



NECTAR COST Action 18202



WG1

**NECTAR for highly hydrolysable and
low-valence state cations**

Montserrat Filella
Olga Iranzo

4th European NECTAR Conference
Milazzo, February 27th 2024



NECTAR COST Action 18202 WG1



Meetings

1) Zoom meetings

2) Presential annual WG1 meetings:

- 25th – 27th August 2021 Lisbon, Portugal

- 24th – 26th August 2022 Ljubljana, Slovenia

- 31st March - 1st April 2022: Université Paris-Saclay, Orsay, France
Organizer: Vladimir SLADKOV

- 28th - 29th September 2023: Ruđer Boškvić Institute, Zagreb, Croatia
Organizer: Elvira Bura-Nakić





NECTAR COST Action 18202 WG1



Webinars and training schools

1) Lunch webinars

- 2 June 2021, 1 pm, **Wolfgang Hummel** (PSI, CH): *Chemical Consistency of Thermodynamic Data*
- 30 June 2021, 1 pm, **Xavier Gaona** (KIT, Germany): *Hydrolysis and solubility constants*

2) Advance school

NECTAR Advanced school on aqua ions and hydrolysis-related equilibria
29th September 2023, Zagreb, Croatia



NECTAR COST Action 18202 WG1



9:00 – 10:00	Montserrat Filella, Xavier Gaona, Taishi Kobayashi	<i>Equilibrium constants for hydrolysable elements: from cradle to plate</i>
10:00 – 11:00	Luis Laglera	<i>Implications of kinetics of ligand exchange in the case of hydrolysable elements</i>
11:00 – 11:30	COFFEE BREAK	
11:30 – 12:30	Premek Lubal	<i>Solution chemistry & complex equilibria of low-valent elements</i>
12:30 – 14:00	LUNCH	
14:00 – 15:00	Wolfgang Hummel	<i>Strategies and practice in the selection of 'best' equilibrium constants</i>
15:00 – 16:00	Stuart Chalk	<i>Application of FAIR principles to equilibrium data</i>
16:00 – 16:30	COFFEE BREAK	
16:30 – 18:00	Montserrat Filella, Wolfgang Hummel, Olga Iranzo, Luis Laglera, Premek Lubal	<i>Open discussion: needs</i>



NECTAR COST Action 18202 WG1



STSMs



University of Wroclaw, **Poland**

University of Ferrara, **Italy**

University of Messina, **Italy**

University of Sassari, **Italy**

Medical University Innsbruck, **Austria**

Pavol Jozef Šafarik University, **Slovakia**

Slovak University of Technology in Bratislava, **Slovakia**

University of Zagreb, **Croatia**

Université de Strasbourg, **France**

Université Paris-Saclay, **France**

Aix-Marseille University, **France**



NECTAR COST Action 18202 WG1



STSMs

Yulia Toporivska (Biological Inorganic Chemistry Group, University of Wroclaw, **Poland**), *New efficient ^{89}Zr chelators for Positron Emission Tomography*, Dipartimento di Scienze Chimiche, Farmaceutiche ed Agrarie, University of Ferrara, **Italy**, 2020.

Andrzej Mular (Biological Inorganic Chemistry Group, University of Wroclaw, **Poland**), *^{68}Ga labelled analogues of desferrioxamine-E for nuclear imaging*, Department of Nuclear Medicine, Medical University Innsbruck, **Austria**, 2021.

Michaela Rendosova (Institute of Chemistry, Pavol Jozef Šafarik University, **Slovakia**), *Exploring of different techniques and computational programs for thermodynamic studies of silver(I) and gallium(III) complexes*, University of Messina, **Italy**, 2021.

Lucija Knezevic (Ruđer Bošković Institute, University of Zagreb, **Croatia**), *Vanadium(IV) and vanadium(V) complexation by succinic acid studied by affinity capillary electrophoresis*. Laboratoire de Physique des 2 Infinis Irène Joliot Curie, Université Paris-Saclay, **France**, 2021.

Andrzej Mular, (Biological Inorganic Chemistry Group, University of Wroclaw, **Poland**), *Investigation of FOXE analogues ability to transport iron into Pseudomonas aeruginosa cells*, CNRS, UMR7242, ESBS, University of Strasbourg, **France**, 2022.



STSMs

NECTAR COST Action 18202 WG1



Bartosz Orzeł (Biological Inorganic Chemistry Group, University of Wrocław, **Poland**), *Exploring the metal coordination chemistry of Fe(II) bacterial transporters with the use of NMR spectroscopy*, Department of Chemistry and Pharmacy, University of Sassari, **Italy**, 2022.

Valentyn Dzyhovskiy, (Biological Inorganic Chemistry Group, University of Wrocław, **Poland**), *Synthesis of the compounds intended to fit to the flavin mononucleotide riboswitches of Staphylococcus aureus*, Department of Chemical, Pharmaceutical and Agricultural Sciences, University of Ferrara, **Italy**, 2022.

Dora Crmarić (Ruđer Bošković Institute, University of Zagreb, **Croatia**), *Understanding copper speciation and redox transformations in copper-thiol complexes*, Institut des Sciences Moléculaires de Marseille, Aix-Marseille University, **France**, 2024.

Alejandro Blanco (Institut des Sciences Moléculaires de Marseille, Aix-Marseille University, **France**), *Study of the stability of Cu(II)/Cu(I) complexes using operando spectroelectrochemistry methods*, Institute of Physical Chemistry and Chemical Physics, Slovak University of Technology in Bratislava, **Slovakia**, 2024.

New collaborations established



NECTAR COST Action 18202 WG1



WG1 subgroups

Highly hydrolysable (HH) cations: Montserrat Filella

Low-valence (LV) state cations: Olga Iranzo



NECTAR COST Action 18202 WG1



WG1 - Low-valence state cations

Cu(I): *Determining Cu(I) concentration and binding constants: methods and crucial factors for accurate values*

In charge: Olga Iranzo

Contributors: Matteo Tegoni, Valentina Borghesani, Premek Lubal, Zuzana Vargová, Peter Rapta, Michel Meyer, Olga Iranzo

Fe(II): *Fe(II) complexes in solution: coordination and stability*

In charge: Elżbieta Gumienna-Kontecka

Contributors: Bartosz Orzel, Kamila Stokowa-Soltys, Valentyn Dzyhovskyi, Elżbieta Gumienna-Kontecka, Sofia Gama, Gabriele Lando, Demetrio Milea, Eva Anna Enyedy, Clemente Bretti, Peter Rapta

Guidelines for good laboratory practice when working with Cu(I) and Fe(II) under both **anaerobic and aerobic conditions**



NECTAR COST Action 18202 WG1



WG1 - Highly hydrolysable cations

- Periodic Table https://www.cost-nectar.eu/pages/wg1_period.html
- "New insights on U(IV) hydrolysis studies"
In charge: Vladimir
- "Chemical speciation modelling and stability constants determination: effective thermodynamic equilibrium vs kinetic stability"
In charge: Demetrio
- "Misuse of the pM concept with emphasis on hydrolysis"
In charge: Sofia