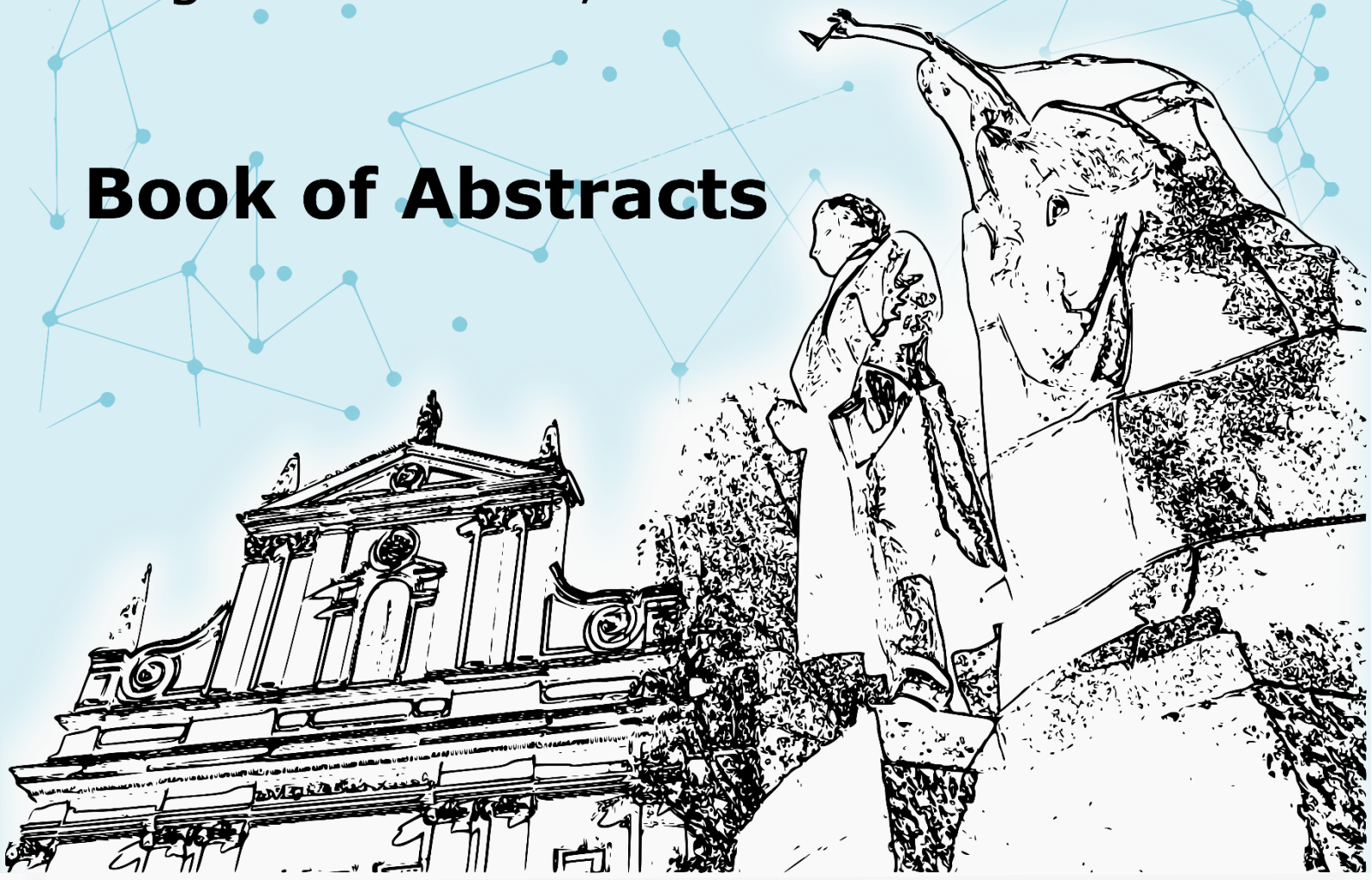
3rd European NECTAR Conference

Ljubljana

August 24th-26th, 2022

Book of Abstracts



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1st Online Edition
Ljubljana, 2022

3rd NECTAR Conference Programme					
August 24th, Wed		August 25th, Thu		August 26th, Fri	
		8:30 - 9:00	Registration	8:30 - 9:00	Registration
		9:00 - 9:30	KN2 (WG4) P. VIKEGARD	9:00 - 9:45	SO/AO Communications
		9:30 - 9:50	OC6 S. BERTO	9:45 - 10:30	Individual WGs Meetings
		9:50 - 10:10	OC7 J. KLADNIK		
		10:10 - 10:30	OC8 T. BOROVIĆ		
		10:30 - 11:00	Coffee Break	10:30 - 11:00	Coffee Break
		11:00 - 11:30	KN3 (WG3) J. TELLINGHUISEN	11:00 - 13:00	Individual WGs Meetings
		11:30 - 11:50	OC9 M. SANADAR		
		11:50 - 12:10	OC10 C. KVARNSTRÖM		
		12:10 - 12:30	OC11 J. MUŠOVIĆ		
		12:30 - 12:50	OC12 Ž. MEDOŠ		
12:00 - 15:00	Registration	12:50 - 15:00	Lunch Break	13:00 - 15:00	Lunch Break
15:00 - 15:20	Opening Ceremony	15:00 - 15:30	KN4 (WG1) J. GALCERAN	15:00 -16:00	WGs Summary Managers Summary Core Group Meeting
15:20 -15:50	KN1 (WG2) P. RAPTA	15:30 -15:50	OC13 L. KNEŽEVIĆ		
15:50 -16:10	OC1 N. RIBEIRO	15:50 -16:10	OC14 E. ZANDA		
16:10 -16:30	OC2 K. STOKOWA-SOŁTYS	16:10 -16:30	OC15 E. BURA-NAKIĆ	16:00 - 16:30	Coffee Break
16:30 - 17:00	Coffee Break	16:30 - 17:00	Coffee Break	16:30 - 18:00	MC Meeting and Closing Ceremony
17:00 - 17:20	OC3 L. ANTONOV	17:00 - 18:00	Poster Session		
17:20 - 17:40	OC4 J. KUBINEC				
17:40 - 18:00	OC5 G. SANTONOCETA				

CONFERENCE PROGRAMME

Wednesday 24th

15:00 - 15:20	**Opening Ceremony**
Chairperson:	Maria Amelia SANTOS - *University of Lisbon, Portugal*
15:20 - 15:50	**KN1 (WG2)** - *In situ* EPR and UV–visible–NIR spectroelectrochemistry as a unique tool for redox mechanism and equilibria studies of biologically active ligands and their metal complexes Peter RAPTA - *Slovak University of Technology in Bratislava, Slovakia*
15:50 - 16:10	**OC1** - Spectroscopic studies on the ethidium bromide/DNA system: a golden standard that still needs information Nádia RIBEIRO – *University of Lisbon, Portugal*
16:10 - 16:30	**OC2** - Interactions of neurokinin B with copper(II) ions and their potential biological consequences Kamila STOKOWA-SOŁTYS - *University of Wroclaw, Poland*
16:30 - 17:00	Coffee Break
Chairperson:	Petr HERMANN - *Charles University in Prague, Czech Republic*
17:00 - 17:20	**OC3** - Favipiravir – tautomeric and complexation properties Liudmil ANTONOV - *Bulgarian Academy of Science, University of Chemical Technology and Metallurgy, Bulgaria*
17:20 - 17:40	**OC4** - Structural and solution study of scandium(III) complexes with phosphonate derivatives of H_4DOTA Jan KUBINEC - *Charles University in Prague, Czech Republic*
17:40 - 18:00	**OC5** - Water-soluble prismarene hosts: molecular recognition of ammonium cations in aqueous solution Giuseppina D. G. SANTONOCETA – *University of Catania, Italy*

Thursday 25th

Chairperson:	Winfried PLASS - *Friedrich Schiller University Jena, Germany*
9:00 - 9:30	**KN2 (WG4)** - A combined microcalorimetric cell for quantifying sorption phenomena followed by dissolution into liquid solvents Peter VIKEGARD - *Waters Sverige AB, Sweden*
9:30 - 9:50	**OC6** - Comparative study on the current tools for optimization of stability constants from potentiometric data Silvia BERTO – *University of Turin, Italy*
9:50 - 10:10	**OC7** - Solution chemical properties and biological activity of organoruthenium(II) complexes with *O*,*O*-, *N*,*O*- and *O*,*S*-ligands Jerneja KLADNIK - *University of Ljubljana, Slovenia*
10:10 - 10:30	**OC8** - The effect of salicylate on the solubility and self-aggregation of caffeine - a thermodynamic and computational approach Teona Teodora BOROVIĆ - *University of Novi Sad, Serbia*
10:30 - 11:00	Coffee Break
Chairperson:	Slobodan GADŽURIĆ - *University of Novi Sad, Serbia*
11:00 - 11:30	**KN3 (WG3)** - A (partial) resolution of binding enthalpy discrepancies in ITC studies of Ba^{2+}/crown ether complexation: the importance of calibration Joel TELLINGHUISEN - *Vanderbilt University, USA*
11:30 - 11:50	**OC9** - Cobalt extraction from chloride/nitrate/sulfate media with phosphonium-based ionic liquids Martina SANADAR - *University of Udine, Italy*
11:50 - 12:10	**OC10** - *In situ* FTIR and Raman spectroelectrochemistry on organic semiconductors in room-temperature ionic liquids Carita KVARNSTRÖM - *University of Turku, Finland*
12:10 - 12:30	**OC11** - Spectrophotometric study of stability constant of 1-butyl-3-methylimidazolium 2-mercaptobenzothiazole and cadmium(II) Jasmina MUŠOVIĆ - *University of Belgrade, Serbia*
12:30 - 12:50	**OC12** - Aggregation of metallacarboranes in aqueous solutions Žiga MEDOŠ - *University of Ljubljana, Slovenia*
12:50 - 15:00	Lunch Break

Chairperson:	Olga IRANZO, *CNRS, University of Aix-Marseille, France*
15:00 - 15:30	**KN4 (WG1)** - Thermodynamics and kinetics of the dissolution of In_2O_3 nanoparticles Josep GALCERAN – *University of Lleida and AGROTECNIO-CERCA, Spain*
15:30 - 15:50	**OC13** - Vanadium(IV) and vanadium(V) complexation with succinic acid by affinity capillary electrophoresis Lucija KNEŽEVIĆ - *Ruđer Bošković Institute, Croatia*
15:50 - 16:10	**OC14** - Complexation studies of U(IV) with hydroxamic acid ligands Emanuele ZANDA - *University of Paris-Saclay, France*
16:10 - 16:30	**OC15** - Study of bathocuproine and Cu(I) electrochemical behavior on Hg electrode surface Elvira BURA-NAKIĆ - *Ruđer Bošković Institute, Croatia*
16:30 - 17:00	Coffee Break
17:00 - 18:00	**Poster Session**
19:30 - 22:30	**Conference Dinner, Ljubljana Castle**

Friday 26th

9:00 - 9:45	**SO/AO Communications**
9:45 - 10:30	**Individual WGs Meetings**
10:30 - 11:00	Coffee Break
11:00 - 13:00	**Individual WGs Meetings**
13:00 - 15:00	Lunch Break
Chairperson:	*Demetrio MILEA – University of Messina, Italy*
15:00 - 16:00	**WGs Summary** **Managers Summary** **Core Group Meeting**
16:00 - 16:30	Coffee Break
16:30 - 18:00	**MC Meeting** **Closing Ceremony**

Comparative study on the current tools for optimization of stability constants from potentiometric data

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Among the participants of COST Action CA18202 NECTAR – Network for Equilibria and Chemical Thermodynamics Advanced Research, a survey was conducted regarding what software is used daily and what problems the users are facing. The results show a high fragmentation in the software used, associated with a common dissatisfaction concerning the user experience, highlighting the need of the development of new IT tools for the management of chemical equilibria in solution by the NECTAR community. Following this line, WG4 is working to meet this need developing a free, multi-platform and open-source software, dedicated to the analysis of potentiometric data, with the aim of making it become the reference software for in solution speciation studies. Towards that goal, we have also undertaken a critical evaluation of the software actually available for the analysis of potentiometric data, in order to identify the strengths and weaknesses of each and to use this knowledge for the development of the new IT products. With this aim, the software Hyperquad [1,2], SUPERQUAD [3], PSEQUAD [4], BSTAC [5], OPIUM [6], Reactlab™ suite [7] and KEV, were tested on an

artificial dataset of six different titrations conducted on a hypothetic hexaprotic acid, in order to optimize the six protonation constants. The results obtained with the different software were analyzed and discussed. Moreover, the data analysis was carried out including some systematic errors in the calculation, quite common in the experimental procedures, in order to stress the impact of systematic errors arising in potentiometry on the refined parameters, and check the sensitivity of the different software in relation to these errors. The systematic errors considered were: carbonation of the base used as titrant, impurity of the solution components (partial salification of the titrated acid, for example), disregarding of the junction potential, the use of a not correct formal potential, changes on the ionic strength during the titration. The discussion of the results was also used to highlight the extent of the effects of systematic errors on the final results and to propose guidelines for the obtention of reliable formation constants.

References:

[1] P. Gans, A. Sabatini, A. Vacca, *Talanta* **1996**, 43, 1739-1753.
[2] http://www.hyperquad.co.uk/HQ2013.htm
[3] P. Gans, A. Sabatini, A. Vacca, *Inorg. Chim. Acta* **1983**, 79, 219-220.
[4] L. Zekany, I. Nagypal, PSEQUAD, a comprehensive program for the evaluation of potentiometric and/or spectrophotometric equilibrium data using analytical derivatives. In *Computational Methods for the Determination of Formation Constants*, D. J. Leggett, Ed. Plenum Press: New York, **1985**, pp. 291-353.
[5] C. De Stefano, P. Mineo, C. Rigano, S. Sammartano, *Annali di Chimica (Rome)* **1993**, 83, 243-277.
[6] https://web.natur.cuni.cz/~kyvala/opium.html
[7] https://jplusconsulting.com/
[8] A.N. Meshkov, G.A. Gamov, *Talanta* **2019**, 198, 200-205.