for free download at the AIQ blog <http://quimica2011.org.br >, researchers have tried to explain chemical reactions present in various health situations at a molecular level, to try to encourage an interest in Chemistry in young people by dealing with everyday topics explained through Chemistry.

AIQ CONFERENCE CYCLE

At the request of the Brazilian Chemistry Society (SBQ) and of the Foundation for Research Support in the State of Sao Paulo (FAPESP), INCT-INOFAR researchers have been part of the Conference Cycle for the International Year of Chemistry (AIQ). Throughout 2011, the cycle had 10 meetings to debate different themes in Chemistry. The entire conference cycle was covered by the FAPESP Research magazine.

The cycle titled *"Medicinal Chemistry: challenges and perspectives"*, which took place at the FAPESP auditorium in Sao Paulo had the presence of INCT-INOFAR researchers Eliezer J. Barreiro (UFRJ) and Luiz Carlos Dias (UNICAMP).

The following month, the *"Biodiversity and Chemistry"* cycle took place. Prof. Vanderlan da Silva Bolzani (UNESP – Araraquara), researcher and member of the INCT-INOFAR Managing and Follow-Up Committee, alongside with Mariluce Moura, FAPESP Research magazine director, coordinated the AIQ conference cycle activities.

In the cycle *"Chemistry sweet, bitter, and fragrant"*, which took place in August, INCT-INOFAR CGA researcher Angelo da Cunha Pinto (UFRJ) talked about how natural products, for example, carbohydrates, terpenes, fragrances, alkaloids, and flavonoids, can inspire new pharmaceuticals.

"Medicine is made of molecules: chemical components are behind diseases, diagnoses, and treatments"
FAPESP Research Magazine
Issue 185, July 2011

"From molecule to organisms: the wealth of biodiversity of Brazilian forests is also revealed in substances"
FAPESP Research Magazine
Issue186, August 2011

"Flavors and perfumes: sweet, fragrant compounds are the lead characters"
FAPESP Research Magazine
Issue 187, September 2011

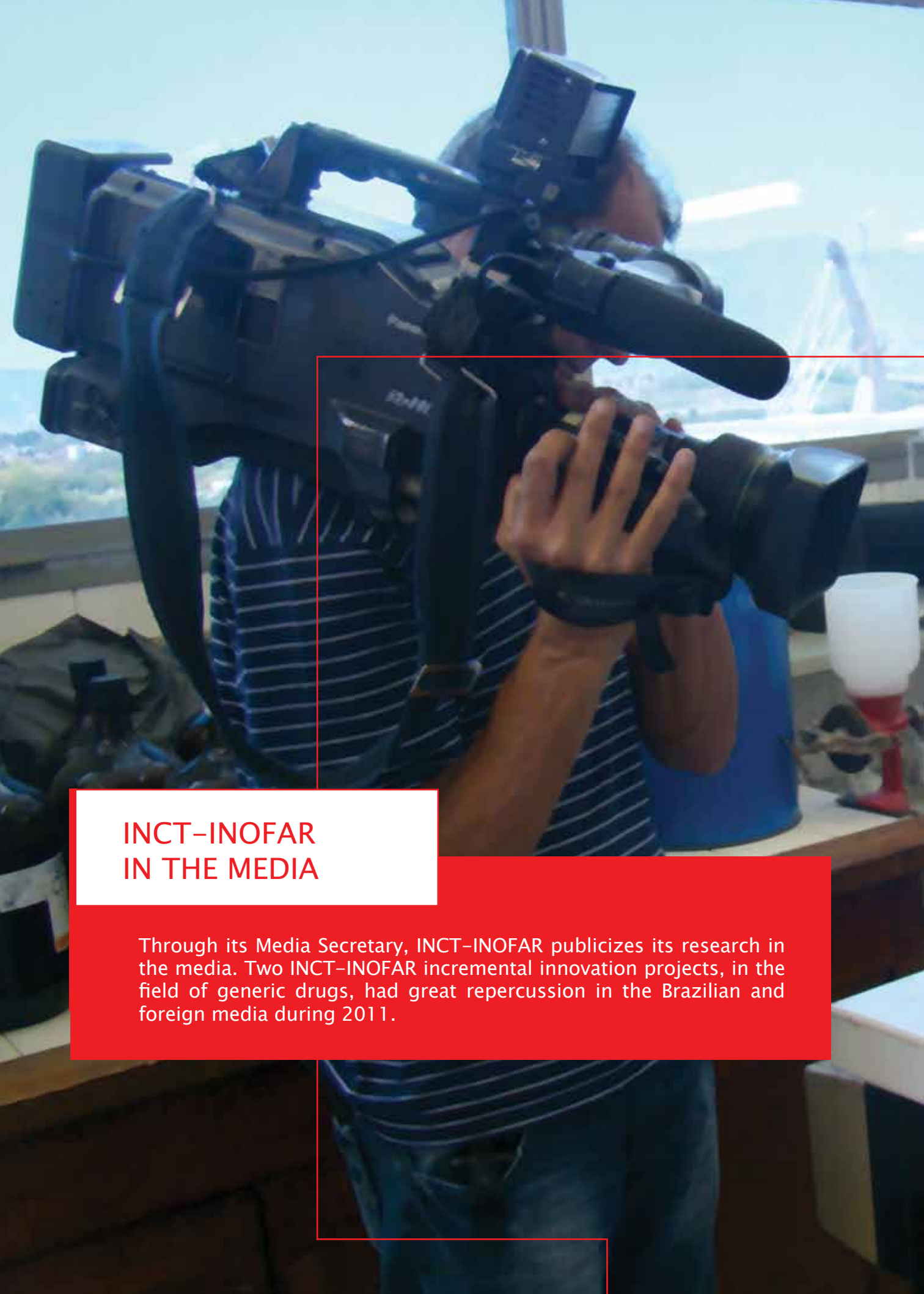
NOBEL PRIZE IN CHEMISTRY CONFERENCE AT UFRJ

Professor Martin Chalfie retells the story of the Green Fluorescent Protein and explains its power to "enlighten life"

INCT-INOFAR was part of the conference with the 2008 Nobel Prize winner, Prof. Martin Chalfie, where he was part of the commencement of the National Week of Science and Technology 2011, at the Complexo do Alemao in Rio de Janeiro. Before the event, the Nobel Prize winner lectured at the Chemistry Graduate Program in UFRJ.

At the conference titled "Fluorescent Proteins (GFP): Enlightening Life", on October 17 2011 at UFRJ, Prof. Martin Chalfie, in a humorous retelling, narrated his scientific trajectory in the studies of GFP to an audience filled with High School students. This is the research field who led him to win the Nobel Prize in Chemistry in 2008, alongside Osamo Shimomura and Roger Tsein. Martin Chalfie is a professor in the Department of Biological Sciences at Columbia University, in the USA.

INCT-INOFAR, through the Pharmaceuticals Portal, covered the Nobel Prize in Chemistry conference at UFRJ.



INCT-INOFAR IN THE MEDIA

Through its Media Secretary, INCT-INOFAR publicizes its research in the media. Two INCT-INOFAR incremental innovation projects, in the field of generic drugs, had great repercussion in the Brazilian and foreign media during 2011.

New synthetic route for atorvastatin – In December 2010, the same month where the Lipitor ®/ Pfizer patent expired in Brazil, INCT-INOFAR researchers announced the discovery of a new synthetic route for the production of its active principle, atorvastatin. A continuous use medication for cholesterol reduction of wide use, Lipitor® is the number one sold pharmaceutical in the world.

INCT-INOFAR produced a hot site to make the media clipping on the discovery available. Interviews with the researchers responsible for the discovery, Prof. Luiz Carlos Dias and Dr. Adriano Siqueira Vieira of the Institute of Chemistry of the State University of Campinas (UNICAMP) on the radio, TV, newspapers, magazines and websites in Brazil and abroad are available.
www.portaldosfarmacos.ccs.ufrj.br/inct/hot_atorvastatina/main.swf


NOTÍCIAS ATORVASTATINA

DESCOBERTO NOVO PROCESSO DE PRODUÇÃO DE MEDICAMENTO CONTRA COLESTEROL

UNICAMP DESCOBRE NOVA ROTA PARA PRODUZIR MEDICAMENTO MAIS VENDIDO NO MUNDO

BRAZIL DEVELOPS LOW-COST LIPITOR

O GENÉRICO BRASILEIRO DO LIPITOR

Descoberta inédita química revolucionária reduz custos contra o colesterol alto

BRASIL PRODUZ DROGA MELHOR CONTRA COLESTEROL

MAIS E MELHORES MEDICAMENTOS

REMÉDIOS A PREÇOS MAIS BARATOS

Alternativa para fármaco mais vendido

At the atorvastatin hot site, all it takes is a click on the headlines to read the articles.

New synthetic route for Sunitinib – Recommended to fight certain types of cancers on the kidneys, stomach, and intestines, Sunitinib is the active principle of Sutent®/ Pfizer, a high price medication – around 11 thousand Reais for a box with 28 pills - that, unfortunately, is not made available in the public health care system (SUS), and which is the target of several lawsuits because of this.

The new synthetic route for Sunitinib was developed by Prof. Angelo da Cunha Pinto, and by Prof. Barbara Vasconcellos da Silva, of the Institute of Chemistry of the Federal University of Rio de Janeiro (UFRJ). After the news was publicized in academic journals, in late September 2011, the Terra Portal in Spain also reported on the discovery.

09/28/2011 Science Journal:
High cost medication may have cheaper generic

09/29/2011 FAPERJ Journal:
Researchers develop process to produce generic chemotherapeutical

09/29/2011 Portal Terra:
Tecnología brasileña reduce costo de medicina contra el cáncer

10/04/2011 ¡Saúde! Portal:
Process developed in Brazil allows for production of generic chemotherapeutical

10/13/2011 Vital Look / UFRJ:
Institute of Chemistry researchers develop generic pharmaceutical to fight certain types of cancer

INCT–INOFAR HIGHLIGHTED

INCT-INOFAR new medication research was the cover of Rio Research Magazine, edited by the Foundation for Research Support of Rio de Janeiro (FAPERJ), in March 2011:
"More and Better Drugs: Research network headquartered in Rio opens new perspectives in the pharmaceutical field for the country"
Rio Research Magazine
Year 5, issue 14, March 2011

In an interview with Medical Research Magazine, Prof. Eliezer J. Barreiro, INCT-INOFAR coordinator, discusses the process of patent recognition in Brazil and talks about the LASSBio 596 molecule, a strong INCT-INOFAR candidate to become a medication used on inflammatory respiratory illnesses, like asthma, chronic obstructive pulmonary disease, and emphysema.
"The roadblocks to pharmaceutical innovation"
Medical Research Magazine
Issue 17, Jan-Mar 2011

In a special report on the International Year of Chemistry, 'Chemistry and Derivates' magazine talked about how the creation of molecules capable of keeping the human body healthy may be one of the most noble applications of Chemistry. INCT-INOFAR coordinator, Prof. Eliezer J. Barreiro, was one of the researchers interviewed in the article.
"Medications: health enhanced by Chemistry advances"
Chemistry and Derivates Magazine
Year XLVI – issue 513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31/08 das 14h às 16h
Agende-se aqui.
EDUCAÇÃO CONTINUADA
EDUCAÇÃO EM SAÚDE

PROMOTION AND PARTICIPATION IN EVENTS

As part of its institutional routine, INCT-INOFAR organizes, promotes, supports, and participates in events in its field of research of pharmaceuticals and medication. It is a way to actively contribute to the publicizing of knowledge in the academic-scientific community, helping Brazil enhance its human resources and advance in studies of new medications.

Periodically, INCT-INOFAR researchers take part in Congresses, Meetings, Seminars, Symposiums, and Workshops, teaching courses, giving conferences, being part of round tables, among other activities. Parallel to these actions, INCT-INOFAR also supports courses and conferences in its field of research. The Institute also invests in events where it searches the cooperation of companies, non-profit organizations, and other institutions, so that new partnerships may be established.

INCT–INOFAR FOLLOW–UP AND EVALUATION MEETINGS

With a goal of strengthening scientific cooperation among its research network and of internally discussing the goals achieved by its subprojects that are most advanced in the chain of innovation in pharmaceuticals and medications, INCT-INOFAR organizes internal events of follow-up and evaluation, every six months.

"The multidisciplinary environment of the INCT-INOFAR evaluation meetings promotes scientific exchange among researchers of different complementary areas in the complex chain of innovation in pharmaceuticals and medications. As the subprojects are presented, criticism and suggestions are added to the scope of each research, optimizing the end results" – evaluates INCT-INOFAR coordinator, Prof. Eliezer J. Barreiro.

I 2011 EVALUATION AND FOLLOW–UP MEETING

The I 2011 Evaluation and Follow-Up Meeting took place on March 17 and 18, 2011, at the Health Sciences Center at UFRJ, which is the Institute's host institution. During the two days of the event, around 30 researchers that supervise the groups associated with INCT-INOFAR had the opportunity to present their research directly to representatives of funding agencies and to experts in the area.

Invited to the meeting under confidentiality and non-disclosure agreements were Gilberto Soares (FINEP), Pedro Palmeira (BNDES), Jerson Lima (FAPERJ), Carlos Gadelha (Ministry of Health), Rogerio Filgueiras (UFRJ Innovation Agency), and Prof. Vitor Ferreira (UFF), who enriched discussion by bringing new contribution to the development of projects.

I 2011 Evaluation and Follow-Up Meeting of INCT-INOFAR .

II 2011 EVALUATION AND FOLLOW-UP MEETING

On November 17 and 18, INCT-INOFAR had its II 2011 Evaluation and Follow-Up Meeting at the Merlin Hotel in Copacabana, Rio de Janeiro. Researchers took turns presenting the Institute's research subprojects in radical innovation that are the most advanced. Among them, pharmaceutical candidates for the recovery of myocardial infarction, new antipsychotic prototypes, substances for the treatment of neuropathic pain, leishmaniasis and Trypanosoma cruzi antiparasitic drugs, antiasthmatics, and vasodilators for arterial and pulmonary hypertension.

In the field of incremental innovation, two projects that successfully achieved new synthetic routes for generic drugs were presented. On this occasion, the trajectories followed to develop a new synthetic route for atorvastatin, the active principle of the cholesterol reducing drug Lipitor®, and of Sunitinib, the active principle in the chemotherapeutic drug Sutent®.

For this second meeting, the INCT-INOFAR Managing and Follow-Up Committee (CGA) brought Mercedes Gonzalez and Hugo Cerecetto, Uruguayan experts in Medicinal Chemistry and professors at the Universidad de la Republica (Udelar) in Montevideo. To further enhance the team of external consultants employed by the Institute, the event also had the presence of Andre Tempone, researcher from the Adolfo Lutz Institute, and of Professor Paulo Ribeiro Costa, from the Natural Products Research Nucleus of UFRJ.

Around 40 INCT-INOFAR researchers were present at the II 2011 Evaluation and Follow-Up Meeting.

34ª ANNUAL MEETING OF THE SBQ

Enhancing the discussions on Chemistry for the development of new pharmaceuticals and medications, INCT-INOFAR researchers were part of the 34th Annual Meeting of the Brazilian Chemistry Society (34th RASBQ), which took place on May 23 to 26, 2011, in the city of Florianopolis, in Santa Catarina.

With a record number of enrollments – 4,500 – the event was the largest Chemistry event in Latin America, and was the stage for some of the main celebrations of the International Year of Chemistry (AIQ) in Brazil.

INCT-INOFAR was present at the 34th Annual Meeting of the SBQ, showcasing its research activities in radical and incremental (generic drugs) pharmaceutical innovation at the stand dedicated to the National Institutes of Science and Technology (INCTs). At this environment, the participants had the opportunity to talk to the INCT-INOFAR researchers in person, and to see the Scientific Awareness and Health Education initiatives carried out by the Institute.

Teaching conferences, mini-courses, giving lectures at theme sessions and presenting papers at coordinated sessions and panels, INCT-INOFAR researchers played important roles at the scientific programming of the 34th RASBQ.

INCT-INOFAR was part of the INCT stands at the 34th SBQ Annual Meeting.

Member of the INCT-INOFAR Managing Committee, Prof. Vanderlan da Silva Bolzani, of the Institute of Chemistry of UNESP-Araraquara – who made her name in the history of Brazilian Chemistry by being, in 2008, the first woman to be elected president of the SBQ – was chosen to give the commencement conference for the event. As an acknowledgement of her scientific trajectory in Chemistry, the professor was also honored at the 34th RASBQ with the Simao Mathias Medal.

"History of the Discovery of Pharmaceuticals" was the theme of the mini-course presented by Prof. Carlos Alberto Manssour Fraga, INCT-INOFAR associate researcher connected to the Evaluation and Synthesis of Bioactive Substances Laboratory (LASSBio®) of UFRJ. Aside from presenting an overview of the chronology of strategies for planning and structurally optimizing prototypes, Manssour presented the history of the discovery of antibacterial pharmaceuticals like penicillin and sulfas and of innovative pharmaceuticals, like sildenafil and imatinib.

Chaired by Prof. Eliezer J. Barreiro (UFRJ), INCT-INOFAR coordinator, the theme session "Pharmaceuticals and Medications" was planned to talk about fundamental concepts of Medicinal Chemistry that have guided pharmaceutical research in the 20th century and the trends for the first decades of the 21st century. In its presentation, professor Barreiro presented the Fischer & Ehrlich paradigm in Modern Medicinal Chemistry.

Lidia Moreira Lima (UFRJ), Nelima Romeiro (UFRJ-Macae), Heloisa Beraldo (UFMG), Carlos Viegas (UNIFAL), Fernando Cunha (USP-Ribeirao Preto), and Luiz Carlos Dias (UNICAMP) were some of the researchers associated with INCT-INOFAR that were also present in the 34th Annual Meeting of the Brazilian Chemistry Society.

5TH ENIFARMED

From August 29 to August 31, 2011, in the city of Sao Paulo, the 5th National Meeting of Innovation in Pharmaceuticals and Medications – ENIFarMed debated the theme "The Health Industrial Complex: Strategic in access to medications".

A consolidated forum to stimulate the direct interaction of P, D&I professionals as well as of companies in the chain of production and of ICTs (Science and Technology Institutes) and Universities, the event aims to establish a common agenda among government and regulatory agencies in Brazil for the advancement of technological innovation in pharmaceuticals and medications in Brazil.

TECHNICAL ACKNOWLEDGEMENT AWARD

INCT-INOFAR received the Technical Acknowledgement Award in the 5th ENIFarMed for the panel "*Total synthesis of atorvastatin calcium*". Authored by Dr. Adriano Siqueira Vieira and Prof. Luiz Carlos Dias, INCT-INOFAR researchers connected to the Institute of Chemistry of UNICAMP, the work was one of 6 projects selected for oral presentation at the event. Among the selection criteria were adequacy of project to a market focus; conceptual and practical basis, and social relevance of the theme.

The award winning paper summarizes the efforts of INCT-INOFAR in the discovery of a new synthetic route for atorvastatin, the active principle of Lipitor®/ Pfizer, the worldwide most sold medication, which had its patent expire in Brazil on December 2010.

The synthetic methodology developed by INCT-INOFAR represents an innovative way to obtain the generic Lipitor®. By reducing stages in the synthetic route, the UNICAMP researchers have made it more efficient and cheaper when compared to the original route described in the Pfizer patent. There is also the advantage of presenting some new intermediates, with simple synthetic access.

Adriano Siqueira and Luiz Carlos Dias
(UNICAMP)


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DEBATE PANEL

To speak on pharmaceutical patents and other barriers that Brazil still needs to overcome to really innovate in the area of pharmaceuticals and medications, INCT-INOFAR coordinator Prof. Eliezer J. Barreiro, was invited by the 5th ENIFarMed to be part of the panel entitled "New Paths in Intellectual Property in the Pharmaceutical Sector".

Moderated by Luciene Amaral and Alexandre Lopes, both from the National Institute for Intellectual Property (INPI), the debate panel also had the presence of Eduardo Pedral Fiuza, from the Institute for Applied Economic Research (IPEA), and of Marcio Falci, Biolab research doctor.

5TH ENIFARMED EXPOSITION FAIR

With a goal of publicizing current projects in its drugs and medicines research network, as well as strategically connecting with the productive sector, INCT- INOFAR set up a stand on the 3rd EXPOFARMED, a business fair associated with the 5th ENIFarMed, as it had done in the previous year. This time, INCT-INOFAR presented the scientific know how of its research group and its actions on Scientific Awareness and Health Education.

INCT-INOFAR stand in the 5th ENIFarMed publicized the institute research to the productive sector, government, regulating agencies and universities.

XIII REGIONAL MEETING SBQ-RIO

With the theme "Challenges in Chemistry at the 'Golden Age' of Rio de Janeiro", the XII Regional Meeting of the Brazilian Chemistry Society – Rio de Janeiro (SBQ-Rio), conducted from July 4 to 7, 2011, at the Military Institute of Engineering (IME), also had INCT-INOFAR researchers among its speakers. As well as taking part in the event, the Institute researchers were also awarded by SBQ-Rio.

WALTER BAPTIST MORS MEDAL

The Walter Baptist Mors medal, created in honor of the renowned Brazilian chemist who was a pioneer of natural products Chemistry, was awarded to the researchers who made the biggest impact in Chemistry in 2010. Prof. Eliezer J. Barreiro, INCT-INOFAR coordinator, Prof. Angelo da Cunha Pinto, member of the Managing and Follow-Up Committee (CGA), Prof. Vitor Francisco Ferreira, scientific consultant for the Institute, and Prof. Francisco Radler de Aquino Neto, INCT-INOFAR UFRJ associate researcher, were awarded with the medal by SBQ-Rio.

ROUND TABLES

On the XIII Regional Meeting of SBQ-Rio, Prof. Eliezer J. Barreiro led the table "Challenges of the Pharmaceutical Industry in Brazil" which had the presence of Dr. Nubia Boechat, Farmanguinhos researcher, and of Tatiana Donato, Servier Laboratories project manager. In their presentations, the presenters talked about issues such as the generics market and the differences between the public and private sector markets in medications.

The round table on perspectives for undergraduate and graduate schools in Chemistry in the state of Rio de Janeiro had the presence of Prof. Luiz Carlos Dias, INCT-INOFAR CGA member. The professor, who is CAPES Chemistry coordinator, defended that it is necessary to advance in the consolidation of graduate schools in the North, Northeast, and Midwest regions, as well as strengthening undergraduate courses in those areas. To him, it is necessary to correct the imbalances, providing extra support to these regions, and encouraging cooperative research done through networks.

SCIENCE FAIR

With a goal of increasing interest in Chemistry among youth, the XIII Regional Meeting - SBQ-Rio promoted a science fair with chemistry presentations. At the INCT-INOFAR stand, the Meeting audience could get to know more about the research activities in the discovery of a 100% Brazilian medication, and the initiatives in the areas of Scientific Awareness and Health Education. At this occasion, INCT-INOFAR also conducted a poll on contraceptive methods and population control. The results of this poll will be the basis for the third booklet produced by the Institute, this time focusing on the correct use of contraceptives.

Soldiers of the Military Institute of Engineering and high school students visited the INCT-INOFAR stand.

INCT–INOFAR INNOVATION MEDAL

At the closing of the XIII Regional Meeting - SBQ-Rio, INCT-INOFAR awarded the first INCT-INOFAR Innovation Medal, an acknowledgement of Institute researchers who actively participated in the Discovery of new synthetic routes for future generic drugs.

Prof. Luiz Carlos Dias and Dr. Adriano Siqueira Vieira of the UNICAMP Institute of Chemistry were awarded the medal for the discovery of a new way to produce atorvastatin, and Prof. Angelo da Cunha Pinto and Dr. Barbara Vasconcellos da Silva, of the UFRJ Institute of Chemistry, for the new synthesis route of Sunitinib.

II FAPERJ FAIR

INCT-INOFAR was present in the II FAPERJ Fair of Science, Technology & Innovation, which took place on the Culture Center for Citizenship Action, in downtown Rio de Janeiro on June 29 and 30. The Fair has the goal of exposing, in a dynamic and fun way, the main advancements in research and innovation in the state supported by the Carlos Chagas Filho Foundation of Research Support in Rio de Janeiro (FAPERJ). As it is headquartered in Rio de Janeiro, INCT-INOFAR has the support of FAPERJ to develop its research activities.

INCT-INOFAR was part of the II FAPERJ Fair with a 16 m2 stand. The space was decorated with posters illustrating the INCT-INOFAR goals and its research structure, as well as the main discoveries of the Institute. In an interactive and dynamic way, researchers associated with the Institute received visitors to the "New Pharmaceuticals" stand presenting the latest INCT-INOFAR innovations in the research for new pharmaceuticals and its main activities in the fields of scientific awareness and health education.

To call the attention of the public present, INCT-INOFAR took large scale medication boxes to demonstrate the care one should have when purchasing medications. In the interaction with visitors, specialists highlighted the meaning of each color band in the packaging (red, black, and no band), as well as presenting the main characteristics of generic drugs.

GA theater group visited the INCT-INOFAR stand at the II FAPERJ Fair

XVII SUMMER SCHOOL IN MEDICINAL CHEMISTRY

Traditionally organized by the Evaluation and Synthesis of Bioactive Substances Laboratory (LASSBio®), the Summer School in Medicinal Chemistry was incorporated by INCT-INOFAR as an extension activity. The event, which is always carried out at UFRJ during summer vacation, offers 5 consecutive days of courses and conferences with renowned Brazilian and foreign experts in the field of Medicinal Pharmaceutical Chemistry.

Since its creation, in 1995, the School has already had over 2,000 participants and has received famous scientists, responsible for the development of innovative medications, like Simon Campbell (sildenafil) and Robin Ganellin (cimetidine), who were able to retell the stories of their discoveries in person.

COURSES OFFERED IN 2011:

- "Introduction to Pharmaceutical Medicinal Chemistry"
  Dr. Eliezer J. Barreiro (UFRJ)
- "Pharmaceuticals Metabolism and Toxicology"
  Dr. Lidia M. Lima (UFRJ)
- "Pharmacology of Pain and Analgesia – new targets for the development of analgesic pharmaceuticals"
  Dr. Thiago M. Cunha (USP/RP)
- "From Gram to Kilogram – challenges of scale transposition"
  Dr. Angelo Machado (UNB)
- "Tutorial: Computational Chemistry and Molecular Modeling"
  Dr. Nelilma C. Romeiro (UFRJ)
- "Highlights in Medicinal Chemistry"
  Dr. Rob Leurs (Vrije Universiteit / ND)

EVENTS ATTENDED BY INCT–INOFAR

December 09, 2011
Workshop "Celebration of the International Year of Chemistry"
Federal University of Parana – PR
Lecture: "*Medicinal Chemistry*"
Prof. Eliezer J. Barreiro

November 30, 2011
2011 – International Year of Chemistry: Chemistry in our lives"
Federal University of Uberlandia – MG
Lecture: "*Medicinal Chemistry and the discovery of pharmaceuticals*"
Mini-Course: "*Pharmaceuticals planning aspects*"
Prof. Eliezer J. Barreiro

November 13, 2011
XXV Regional Meeting of the Brazilian Chemistry Society
University of Lavras – MG
Lecture: "*Medicinal Chemistry and the discovery of new pharmaceuticals: the case of INCT-INOFAR*"
Prof. Eliezer J. Barreiro

November 10, 2011
II Symposium on Planning and Developing New Pharmaceuticals for Neglected Diseases
University of Sao Paulo – SP
Round Table: *"Neglected diseases policies"*
Prof. Eliezer J. Barreiro

October 31 to November 4, 2011
I Escuela Internacional de Química Medicinal y Farmacologia
Universidad de La Republica – Montevideo – Uruguay
Prof. Eliezer J. Barreiro
Prof. Lidia Moreira Lima
Prof. Angelo da Cunha Pinto

October 27, 2011
36th Congress of the Brazilian Society of Pharmaceutical Medicine
Hotel Macksoud Plaza – Sao Paulo – SP
Session: "*PP Partnership in Health – Academia and Industry: cooperation projects and INCT-INOFAR perspectives*"
Prof. Eliezer J. Barreiro

October 6, 2011
AIQ 2011
Department of Chemistry of the Federal University of Vicosa - MG
Lecture: "*Pharmaceutical innovation in Brazil: National Institute of Science and Technology in Pharmaceuticals and Medications*"
Prof. Eliezer J. Barreiro

September 30, 2011
Chemistry Graduate Program
Military Institute of Engineering – RJ
Lecture: "*INCT-INOFAR*"
Prof. Eliezer J. Barreiro

September 30, 2011
Symposium on Development of Phytotherapeuticals
Federal University of Rio de Janeiro – RJ
Commencement Speech
Prof. Eliezer J. Barreiro

September 26 and 27, 2011
XIV "Prof. Edson Rodrigues" Chemistry Week
University of Sao Paulo – Sao Carlos – SP
Mini-course: "*Pharmaceuticals planning*"
Prof. Eliezer J. Barreiro

September 19, 2011
Session Track*: *Global External Research & Development Directors; INCT-INOFAR & Eli Lilly and Company (Dr. Yetunde Taiwo)
Lilly Research Laboratories
Prof. Eliezer J. Barreiro
Prof. Marco Aurelio Martins

September 12 to 16, 2011
XXII Chemistry Academic Week - UFF
Federal University of Rio de Janeiro - RJ
Mini-course: *"Pharmaceuticals"*
Prof. Eliezer J. Barreiro

September 01 to 05, 2011
14th *Brazilian Meeting on Organic Synthesis* – BMOS
Brasilia- DF
Lecture: "*Adventures in the exciting area of total synthesis of bioactive products*"
Prof. Luiz Carlos Dias

August 31, 2011
I International Symposium on Inflammation
Rio de Janeiro, Brazil
Lecture: Chair person at symposium "*Inflammation and cancer*".
Prof. Marco Aurelio Martins

August 29 to 31, 2011
5th National Meeting of Innovation in Pharmaceuticals and Medications (ENIFarMed) and 3rd ExpoFarmed
Reboucas Convention Center – Sao Paulo
Debate Panel: "Intellectual Property"
Prof. Eliezer J. Barreiro
INCT-INOFAR Stand
- Prof. Lidia Moreira Lima, Prof. Angelo C. Pinto and Prof. Roberto Takashi Sudo
"Technical Acknowledgement" Award – Presentation of poster "Total Synthesis of Atorvastatin Calcium"
- Prof. Luiz Carlos Dias and Dr. Adriano Siqueira Vieira

August 25, 2011
XXII Brazilian Parasitology Congress
Reboucas Convention Center – Sao Paulo
Round Table: *"Challenges in pharmaceutical research for neglected diseases"*
Prof. Eliezer J. Barreiro

August 24, 2011
PGQu Seminars
Institute of Chemistry – Federal University of Rio de Janeiro – RJ
Lecture: *"The National Institute of Science and Technology in Drugs and Medicines - INCT-INOFAR: Who we are? What do we do?"*
Prof. Eliezer J. Barreiro

August 17, 2011
Sao Paulo Advanced School on Natural Products, Medicinal Chemistry and Organic Synthesis Integrated Solutions for Tomorrow's World
UNICAMP – Campinas – SP
Lecture: "*Recent progress towards the total synthesis of bioactive compounds*"
Prof. Luiz Carlos Dias

August 16, 2011
Sao Paulo School of Advanced Science
State University of Campinas - SP
Lecture: *"New insights for multifactorial disease therapy – the design of new symbiotic leads"*
Prof. Eliezer J. Barreiro

August 05, 2011
Forum Permanente UNICAMP
State University of Campinas - SP
Round Table: *"The triple helix and Pasteur quadrant as models for the 21st century university"*
Prof. Eliezer J. Barreiro

August 01, 2011
43rd IUPAC World Chemistry Congress, CLI400
San Juan – Puerto Rico
Lecture: "*Modern medicinal chemistry: natural products and synthesis molecules as valuable tools*"
Prof. Luiz Carlos Dias

July 27 to 29, 2011
II International Symposium On Drug Discovery
Faculty of Pharmaceutical Sciences– UNESP – Araraquara - SP
Lecture: "University & pharmaceutical companies interactions"
Prof. Eliezer J. Barreiro

July 11 to 15, 2011
63rd SBPC Annual Meeting
Federal University of Goiania – GO
Mini-course: *"Planning of new pharmaceutical candidates"*
Round Table: *"Production of new pharmaceuticals in Brazil: obstacles and challenges"*
Meeting with INCT Coordinators
Prof. Eliezer J. Barreiro

July 05, 2011
XII SBQ Regional Meeting – Rio de Janeiro
Military Institute of Engineering – RJ
Round Table: *"Challenges of the pharmaceutical industry in Brazil"*
Prof. Eliezer J. Barreiro

June 29 and 30, 2011
II FAPERJ Fair of Science, Technology, and Innovation 2011
Culture Center of Citizenship Action – RJ
Prof. Eliezer J. Barreiro

June 25 to 29, 2011
10th World Congress on Inflammation
Paris, France
Lecture: Chair person and presentation of paper on symposium: "*New trends in the control of lung inflammation*"
Prof. Marco Aurelio Martins
Lecture: Presentation of paper on symposium New Therapeutic Targets in Inflammation "*Suppressive effect of c-jun nh2-terminal kinase (jnk) inhibitor sp600125 on experimental silicosis in mice*"
Prof. Patricia Machado R. S. Martins

June 08, 2011
AIQ 2011 Conference Cycle
FAPESP Auditorium – SP
Round Table: *"Medicinal Chemistry: challenges and perspectives"*
Prof. Eliezer J. Barreiro

June 01, 2011
1st Pharmaceutical Journey
State University of the West Side – RJ
Mini Course: *"Topics of pharmaceutical interest"*
Prof. Eliezer J. Barreiro

May 23 to 26, 2011
34th Annual Meeting of the Brazilian Society of Chemistry
Costao do Santinho – Florianopolis – SC
Lecture: *"The Fischer & Ehrlich paradigm in modern Medicinal Chemistry"*
Prof. Eliezer J. Barreiro

May 13 to 18, 2011
American Thoracic Society International Conference
Denver, USA
Paper presentation on poster session
Prof. Marco Aurelio Martins
Presentation of paper on session *Poster Discussion: Scarring in the lung: principles and perspectives* – "*Effect of annexin-1 n-terminal derived peptide ac 2-26 on the acute phase of silicosis in mice.*"
Prof. Patricia Machado R. S. Martins

May 11, 2011
Integration Week – Faculty of Pharmacy
Federal University of Goiania - GO
Lecture: ***"Development of new pharmaceuticals: from bench to pharmacy shelf"***
Prof. Eliezer J. Barreiro

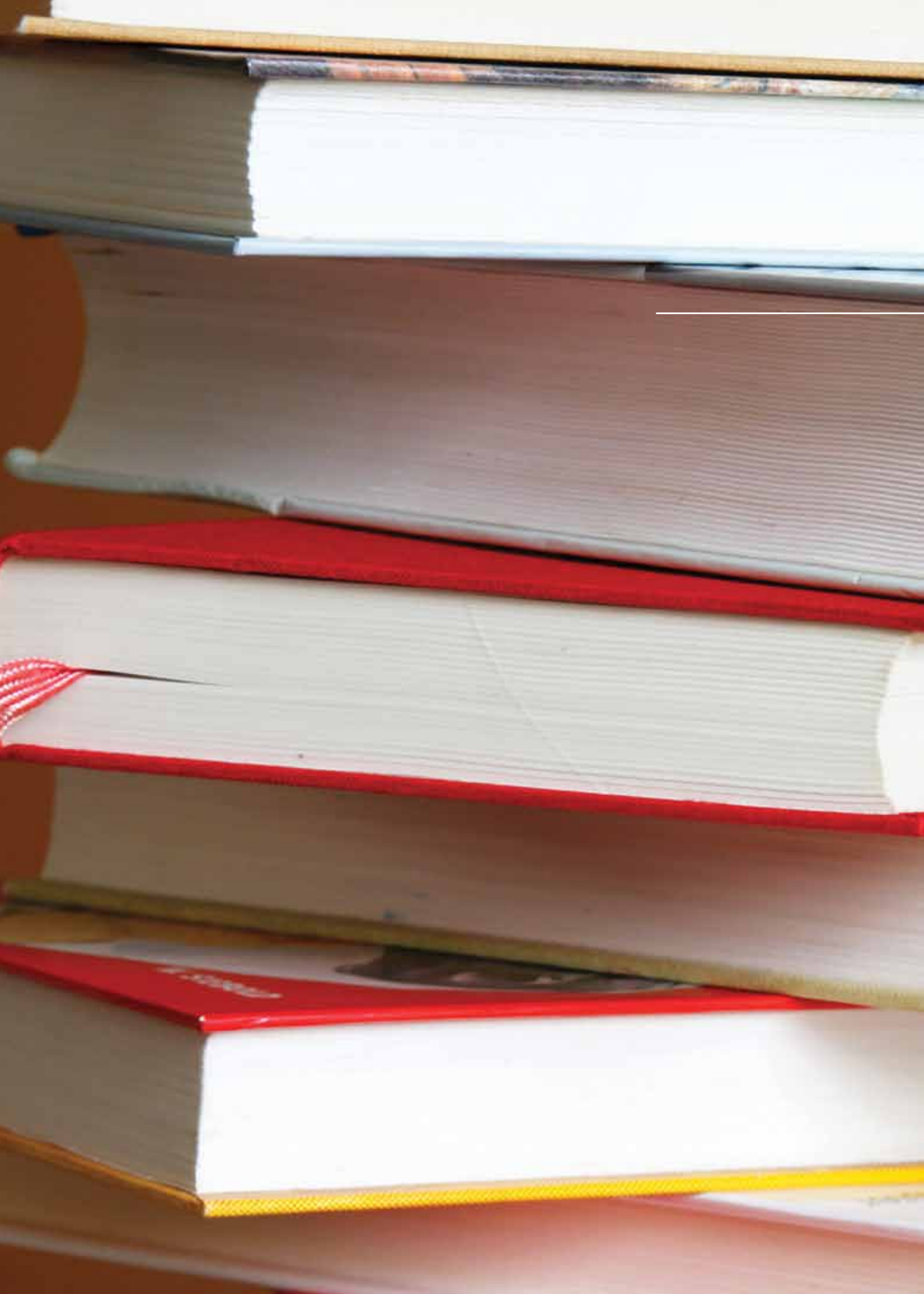
May 09, 2011
I Education and Science Meeting: Biodiversity and Sustainability of the Northern Amazon
State University of Roraima – RR
Round Table: ***"The importance of Medicinal Chemistry on the development of pharmaceuticals"***
Prof. Eliezer J. Barreiro

April 26, 2011
Federal Rural University of Rio de Janeiro - RJ
Chemistry Academic Week
Lecture: ***"On the process of innovation in new pharmaceuticals"***
Prof. Eliezer J. Barreiro

April 25, 2011
Servier Laboratories of Brazil – Rio de Janeiro – RJ
Lecture: ***"Opportunities in pharmaceutical innovation: INCT-INOFAR"***
Prof. Eliezer J. Barreiro

April 15, 2011
EMS Scientific Committee Meeting
Renaissance Hotel – Sao Paulo - SP
Lecture: ***"Opportunities in pharmaceutical innovation: INCT-INOFAR"***
Prof. Eliezer J. Barreiro

February 15, 2011
III International Workshop on Organic Chemistry
UNICAMP – Campinas – SP
Lecture: ***"Recent progress towards the total synthesis of bioactive products"***
Prof. Luiz Carlos Dias



INCT–INOFAR PUBLICATIONS

NATIONAL JOURNALS

1] ANTUNES, A. M. S., GALERA, P., RUBINSTEIN, L. Prospectiva para a indústria química do Brasil: uma visão para o futuro. **Economia & tecnologia**, ano 7, v.26, p.117 - 127, 2011.

2] doi> ANTUNES, M. A.; ROCCO, P. R. M.. Elastase-induced pulmonary emphysema: insights from experimental models. **An. Acad. Bras. Ciênc.** v. 83, p. 1385-1396, 2011.

3] AQUINO NETO, F. R.. Dopagem: ética no esporte e saúde dos atletas**. Ciência Hoje**, v. 48, p. 136-141, 2011.

4] BARBOSA, M. C. M.; BARBOSA, A.P.; ROCCO, P. R. M. Diagnóstico da síndrome do desconforto respiratório agudo na criança. **Pulmão RJ**, v.20, p.7-12, 2011.

5] doi> BRAZ, A. S. ; PAULA, A. P.; DINIZ, M. F. F. M.; ALMEIDA, R. N. Non-pharmacological therapy and complementary and alternative medicine in fibromyalgia. **Revista Brasileira de Reumatologia**, v. 51, p. 269-282, 2011

6] doi> DIAS, M. O.; HAMERSKI, H.; PINTO, A. C.. Separação semipreparativa de α e β-amirina por cromatografia líquida de alta eficiência. **Química Nova**, v. 34, p. 704-706, 2011.

7] doi>DINIZ, M. F. F. M.; OLIVEIRA, S. M. S.; COSTA, M. J. C.; SIQUEIRA JUNIOR, J. P.; FALCÃO-SILVA, V. S. Modulation of drug resistance in Staphylococcus aureus by extract of mango (Mangifera indica) peel. **Revista Brasileira de Farmacognosia**, v. 1, p. 190-193, 2011.

8] doi>FERREIRA, P. M. P.; FARIAS, D. F.; VIANA, M. P.; SOUZA, T. M.; VASCONCELOS, I. M.; SOARES, B. M.; PESSOA, C. O.; COSTA-LOTUFO, L. V.; MORAES , M. O.; CARVALHO, A. F. U. Study of the antiproliferative potential of seed extracts from Northeastern Brazilian plants. **Anais da Academia Brasileira de Ciências**, v. 83, p. 1-14, 2011.

9] FREITAS, A. P. F.; LUCERA, C. T.; CERQUEIRA, G. S.; OLIVEIRA, T. L.; DINIZ, M. F. F. M.. Levantamento de plantas medicinais utilizadas no sertão paraibano: um estudo transversal. **Conceitos** (João Pessoa), v. 1, p. 15-20, 2011.

10] GOSMANN, G.; PROVENSI, G.; COMUNELLO, L. N.; RATES, S. M. K. Composiçao química e aspectos farmacológicos de espécies de Passiflora L.. **Revista Brasileira de Biociências** (Online), v. 9, p. 88-99, 2011.

11] doi>GOTARDO, M. A.; HYSSA, J. T.; CARVALHO, R. S.; DE-CARVALHO, R. R.; GUEIROS, L. S.; SIQUEIRA, C. M.; SARPA, M.; DE-OLIVEIRA, A. C.; PAUMGARTTEN, F. J.. Modulation of expression and activity of cytochrome P450s and alteration of praziquantel kinetics during murine schistosomiasis. **Mem Inst Oswaldo Cruz**. v.106, p.212-219, 2011.

12] LIMA, C. M. B. L.; CAVALCANTI, M. G. S.; FREITAS, F. I. S.; MORAIS, L. C. S. L.; DINIZ, M. F. F. M.. Avaliação do tratamento com o óleo essencial do Allium sativum (alho) em pacientes parasitados. **Revista Brasileira de Análises Clínicas**, v. 43, p. 076-080, 2011

13] doi> LIMA, C. M. B. L.; FREITAS, F. I. S.; MORAIS, L. C. S. L.; CAVALCANTI, M. G. S.; SILVA, L. F.; PADILHA, R. J. R.; BARBOSA, C. G. S.; SANTOS, F. A. B.; ALVES, L. C.; DINIZ, M. F. F. M.. Ultrastructural study on the morphological changes to male worms of Schistosoma mansoni after in vitro exposure to allicin. **Revista da Sociedade Brasileira de Medicina Tropical**, v. 44, p. 327-330, 2011.

14] doi>LIMA, R. A.; SCHANAIDER, A.; SANTANA, M. C. E.; OLIVEIRA, M. G.; CAPELOZZI, V. L.; ROCCO, P. R. M.. Desenvolvimento de um novo modelo experimental de síndrome do compartimento abdominal. R**ev. Col. Bras. Cir.,** v. 38, p. 417-421, 2011.

15] MAGALHAES, J. L., BOECHAT. N., ANTUNES, A. M. S. Laboratórios farmacêuticos oficiais e sua relevância para saúde pública do Brasil. RECIIS. **Revista eletrônica de comunicação, informação & inovação em saúde,** v.5, p.85-99, 2011.

16] doi> MENDONÇA, M. C. L., FERREIRA, A. M. A., SANTOS, M. G. M., OVIEDO, E. C., BELLO, M. S. D., SIQUEIRA, M. M., MACEIRA, J. M. P., HUBINGER, M. G, COUCEIRO, J. N. S. S.. Genotyping of Human parvovirus B19 in clinical samples from Brazil and Paraguay using HMA (Heteroduplex Mobility Assay), SSCP (Single-Stranded Conformation Polymorphism) and nucleotide sequencing. **Memórias do Instituto Oswaldo Cruz**, v.106, p.502- 504, 2011.

17] doi> MEDEI, E.; RAIMUNDO, J. M.; NASCIMENTO, J. H. M.; SUDO, R. T.; ZAPATA-SUDO, G. Inhibition of L-type calcium current by tramadol and enantiomers in cardiac myocytes from rats. **Arq. Bras. Cardiol**., v. 97, p. 324-331, 2011.

18] doi> MORANO, J. A. C. O. D.; CORDEIRO, N.; GUIMARÃES, S. B.; JAMACARU, F. V. F.; MORAES, M. O. Experimental model of ultrasound thermotherapy in rats inoculated with Walker-236 tumor. **Acta Cirurgica Brasileira**, v. 26, p. 01-06, 2011

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21] doi> PAUMGARTTEN, F. J. Pharmacological treatment of obesity: a public health perspective. **Cad Saude Publica.** 2011, v.27, n.3, p.404-405.

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25] doi> UEKANE, T. M.; AQUINO NETO, F. R.; GOMES, L. N. F. Development and validation of a method for the analysis of tetracyclines in chicken-muscle by liquid chromatography-electrospray-mass spectrometry in tandem (LC-ESI-MS/MS). **Química Nova**, v. 34, p. 43-48, 2011.

26] VIEGAS, F.P.D.; SIMOES, M. C. R.; ROCHA, M. D.; CASTELLI, M. R.; MOREIRA, M. S.; VIEGAS JR., C.. Doença de Alzheimer: caracterização, evolução e implicações do processo neuro-inflamatório. **Revista Virtual de Química**, v. 3, p. 286-306, 2011.

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1] doi> BARREIRO, E. J.; KUMMERLE, A. E.; FRAGA, C. A. M.. The methylation effect in medicinal Chemistry. Chemical Reviews, v. 111, p. 5215-5246, 2011.

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4] doi> ABREU, S. C.; ANTUNES, L. A.; PELOSI, P.; MORALES, M.; ROCCO, P. R. M. Mechanisms of cellular therapy in respiratory diseases. Intensive Care Med. v. 37, p.1421-1431, 2011.

5] doi> ARAUJO, J. Q.; LIMA, J. A.; PINTO, A. C.; ALENCASTRO, R. B.; ALBUQUERQUE, M. G.. Docking of the alkaloid geissospermine into acetylcholinesterase: a natural scaffold targeting the treatment of Alzheimer s disease. Journal of Molecular Modeling, v. 17, p. 1401-1412, 2011.

6] doi> AVILA, C. M.; LOPES, A. B.; GONÇALVES, A. S.; SILVA, L. L.; ROMEIRO, N. C.; MIRANDA, A. L. P.; SANT'ANNA, C. M. R.; BARREIRO, E. J.; FRAGA, C. A. M.. Structure-based design and biological profile of (E)-N-(4-Nitrobenzylidene)-2-naphthohydrazide, a novel small molecule inhibitor of IKKβ-kinase. European Journal of Medicinal Chemistry, v. 46, p. 1245-1253, 2011.

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8] doi> BARROS, F. W. A.; BANDEIRA, P. N.; LIMA, D. J. B.; MEIRA, A. S.; DE FARIAS, S. S.; ALBUQUERQUE, M. R. J. R.; SANTOS, H. S.; LEMOS, T. L. G.; MORAES , M. O.; COSTA-LOTUFO, L.V.. Amyrin esters induce cell death by apoptosis in HL-60 leukemia cells. Bioorganic & Medicinal Chemistry, v. 19, p. 1268-1276, 2011.

9] doi> BRAGA, R. C.; TÔRRES, A. C. B.; PERSIANO, C. B.; ALVES, R. O.; FRAGA, C. A. M.; BARREIRO, E. J.; OLIVEIRA, V.. Determination of the cardioactive prototype LASSBio-294 and its metabolites in dog plasma by LC MS/MS: Application for a pharmacokinetic study. Journal of Pharmaceutical and Biomedical Analysis, v. 55, p. 1024-1030, 2011.

10] doi> BUARQUE, C. D.; MILITÃO, G. C. G.; LIMA, D. J. B.; COSTA-LOTUFO, L. V.; PESSOA, C. O.; MORAES , M. O.; CUNHA-JÚNIOR, E. F.; TORRES-SANTOS, E. C.; NETTO, C. D.; COSTA, P. R. R. Pterocarpanquinones, aza-pterocarpanquinone and derivates: Synthesis, antineoplasic activity on human malignant cell lines and antileishmanial activity on Leishmania amazonensis. Bioorganic & Medicinal Chemistry, v. 19, p. 6885-6891, 2011.

11] doi> CARVALHO, A. A.; FINGER, D.; MACHADO, C. S.; SCHMIDT, E. M.; COSTA, P. M.; ALVES, A. P. N. N.; MORAIS, T. M. F.; QUEIROZ, M. G. R.; QUINÁIA, S. P.; ROSA, M. R.; MORAES, M. O.. In vivo antitumoural activity and composition of an oil extract of Brazilian propolis. Food Chemistry, v. 126, p. 1239-1245, 2011.

12] doi> CARVALHO, T. T.; FLAUZINO, T.; OTAGUIRI, E. S.; BATISTELA, A. P.; ZARPELON, A. C.; CUNHA, T. M.; FERREIRA, S. H.; CUNHA, F. Q.; VERRI JR., W. A.. Granulocyte-Colony Stimulating Factor (G-CSF) induces mechanical hyperalgesia via spinal activation of MAP kinases and PI3K in mice. Pharmacology, Biochemistry and Behavior, v. 98, p. 188-195, 2011.

13] doi> CARVALHO, V. F.; FLORIM, L. T.; BARRETO, E. O.; TORRES, R. C.; MEUSERBATISTA, M.; AMENDOEIRA, F. C.; CORDEIRO, R. S. B.; Martins, M. A.; E SILVA, P. M. R.. Inhibition of advanced glycation end products by aminoguanidine restores mast cell numbers and reactivity in alloxan-diabetic rats. European Journal of Pharmacology, v. 669, n. 1-3, p. 143-148, 2011.

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Newly Isolated Bacillus circulans BL32. American Journal of Food Technology, v. 6, p. 460-471, 2011.

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28] Natália Araújo Touza. Caracterização da inibição da Na,K-ATPase por bufadienólidos endógenos e semi-sintéticos. 2011. Dissertação (Mestrado em Ciências Biológicas (Farmacologia e Química Medicinal) - Universidade Federal do Rio de Janeiro, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior. Orientador: Francois Germain Noel.

29] Ramon Borges da Silva. Síntese e avaliação do perfil tripanocida dos novos derivados imidazólicos trissubstituídos planejados como potenciais agentes anti-chagásicos. 2011. Dissertação (Mestrado em Química) - Universidade Federal do Rio de Janeiro, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior. Orientador: Carlos Alberto Manssour Fraga.

30] Raphael Trevizani. Biblioteca de fragmentos para a predição de estruturas de proteínas. 2011. Dissertação (Mestrado em Modelagem Computacional) - Laboratório Nacional de Computação Científica, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior. Orientador: Laurent Emmanuel Dardenne.

31] Raquel Cenachi Madalosso. Avaliação da toxicidade aguda e da atividade gastroprotetora de extratos de *campanesia lineatifolia* Ruiz & Pav. em roedores. 2011. Dissertação (Mestrado em Programa de Pós-Graduação em Ciências Framacêutica) - Universidade Federal de Minas Gerais, Fundação de Amparo à Pesquisa do Estado de Minas Gerais. Co-Orientador: Carlos Alberto Tagliati.

32] Raquel Souza Santos. Efeitos respiratórios do ácido oleanólico nos processos inflamatório e oxidativo em modelo experimental de lesão pulmonar aguda. 2011. Dissertação (Mestrado em Ciências Biológicas (Fisiologia)) - Universidade Federal do Rio de Janeiro, Fundação Carlos Chagas Filho de Amparo à Pesq. do Estado do Rio de Janeiro. Orientador: Patricia Rieken Macedo Rocco.

33] Renato Mazon Lima Verde Leal. Estudo do efeito protetor da N-aceitlcisteína sobre a esteato-hepatite induzida por irinotecano em camundongos. Início: 2011. Dissertação (Mestrado em Cirurgia) - Universidade Federal do Ceará. (Orientador).

34] Rodrigo José Avila Cartaxo. Metodologia de priorização para produção nacional dos medicamentos pertencentes à lista do Sistema Único de Saúde - SUS. 2011. Dissertação (Mestrado em Mestrado Profissional em Propr Intelec e Ino) - Instituto Nacional da Propriedade Industrial. Orientador: Adelaide Maria de Souza Antunes.

35] Rosina Maria Carvalho Muniz. Avaliação da prevalência de patologias orais e sua relação com a capacidade-tampão salivar e a flora oral no paciente bariátrico. 2011. Dissertação (Mestrado em Pós-Graduação em Farmacologia) - Universidade Federal do Ceará. Orientador: Manoel Odorico de Moraes Filho.

36] Simone Abrantes Saraiva. Impacto da obesidade no remodelamento da via aérea e parenquima pulmonar em modelo murino de asma alérgica crônica. 2011. Dissertação (Mestrado em Clínica Médica) - Universidade Federal do Rio de Janeiro. Orientador: Patricia Rieken Macedo Rocco.

37] Thais Andrade Soares. Síntese e avaliação farmacológica de derivados indolil N-acilidrazônicos planejados como ligantes canabinóides. 2011. Dissertação (Mestrado em Química) - Universidade Federal do Rio de Janeiro, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior. Orientador: Carlos Alberto Manssour Fraga.

38] Thiago Stevanatto Sampaio. Desenho, síntese e avaliação farmacológica de novos protótipos análogos ao imatinibe. 2011. Dissertação (Mestrado em Farmacologia e Química Medicinal) - Universidade Federal do Rio de Janeiro, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior. Orientador: Eliezer Jesus de Lacerda Barreiro.

39] Vitor Sueth Santiago. Síntese e avaliação farmacológica de novos análogos sacarínicos do protótipo antiinflamatório LASSBio-468. 2011. Dissertação (Mestrado em Química) - Universidade Federal do Rio de Janeiro, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior. Orientador: Carlos Alberto Manssour Fraga.

FINISHED DOCTORAL THESES 2011

1] Adriana Andrade Carvalho. Avaliação do potencial antimetastatico e antiangiogênico da biflorina. 2011. Tese (Doutorado em Pós Graduação Em Farmacologia) - Universidade Federal do Ceará, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior. Orientador: Manoel Odorico de Moraes Filho.

2] Caliandra Maria Bezerra Luna Lima. Investigação da atividade anti-parasitária do *allium sativum* L. *in vitro* e *in vivo*. 2011. Tese (Doutorado em Produtos Naturais e Sintéticos Bioativos) - Universidade Federal da Paraíba. Orientador: Margareth de Fátima Formiga Melo Diniz.

3] Carlos Augusto Ciarlini Teixeira. Estudo das características clínicas e evolutivas e das características epidemiológicas de 146 pacientes com esclerose múltipla observadas e acompanhadas em Fortaleza, Ceará, Brasil entre os anos 1979 e 2010. 2011. Tese (Doutorado em Programa de Pós-Graduação em Farmacologia) - Universidade Federal do Ceará. Orientador: Manoel Odorico de Moraes Filho.

4] Carmelita Gomes da Silva. Aspectos químicos de vellozia kolbekii Alves (Velloziaceae) e estudo das atividades antioxidante, citotóxica e antibacteriana. 2011. Tese (Doutorado em Química) - Universidade Federal do Rio de Janeiro, Conselho Nacional de Desenvolvimento Científico e Tecnológico. Orientador: Claudia Moraes de Rezende.

5] Cristiane Ribeiro Pereira. Papel da NADPH oxidase na proliferação e apoptose de células de melanoma humano. 2011. Tese (Doutorado em Biologia (Biociências Nucleares)) - Universidade do Estado do Rio de Janeiro, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior. Orientador: Thereza Christina Barja Fidalgo.

6] Daniele Gabriel Costa. Melhora da disfunção ventricular após tratamento com derivado tienilhidrazona pós-infarto do miocárdio. 2011. Tese (Doutorado em Ciências Biológicas (Farmacologia e Química Medicinal)) - Universidade Federal do Rio de Janeiro, Fundação Carlos Chagas Filho de Amparo à Pesq. do Estado do Rio de Janeiro. Orientador: Gisele Zapata-Sudo.

7] Débora Costa Reis. Estudo do perfil farmacológico de novas tiossemicarbazonas e novos complexos de bismuto(III) e antimônio(III). 2011. Tese (Doutorado em Química) - Universidade Federal de Minas Gerais, Conselho Nacional de Desenvolvimento Científico e Tecnológico. Orientador: Heloisa de Oliveira Beraldo.

8] Elias Borges Nascimento Júnior. Avaliação do papel da 5-hidroxitriptamina no processamento nociceptivo periférico da resposta nociceptiva. 2011. Tese (Doutorado em Ciências Farmacêuticas) - Universidade Federal de Minas Gerais. Orientador: Márcio de Matos Coelho.

9] Elisabete Barros. Estudo dos constituintes voláteis de vinhos brancos brasileiros. 2011. Tese (Doutorado em Ciência de Alimentos- Universidade Federal do Rio de Janeiro) - Universidade Federal do Rio de Janeiro, Conselho Nacional de Desenvolvimento Científico e Tecnológico. Co-Orientador: Claudia Moraes de Rezende.

10] Gabrille Dias Salton. Importância de motivos conservados do fator de início de tradução 2 (eIF2) na síntese de proteínas e na distribuição subcelular desse fator em células humanas. 2011. Tese (Doutorado em Biologia Celular e Molecular) - Universidade Federal do Rio Grande do Sul, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior. Orientador: João Antonio Pegas Henriques.

11] Henrique de Paula Lemos. Interdependência entre vias supressoras do IFN-gama e das enzimas indoleamina (2,3) - dioxigenas (IDO) e heme oxigenase- 1 (HO-1) na artrite induzida por antigeno e na encefalomielite autoimune experimental. 2011. Tese (Doutorado em Farmacologia) - Faculdade de Medicina de Ribeirão Preto-USP, Fundação de Amparo à Pesquisa do Estado de São Paulo. Orientador: Fernando de Queiroz Cunha.

12] Igara Oliveira Lima. Atividade antifúngica e toxicidade dos monoterpenos citral e carvacrol. 2011. Tese (Doutorado em Produtos Naturais e Sintéticos Bioativos) - Universidade Federal da Paraíba, Conselho Nacional de Desenvolvimento Científico e Tecnológico. Orientador: Margareth de Fátima Formiga Melo Diniz.

13] Jana Luiza Toscano Mendes de Oliveira. Investigação da toxidade geral e oftalmológica do óleo essencial de *origanum vulgari* L. (LAMIACEAE). 2011. Tese (Doutorado em Produtos Naturais e Sintéticos Bioativos) - Universidade Federal da Paraíba. Orientador: Margareth de Fátima Formiga Melo Diniz.

14] Jean Pierre Barros Thibaut. Caracterização do mecanismo de ação esquistossomicida do 3-metilclonazepam e de novas benzodiazepinas. 2011. Tese (Doutorado em Ciências Biológicas (Farmacologia e Química Medicinal)) - Universidade Federal do Rio de Janeiro, Fundação Carlos Chagas Filho de Amparo à Pesq. do Estado do Rio de Janeiro. Orientador: Francois Germain Noel.

15] João Alfredo de Moraes Gomes da Silva. Modulação redox da resposta de células musculares lisas ao heme. 2011. Tese (Doutorado em Biologia) - Universidade do Estado do Rio de Janeiro, Conselho Nacional de Desenvolvimento Científico e Tecnológico. Orientador: Thereza Christina Barja Fidalgo.

INCT-INOFAR Publications

16] João Eucliodes Fernandes Braga. Ensaios farmalógicos clínicos com o extrato das raízes do *panax ginseng* C.A. Meyer no controle da ansiedade. 2011. Tese (Doutorado em Produtos Naturais e Sintéticos Bioativos) - Universidade Federal da Paraíba. Co-Orientador: Margareth de Fátima Formiga Melo Diniz.

17] Juliana Arcanjo Lino. Mediadores e mecanismos moleculares envolvidos no efeito protetor da amifostina na neuropatia sensitiva periférica experimental induzida por oxaliplatina. Início: 2011. Tese (Doutorado em Farmacologia) - Universidade Federal do Ceará. (Orientador).

18] Luiz Felipe Prota. Expressão do CFTR e sua modulação pela dexametasona em células brônquicas. 2011. Tese (Doutorado em Ciências Biológicas (Fisiologia)) - Universidade Federal do Rio de Janeiro, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior. Co-Orientador: Patricia Rieken Macedo Rocco.

19] Maria Lucia Abranches da Silva. A proteção patentária do segundo uso médico de compostos químico-farmacêuticos. 2011. Tese (Doutorado em Tec de Processos Químicos e Bioquimicos) - Escola de Química - UFRJ. Orientador: Adelaide Maria de Souza Antunes.

20] Maria Tereza A. Pessoa Morano. Impacto da reabilitação pulmonar nos marcadores inflamatórios pré-operatórios e nas complicações pulmonares pós-operatórias de pacientes com câncer de pulmão, candidatos a ressecção pulmonar de complicações respiratórias no pós-operatório na rececção cirurgica por neoplasia de pulmão. 2011. Tese (Doutorado em Cirurgia) - Universidade Federal do Ceará. Orientador: Manoel Odorico de Moraes Filho.

21] Marina Vieira Martins. Avaliação do perfil leishmanicida de novos derivados hidrazídicos. 2011. Tese (Doutorado em Ciências Biológicas (Farmacologia e Química Medicinal)) - Universidade Federal do Rio de Janeiro, Conselho Nacional de Desenvolvimento Científico e Tecnológico. Orientador: Eliezer Jesus de Lacerda Barreiro.

22] Marine Raquel Diniz da Rosa. Interferência do óleo essencial *citrus aurantium* L. sobre a ansiedade de trabalhadores expostos ao ruído ocupacional. 2011. Tese (Doutorado em Produtos Naturais e Sintéticos Bioativos) - Universidade Federal da Paraíba. Orientador: Margareth de Fátima Formiga Melo Diniz.

23] Miriana da Silva Machado. Avaliação dos mecanismos de ação dos novos agentes zalypsis, tryptamicidin e 3'3-ditrifluormetildifenil disseleneto. 2011. Tese (Doutorado em Ciências Biológicas (Bioquímica)) - Universidade Federal do Rio Grande do Sul. Orientador: João Antonio Pegas Henriques.

24] Paola Hernández. N-acylhydtazonas Bioactivas. 2011. Tese (Doutorado em Química) - Universidad de La Republica. Co-Orientador: Eliezer Jesus de Lacerda Barreiro.

25] Patricia Gonçalves Trentin. Estudo da inflamação pulmonar crônica induzida por sílica em camundongos: busca por uma terapia. 2011. Tese (Doutorado em Biologia Celular e Molecular) - Fundação Oswaldo Cruz, Conselho Nacional de Desenvolvimento Científico e Tecnológico. Co-Orientador: Marco Aurélio Martins.

26] Priscilla Christina Olsen. Estudo do modo de ação antiinflamatório do composto JMF2-1 e sua potencial aplicabilidade no controle da asma. 2011. Tese (Doutorado em Biologia Celular e Molecular) - Fundação Oswaldo Cruz, Conselho Nacional de Desenvolvimento Científico e Tecnológico. Orientador: Marco Aurélio Martins.

27] Priscila Vanessa Zabala Capriles Goliatt. Desenvolvimento e implementação de um modelo coarse-grained para predição de estruturas de proteínas. 2011. Tese (Doutorado em Modelagem Computacional) - Laboratório Nacional de Computação Científica, Conselho Nacional de Desenvolvimento Científico e Tecnológico. Orientador: Laurent Emmanuel Dardenne.

28] Queli Cruz Bastos. Proteção dos compostos químicos - farmacêuticos por patentes - Markush. 2011. Tese (Doutorado em Tec de Processos Químicos e Bioquimicos) - Escola de Química - UFRJ. Orientador: Adelaide Maria de Souza Antunes.

29] Rafaela Sabato Guerrante. Estratégia de inovação e tecnologia em sementes. 2011. Tese (Doutorado em Tec de Processos Químicos e Bioquimicos) - Escola de Química - UFRJ. Orientador: Adelaide Maria de Souza Antunes.

30] Rebecca Soares Nicolich. Controle de resíduos de hormônio do crescimento recombinante em alimentos. 2011. Tese (Doutorado em Química) - Universidade Federal do Rio de Janeiro, Conselho Nacional de Desenvolvimento Científico e Tecnológico. Orientador: Francisco Radler de Aquino Neto.

31] Renata Barbosa Lacerda. Estudos de novos protótipos de fármacos antiinflamatórios simbióticos. 2012. Tese (Doutorado em Química) - Universidade Federal do Rio de Janeiro, Conselho Nacional de Desenvolvimento Científico e Tecnológico. Co-Orientador: Eliezer Jesus de Lacerda Barreiro.

32] Renata Bessa Pontes. Mecanismos envolvidos na patogênese da neurotoxicidade experimental induzida pelo agente antineoplásico oxaliplatina: papel de receptores (TRPA1, TRPM8, TRPV1 E NMDA) e de. Início: 2011. Tese (Doutorado em Farmacologia) - Universidade Federal do Ceará. (Orientador).

33] Renato Saldanha Bastos. Síntese e avaliação de semicarbazonas, tiossemicarbazonas e produtos de mannich derivados de isatinas como antivirais e caracterização espectroscópica de isonitrosoacetanilidas. 2011. Tese (Doutorado em Química) - Universidade Federal do Rio de Janeiro, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior. Orientador: Angelo da Cunha Pinto.

34] Ricardo Antonio Correia Lima. Novo modelo experimental de síndrome do compartimento abdominal: repercussões renais, hepáticas, pulmonares e do intestino delgado. 2011. Tese (Doutorado em Medicina (Cirurgia Geral)) - Universidade Federal do Rio de Janeiro. Orientador: Patricia Rieken Macedo Rocco.

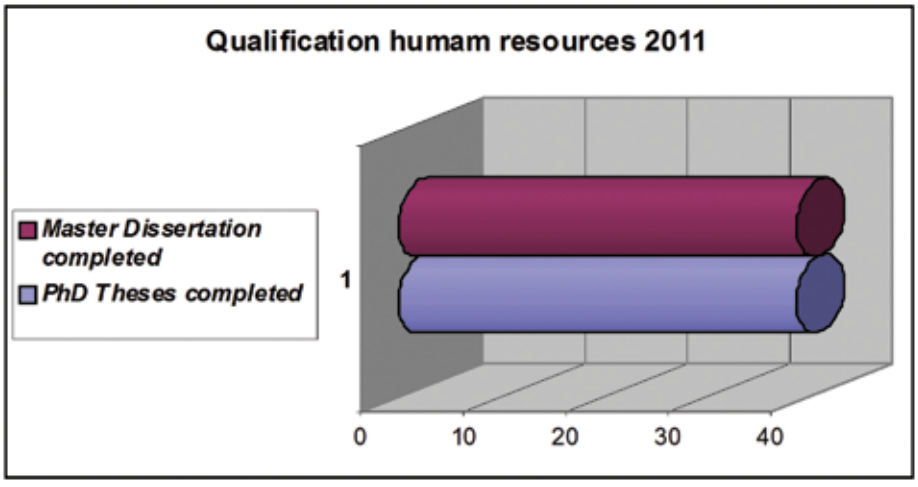
35] Rodolfo do Couto Maia. Novos derivados N-acilidrazônicos candidatos a protótipos úteis no tratamento da dor crônica inflamatória e neuropática. 2012. Tese (Doutorado em Química) - Universidade Federal do Rio de Janeiro, Conselho Nacional de Desenvolvimento Científico e Tecnológico. Orientador: Carlos Alberto Manssour Fraga.

36] Samir D'Aquino Carvalho. Síntese e avaliação do perfil tripanocida N-acilidrazonas cinâmicas planejadas como potenciais agentes anti-chagásicos. 2011. Tese (Doutorado em Química) - Universidade Federal do Rio de Janeiro. Orientador: Carlos Alberto Manssour Fraga.

37] Sharlene Lopes Pereira. Avaliação farmacológica do derivado N-acilidrazônico LASSBio-1289 em modelos de hipertensão arterial e hipertensão arterial pulmonar. 2011. Tese (Doutorado em Ciências Biológicas (Farmacologia e Química Medicinal) - Universidade Federal do Rio de Janeiro, Fundação Carlos Chagas Filho de Amparo à Pesq. do Estado do Rio de Janeiro. Orientador: Gisele Zapata-Sudo.

38] Sócrates Golzio dos Santos. Desenvolvimento bioanalítico para estudo farmacocinético e metabolômico das riparinas I e III- Anoba riparia (NEES) Mez. 2011. Tese (Doutorado em Produtos Naturais e Sintéticos Bioativos) - Universidade Federal da Paraíba. Co-Orientador: Margareth de Fátima Formiga Melo Diniz.

39] Walter Mendes de Oliveira Júnior. Efeito antinociceptivo do farnesol e avaliação histopatológica de tecidos cerebrais de camundongos tratados. 2011. Tese (Doutorado em Produtos Naturais e Sintéticos Bioativos) - Universidade Federal da Paraíba. Co-Orientador: Margareth de Fátima Formiga Melo Diniz.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INCT-INOFAR SCHOLARS

UNICAMP

Adriano Siqueira Vieira
CNPq Junior Post-Doctorate Scholarship
Time: August 2010 to March 2012
Project: "*Atorvastatin synthesis*"
Supervisor: Prof. Dr. Luiz Carlos Dias
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Leila de Souza Conegero
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Time: July 2010 to January 2011
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UFG

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CNPq Technical Support Scholarship – AT NM
Time: January to June 2011
Project: "*In silico prediction and in vitro production of pharmaceutical prototype candidates through bioconversion of human metabolites*"
Supervisor: Prof. Dr. Valeria de Oliveira
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Project: *"Semicarbazone Benzaldehyde (BS)"*
Supervisor: Prof. Dr. Carlos Alberto Tagliatti
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Time: July 2010 to June 2011
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CNPq Technical Support Scholarship – AT NS
Time: May to December 2011
Project: "*Scientific awareness and health education at INCT-INOFAR"*
Supervisor: Prof. Dr. Eliezer J. Barreiro

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CAPES Master Scholarship
Time: March 2010 to February 2012
Project: *"Design, synthesis and pharmacological evaluation of new antitumor ß –tubulin inhibitor prototypes*"
Supervisor: Prof. Dr. Lidia Moreira Lima
LASSBio

Carlos Eduardo da Silva Monteiro
CNPq Technological Development Scholarship – DTI-3
Time: January to February 2011
Project: "*Multitarget activation: strategy for symptomatic treatment of neuropathic pain*"
Supervisor: Prof. Roberto Takashi Sudo
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Clemilson Berto Junior
CAPES Master Scholarship
Time: October 2011 to January 2013
Project: "*Evaluation of teratogenic potential of LASSBio 596 and LASSBio 468 prototypes, antiasthma pharmaceutical candidates*"
Supervisor: Prof. Dr. Aloa Machado
LASSBio

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Project: "Qnit"
Supervisor: Prof. Dr. Claudia Rezende
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Project: "*Sunitinib synthesis*"
Supervisor: Prof. Dr. Angelo da Cunha Pinto
Institute of Chemistry (IQ)

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Time: October 2010 to September 2011
CNPq Technological Development Scholarship – DTI-1
Time: October 2011 to September 2012
Project: *"Scientific awareness and health education at INCT-INOFAR"*
Supervisor: Prof. Dr. Eliezer J. Barreiro

Luciano da Silva Santos
CNPq Scientific Initiation Scholarship - IC
Time: August to October 2011
CNPq Technical Support Scholarship – AT NS
Time: November 2011 to February 2012
Project: "*Synthesis and pharmacological activity of new ferrocene-N-acylhydrazone derivates*"
Supervisor: Prof. Dr. Lidia Moreira Lima
LASSBio

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Project: "*In vitro metabolism of new leishmanicide and tripanomicide pharmaceutical prototypes"*
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LASSBio

Natalia Medeiros de Lima
CNPq Technical Support Scholarship – AT NS
Time: August 2010 to July 2011
Project: *"Scientific awareness and health education at INCT-INOFAR"*
Supervisor: Prof. Dr. Eliezer J. Barreiro

Pedro Gabriel D. L. Pereira
CNPq Scientific Initiation Scholarship - IC
Time: August to October 2011
Project: "*Synthesis of cyclodextrin complexes of LASSBio-596 salts*"
Supervisor: Prof. Dr. Lidia Moreira Lima
LASSBio

Roberta Tesch
CAPES Master Scholarship
Time: March to April 2011
Project: "*Studies of molecular modeling and structural planning of new ligands to adenosine receptors*"
Supervisor: Prof. Dr. Carlos Alberto Manssour Fraga
LASSBio

Rodolfo Do Couto Maia
CAPES Exchange Doctorate Scholarship (Dsw)
Time: February to July 2011
Project: "*Synthesis and evaluation of antitumor activity of a new family of pyrazole-pyridone family*"
Supervisor: Prof. Dr. Carlos Alberto Manssour Fraga
LASSBio

Tais Rubia Dos Santos
CNPq Scientific Initiation Scholarship - IC
Time: September to November 2011
Project: *"Planning, synthesis and pharmacological evaluation of new leflunomide analogs*"
Supervisor: Prof. Dr. Lidia Moreira Lima
LASSBio

USP- RIBEIRAO PRETO

Giuliana Bertozi Francisco
CNPq Technical Support Scholarship – AT NM
Time: September 2010 to December 2011
Project: *"Semicarbazone Benzaldehyde (BS)"*
Supervisor: Prof. Dr. Fernando de Queiroz Cunha
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Vice-Coordinator

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4] Angelo da Cunha Pinto (UFRJ) *CV-Lattes*

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33] Valeria de Oliveira (UFG) *CV-Lattes*

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