



ISMEC2012

International Symposium on Metal Complexes 2012

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**CONFERENCE PROGRAMME**

**Monday, June 18<sup>th</sup>**

14.00 - 16.25 Registration of participants

16.25 – 16.55 Coffee break

**Auditorium 3**

Chairman: **Margarida C. dos Santos**

16.55 – 17.30 Welcome words

**KN1** - The chemistry behind the use of bioassays to assess metal toxicity: pH influence, complexation equilibria

*Isabel Villaescusa*

17.30 – 17.50 **OC1** - Metal leaching capacity of rainwater in an abandoned lead-zinc mine

*Ainhoa Tirapu, Leire Kortazar, Naiara Goienaga, Maitane Olivares, Jose Antonio Carrero, Juan Manuel Madariaga, Luis Ángel Fernández*

17.50 – 18.10 **OC2** - Characterization of the interactions between proteinaceous binders and inorganic pigments in paint reconstructions

*Ilaria Bonaduce, Emilia Bramanti, Maria Perla Colombini, Celia Duce, Lisa Ghezzi, Alessio Spepi, Maria Rosaria Tinè*

18.10 – 18.30 **OC3** - Insights on the U(VI) speciation with bacterial isolates from Äspö and Mont Terri

19.00 – 20.00 Welcome reception

**Tuesday, June 19<sup>th</sup>**

8.00 – 9.00 Registration of participants

**Auditorium 3**

9.00 – 9.15 Opening ceremony

Chairman: **Guido Crisponi**

9.15 – 10.10 **PL1** - Redox metals in neurodegenerative diseases, and therapeutic perspectives

*Robert R. Crichton, Roberta J. Ward, David T. Dexter*

Chairman: **Chris Exley**

10.10 – 10.30 **OC4** - Histidine-rich branched peptides as copper and zinc chelators with potential therapeutic application in Alzheimer's disease

*Andrea Lakatos, Béla Gyurcsik, Nóra V. Nagy, Zita Csendes, Edit Wéber, Livia Fülöp, Tamás Kiss*

10.30 – 10.50 **OC5** - Biomimetic analogues of siderophores as structural probes for microbial iron uptake processes

*Agnieszka Szebesczyk, Jenny Kolsenik, Evgenia Olshvang, Abraham Shanzer, Elzbieta Gumienna-Kontecka*

10.50 – 11.20 Coffee break

	Chairman: <b>Roberta Ward</b>	16.20 – 16.40	<b>OC9</b> - Actinide complexes incorporating environmentally relevant chelators: a structural, thermodynamic, and kinetic prospect <i><u>Michel Meyer</u></i>
11.20 – 11.50	<b>KN2</b> - Structural and thermodynamic aspects of thiol binding to metal ions in excentric proteins <i><u>Henryk Kozłowski, Karolina Krzywoszynska, Slawomir Potocki, Magdalena Rowinska-Zyrek, Danuta Witkowska</u></i>	16.40 – 17.10	Coffee break
	Chairman: <b>Manuel Valiente</b>		Chairman: <b>Alexander Shestakov</b>
11.50 – 12.10	<b>OC6</b> - A peptidic turn with high affinity for heavy metal ions <i>Sara Pires, Murat Sezer, Cláudio M. Soares, Lars Hemmingsen, <u>Olga Iranzo</u></i>	17.10 – 17.40	<b>KN4</b> - Modeling of molecular properties. Fundamental principles and case studies with transition metal compounds <i><u>Peter Comba</u></i>
12.10 – 12.30	<b>OC7</b> - Microprotonation and Na(I)/Mg(II)-interaction of inositol 1,3,4,5,6-pentakis phosphate: <sup>31</sup> P NMR and computational insights <i><u>Nicolás Veiga, Julia Torres, Israel Macho, Kerman Gómez, Gabriel González, Carlos Kremer</u></i>	17.40 – 18.00	<b>OC10</b> - Computational studies of cesium-137 recognition by cucurbituril <i><u>Fabio Pichierri</u></i>
12.30 – 14.30	Lunch break, exhibition and poster viewing	18.00 – 18.20	<b>OC11</b> - Protonation sequence of zoledronic acid: a DFT and QTAIM study <i><u>Ignacy Cukrowski, Anindita Sarkar, Anton van Aswegen, David Liles</u></i>
	Chairman: <b>Chris Orvig</b>		
14.30 – 15.30	<b>PL2</b> - Metal ion selective sequestering agents, with selective properties <i><u>Kenneth N. Raymond</u></i>	18.20 – 19.30	Poster session 1
	Chairman: <b>Etelka Farkas</b>	19.30 – 20.30	GTC Meeting
15.30 – 16.00	<b>KN3</b> - Metal complexes defining aluminium's exposome <i><u>Chris Exley</u></i>		<b>Room 2</b>
16.00 – 16.20	<b>OC8</b> - Siderophores - transport properties and environmental stability <i><u>Günther Winkelmann</u></i>	10.10 – 10.30	Chairman: <b>Elia Grueso</b> <b>OC31</b> - The mechanism of the reaction of gold(III) ion with pyridine-2-azo-p-dimethylaniline in water and SDS <i><u>Sabriye Aydinoğlu, Tarita Biver, Fernando Secco, Marcella Venturini</u></i>

10.30 – 10.50 **OC32** - New synthesis of dinuclear metal complexes which include gold(III), ruthenium(II) and platinum(II), induce apoptosis in cancer cells via activation of mitochondrial pathway

*R. Beklem Bostancioglu, A. Tansu Koparal, Kadriye Benkli*

10.50 – 11.20 *Coffee break*

Chairman: **Alessandro de Robertis**

11.50 – 12.10 **OC33** - Tuning the hydrolytic properties of half-sandwich type organometallic cations in aqueous solution

*Péter Buglyó, Linda Biró, Eugenio Garribba, Zsolt Bihari*

12.10 – 12.30 **OC34** - The leaving group of ruthenium arene complexes plays an essential role in biological activity

*Natalia Busto, Begoña García, José M. Leal, Héctor J. Lozano, Jesús Valladolid, Gustavo A. Espino, Tarita Biver*

12.30 – 14.30 *Lunch break, exhibition and poster viewing*

Chairman: **Igor Nikolayenko**

16.00 – 16.20 **OC35** - Synergistic effects of copper(II) complexes and cisplatin: an application of artificial neural networks and experimental design

*Tiziana Pivetta, Francesco Isaia, Federica Trudu, Alessandra Pani, Matteo Manca, Daniela Perra, Filippo Amato, Josef Havel*

16.20 – 16.40 **OC36** - Reliability of protonation constants and chemical model of drugs using SQUAD(84) and SPECFIT/32 regression analysis of pH-UV/VIS spectra

*Milan Meloun*

Chairman: **Marian Olazabal**

17.40 – 18.00 **OC37** - Aqueous complexation and interactions of Nd(III) and Am(III) with citrate in perchlorate media

*M. Alex Brown, Alena Paulenova, Artem V. Gelis*

18.00 – 18.20 **OC38** - Neurotoxic effect of nano-alumina on SD rats *in vivo*

*Qinli Zhang, Meiqin Li, Li Xu, Xia Jiao, Qiao Niu*

**Wednesday, June 20<sup>th</sup>**

**Auditorium 3**

Chairman: **Maria Rangel**

9.10 – 10.10 **PL3** - Therapeutic and diagnostic metal complexes in medicinal inorganic chemistry

*Chris Orvig*

Chairman: **Enrique García-España**

10.10 – 10.30 **OC12** - (Thio)pyrone-derived organometallics: an approach for new metal-based anticancer drugs

*Wolfgang Kandioller, Samuel M. Meier, Michael A. Jakupec, Bernhard K. Keppler, Christian G. Hartinger*

10.30 – 10.50 **OC13** - Solution and biological behaviour of fluoroquinolones metalloantibiotics: a route to counteract bacterial resistance?

*Maria J. Feio, Paula Gameiro*

10.50 – 11.20 *Coffee break*

- Chairman: **Juan Nicolás-Gutiérrez**
- 11.20 – 11.50 **KN5** - Cation, anion and ion-pair binding with branched polyamines  
*Carla Bazzicalupi, Antonio Bianchi, Claudia Giorgi, Barbara Valtancoli*
- 11.50 – 12.10 **OC14** - Supramolecular chirogenesis with schiff base complexes: a gateway for determination of absolute configurations  
*Martha V. Escárcega-Bobadilla, Giovanni Salassa, Sander J. Wezenberg, Arjan W. Kleij*
- 12.10 – 12.30 **OC15** - Complex formation equilibria of copper(II) with triethylenetetramine and its human acetyl metabolites.  
*Guido Crisponi, Valeria M. Nurchi, Miriam Crespo-Alonso, Garth J. S. Cooper*
- 12.30 – 12.50 **OC16** - Metal complexes of the antitumor drug Triapine and related thiosemicarbazones  
*Éva A. Enyedý, Christian R. Kowol, Nóra V. Nagy, Éva Zsigó, Tamás Jakusch, Vladimir B. Arion, Bernhard K. Keppler, Tamás Kiss*
- 12.50 – 14.45 *Lunch break*
- 15.00 – 20.00 *Excursion*

### Room2

Chairman: **Plinio di Bernardo**

- 10.10 – 10.30 **OC39** - Speciation of vanadyl complexes with simple organic ligands in aqueous solutions  
*Nadira Batool, Danielle Meyrick, Peter May*

- 10.30 – 10.50 **OC40** - Thermodynamic studies on new copper(I) and silver(I) phosphine complexes with potential antitumor activity  
*Francesco Endrizzi, Plinio DI Bernardo, Pierluigi Zanonato, Francesco Tisato, Marina Porchia*

10.50 – 11.20 *Coffee break*

Chairman: **Rita Delgado**

- 11.50 – 12.10 **OC41** - Molecular recognition patterns in ternary copper(II) complexes with deaza-adenine and amino-polycarboxylate ligands  
*Alicia Domínguez-Martín, Duane Choquesillo-Lazarte, Jose A. Dobado, Isaac Vidal, Josefã M. González-Pérez, Alfonso Castiñeiras, Juan Nicolás-Gutiérrez*

- 12.10 – 12.30 **OC42** - MALDI and SALDI TOF mass spectrometry - fast and efficient way to search for supramolecular complex formation and new drug carriers  
*Filippo Amato, Eladia Maria Peña-Méndez, Tiziana Pivetta, Reddy Nagender Panyala, Josef Havel*

- 12.30 – 12.50 **OC43** - Supramolecular systems connecting flavylum moieties with metal complexes  
*Ana M. Diniz, Fernando Pina, A. Jorge Parola*

**Thursday, June 21<sup>st</sup>**

### Auditorium 3

Chairman: **Marilena Tolazzi**

- 9.10 – 10.10 **PL4** - Metal-based chelates and nanosystems for multimodal molecular imaging applications

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Carlos F.G.C. Geraldes

Chairman: **João P. André**

10.10 – 10.30 **OC17** - Equilibrium, kinetic, relaxation and structural properties of H<sub>3</sub>DO3A-sulfonamide ligand and its Ca<sup>2+</sup>, Zn<sup>2+</sup>, Cu<sup>2+</sup> and Ln<sup>3+</sup>-complexes

Zsolt Baranyai, Anett Takács, Balázs Podolyák, Mihály Purgel, Roberta Napolitano, Silvio Aime, Ernő Brücher, Imre Tóth

10.30 – 10.50 **OC18** - Monopicolinate cyclen and cyclam derivatives for stable copper(II) complexation

Luís M. P. Lima, David Esteban-Gómez, Rita Delgado, Carlos Platas-Iglesias, Raphaël Tripier

10.50 – 11.20 *Coffee break*

Chairman: **Antonio Bianchi**

11.20 – 11.50 **KN6** - Macrobicyclic architectures for recognition of anions

Rita Delgado, Pedro Mateus

11.50 – 12.10 **OC19** - Mn(II) chelates with potential interest for MRI

Arsénio de Sá, Célia S. Bonnet, Carlos F. G. C. Geraldes, Eva Tóth, Paula M.T. Ferreira, João P. André

12.10 – 12.30 **OC20** - Binding properties of *p*-*tert*-butylcalix[4]arene derivatives and their application in ion selective electrodes

Véronique Hubscher-Bruder, Joanna Kulesza, Françoise Arnaud-Neu, Maria Bochenska

12.30 – 14.30 *Lunch break, exhibition and poster viewing*

Chairman: **Fernando Pina**

14.30 – 15.30

**PL5** - Luminescent silica nanoparticles: extending the frontiers of brightness

Sara Bonacchi, Damiano Genovese, Riccardo Juris, Marco Montalti, Enrico Rampazzo, Nelsi Zaccheroni, Luca Prodi

Chairman: **Carlos Geraldes**

15.30 – 16.00

**KN7** - Cation and anion coordination and self-assembling capabilities of 1H-pyrazole containing ligands. Surface modification of nanoparticles

Enrique García-España, Javier Pitarch, Felipe Reviriego, Salvador Blasco, M. Paz Clares, Raquel Belda, José M. Llinares, Javier Alarcón, Estefanía Delgado-Pinar, Pilar Navarro

16.00 – 16.20

**OC21** - BODIPY-phosphane as a versatile tool for an easy access to new metal-based theranostics

Semra Tasan, Olivier Zava, Julien Pierron, Benoît Bertrand, Claire Bernhard, Christine Goze, Michel Picquet, Pierre Le Gendre, Franck Denat, Angela Casini, Ewen Bodio

16.20 – 16.40

**OC22** - Effect of ethanol on gold nanoparticles-induced DNA compaction: thermodynamic, kinetic and conformational aspects of the interaction

Consuelo Cerrillos, Pilar Pérez-Tejeda, Rafael Prado-Gotor, Elia Grueso

16.40 – 17.10

*Coffee break*

Chairman: **Maurizio Remelli**

17.10 – 17.40

**KN8** - Interaction of hydroxamic acids with metals: from simple complexes to metallacrowns

	<i>Maria Rosa Beccia, Tarita Biver, Begoña García, José Maria Leal, Fernando Secco, Matteo Tegoni, Marcella Venturini</i>	10.50 – 11.20	Coffee break
17.40 – 18.00	<b>OC23</b> - Factors affecting the thermodynamic and redox stability of manganese(II) – and cobalt(II) – hydroxamate complexes <i>Etelka Farkas, Orsolya Szabó</i>		Chairman: <b>Jose Maria Leal</b>
18.00 – 18.20	<b>OC24</b> - Kinetic study of metal complexes with tetraazamacrocyclic ligands with carboxylate/phosphonate pendant arms <i>Přemysl Lubal, Petr Hermann, Jan Kotek, M. Paula C. Campello, Isabel Santos</i>	11.50 – 12.10	<b>OC46</b> - Multinuclear cytotoxic metallodrugs: synthesis and biological properties of novel bimetallic ruthenium-titanium and gold-titanium complexes <i>Margot Wenzel, Benoît Bertrand, Philippe Richard, Michael Groessl, Olivier Zava, Pierre Le Gendre, Michel Picquet, Angela casini</i>
18.20 – 19.30	Poster session 2	12.10 – 12.30	<b>OC47</b> - New polydentate Ru(III)-Salan complexes: synthesis, characterization, anti-tumour activity and interaction with human serum proteins <i>Cristina P. Matos, Andreia Valente, Fernanda Marques, Pedro Adão, Rodrigo F. M. Almeida, João Costa Pessoa, M. Helena Garcia, Ana Isabel Tomaz</i>
20.30	Social dinner		
	<b>Room2</b>		
	Chairman: <b>Katalin Várnagy</b>	12.30 – 14.30	Lunch break, exhibition and poster viewing  Chairman: <b>Barbara Barszcz</b>
10.10 – 10.30	<b>OC44</b> - Interaction of vanadate, niobate, molybdate and tungstate oxometalates with calcium pump from sarcoplasmic reticulum: Ca <sup>2+</sup> -ATPase conformational changes <i>Manuel Aureliano, Gil Fraqueza, C. André Ohlin, William H. Casey, M. Paula M. Marques, Luís A.E. Carvalho</i>	16.00 – 16.20	<b>OC48</b> - Tuning structure and properties of Pd and Pt camphorimine complexes <i>M. Fernanda N. N. Carvalho, Ana S.D. Ferreira, Adelino M. Galvão</i>
10.30 – 10.50	<b>OC45</b> - Magnesium and nickel metal ions can induce poly(rU)poly(rA)poly(rU) triplexes formation or quadruplexes stabilization <i>Maria Rosa Beccia, Tarita Biver, Natalia Busto, Begoña García, José Maria Leal, Luisa Menichetti, Fernando Secco, Marcella Venturini</i>	16.20 – 16.40	<b>OC49</b> - How CO releasing molecules CO-RMs interact with proteins <i>Teresa Santos-Silva, Abhik Mukhopadhyay, Marino F. A. Santos, João D. Seixas, Ana C. Coelho, Patrícia M. Reis, Maria J. Romão, Carlos C. Romão</i>  Chairman: <b>Andrea Gómez-Zavaglia</b>
		17.40 – 18.00	<b>OC50</b> - Mechanism of sulfide ion incorporation into the metal cluster of metallothioneins

	<i>Tamara Huber, Eva Freisinger</i>	10.40 – 11.10	<i>Coffee break</i>
18.00 – 18.20	<b>OC51</b> - Orange proteins in sulphate reducing bacteria: Mo-Cu heterometallic clusters in proteins involved in cell division <i>Marta. S.P. Carepo, Raquel Grazina, Cíntia.C.S. Carreira, Corrine Aubert, Allan Dolla, José J.G. Moura, Isabel Moura</i>		Chairman: <b>Raffaella Biesuz</b>
		11.10 – 11.40	<b>KN10</b> - Chemical speciation in environment and biomedicine: examples to technological development <i>Manuel Valiente</i>
<b>Friday, June 22<sup>nd</sup></b>			
<b>Auditorium 3</b>			
	Chairman: <b>Begoña García</b>		
9.10 – 9.40	<b>KN9</b> - Mechanistic modelling of An and Ln extraction by ILs: a first step towards a general model <i>Isabelle Billard</i>		
9.40 – 10.00	<b>OC25</b> - Novel functional materials as Ionic Liquids based on metal complexes <i>Luis C. Branco, Fernando Pina</i>		Chairman: <b>Maurizio Remelli</b>
10.00 – 10.20	<b>OC26</b> - Grafted squaramide nanoparticle systems for sulfate recognition in pure water <i>Estefanía Delgado-Pinar, Esther Carbonell, Carmen Rotger, Antoni Costa, M. Neus Piña, Hermas R. Jiménez, Javier Alarcón, Enrique García-España</i>		12.20 – 12.45 <b>OC30 (Pulidori award)</b> - Molecular reorganisations in polytopic receptors <i>Jorge González, Raquel Gavara, Carmen E. Castillo, J. M. Llinares, H. Jimenez, M. A. Mañez, Fernando Pina, M. G. Basallote, Enrique García-España</i>
10.20 – 10.40	<b>OC27</b> - Thermodynamics of protonation and metallation of the TPTZ ligand with a variety of cations <i>Igor V. Nikolayenko, Robert D. Hancock, Galen C. Littman</i>		12.45 – 13.15 <i>Closing remarks and presentation of ISMEC2013</i>