Preliminary program

November, 9 (Sunday)		
Timetable	**Activity**	**Speaker**
9 am – 6 pm	**Registration**	
9 am-12 pm 2-5 pm	**Short course** Metodologias de Ressonância Magnética Nuclear em Química Medicinal	José Daniel Figueroa Villar
9 am-12 pm	**Workshop pre-symposium** Virtual Screening: How to do it better and how to know you are doing better	Paul Hawkins
2-5 pm	**Workshop pre-symposium** Beyond the Rule of 5	Tudor Oprea, Peter Kenny
6-7 pm	**Opening Ceremony**	
7-8 pm	**Opening Conference** Structural Biology and Structural Genomics for Rational Drug Design	Kurt Wüthrich
8 pm	Welcome reception	

November, 10 (Monday)

Timetable	Activity	Speaker
	Target-based drug design	
9-9:15 am	Overview and introduction	Cristiano Guimarães
9:15-10 am	Simulation and informatics for chemical insight and design	Michael Gilson
10-10:45 am	Prion-Like Neurodegenerative Diseases and Cancer: New Targets to Chemotherapy	Jerson Lima
10:45-11 am	Coffee break	
11-11:45 am	Illuminating Ligand-Receptor Interactions: New Insights into GPCR Pharmacology using Fluorescent Ligands	Barrie Kellam
11:45 am-12:30 pm	Methodological improvements in docking: are we actually getting better?	Paul Hawkins
12:30-2:30 pm	Lunch	
	ADME-Tox in Drug Discovery	
2:30-2:45 pm	Overview and introduction	Antonia T. do Amaral
2:45-3:30 pm	Human Metabolism Prediction: Facts or Fantasy?	Gabriele Cruciani
3:30-4:15 pm	Accident and misadventure in property-based design	Peter Kenny
4:15-4:30 pm	Coffee break	
4:30-5:15 pm	Informatics and modeling supports drug safety	Catrin Hasselgren
	Oral presentations	
5:15-5:30 pm	Cation-π interactions play a key role in the binding of new CREBBP bromodomain inhibitors	Wilian Cortopassi
5:30-5:45 pm	C-7 Substituted artemisinin derivatives	Paulo Carvalho
5:45-6 pm	Design and Synthesis of Rac1 inhibitors as Potential Antitumor Agents	Maria Julieta Comin
6-7:30 pm	Poster session I	

November, 11 (Tuesday)

Timetable	Activity	Speaker
	Open Innovation in Cheminformatics (Sponsored by the Royal Society of Chemistry)	
9-9:15 am	Overview and introduction	Claudio Cavasotto
9:15-10 am	Drug Repurposing from an Academic Perspective	Tudor Oprea
10-10:45 am	Serving the Medicinal Chemistry Community with Royal Society of Chemistry Cheminformatics Platforms	Antony Williams
10:45-11 am	Coffee break	
11-11:45 am	Using Bioactivity Databases and Computer Algorithms for Target Deconvolution and Compound Design	Andreas Bender
11:45 am-12:15 pm	Incorporating quantum-mechanical methods in structure-based drug discovery	Claudio Cavasotto
12:15-2:30 pm	Lunch	
	Synthesis & Drug Design	
2:30-2:45 pm	Overview and introduction	Antonio Burtoloso
2:45-3:30 pm	Discovery of the Smoothened Inhibitors LEQ506 and LDE225 for the Treatment of Hedgehog-Dependent Tumors	Stefan Peukert
3:30-4:15 pm	Synthesis and Biological Activity of Natural Products and Derivatives	Ronaldo Pilli
4:15-4:30 pm	Coffee break	
4:30-5:15 pm	(Synthetic) Approaches to Lead Identification	Hans P. Wessel
	Oral presentations	
5:15-5:30 pm	The first crystal structures of fragment-like inhibitors bound to cruzain provides new insights for novel inhibitors design	William Fernandes
5:30-5:45 pm	Understanding miltefosine-membrane interactions using molecular dynamics simulations	Matheus Malta de Sá
5:45-6 pm	Association of the anti-tuberculosis drug rifampicin with PAMAM dendrimer: a molecular dynamics simulation study	Bruno Horta
6-7:30 pm	Poster session II	

November, 12 (Wednesday)

Timetable	Activity	Speaker
	Brazilian-Portuguese-Spanish Meeting on Medicinal Chemistry	
9-9:15 am	Overview and introduction	José Daniel Figueroa Villar
9:15-9:45 am	DockThor: a Brazilian Receptor-Ligand Docking Program	Laurent Dardenne
9:45-10:15 am	Chemogenomic approaches to single and dual-stage antimalarial agents	Rui Moreira
10:15-10:45 am	Progress and Pitfalls in the Modeling and Simulation of Tubulin-Drug Interactions	Federico Gago
10:45-11 am	Coffee-break	
11-11:30 am	Research, Development & Innovation at Aché.	Cristiano Guimarães
11:30 am-12 pm	New Synthetic Routes of Nitrogen and Oxygen Heterocycles	Artur Silva
12-12:30 pm	Discovery of Novel EP1 Ligands for the Treatment of Pain	Antoni Torrens
12:30-2:30 pm	Lunch	
	New Approaches in Drug Discovery	
2:30-2:45 pm	Overview and introduction	Andrei Leitão
2:45-3:30 pm	The Emergence of Drug Discovery in Academia: Case studies in Neurodegenerative Disease	Marcie Ann Glicksman
3:30-4:15 pm	Human Cell Systems Biology for Drug Discovery and Chemical Safety	Ellen L. Berg
4:15-4:30 pm	Coffee-break	
4:30-5:15 pm	Enabling the Best Structure-Based Design Engine: An Expert Scientist	Jeffrey Blaney
5:15-7 pm	Round table	
7-8 pm	Closing remarks	