
# Next Generation Ambassadors of Chemistry Symposium

## Sunday, August 10, 2014

### Moscone Center, South Bldg.
### South Lobby, Esplanade Room 300

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## *Brazilian Chemical Society (SBQ)*

### Welcome Address

Dear Colleagues,

On behalf of the Brazilian Chemical Society (SBQ), I am delighted to welcome you to the Next Generation Ambassadors of Chemistry Symposium at the 248th ACS National Meeting in San Francisco, California. SBQ is very proud to once again partner with the American Chemical Society (ACS) to bring young scientists to exchange ideas and explore collaborations. This rewarding and unique experience will not only inspire and motivate our best talents, but also enrich their life and promote a culture of international collaboration that will further contribute to their scientific careers.

As we approach the middle of the second decade of this century, we know that we have many challenging chemistry problems to solve and it is essential to view globalization as an opportunity to increase worldwide prosperity. It is particularly important to stimulate and promote our ability to create and use new scientific information to advance the health and quality of life for all people around the world.

On behalf of the Brazilian Chemical Society I would like to thank the National Council for Scientific and Technological Development / Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) through its Science without Borders program / Ciência sem Fronteiras (CsF), whose main goal is to promote the consolidation and expansion of science, technology and innovation in Brazil by means of international exchange and mobility. The program has allowed a huge number of students to further their education in the best universities and research institutes of the world. I would also like to express my sincere thanks to ACS and all the organizers for making this wonderful symposium possible. The 248th ACS National Meeting offers an amazingly rich variety of opportunities to meet and network with colleagues from around the world with a wide range of research interests, expertise and perspectives.

I encourage you to take full advantage of the exciting opportunities in a productive way and make new contacts that will help you to grow personally and professionally. Enjoy the symposium and the meeting, as well as your stay in the beautiful city of San Francisco.

Sincerely,

Adriano D. Andricopulo

2014 President, Brazilian Chemical Society

# *American Chemical Society (ACS)*

## Welcome Address

**Prezados participantes, boa tarde**
*Dear participants, good afternoon*

Friends and fellow members of the global scientific community, on behalf of the American Chemical Society, I am delighted to welcome all of you and I wish to thank the Brazilian Chemical Society and the ACS Committee on International Activities for once again demonstrating innovation through collaboration on putting together this symposium. I would like to thank the Brazilian National Council for Scientific and Technological Development / **Conselho Nacional de Desenvolvimento Científico e Tecnológico** (CNPq) and the ACS for funding this event.

Primarily I would like to thank you for the invitation and the opportunity to speak before a privileged group of Brazilian post doctorates. In this last month of May, I was invited to attend the annual meeting of the Brazilian Chemical Society, and even after confirming my presence, unfortunately, I could not attend. **Foi uma lástima e mais uma vez, minhas sinceras desculpas.** *It was unfortunate, and once again, my sincere apologies.*

Now, this opportunity to meet with all of you today will be of immense value to continue the collaboration and exchange of knowledge between the American Chemical Society and the Brazilian Chemical Society.

As President of the ACS, I am honored to represent more than 161,000 ACS members, of which more than 15% live or work outside of the US and by the last count, more than 300 live in Brazil. I am always appreciative of the opportunity to interact and engage with young, talented, and energetic scientists and engineers such as you who represent the future of the science.

Our commitment to international collaboration is in line with our mission at ACS; to advance the broader chemistry enterprise and its practitioners for the benefit of Earth and its people. My hope is that this is a beginning of many great exchanges and collaboration in the future.

Today's activity marks a continuation of a commitment between the two societies. We believe that chemistry's contributions toward global concerns must be prominent. It is wonderful that we have a group of scientists with research interests spanning across so many disciplines represented at this meeting: analytical chemistry, physical chemistry, organic chemistry, biochemistry, computational chemistry and bioinformatics and many others. All of them play critical roles in addressing the many global problems that confront us – whether in health, energy, the environment, etc.

I would like to thank you for your personal commitment of time to participate in this symposium today. This is the beginning for some of you and the continuation for many of us of a lifelong learning process. I encourage you to take advantage of this opportunity to network and interact with your peers. It is, sometimes, the random collisions between individuals at forums like this that inspire some of the best scientific and engineering breakthroughs.

**Eu espero que todos tenham uma sessão bastante produtiva e que aproveitem o seu tempo aqui em San Francisco.** *I wish you all have a very productive session and enjoy your time here in San Francisco.*

**Sejam bem vindos e muito obrigado,**
*Welcome and thank you,*

Tom Barton
2014, ACS President

# Next Generation Ambassadors of Chemistry Symposium Agenda

| Day | Date / Time | Activity | Location |
|---|---|---|---|
| Saturday | **August 09** | Arrival in San Francisco | Check in at Hotel<br>Hilton SF Union Square |
| Sunday | **August 10** | | |
| | **8 AM – 12 PM** | Professional Development Session 1<br>*Facilitators: H.N. Cheng and Bradley Miller*<br>▪ Communicating Science to the General Public<br>▪ Global Career Pathways/Fostering Innovation and Entrepreneurship | Hilton SF Union Square<br>Franciscan A |
| | **1 PM – 5:30 PM** | **"Next Generation Ambassadors of Chemistry Symposium"**<br><br>1:00 PM – Welcome remarks – ACS and SBQ<br>1:05 PM – Oral presentations start<br>4:45 PM – Networking and poster session start<br><br>4:45 PM – 5:30 – ACS video production team will be interviewing and filming participants to produce video about the symposium during the networking and poster session. | The Moscone Center<br>South building, South Lobby<br>Esplanade Ballroom 300 |
| | **5:30 PM – 8 PM** | IAC International Reception | Hilton SF Union Square<br>Grand Ballroom A |
| Monday | **August 11** | | |
| | **8 AM – 5 PM** | IAC International Innovation and Collaboration Symposium | The Moscone Center<br>South building, South Lobby<br>Esplanade Ballroom 300 |
| | **3 PM** | **New Member Reception** Networking with the Rockstars of Chemistry | The Moscone Center<br>South building, Room 105 |
| Tuesday | **August 12** | | |
| | **8 AM – 5 PM** | Asia-America Chemical Symposium: *Global Stewardship and Chemistry Innovations for Sustainable Agriculture and Food Products* | The Moscone Center<br>South building, South Lobby<br>Esplanade Ballroom 300 |
| | **11:00 AM** | Prof. Luiz F. Silva Jr. presentation: (ORGN Division)<br>PAPER ID: 23888 - *"Hypervalent iodine in synthetic organic chemistry: Electrophilic alkynylation and rearrangement reactions"* | Moscone Center<br>West Building, Room 3011 |

| | | | |
|---|---|---|---|
| Wednesday | **August 13** | | |
| | **8 AM – 12 PM** | Professional Development Session 2<br>*Facilitators: Timothy Hanks and Luiz F. Silva Jr*<br>▪ Principles of Peer Review and Scientific Manuscript Development<br>▪ Funding Proposal Writing | Hilton SF Union Square<br>Franciscan B |
| | **12 PM to 2 PM** | Lunch, Certificate and Final Remarks Session | |

## Presentation order and time

| Start Time | End Time | Presenter | Duration |
|---|---|---|---|
| 1:00 | 1:05 | Opening Remarks | 0:05 |
| 1:05 | 1:20 | Raphael Nagao de Sousa<br>*Elucidation of reaction mechanisms far from thermodynamic equilibrium* | 0:15 |
| 1:20 | 1:35 | Gabriel Costa Alverni da Hora<br>*Molecular dynamics studies of a pediocin-plantaricin hybrid peptide in POPG:POPC bilayers* | 0:15 |
| 1:35 | 1:50 | Maria José Fonseca Costa<br>*Microwave-assisted single-surfactant templating synthesis of mesoporous zeolites* | 0:15 |
| 1:50 | 2:05 | Jeronimo Lameira Silva<br>*Molecular origin of the activation of GTPase: Paradynamics (PD) study* | 0:15 |
| 2:05 | 2:20 | Alexandre Amormino dos Santos Goncalves<br>*One-pot synthesis of mesoporous Ti-Ni-Al ternary oxides as a strategy to develop highly selective catalysts for steam reforming of ethanol* | 0:15 |
| 2:20 | 2:35 | Vinícius Alves<br>*Pred-hERG: A novel web-accessible computational tool for predicting cardiac toxicity of drug candidates* | 0:15 |

# Next Generation Ambassadors of Chemistry Symposium Agenda

| Start Time | End Time | Presenter | Duration |
|---|---|---|---|
| 2:35 | 2:50 | João Luiz Baldim Zanin<br>*New strategy to access the Burkholderia diversity from environmental samples* | 0:15 |
| 2:50 | 3:00 | Coffee Break | 0:10 |
| 3:00 | 3:15 | Richard Piffer Soares de Campos<br>*Microfluidic devices for cell manipulation and detection of cell components* | 0:15 |
| 3:15 | 3:30 | Luiza Magalhães Fiuza Gomes<br>*Development of 8-hydroxyquinoline derivatives as possible therapeutics for the treatment of Alzheimer's disease* | 0:15 |
| 3:30 | 3:45 | Rodrigo Villegas Salvatierra<br>*Lithium ion battery based on thin films of graphene nanoribbons, conjugated polymers, and silicon nanoparticles* | 0:15 |
| 3:45 | 4:00 | Rita de Cassia Pessotti<br>*Actinobacterial interaction triggers antibiotic production against a multidrug resistant strain* | 0:15 |
| 4:00 | 4:15 | Lucas Gontijo Silva Maia<br>*Functional analysis of a nodule-specific GRF zinc finger transcription factor in the model legume, Medicago truncatula* | 0:15 |
| 4:15 | 4:30 | Diogo Montes Vidal<br>*Identification and synthesis of the aggregation pheromone of Homalinotus depressus (Coleoptera: Curculionidae)* | 0:15 |
| 4:30 | 4:45 | Carla Grazieli Azevedo da Silva<br>*Characterization of different stationary phases using supercritical fluid chromatography (SFC) and ultra-high performance supercritical fluid chromatography (UHPSFC)* | 0:15 |
| 4:45 | 5:30 | Concluding Remarks, Networking and Poster Session | 0:45 |

## *Professional Development Session 1 Facilitators*

- Communicating Science to the General Public
- Global Career Pathways / Fostering Innovation and Entrepreneurship

### *H.N. Cheng*

H. N. Cheng obtained his B.S. from UCLA and his Ph.D. from the University of Illinois at Urbana-Champaign. He is currently a research scientist at USDA Southern Regional Research Center in New Orleans, where he is engaged in improved utilization of agricultural products and byproducts. Prior to 2009, he was Senior Research Fellow at Hercules Incorporated in Wilmington, Delaware, where he held various R&D and managerial positions, including new business development, polymer chemistry, analytical chemistry, nutrition, biocatalysis, and pulp and paper technology. He has authored or co-authored 165 papers and 24 patent publications. He has organized 25 symposia at national meetings since 1997 and has edited 8 books. He also serves as an associate editor of the *International Journal of Polymer Analysis & Characterization*, and a member of the governing board of the International Symposium on Polymer Analysis and Characterization.

Dr. Cheng is known for his research in polymer chemistry, renewable materials, biocatalysis, and polymer NMR. He was elected a Fellow of the American Chemical Society (ACS) (2009), and a Fellow of the ACS Polymer Chemistry Division (2010). He was the recipient of Tillmans-Skolnick Award for Outstanding Service from the ACS Delaware Section (2006), Distinguished Service Award from ACS Polymer Division (2005), and ACS Delaware Section Award for research excellence (1994). Dr. Cheng is active professionally and has served in a large number of professional committees and task forces. In 2013 at the ACS, he serves as the Chair of the ACS Louisiana Section, the Chair of the International Activities Committee, a member of ACS Polymer Chemistry Division executive committee and co-chair of ACS Polymer Division Workshop Committee, among several other activities.

### *Bradley Miller*

Bradley Miller, Director of the American Chemical Society (ACS) Office of International Activities, has worked for ACS since 1999 developing programs, products, and services to advance chemical sciences through collaborations in Africa, Asia, Europe, Latin America and the Middle East. At ACS, the world's largest single disciplinary scientific society, he works to create opportunities for chemistry to address global challenges through in-person and web-based scientific network development and research and educational exchange. In 2009, Miller was appointed to co-chair the ACS International Year of Chemistry Staff Working Group. In 2006 Miller was recipient of an NSF Discovery Corps Fellowship to catalyze and sustain US/Brazil collaboration in chemistry of biomass conversions to biofuels. He has worked for university-based international programs, for a higher education association focused on principles of quality assurance for transnational educational offerings, and for a private voluntary organization dedicated to international allied-health sciences. With a Ph.D. from the University of Arizona (and research interests / experience in scientific, professional and academic mobility), a master's degree from the University of Northern Colorado and a baccalaureate degree from University of Virginia - Wise, Brad speaks French, Spanish and Portuguese and has published nine articles and book chapters. Brad and his wife, Rebecca, live in Gerrardstown, WV.

## *Professional Development Session 2 Facilitators*

- Principles of Peer Review and Scientific Manuscript Development
- Funding Proposal Writing

### *Timothy Hanks*

Professor Tim Hanks received a B.S. in Chemistry from the South Dakota School of Mines and Technology and a PhD in Organic Chemistry from Montana State University. After working as a Postdoctoral Research Associate at the University of Minnesota, he moved to South Carolina, joining the Chemistry Department at Furman University in 1990. He is currently Professor of Chemistry at Furman and also an Adjunct Professor in the Chemistry Department at Clemson University. He has held positions as a Visiting Professor in the Clemson School of Materials Science, and Visiting Scientist at Départment du Recherche Fondamentale sur la Matiére Condensée, Commissariat á l'Energie Atomique in Grenoble, France. In 2011 he spent six months as a Fulbright Senior Scholar and Visiting Scientist at the Intelligent Polymer Research Institute at the University of Wollongong, Australia. Dr. Hanks is the Awards Chair and an Alternate Councilor for the Western Carolinas Section of the ACS and a member of the ACS International Activities Committee. He has organized two Southeast Regional ACS meetings and is currently the Chair Elect of the SERMACS Board. He is also a recipient of the Ann Nalley Volunteer Services Award for the Southeast Region.

Dr. Hanks research interests focus on mechanisms of self-assembly and the construction of functional materials from highly conjugated polymers. Current projects include the synthesis of anti-biofouling coatings for ocean vessels and medical implants, biosensors for detecting food pathogens, and the fabrication of 3D scaffolds from electrically conducting hydrogels for tissue engineering applications. He has published 67 research papers and book chapters in professional publications.

### *Luiz F. Silva Jr.*

Luiz F. Silva, Jr. was born in São Paulo, Brazil, in 1971. He studied chemistry at the University of São Paulo, where he received his B.Sc. in 1993. In 1994, he joined the group of Professor Helena M. C. Ferraz, at the University of São Paulo, receiving his Ph.D. in 1999. He then worked one year as a postdoctoral research associate with Professor Gary A. Molander, at the University of Pennsylvania. He returned to Brazil to work as a postdoctoral research associate in the group of Professor Ferraz. In April of 2002, he accepted an appointment at the University of São Paulo, as Assistant Professor of Chemistry. In January of 2008, he became Associate Professor I at the same Department. In 2012, he was promoted to Associate Professor III. He has been working at the Brazilian Chemical Society since 2004 and will be the general secretary at this society from 06/2014 to 05/2016. His current research interests are focus mainly on the total synthesis of natural products and on the study of reactions promoted by hypervalent iodine reagents. His researcher ID is E-9749-2001. Further information concerning current research projects can be obtained at his website at http://www.iq.usp.br/luizfsjr/.

## *Dr. Alexandre Amormino dos Santos Gonçalves*

Alexandre Amormino S. Gonçalves was born in Belo Horizonte, Minas Gerais, Brazil in 1986. He graduated in 2010 with a BSc in Industrial Chemistry, with a minor in Environmental Chemistry at the Federal University of Ouro Preto, MG, Brazil. During that time, he worked for three years in a specialized water waste treatment lab, focusing primarily on analytical chemistry. After Alexandre completed his BSc, he pursued a M.Sc. in Chemical Engineering at the Federal University of São Carlos-SP in Brazil, receiving his degree in 2012. While studying for his M. Sc., he worked on the development of Heterogeneous Catalysts for petrochemical refining, focusing on Material Science and Catalysis. In 2012, Alexandre joined Professor Mietek Jaroniec's team at Kent State University, in Kent, OH, where is a Ph.D. candidate in Physical Chemistry, working also as a teaching assistant. Alexandre is currently developing his doctoratal dissertation on the development of nanostructured bifunctional metal oxides for catalytic applications on the production of clean and alternative fuels. Further information can be found here: www.linkedin.com/in/alexandreamormino/.

## *Abstract*

**Presenting Author**: Alexandre Amormino dos Santos Gonçalves[1]
**Additional Author(s)**: Patrícia Brigida Faustino[2], José Mansur Assaf[3], and Mietek Jaroniec[4]

### *One-pot synthesis of mesoporous Ti-Ni-Al ternary oxides as a strategy to develop highly selective catalysts for steam reforming of ethanol*

One-pot synthesis of nanostructured ternary oxides (Ni, Al and Ti) was designed and facilely performed via evaporation induced self-assembly (EISA) strategy [1], while Ti- and Ni-containing precursors were added during preparation of ordered mesoporous alumina (OMA) [2,3]. The resulting materials showed improved textural and adsorption properties, and were applied as catalysts in the Steam Reforming of Ethanol (SRE) for H2 production. These materials were characterized by X-ray diffraction, N2, CO2 and NH3 adsorption, and temperature-programmed reduction of H2 (TPR-H2). N2 physisorption analysis showed uniform mesoporosity of NiO-Al2O3, while the addition of Titania precursor caused an expansion of the pore size distribution and an enlargement of the specific surface area for the catalysts calcined at 400 oC and its reduction when calcination was carried out at 700 oC. X-ray diffraction analysis indicated that the addition of titania precursor altered the mesostructure from ordered to disordered, along with the crystallization of TiO2 and NiO for the samples calcined at 700 oC. All materials showed large pore volumes (0.35-0.58 cm3/g), large pore sizes (7-9.5 nm), and high specific surface areas (205-310 m2/g). CO2 and NH3 adsorption measurements indicated a decrease in the basicity and acidity with addition of titania precursor. The H2-TPR showed a shift in the maximum of reduction temperature to higher temperatures. Modification of Ni-Al mixed oxides with titania plays a dual role in promoting catalytic activity of the resulting composite. The presence of titania hinders the reduction of NiO during reduction processes, thus decreases conversion, while the change in acidity changes the reaction pathways and provides catalysts with higher selectivity [4]. Although a balance between these effects results in similar performance toward H2 production: 5.1-5.35 moles of H2 per mole of ethanol (6 moles of H2 is the theoretical value). Studies of these catalysts are important because of their potential for steam reforming of ethanol, which is one of crucial processes for cleaner and more efficient production of gas products.

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## *Dr. Carla Grazieli Azevedo da Silva*

Carla G. A. da Silva was born in Porto Alegre, Brazil, in 1978. She studied chemistry at the University of Rio Grande do Sul, where she received her B.Sc. in 2004 and master's degree in analytical and environmental chemistry in 2007. In 2009, she joined the group of Professor Carol H. Collins, at the University of Campinas, receiving her Ph.D. in sciences (emphasis on analytical chemistry) in 2013. Since then she has been a postdoctoral research associate with Professor Carla B. G. Bottoli, also in analytical chemistry, at the University of Campinas. In 2012, she made a doctoral internship in France in the group of Dr. Eric Lesellier and Dr. Caroline West. She has a strong background in gas, liquid and supercritical fluid chromatography, especially in the development of new stationary phases for use in these techniques. Her current research interests are focused mainly on the development of new capillary stationary phases for nanoLC and in separations using supercritical fluid chromatography. Further information concerning current research projects can be obtained at her website at http://lattes.cnpq.br/5527638997019193.

## *Abstract*

**Presenting Author**: Carla Grazieli Azevedo da Silva[5]
**Additional Author(s)**: Carol H. Collins[6], Isabel Cristina Sales Fontes Jardim[7], Eric Lesellier[8], and Caroline West[9]

### *Characterization of different stationary phases using supercritical fluid chromatography (SFC) and ultra-high performance supercritical fluid chromatography (UHPSFC)*

The present study investigated the effect of different stationary phase (SP) chemistries and particle sizes for separations using SFC and UHPSFC. Linear solvation energy relationships (LSERs), namely the solvation parameter model based on Abraham descriptors, where several neutral, acidic and basic aromatic compounds are separated using the same mobile phase (CO2 with 10% methanol as organic modifier, 25ºC, 15.0 MPa backpressure) were used for the evaluations. The SP presented different chemical properties: polar ones such as silica, zirconized silica and titanized silica, classical C8 or C18 SP, particles with alkyl C4, C8, C18 groups and aromatic and fluorinated phases. In addition, separations with other type of polar organic modifiers were performed. The SP presented varied profiles and selectivities and the results showed that the model could be applied to SP with different ranges of polarities.

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## *Dr. Diogo Vidal*

Diogo Montes Vidal was born in Curitiba, Brazil, 1987. He graduated in Chemistry from the Federal University of Parana in 2009 (UFPR). In 2009 he joined the group of Professor Walter Leal at UC Davis, as a part of Sustainable Crop Protection in Agriculture Program (FIPSE/USA-CAPES/Brazil) to work with pheromone binding proteins. He holds a Master of Organic Chemistry from UFPR (2012) and was advised by Professor Paulo H. G. Zarbin. Since 2012, he is a PhD student at UFPR (CNPq fellowship holder), advised by Professor Zarbin. His research interests are focused mainly on organic synthesis, pheromone chemistry, identification of natural products and chemical ecology. His researcher ID is G-4262-2011. Further information about research projects and publications can be obtained at the following website: quimica.ufpr.br/semioquimicos.

## *Abstract*

**Presenting Author:** Diogo Montes Vidal[10]
**Additional Author(s):** Paulo Henrique Gorgatti Zarbin[11] and Marcos Antonio Barbosa Moreira[12]

### ***Identification and synthesis of the aggregation pheromone of Homalinotus depressus (Coleoptera: Curculionidae)***

Since 2005, the populations of *Homalinotus depressus* (Coleoptera: Curculionidae) is constantly increasing in the Brazilian northern region, leading to large financial losses to coconut production. Due to biological aspects of the species, the use of pheromones in pest management programs is promising. The behavioral responses of *H. depressus* to conspecifics aeration extracts suggested the presence of a male-produced aggregation pheromone. GC analyses of these extracts revealed the presence of three male-specific compounds. Analytical datasets suggested the identity of the minor component as isophorone which was confirmed by co-injection with an analytical standard. Several reactions were proposed starting from isophorone in order to identify the remaining components. The epoxydation reaction resulted in epoxyisophorone, which co-eluted with one of the male-specific compounds. FTIR spectrum for the major compound showed an O-H stretch band at 3300cm$^{-1}$ suggesting the presence of a hydroxyl group. Mass spectrum showed a molecular ion at *m/z*156 indicating two additional mass units, when compared to epoxyisophorone. By $NaBH_4$ reduction of epoxyisophorone we identified the major compound as epoxyisophorol. We prepared a mixture of *syn* and *anti* stereoisomers and their respective retention times, and NMR data revealed the natural major compound as one of the *syn* enantiomers. *Syn*-enantiopure compounds were obtained in high enantiomeric excesses by biocalalysis reactions and the absolute configuration was determined as (1*S*,2*S*,6*R*)-epoxyisophorol. Y-tube olfactometer bioassays demonstrated that the synthetic major compound is as attractive as male volatiles. Field bioassays employing the major compound in different stereoisomeric compositions are underway.

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## *Gabriel Costa Alverni da Hora*

Gabriel Costa A. da Hora was born in Recife, Brazil in 1986. He studied Chemistry at the Federal University of Pernambuco (UFPE) from 2005 to 2008 where he received his B.Sc. In 2009, he got his Master degree in the Theoretical and Computational Chemistry group with Professor João Bosco P. da Silva and Professor Ricardo L. Longo. He studied the conformations, reactions, hydration and hydrolysis of arsenic trioxide isomers using Density Functional Theory (DFT). After receiving his M.Sc. in the end of 2011, he started to work with Professor Thereza A. Soares in the Biomaterials Group at the Fundamental Chemistry Department (UFPE) to obtain his Ph.D. degree. He is working on projects in the Biochemistry fields, focused on hydrogen production via enzymatic catalysis from Hydrogenases using DFT approach and interaction of antimicrobial peptides with phospholipids membrane using Molecular Dynamics. His current research also includes collaboration with Professor Roland Faller in Davis, California, working with the development of a coarse-grained model for polymer brushes, which present cell adhesion properties. Further information concerning current research projects can be obtained at his website at http://biomat.dqf.ufpe.br/Welcome.html.

## *Abstract*

**Presenting Author:** Gabriel Costa Alverni da Hora, MSc[13]
**Additional Author(s):** Thereza Amélia Soares, PhD[14]

### *Molecular dynamics studies of a pediocin-plantaricin hybrid peptide in POPG:POPC bilayers*

A new antimicrobial hybrid peptide sequence has been synthesized from pediocin A (N-terminal) and plantaricin 149A (C-terminal). Previous studies of circular dichroism and fluorescence spectroscopic studies have shown a disordered to ordered conformational transition of the peptide upon binding to POPG but not to POPC. Optical microscopy measurements have indicated that at low concentrations the peptide causes the disruption of POPG membrane of vesicles and formation of small, heterogeneous complexes of phospholipids and peptides. In order to analyze action mechanism of the hybrid peptide, molecular dynamics (MD) simulations were carried out using the GROMOS parameter set 54A7 (atomistic level) and MARTINI (coarse-grain level). The peptide concentration was taken into account. The systems were analyzed with respect to time-dependent (peptide secondary structure map and lipid tilt angle), and average properties (density profiles and deuterium order parameters). Our MD simulations show that the peptide adsorbs on both PG and PC membranes via electrostatic interactions. Only upon binding to the PG surface there is an increase of helical content compared to the peptide in solution. Higher helical content is also observed for the single peptide embedded in PG compared to PC membranes which is in agreement with experimental data. The density of the membrane medium makes conformational transition of the peptide embedded slower than on the surface of the membrane. The results suggest a mechanism of membrane disruption without deep penetration of the peptide, but only from a given peptide concentration threshold. Evidence for that comes from increased disorder of the membrane and persistent interactions between the peptide and membrane headgroups throughout the membrane disruption process. Our findings suggest that the hybrid peptide disrupt the membrane via a carpet-like mechanism (in a V-shape) which has also been postulated for the action of Pediocin A and Plantaricin 149A.

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## *Dr. Jeronimo Lameira Silva*

Jerônimo Lameira Silva was born in Belém, Pará, Brazil, in 1981. He received his degree in Chemistry at the Universidade Federal do Pará (UFPA) in 2004. He earned his MSc in 2006 working with Cláudio Nahum. In 2008, He earned his PhD degree in Physical Chemistry at UFPA working with Cláudio Nahum and Vicent Moliner (Universitat Jaume I). In 2008 He joined the Faculty of Biotechnology at UFPA, where he has a position as Associate Professor II. In 2012 he received a fellowship from Programa Ciência Sem Fronteira (CNPq) to work as postdoctoral researcher with Arieh Warshel at the University of Southern California. He works on computational chemistry and bioinformatics and his current research is focused on the application of computational methods to study enzymatic catalysis. More information concerning current research projects and publications can be obtained at http://lattes.cnpq.br/7711489635465954.

## *Abstract*

**Presenting Author:** Jerônimo Lameira[15]
**Additional Author(s)[16]:** Nikolay V. Plotnikov, B. Ram Prasad, and Arieh Warshela

### *Molecular origin of the activation of GTPase: paradynamics (PD) study*

Despite the recent advancements in computational power, and in the theoretical approaches, obtaining reliable QM(ab-initio)/MM free energy results in condensed phase remain highly challenging. To this end, our recently proposed paradynamics (PD) approach (Nikolay V. Plotnikov and Arieh Warshel, J. Phys. Chem. B. 2012, 116, 10342-10356), to carry out the QM/MM free energy calculations in condensed phases, appears to be very promising and computationally tractable. In order to establish the reliability and the applicability of the PD approach, we estimated the activation free energy barriers associated with the proton transfer pathways (direct vs second water mediated) in the hydrated metaphosphate, which is used as a representative model for the intermediate state along the minimum free energy pathway corresponding to the free energy surface of the phosphate monoester hydrolysis in aqueous solution. The results obtained are quite encouraging and are in very good agreement with the corresponding estimates obtained recently using other QM(ai)/MM approaches (Nikolay V. Plotnikov et al. J. Phys. Chem. B. 2013, 117, 12807-128019). We are now exploring the molecular origin of the activation of GTPase in RasGap using the PD approach.

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## *Dr. João Francisco Ventrici de Souza*

Joao received his bachelor's degree in Chemistry at Universidade de Sao Paulo, Ribeirao Preto in 2009. As an undergraduate student he worked with biomembrane models in interaction with sugars such as sucrose and glucose. The following year he started his Master's studies in Chemistry at the same University, receiving the degree in 2012. His focus, at that time, was on biomembrane models in interaction with particulate material from the burning of sugar cane leaves. He is a PhD student in the Department of Chemistry and in the Department of Chemical Engineering and Materials Science at University of California, Davis. Since 2012 he has been working under the orientation of Professor Gang-yu Liu and Professor Tonya Kuhl in two main projects: one, the pulmonary surfactant models interaction with cholesterol and potential cholesterol withdrawers from the biomembranes; and the other is the development of a 3D nanoprinting technique using Atomic Force Microscopy (AFM) and hydrogels.

## *Abstract*

**Presenting Author:** Joao Ventrici[17]
**Additional Author(s):** Tonya Kuhl[18] and Gang-yu Liu[19]

### *Cholesterol withdrawal from lipid monolayers**

Cholesterol is one of the components of cell membranes. This lipid grants the membranes some physical-chemistry properties fundamental for their well-functioning. When the concentration of cholesterol in the membranes is increased, the result is the change in both the morphology and properties of the membrane, leading to problems regarding the elasticity of the system. Previous studies made by our group have showed the effect of the cholesterol concentration increase on the viscoelastic properties of lipid monolayers. In this study, the effect of cucurbituryls (CBs) is studied on membrane models containing high amounts of cholesterol. Atomic Force Microscopy (AFM) and Confocal Fluorescence Microscopy are used to assess morphological behavior of supported lipid monolayers before and after CB treatment. The effect of the presence of high concentration of cholesterol on the lipid layers is observed. Also, a considerable recover of morphological aspects of the monolayers were observed when CB is employed.

**Poster presentation only.*

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## *Dr. João Luiz Baldim Zanin*

Joao Baldim Z. was born in Minas Gerais, Brazil in 1987. He studied chemistry at Vale do Rio Verde University and Federal University of Lavras (UFLA), where he received his B.Sc and Specialization in 2007 and 2009, respectively. In 2010, he joined the group of Marisi Gomes Soares doing research in Natural Products and biological activities at Federal University of Alfenas (UNIFAL – MG) where he received his Masters. At the same time, he worked in the group of João Batista Fernandes at Federal University of São Carlos (UFSCar – SP) as an intern student doing research on interactions between Natural Products and insects to discover new natural methods to be used in agriculture. In 2012 he started his Ph.D. at Federal University of Alfenas. In 2013 he started work at the University of California, Santa Cruz (UCSC) in the group of Roger Linington, doing research on new methods to discover and access the biodiversity in natural products from microbial sources. His current research interests are focused mainly on new methods to access next-generation antibiotics with unique molecular architectures and biological modes of action for the treatment of drug resistant infections and on the interaction between plants and microorganisms to induce the production of new molecules from silent bacterial gene clusters.

## *Abstract*

**Presenting Author:** Joao Luiz Baldim Zanin[20]
**Additional Author(s):** Roger Linington[21], Jessica Ochoa[22], Weng Ruh Wong[23], Emerson Glassey[24] and Marisi Gomes Soares[25]

### *New strategy to access the Burkholderia diversity from environmental samples*

Since the first discovery of antibiotics from microorganisms, the use of bacteria as a source of chemical diversity has provided a wide number of natural products with both a broad array of biological activities and unique scaffolds and/or novel mechanisms of action. However, in recent decades the number of new antibacterial agents approved for clinical use has declined sharply. Coupled with an increase in prevalence of resistant pathogenic strains in hospital settings, this has become a significant crisis for the global healthcare community. In the field of natural products, Actinobacteria, as a main source of natural products, have been the most well studied family, providing numerous novel antibacterial agents to overcome the antibiotic resistance. However, increasing instances of rediscovery of common scaffolds suggests that there is a diminishing return to the continued use of the same discovery strategies in the face of rising antibiotic resistance. Recent genomic evidence suggests that there are a significant number of natural products clusters in Proterobacteria, still unexplored reservoirs of natural products diversity. The Burkholderia genus, being part of this phylum, has been recognized to contain a substantial number of clusters encoding putatively novel natural products, but to date has not been well studied. Since there are few efficient methods to isolate Burkholderia species from environmental sources, this project aims to develop a new isolation method using genomic, metagenomic and metabolic information to take advantage of unique properties of Burkholderia metabolism. This approach relies on examination of important metabolic properties, including antibiotic resistance, metal resistance, as well as the carbon and nitrogen metabolism profiles from Burkholderia and untargeted species in bacterial communities. Thus, this strategy can generate the possibility to construct a differential culture media to access this genus in diverse types of environmental samples. Ultimately, the objective of this research program is to examine environmental samples of the genus Burkholderia in order to discover next-generation antibiotics with unique molecular architectures and biological modes of action for the treatment of drug resistant infections.

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## *Dr. Lucas Gontijo Silva Maia*

Lucas Gontijo Silva Maia was born in Minas Gerais, Brazil in 1984. He received his Bachelor degree in biological science at the Lavras Federal University in July 2010, where he had the orientation of the Magno Antonio Patto Ramalho professor and studied quantitative genetic of annual plants, common beans. In July of 2013 he defended his Master in Agronomy/Plant Physiology by the same university, in which he worked with the characterization of mutant in the novel of nodule development and nitrogen fixation with the model plant Medicago truncatula, by the orientation of the Professor Vagner Augusto Benedito. In the August of the same year he started his Ph.D. in Genetics & Developmental Biology at the West Virginia University sponsored by CAPEs. In this Ph.D., he is working with functional characterization of Transcription Factor gene, important to the nodulation and nodule development in the model plant Medicago truncatula by the orientation of Professor Vagner Augusto Benedito.

## *Abstract*

**Presenting Author:** Lucas Gontijo Silva Maia[26]
**Additional Author(s):** Michael Udvardi[27] and Vagner Augusto Benedito[28]

### *Functional analysis of a nodule-specific GRF Zinc Finger transcription factor in the model legume, Medicago truncatula*

Nitrogen is an element required for all living organisms and a constituent of amino acids, nucleic acids and signal molecules. Despite its importance and abundance, N is largely limiting because most of it is in a highly stable form, the gas dinitrogen (N2), which composes 78% of the Earth's atmosphere. This molecule has a triple covalent bond that requires 92.4 kJ/mol of energy to break. Diazotrophic bacteria evolved an enzymatic complex, nitrogenase, which reduces N2 into ammonia (NH3). Those bacteria can interact symbiotically with plants, making them nitrogen self-sufficient. This interaction, known as symbiotic nitrogen fixation (SNF), develops a “de novo” organ called a nodule. Within the nodule, rhizobia provide reduced nitrogen to the plant and the host plant feeds and provides an optimum environment for bacteria to thrive and fix nitrogen. Both organisms genetically control the nodulation, or nodule organogenesis, by an intricate genetic regulatory network, in which transcription factors (TFs) are essential. The gene Medtr7g086040.1 codes for a novel GRF zinc finger transcription factor (MtGRF) that is highly expressed and specific to root nodules of Medicago truncatula. Zinc Finger TFs have a binding domain that allows affinity to specific DNA regions and RNA polymerases to regulate gene expression. This gene is expressed from early stages of nodule development (4 days post inoculation) and its expression is sustained in mature nodules. Three insertional mutant lines have been identified in the Tnt1 mutant collection at Noble Foundation. Homozygous plants of an analyzed mutant developed nodules that are capable of growing, but remain non-functional. This suggests an important role of this transcription factor in controlling the regulatory gene network associated with SNF. Furthermore, mutants and genetically modified organisms are being used to understand SNF and the chemistry behind the regulation of gene expression through the affinity of TFs binding to DNA.

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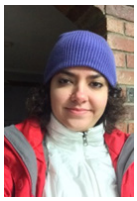

## *Dr. Luiza Gomes*

Luiza M. F. Gomes was born in Belo Horizonte, Brazil, in 1988. In 2006, she started her undergraduate studies at Federal University of Minas Gerais (UFMG). During this time she earned a grant for developing two research projects at the Center of the Development of Nuclear Energy (CDTN) where she spent two years focusing on material chemistry and one year focusing on analytical chemistry. She received her B.Sc. in 2011 and immediately after she joined Heloisa Beraldo's group at UFMG as a master student, working on the synthesis of new Schiff bases as therapeutics for Alzheimer's diseases and Osteoporosis. Luiza received her M.Sc. in 2013 and was awarded a scholarship from the Brazilian government through the Science without Borders program/CAPES to do her PhD in the group of Professor Tim Storr at Simon Fraser University, Canada. The main focus of her current research project in this group is the development of new compounds as therapeutic agents for the treatment of neurodegenerative diseases, especially Alzheimer's disease. Further information about Luiza and her activities on research in Storr's group can be found in the following link: http://bioinorganicchemistrylaboratory.weebly.com/index.html

## *Abstract*

**Presenting Author:** Luiza M.F. Gomes[29]
**Additional Author(s):** Rafael P. Vieira[30], Heloisa Beraldo[31] and Tim Storr[32]

### *Development of 8-hydroxyquinoline derivatives as possible therapeutics for the treatment of Alzheimer's disease*

Alzheimer's disease (AD) is a neurodegenerative disorder that affects approximately 6 million people in North America. AD causes a loss of cognition and eventually leads to death. The dominant theory for AD is the Amyloid Hypothesis, postulating that amyloid-(A) plaques, or partially aggregated soluble A, trigger a neurotoxic cascade causing AD pathology. High concentrations of metal ions, such as Cu(II) and Zn(II), have been found in A plaques in the brain of AD patients. The formation of A plaques, toxic oligomers, and reactive oxygen species (ROS) are related to the presence of these metals, especially redox-active Cu(II) and Fe(III). Oxidative stress caused by ROS in AD brain leads to cell death. A promising therapeutic approach is the use of metal-protein attenuating compounds (MPAC) for AD treatment. MPACs 8-hydroxiquinoline derivatives, such as PBT2, target the metal-A interaction in the extracellular environment and normalize the distribution of metal ions and A peptide in biological fluids. We have synthesized a series of 8-hydroxyquinoline Schiff-bases and evaluated their antioxidant potential and their effect on the process of aggregation of the A peptide. We have shown that these compounds act as antioxidants, and in addition compete with the A peptide for Cu ions restricting formation of toxic metal-containing oligomer species.

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## *Dr. Maria Jose Fonseca Costa*

Maria JF Costa was born in Rio de Janeiro, Brazil, in 1981. She studied chemistry at the Federal University of Rio Grande do Norte, where she received her B.Sc. in 2005. In 2006, she joined Professor Antonio S. Araujo's group, at the Institute of Chemistry at Federal University of Rio Grande do Norte, Natal, Brazil where she received her Master's degree and Ph.D. in 2008 and 2013, respectively. She got a partial completion of her PhD research at Kent State University, Ohio. Currently, she is working as a postdoctoral research associate with Professor Mietek Jaroniec at the Physical Chemistry Division in the Department of Chemistry & Biochemistry at Kent State University, Ohio. Her research involves the synthesis of novel micro-mesoporous materials, such as hybrid AlMCM-41/ZSM-5, that can be used in environmental and energy-related applications. She has expertise in the following materials characterization techniques: physisorption, wide and small-angle powder X-ray diffraction (WAXRD, SAXRD), thermogravimetry (TG/DTG), pyrolysis (Py) coupled with gas chromatography (GC) and mass spectrometry (MS), and scanning electron microscopy (SEM). Further information concerning current research and academic experience can be obtained at her profile: www.linkedin.com/profile/view?id=92054411 (EN)|lattes.cnpq.br/8127030694190277 (PT)

## *Abstract*

**Presenting Author:** Maria José Fonseca Costa[33]
**Additional Author(s):** Antonio Souza Araujo[34] and Mietek Jaroniec[35]

### *Microwave-assisted single-surfactant templating synthesis of mesoporous zeolites*

A novel single-surfactant templating was explored for the synthesis of mesoporous zeolites under hydrothermal conditions and microwave irradiation. The latter was employed for easy programming of temperature and time over a wide range of conditions, allowing a significant reduction of the synthesis time from days to hours. The 16CTAB:12$Na_2O$:100$SiO_2$:2$Al_2O_3$:2500$H_2O$ molar composition was studied. Two different synthesis routes were examined: one-pot synthesis (OS) and two-step synthesis (TS) using different crystallization time. Mesopores were created by using cetyltrimethylammonium bromide (CTAB) surfactant as a soft template and the crystalline microporous framework was formed in the absence of organic molecular template. The XRD analysis of the samples prepared at different crystallization times revealed the formation of the MOR/MFI type of microporous structures with different degree of mesoporosity. The resulting materials were stable and suitable for catalytic applications involving larger molecules, such as catalytic cracking used for conversion of heavy oil fractions into light liquid hydrocarbons. These materials were characterized by using powder X-ray diffraction, and nitrogen and carbon dioxide adsorption. The XRD analysis was employed to identify the crystalline phases in the materials studied, while adsorption isotherms were used to evaluate their surface area and porosity. A detailed characterization of the samples studied revealed that their properties are comparable with those reported in literature for the samples obtained by dual templating or conventional autoclave heating. Namely, the resulting materials are hybrid micro-mesoporous structures consisting of zeolitic crystallites (ZSM-5 and Mordenite-type crystalline domains) co-existing with the amorphous domains of hexagonally ordered mesoporous silica, MCM-41. The catalytic testing of these materials involved pyrolysis of VGO (vacuum gasoil) physically mixed with 10 wt.% of the catalyst at 500ºC coupled with a GC-MS system (helium used as a carrier gas); the recorded spectrum for catalytic pyrolysis of VGO is shown in Figure 1 in comparison to the spectrum obtained for pyrolysis of VGO alone (without catalyst). The latter spectrum reflecting the pyrolysis of VGO alone is located in a wide range of hydrocarbons, typically C17–C41, while the spectrum for catalytic pyrolysis of VGO shows the light fraction of hydrocarbons in the range of liquefied petroleum gas (C3–C5), gasoline (C6–C10) and diesel (C11–C16), indicating that the mesoporous zeolitic materials prepared via single surfactant templating under microwave irradiation are effective catalysts for pyrolysis of VGO.

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## *Dr. Raphael Nagao de Sousa*

Raphael Nagao was born in São Paulo, Brazil in 1984. He received his B.Sc, M.Sc and Ph.D. at the Institute of Chemistry of São Carlos at University of São Paulo, São Paulo, Brazil. He joined the Electrochemistry Group at USP in 2004 under the supervision of Prof. Dr. Hamilton Varela and remained with this group until the defense of his doctoral thesis in 2013. Meanwhile, he participated in a fourteen-month long scientific program in the Department of Chemistry and Volen Center for Complex Systems at Brandeis University, Massachusetts, USA, under the supervision of Prof. Dr. Irving R. Epstein. Currently he is a postdoctoral fellow in the Department of Chemistry, College of Arts and Sciences at Saint Louis University, Missouri, USA, under the supervision of Prof. Dr. István Z. Kiss. He has experience in Physical-Chemistry with emphasis in Electrochemistry, Thermodynamics and Chemical Kinetics. His research interests are mainly focused on the study of Complex Systems, particularly, in the field of nonlinear dynamics, oscillating (electro)chemical reactions, emergency of self-organized pattern, chaos, and complex networks. Up to now, he has published 13 articles in scientific journals (h factor = 5 with 86 citations, Scopus – 06/14/2014) and more than 40 contributions in conferences. Researcher ID: J-9148-2013.

## *Abstract*

**Presenting Author:** Dr. Raphael Nagao[36]
**Additional Author(s):** Prof. Dr. Hamilton Varela[37]

### *Elucidation of Reaction Mechanisms Far From Thermodynamic Equilibrium*

The spontaneous formation of self-organized spatiotemporal patterns under far from thermodynamic equilibrium regime is a characteristic behavior in reaction-transport systems. Targets, waves, spirals, spots and stripes are some typical examples of these chemical self-organized patterns. The emergency of these structures are described by the coupling between the local chemical kinetics, which usually shows oscillatory time-series, and the exchange of spatial information by mass transport. In this work, two fronts will be presented using the nonlinear chemical dynamics in the elucidation of reaction mechanisms under far from thermodynamic equilibrium regime: (a) the investigation of the chemical nature and effect of the drift in the transient time-series in electrochemical oscillators. The analysis of the temporal evolution of the bifurcation parameter was based on an empiric method of stabilization, being the slow accumulation of oxygenated species the main responsible for the drift; (b) the decoupling of the parallel electrochemical routes for CO2 production by a combination of experiments, modeling and numerical simulations during the oscillatory electro-oxidation of methanol on polycrystalline platinum. The effect of perchlorate and sulfate anions in the parallel reactions was investigated by the global production of CO2 and HCOOCH3. Remarkably, sulfate anions inhibited more strongly the catalytic activity from direct pathway in contrast to the small alteration in the indirect pathway. The main idea presented converges in the obtainment of chemical kinetic information which is not observed in conditions close to the thermodynamic equilibrium. This interpretation might be used as an alternative methodology in the study of electrocatalysis in complex chemical reactions.

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## *Richard Piffer Soares de Campos*

Richard P. S. de Campos was born in Limeira, São Paulo, Brazil, in 1984. He studied chemistry at the Paulista State University, where he majored in 2008. In 2010, he joined the group of Professor José Alberto Fracassi da Silva at State University of Campinas, receiving his mastering degree in February of 2012. In the same year, he joined the Ph.D. program of State University of Campinas under the orientation of Dr. da Silva. Currently he is working at Dr. Susan Lunte's laboratory at The University of Kansas, USA, as part of the Ph.D. exchange program Science without Borders, from CNPq. His research interests are in the microfluidics field, with special focus on the development of alternative materials and its bioanalytical applications. He worked with alternative microchip substrates and its applications, PDMS surface modification and development of alternative methods for microfabrication. Nowadays his research is focused on the determination of reactive oxygen species towards electrochemical and fluorescence detection as well as the development of a single cell monitoring system.

## *Abstract*

**Presenting Author:** Richard Piffer Soares de Campos[38]
**Additional Author(s):** José Alberto Fracassi da Silva[39], Susan Lunte[40] and Joseph M. Siegel[41]

### *Microfluidic devices for cell manipulation and detection of cell components*

Cells are the fundamental unit of life and make up the basic structure of all living organisms, and dysregulation of cell physiology can result in many different diseases states. Many times this dysregulation occurs in only a few cells in a cell population. Asynchronous physiological processes that take place on a small time scale are not adequately described by analyzing the average of a cell population, leading to an erroneous or incomplete understanding of the biochemical process. This becomes relevant on issues such as differences in cellular responses to external stimuli and for intracellular reactions. Currently, there is a focus on the development and use of methods that make it possible to detect biochemical differences between individual cells within a cell population. Micro total analysis systems (μTAS) are a great tool for both the analysis of cell lysates and in investigations of cellular heterogeneity. The size of the channels used in μTAS allows for the manipulation and separation of each cell individually. Additionally, it is possible to integrate several analytical steps into a single device which reduces cost as well as overall analysis time. Separation, detection and quantification of intracellular components can be accomplished by microchip electrophoresis (ME) coupled to sufficiently sensitive detection methods. In this research, microfluidic devices that can be used for cell manipulation and analysis are being developed. These devices currently can be used for bulk cell analysis and are now being modified to allow for the manipulation of individual cells within the chip. Conductivity and fluorescence detection methods are being developed for detection of cells and intracellular components. Specifically, this research is developing a method for monitoring intracellular superoxide in single RAW 264.7 macrophages using ME-LIF. Concurrently, the use of conductivity to monitor cell migration through the channel prior to lysis will be evaluated.

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## *Dr. Rita de Cassia Pessotti*

Rita de Cassia Pessotti was born in Ribeirao Preto, SP, Brazil. She studied Biological Sciences at the University of Sao Paulo (USP-Ribeirao Preto) from 2005 to 2011. In 2008 she did an undergraduate international exchange program at the University of Tübingen (Tübingen, Germany) for seven months. In Germany she did short-term internships at the University of Tübingen under the supervision of Prof. Nico Michiel, and at Friedrich-Miescher Laboratory (Max Planck Society) with Dr. Dmitri Ivanov. In 2009 she joined Prof. Monica T. Pupo's group (USP-Ribeirao Preto) as an undergraduate student, where she started her research on microbial natural products. After finishing her bachelor's degree in 2011, she started her Ph.D. training in the same group. The focus of her project is exploring innovative approaches to increase the probability of finding novel bioactive compounds, specifically metagenomics and interspecies interactions. In 2013 she joined Prof. Roberto Kolter's group as a visiting Ph.D. student at Harvard Medical School (Boston, USA) where she is currently working on complex actinobacterial interactions, with the aim of isolating natural products and understanding the chemistry and biology of those interactions.

## *Abstract*

**Presenting Author:** Rita de Cassia Pessotti[42]
**Additional Author(s):** Matthew Francis Traxler[43], David John Dietrich[44], Roberto Kolter[45], Monica T. Pupo[46], and Jon Clardy[47]

### *Actinobacterial interaction triggers antibiotic production against a multi-drug resistant strain*

Increasing drug resistance among microbial pathogens threatens public health and creates a need for new antibiotics. Microbes have been an important source, but increasing rediscovery rates – among other factors – have led to diminished exploration of this source3. Interspecies interactions, especially those that mimic natural ones, can reveal new antibiotics that previous studies missed2. Several actinobacterial strains isolated from plant roots and soil were cultured in pairs to influence secondary metabolism and tested with indicator strains. Pairs were cultivated on R2YE, ISP2 and TSA solid medium for seven days (30 °C). Antibiotic production and other phenotypes were analyzed with soft-LB-agar overlays inoculated with an indicator strain and incubated again overnight. Activity was analyzed by visualization of inhibition halos. Other developmental changes such as induced/inhibited sporulation and inhibited growth were also noted. One promising interaction was chosen for the follow up study: the Krasilnikovia sp. T082 and Streptomyces sp. SPB78 pair, which triggers antibiotic production by T082 against a multi-resistant strain (Amycolaptosis sp. AA4). This activity was also observed in liquid medium (TSB). It was shown that SPB78 cell-free supernatant also triggers this activity through the production of very polar small molecules. The active molecule and method of induction are being investigated.

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## *Dr. Rodrigo Villegas Salvatierra*

Rodrigo V. Salvatierra was born in São Paulo, Brazil in 1983. He studied chemistry at the University of São Paulo (USP) where he received his B.Sc. in 2006. In 2008, he started to work at the group of Prof. Dr. Aldo J. G. Zarbin at the Federal University of Paraná (Curitiba, Brazil), receiving his Master's degree in 2010 and his Ph.D. in 2014. Currently, he is working as a postdoctoral research associate in the group of Prof. Dr. James M. Tour at Rice University (Houston, US). He has experience in the synthesis and characterization of hybrid materials involving carbon nanostructures (like graphene and carbon nanotubes), conjugated polymers and metallic nanostructures for application as transparent electrodes and devices for energy generation and storage. Now, his postdoctoral project is focused on the syntheses of high capacity lithium ion batteries anodes using silicon nanostructures and graphene nanoribbons. Researcher ID L-9380-2013.

## *Abstract*

**Presenting Author:** Rodrigo V. Salvatierra[48]
**Additional Author(s):** James M. Tour[49]

### *Lithium ion battery based on thin films of graphene nanoribbons, conjugated polymers and silicon nanoparticles*

Silicon is a promising material for novel rechargeable Li-ion batteries due to its high specific capacity and the natural abundance of the element Si. However, to be implemented, the Si-based anode must overcome problems related to the huge volume expansion upon Li insertion. This can be attained by creating nanostructured Si and also implementing it in nanocomposites including carbon nanomaterials and conjugated polymers. This work reports on the synthesis of hybrid materials (nanocomposites) comprising graphene nanoribbons (GNR), silicon nanoparticles and conjugated polymers, like polyaniline. In this hybrid material, it is expected that GNR act as a conductive template for Si nanoparticles, while the fibers of polyaniline can provide a flexible and ionic conductor through the material. Combining these nanostructures with the high specific capacity of Si, the hybrid material can be assembled as a thin film and compose a thin film Li-ion battery with improved features, like flexibility and low weight, along with very high capacity.

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## *Vinícius Alves*

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## *Abstract*

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### *Pred-hERG: A novel web-accessible computational tool for predicting cardiac toxicity of drug candidates*

Several non-cardiovascular drugs have been withdrawn from the market due to their critical side effect of inhibiting the human ether-à-go-go related gene (hERG) K+ channels, which may lead to heart arrhythmia and death. Thus, hERG safety testing is an indispensable process that is required by the US FDA. There is considerable interest in developing computational tools to filter out potential hERG blockers in early stages of drug discovery. In this work, we describe the development of a new tool for the rapid identification of potential cardiotoxic compounds by hERG inhibition. We have compiled the largest publicly available dataset of hERG binding, containing 11,958 compounds from the ChEMBL database. Once curated, this dataset contained 4,980 compounds for modeling. Several types of QSAR models have been developed and validated according to the OECD principles. The external classification accuracies discriminating blockers from non-blockers were 0.83-0.93 on external set. Model interpretation revealed several SAR rules, which can guide structural optimization of some hERG blockers into non-blockers. Virtual screening of the WDI chemical library using selected QSAR models identified 4,945 compounds as potential hERG blockers. The developed models can reliably identify blockers and non-blockers, which could be useful for the scientific community. A freely accessible web server has been developed allowing users to identify putative hERG blockers and non-blockers in chemical libraries of their interest (http://labmol.farmacia.ufg.br/predherg).

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*Acknowledgements*

*Thank you to our sponsors, organizers and supporters:*

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