

Sunday – September 1st

14:00

Check-in at the hotel (Pousada dos Pirineus)

15:00 – 18:00

Registration

18:00 - 19:00

Cultural presentation: Cavahadas Parade

19:00 – 19:30

Opening Ceremony

Opening conference

Chair: Carolina Horta Andrade (UFG)

19:30 – 20:30

Discovery of Drugs to treat Neglected Diseases

Peter Warner

(Bill & Melinda Gates Foundation, USA)

20:30 – 22:30

Welcome reception

Monday – September 2nd

Session 1 - Integrating Academia into novel models for drug discovery

Chair: Glaucius Oliva (USP)

09:00 – 10:40

Plenary Lecture (PL)1: Open Source Drug Discovery for Kids Rare Diseases

Aled Edwards

(CEO, Structural Genomics Consortium – SGC - University of Toronto, Canada)

PL2: Novel collaborative approaches boosting R&D for neglected tropical diseases

Jadel Kratz

(Drugs for Neglected Diseases initiative (DNDi), Latin America)

PL3: Plasmodium Kinases – Novel Targets for Antimalarial Drug Discovery

Greg Basarab

(Drug Discovery and Development Centre - H3D - University of Cape Town, South Africa)

Flash Presentation (FP)1: Aryl Benzimidazoles: A new lead in malaria drug discovery

Malkeet Kumar (UNICAMP)

10:40 – 11:00

Coffee-break

Session 2 - Exploring different screening approaches to find drug candidates from fragments and small molecule libraries

Chair: Floriano Paes Silva-Junior (FIOCRUZ)

PL4: Fragment-based discovery of Schistosoma mansoni Thioredoxin Glutathione Reductase (SmTGR) inhibitors: Second generation of structurally optimized leads identified by X-ray crystallography

Nickolas Furnham

(London School of Hygiene & Tropical Medicine, UK)

PL5: Searching for new malaria transmission-blocking compounds

Daniel Bargieri

(Department of Parasitology, Institute of Biomedical Sciences, University of São Paulo)

PL6: Identifying Novel Inhibitor Scaffolds for the Mycobacterium tuberculosis Dihydrofolate Reductase Using a Fragment-Based Drug Discovery Approach

Marcio Dias

(University of São Paulo, Brazil)

11:00 – 12:40

FP2: Anti-Trypanosomal Activity of Cyclic Amine-Chalcone Hybrids

Jefferson R.S. Oliveira (UFMS)

12:40 – 14:00

Lunch

Exhibitor Talk: Shimadzu

Overcome the challenges of chromatography: Discover the new Shimadzu Benchmark!

13:10 – 14:00

Luísa Barrella Ambrosio

14:00 – 15:30

S3 - BrazMedChem 2019 Awards

Chair: Marcelo Castilho (UFBA)

PL7: Early Career Award

Prof. Dr. Luis Octavio Regasini (UNESP)

Potential Antineoplastic and Anti-Infective of α,β -Unsaturated Ketones: A contribution of the Electrophilic Compounds

PL8: Vanguard Researcher

Profa. Dra. Lídia Moreira Lima (UFRJ)

Discovery of new small molecules designed as antitumor candidates

PL9: Senior Researcher

Prof. Dr. Carlos Alberto Manssour Fraga (UFRJ)

Discovery of Novel Kinase Inhibitors Belonging to Isosteric N-Acylhydrazone or N-Sulfonylhydrazone Classes

15:30 – 15:50

Coffee-break

S4 - Targeting Epigenetics and Genetics for Drug Discovery

Chair: Fabio T M Costa (UNICAMP)

PL10: Heavy metal fans: Targeting the zinc-dependent histone

A Ganesan

(University of East Anglia, UK)

PL11: Epigenetic Drug Discovery: A Focus on Activity Landscape Modeling

Jose Medina-Franco

(Universidad Nacional Autónoma de México, México)

PL12: New molecules against Plasmodium vivax using yeast surrogate genetics

Per Sunnerhagen

(University of Gothenburg, Sweden)

15:50 – 17:30

FP3: Integrative Target Prediction, Molecular docking and Experimental Evaluation of the Antidepressant-like effects of Doxycycline

Adriano Maia Chaves-Filho (UFC)

Interactive Session I: Women in Medicinal Chemistry: Why so Few?

17:30 – 19:00

- **Vanderlan Bolzani** - Sao Paulo State University, Brazil (**Chair**)
- **Gunda Georg** - University of Minnesota, USA
- **Sylvie Garneau-Tsodikova** - University of Kentucky, USA
- **Maria Cristian Nonato** - University of São Paulo, Brazil

19:00 – 20:30

Poster Session I

Tuesday - September 3rd

S5 - The new age of Natural Products for Drug Discovery

Chair: Angelo de Fátima (UFMG)

PL13: MedChemComm Emerging Investigator Lectureship: Chemical Physiology of Antibody Conjugates and Natural Products

Gonçalo Bernardes

(University of Cambridge, UK. Instituto de Medicina Molecular, Lisbon, Portugal)

PL14: Antimicrobial drug discovery

Sylvie Garneau-Tsodikova

(University of Kentucky, USA - Associate Editor for MedChemComm)

PL15: Chemical warfare in Nature inspires the discovery of antimicrobials

Mônica T. Pupo

(University of Sao Paulo, Brazil)

FP4: Novel 8-hydroxyquinoline derivatives are potential candidates for treatment of fungal infections: toxicity, irritability and PK/PD modeling studies

Angelica R. Joaquim (UFRGS)

09:00 – 10:40

10:40 – 11:00

Coffee-break

S6 - Rethinking academia facilities to Drug Discovery

Chair: Arthur E. Kummerle (UFRRJ)

PL16: Drug Discovery in Academia: The Institute for Therapeutics Discovery and Development at the University of Minnesota, USA

Gunda Georg

(Institute for Therapeutics Discovery and Development, University of Minnesota, USA)

PL18: Collaborative research and innovation in drug discovery against arboviruses circulating in Brazil

Glaucius Oliva

(Center for Research and Innovation in Biodiversity and Drug Discovery (CIBFar/CEPID), University of São Paulo, Brazil.)

PL17: Discovery of Chemical Probes for New Targets

Paul Brennan

11:00 – 12:40

(Structural Genomics Consortium - Target Discovery Institute – University of Oxford, UK)

FP5: An Open Science, Medicinal Chemistry Program to Develop New Therapeutics Against Non-Tuberculous Mycobacteria

Gustavo Riboldi (UNICAMP)

12:40 – 14:00

Lunch

Exhibitor Talk: Clarivate Analytics

13:10 – 14:00

Integrity: A tool to aid the Drug Discovery for Medicinal Chemists.

Sergio Delarcina

S7 - Special Section in Tribute to Prof Antony (Tony) Hopfinger

Chair: Elizabeth I. Ferreira (USP)

PL19: The development and application of receptor independent 4D-QSAR

Magaly G. Albuquerque

(Federal University of Rio de Janeiro, RJ, Brazil)

PL20: FEFF-QSAR-3D

Nililma C. Romeiro

(Federal University of Rio de Janeiro, Macaé, Brazil)

14:00 – 15:30

PL21: Structure-Based QSAR Analysis of a Set of 4-Hydroxy-5,6-dihydropyrone as Inhibitors of HIV-1 Protease: An Application of the Receptor-Dependent (RD) 4D-QSAR

Oswaldo A. Santos-Filho

(Federal University of Rio de Janeiro, RJ, Brazil)

PL22: Highlights from Learnings and Experiences with Prof. Tony Hopfinger

Mario Cardozo

(Nurix, Inc., USA)

15:30 – 15:50

Coffee-break

S8 - The evolution of Computer-Assisted Drug Discovery

Chair: Marcus T. Scotti (UFPB)

PL23: The Next Era of Pharmaceutical Research: From Bayesian Models to Deep Learning

Sean Ekins

(CEO of Collaborations Pharmaceuticals, Inc., USA)

15:50 – 17:30

PL24: Protein-Ligand Docking: Pose and Binding Affinity Prediction

Laurent Dardenne

(LNCC, Brazil)

PL25: Design of an Artificial Intelligence System for Drug Discovery

Rodolpho Braga

(Co-founder and CTO, inSilicAll, Brazil)

FP6: Rescuing poorly soluble drugs: a cheminformatics approach for polymeric micelle-drug formulations

Vinicius Medeiros Alves (University of North Carolina, USA)

Interactive Session II: Scientific Publishing

17:30 – 18:30

- **Paulo César Vieira** - Editor-in-chief for the Journal of the Brazilian Chemical Society, SBQ - **Chair**
- **Gunda Georg** - Editor-in-Chief for the Journal of Medicinal Chemistry, ACS.
- **Sylvie Garneau-Tsodikova** - Associate Editor for MedChemComm, RSC.
- **José Medina-Franco** - Editor of Frontiers in Chemistry. Past Associate Editor of RSC Advances

20:00 – 00:00

Party

Wednesday – September 4th

S9 – From library development to mechanism of action: The early stages in drug discovery

Chair: Cedric S. Graebin (UFRJ)

PL26: The transporter-mediated uptake of drugs is the rule

Elizabeth Bisland

(State University of Campinas)

09:00 – 10:40

PL27: Design, Synthesis and Biological evaluation for the discovery of drug candidates for Sickle Cell Disease

Chung Man-Chin

(University of São Paulo State, Araraquara, Brazil)

PL28: Exploring different facets of catalysis towards bioactive quinoidal compounds: The complexity of simple and powerful molecules

Eufrânio N. da Silva Júnior

(Federal University of Minas Gerais, Brazil)

FP7: Pteridine scaffold as candidate for MRCK γ kinase inhibitor

Stanley Vasconcelos (SGC - UNICAMP)

10:40 – 11:00

Coffee-break

11:00 – 12:30

Poster Session II

11:00 – 13:00

Science promoting activity with the local community

12:30 – 14:00

Lunch

Round Table - Cases of success between Academia and Industry

14:00 – 15:30

- **Katlin Massirer** (SGC-Unicamp, Brazil) - **Chair**
- **Carine Drewes** (EUROFARMA, Brazil)
- **Hatylas Zaneti de Azevedo** (Aché, Brazil)
- **Fabio Barros** (Instituto Vita Nova, Brazil)
- **Paulo Lacativa** (Biozeus, Brazil)

15:30 – 15:50

Coffee-break

S10 – Challenging Projects in drug discovery

Chair: Rafaela Ferreira (UFMG)

PL29: Impact of Computational Chemistry on Challenging Drug Discovery Projects: Structure-Based Design of potent Protein-Protein Interaction Inhibitors and Modulators

Mario Cardozo
(Nurix, Inc., USA)

15:50 – 17:30

PL30: Fragment screening against human prion protein

Maria Cristina Nonato
(University of São Paulo, Brazil)

PL31: Identifying novel drugs for the treatment of rhabdomyosarcoma

Sharon Prince
(University of Cape Town, South Africa)

FP8: Structure-based design and synthesis of new benzothiophene derivatives as potent PRPF4 kinase inhibitors

Natanael Dante Segretti (Aché, Brazil)

Closing Ceremony

17:30 – 18:30

Poster Prizes

Announcement of 10th BrazMedChem 2021