COST Action CA18202 – NECTAR

Network for Equilibria and Chemical Thermodynamics Advanced Research

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EUROPEAN COOPERATION
IN SCIENCE & TECHNOLOGY

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NECTAR
NETWORK FOR EQUILIBRIA AND CHEMICAL THERMODYNAMICS ADVANCED RESEARCH

NECTAR CA18202

Network for Equilibria and Chemical Thermodynamics Advanced Research
COST ACTION 18202

The thermodynamic study of chemical equilibria represents the core of many important branches of chemistry. Coordination and supramolecular chemistry, chemical speciation, molecular modelling, drug design are just few examples.

The importance of chemical equilibria, and chemical thermodynamics in general, results from the simple assertion that many properties of elements and compounds depend mainly on their interactions in a given system: the biological activity of an element or molecule, or their environmental impact can be explained by a detailed study of these interactions, whose nature and strength can be evaluated by chemical equilibrium and other thermodynamic studies. For example, speciation modelling based on chemical equilibrium data is commonly used in to improve commercial products performances, investigate the mobility of pollutants and toxicants in the environment, optimize industrial processes, explain the mechanisms of action of biologically active substances. Furthermore, advanced thermodynamic studies yield deeper insights into the mechanisms of these interactions.

NECTAR will combine the expertise of the large community of specialists working in this field, creating a network based on the stimulating collaboration between them, promoting knowledge exchange, and achieving high technological progress. All this will be accomplished through a fruitful collaboration between young researchers and experienced scientists, taking into consideration gender balance and maximal geographical distribution. Innovative and integrated theoretical and experimental approaches will be established and optimized.

Overall, the outstanding quality of obtained results will serve as benchmark for next decades, allowing their application in the above-mentioned fields and substantially impacting on life quality of next generations.

https://www.cost.eu/actions/CA18202/ **https://www.cost-nectar.eu/**

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NECTAR CA18202

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COST ACTION 18202

Main Aim / Objective of the Action:

Provide a scientific and technological platform to gather together, under a unique network, a critical mass of European research groups with a strong expertise in chemical equilibria with industrial stakeholders, with the valuable reinforcement of international partners and European enterprises.

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Objectives of the Action:

Give response to actual scientific and technological challenges. In the wide field of equilibrium thermodynamics, particular attention will be paid to four specific areas: i) biology and medicine; ii) environmental science; iii) technology and industry; iv) modelling and software development.

Develop new technologies. The multidisciplinarity and diversity of expertise within NECTAR will bring about a demand for developing new technological solutions, which will successfully combine all stakeholders' interests.

Identify new industrial stakeholders and applications. One of NECTAR's aims is to enlarge the perception about the potential of the use of different thermodynamic studies on specific industrial and technological applications (including environmental and biological/medical).

Promoting mobility and multidisciplinary training between the different participants of the Action.

Transfering knowledge and promoting industrial awareness.

Supporting a high proportion of ECIs, ITCs and assuring gender balance in the COST Action.

Promoting the sustainability of the network beyond the Action.

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NECTAR CA18202

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COST ACTION 18202

Fact Sheet

Start of Action: 02/10/2019

End of Action: 01/04/2024

31 Member Countries (19 ITC)

249 Active Participants (~ 55% female, ~ 30% ECI)

Working Groups:

WG1 NECTAR for highly hydrolysable (HHC) and/or low-valence state (LVC) cations

WG2 NECTAR for strong and/or multifunctional ligands, macromolecules, polyelectrolytes

WG3 NECTAR for multicomponent solutions and complex matrices

WG4 NECTAR tools, services and facilities

WG5 NECTAR for the future: new trends and exploitation of results

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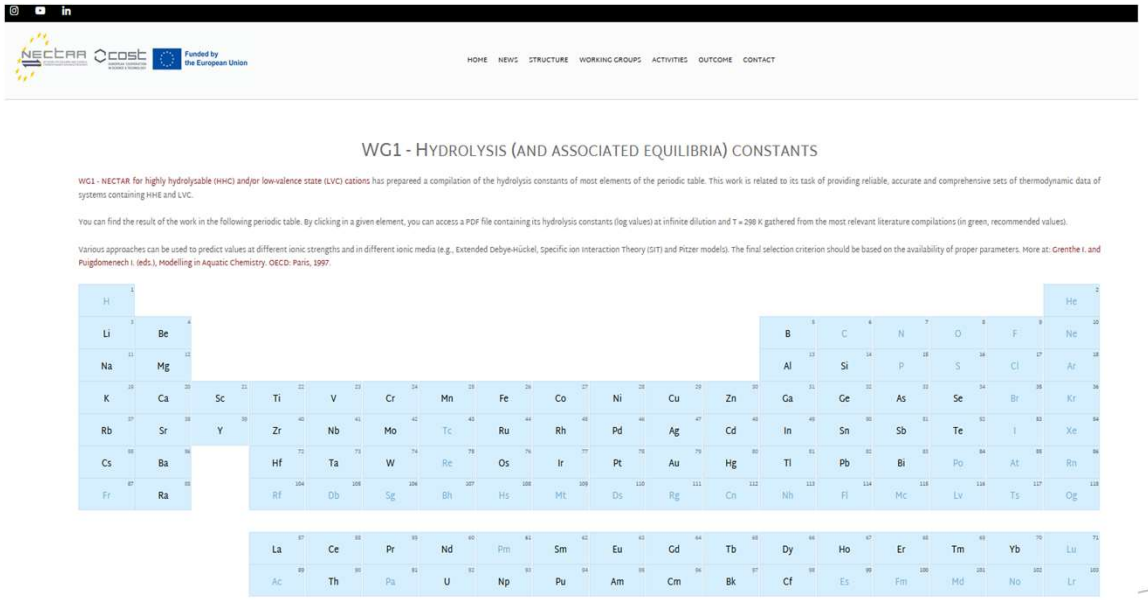
WG1

Main outcomes:

Compilation and critical assessment of hydrolysis constants and solubility products for some selected elements:

- Online "Periodic Table" release concerning acid-base properties of elements - database on cations hydrolysis.



https://www.cost-nectar.eu/pages/wg1_period.html

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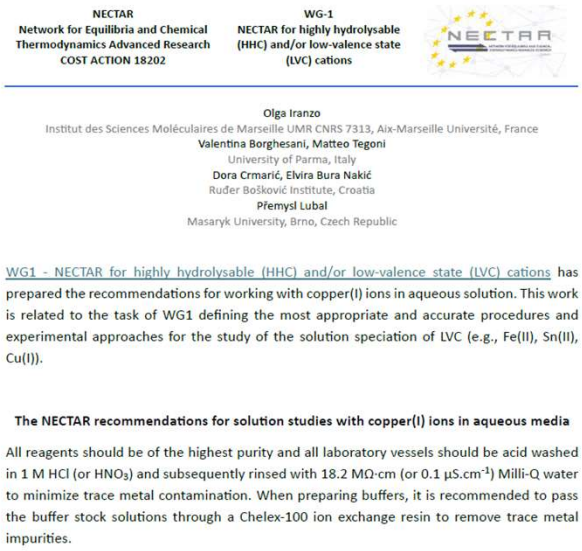
WG1

Main outcomes:

Development and testing of recommended procedures for the accurate determination of stability constants for some selected systems:

- Online release of guidelines on Cu(I) thermodynamic studies.



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WG-1
NECTAR for highly hydrolysable (HHC) and/or low-valence state (LVC) cations

Olga Iranzo
Institut des Sciences Moléculaires de Marseille UMR CNRS 7313, Aix-Marseille Université, France
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University of Parma, Italy
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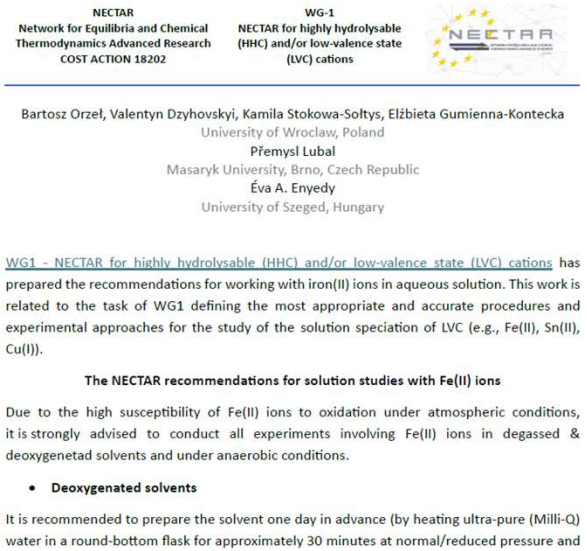
Masaryk University, Brno, Czech Republic

WG1 - NECTAR for highly hydrolysable (HHC) and/or low-valence state (LVC) cations has prepared the recommendations for working with copper(I) ions in aqueous solution. This work is related to the task of WG1 defining the most appropriate and accurate procedures and experimental approaches for the study of the solution speciation of LVC (e.g., Fe(II), Sn(II), Cu(I)).

The NECTAR recommendations for solution studies with copper(I) ions in aqueous media

All reagents should be of the highest purity and all laboratory vessels should be acid washed in 1 M HCl (or HNO_3) and subsequently rinsed with 18.2 MΩ·cm (or 0.1 $\mu S.cm^{-1}$) Milli-Q water to minimize trace metal contamination. When preparing buffers, it is recommended to pass the buffer stock solutions through a Chelex-100 ion exchange resin to remove trace metal impurities.

- Online release of guidelines on Fe(II) thermodynamic studies.



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WG-1
NECTAR for highly hydrolysable (HHC) and/or low-valence state (LVC) cations

Bartosz Orzeł, Valentyn Dzyhovskyi, Kamila Stokowa-Sołtys, Elżbieta Gumienna-Kontecka
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Masaryk University, Brno, Czech Republic
Éva A. Enyedy
University of Szeged, Hungary

WG1 - NECTAR for highly hydrolysable (HHC) and/or low-valence state (LVC) cations has prepared the recommendations for working with iron(II) ions in aqueous solution. This work is related to the task of WG1 defining the most appropriate and accurate procedures and experimental approaches for the study of the solution speciation of LVC (e.g., Fe(II), Sn(II), Cu(I)).

The NECTAR recommendations for solution studies with Fe(II) ions

Due to the high susceptibility of Fe(II) ions to oxidation under atmospheric conditions, it is strongly advised to conduct all experiments involving Fe(II) ions in degassed & deoxygenetad solvents and under anaerobic conditions.

- **Deoxygenated solvents**

It is recommended to prepare the solvent one day in advance (by heating ultra-pure (Milli-Q) water in a round-bottom flask for approximately 30 minutes at normal/reduced pressure and then bubbling argon gas through the liquid, and store the solution in a glove box until the next day.

https://www.cost-nectar.eu/pages/guides.html

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WG2

Main outcomes:

Development and testing of recommended procedures for the accurate determination of stability constants for some selected systems:

- Guidelines and recommended procedures for potentiometric measurements of strong ligand/metal interactions.
- Guidelines and recommended procedures for DNA interaction studies

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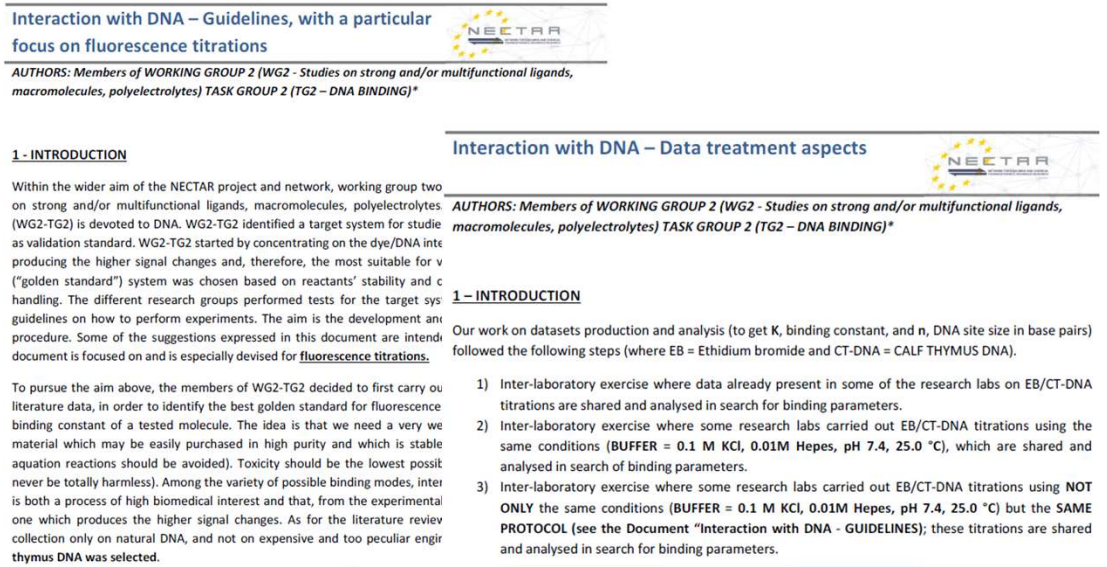
WG-2
NECTAR for strong and/or multifunctional ligands, macromolecules, polyelectrolytes

31 March 2024

Matteo Marafante, Silvia Berto
Università degli Studi di Torino, Italy
Gabriele Lando, Clemente Bretti, Concetta De Stefano, Demetrio Milea
Università degli Studi di Messina, Italy
Antonio Bianchi
Università degli Studi di Firenze, Italy
Katalin Varnágy
University of Debrecen, Hungary
Enrique Garcia-España
University of Valencia, Spain
Jana Havlíčková, Vojtěch Kubíček, Petr Hermann
Univerita Karlova (Charles Univesity Prague), Czech Republic

Recommended procedures for potentiometric determination of equilibrium constants of polydentate ligands and their metal ion complexes

Content: *Page*



Interaction with DNA – Guidelines, with a particular focus on fluorescence titrations

*AUTHORS: Members of WORKING GROUP 2 (WG2 - Studies on strong and/or multifunctional ligands, macromolecules, polyelectrolytes) TASK GROUP 2 (TG2 – DNA BINDING)**

1 - INTRODUCTION

Within the wider aim of the NECTAR project and network, working group two on strong and/or multifunctional ligands, macromolecules, polyelectrolytes (WG2-TG2) is devoted to DNA. WG2-TG2 identified a target system for studie as validation standard. WG2-TG2 started by concentrating on the dye/DNA inte producing the higher signal changes and, therefore, the most suitable for v ("golden standard") system was chosen based on reactants' stability and c handling. The different research groups performed tests for the target sys guidelines on how to perform experiments. The aim is the development an procedure. Some of the suggestions expressed in this document are intend document is focused on and is especially devised for **fluorescence titrations.**

To pursue the aim above, the members of WG2-TG2 decided to first carry ou literature data, in order to identify the best golden standard for fluorescence binding constant of a tested molecule. The idea is that we need a very we material which may be easily purchased in high purity and which is stable aquation reactions should be avoided). Toxicity should be the lowest possit never be totally harmless). Among the variety of possible binding modes, inter is both a process of high biomedical interest and that, from the experimental one which produces the higher signal changes. As for the literature reviev collection only on natural DNA, and not on expensive and too peculiar engir **thymus DNA was selected.**

Interaction with DNA – Data treatment aspects

*AUTHORS: Members of WORKING GROUP 2 (WG2 - Studies on strong and/or multifunctional ligands, macromolecules, polyelectrolytes) TASK GROUP 2 (TG2 – DNA BINDING)**

1 – INTRODUCTION

Our work on datasets production and analysis (to get **K**, binding constant, and **n**, DNA site size in base pairs) followed the following steps (where EB = Ethidium bromide and CT-DNA = CALF THYMUS DNA).

1) Inter-laboratory exercise where data already present in some of the research labs on EB/CT-DNA titrations are shared and analysed in search for binding parameters.
2) Inter-laboratory exercise where some research labs carried out EB/CT-DNA titrations using the same conditions (**BUFFER = 0.1 M KCl, 0.01M Hepes, pH 7.4, 25.0 °C**), which are shared and analysed in search of binding parameters.
3) Inter-laboratory exercise where some research labs carried out EB/CT-DNA titrations using **NOT ONLY** the same conditions (**BUFFER = 0.1 M KCl, 0.01M Hepes, pH 7.4, 25.0 °C**) but the **SAME PROTOCOL (see the Document "Interaction with DNA - GUIDELINES)**; these titrations are shared and analysed in search for binding parameters.

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WG2

Main outcomes:

Development and testing of recommended procedures for the accurate determination of stability constants for some selected systems:

- Guidelines for proper data collection and analysis in isothermal titration calorimetry experiments

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Working Group 2, Task Group 5

Recommended procedure for proper data collection and analysis in isothermal titration calorimetry experiments: the case of multiple host-guest equilibria

April 2024

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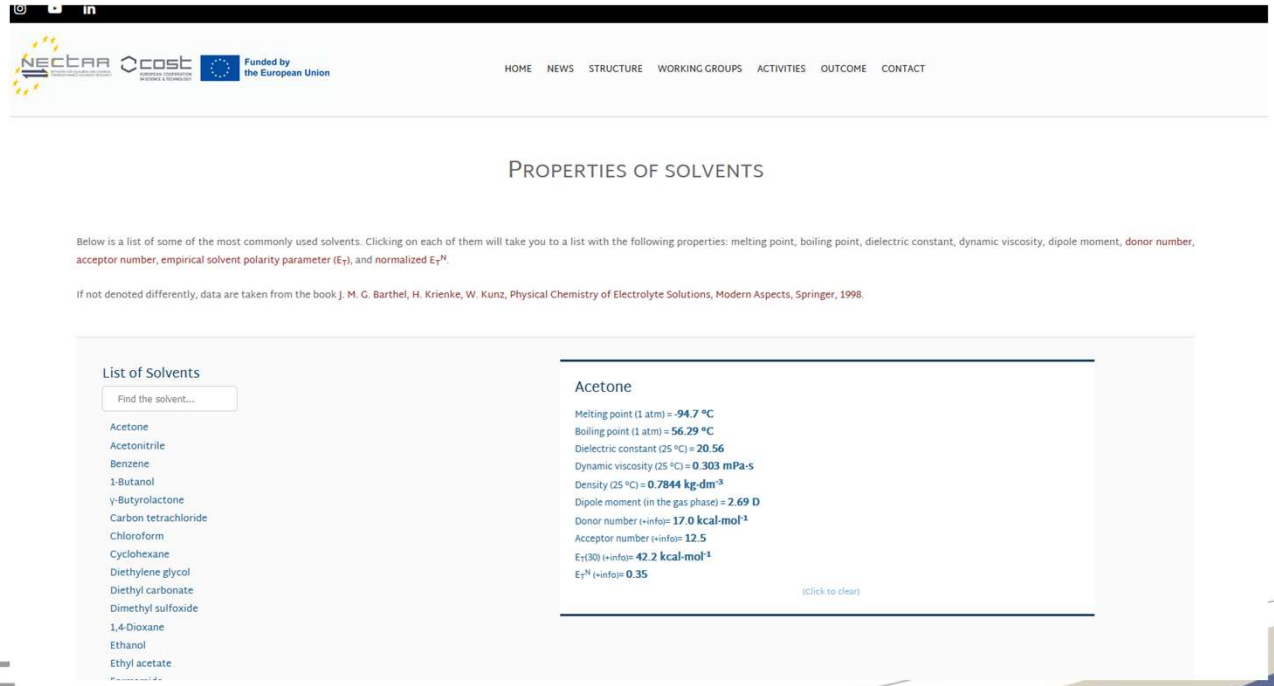
WG3

Main outcomes:

Development of methodologies for thermodynamic studies of non-aqueous solutions:

- Online release of a database of chemical and physical properties of non aqueous solvents.



https://www.cost-nectar.eu/pages/wg3_prop-solv.html

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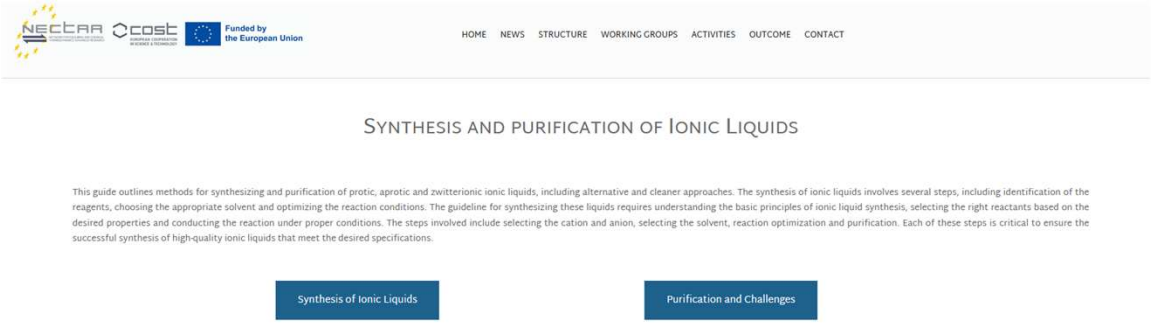
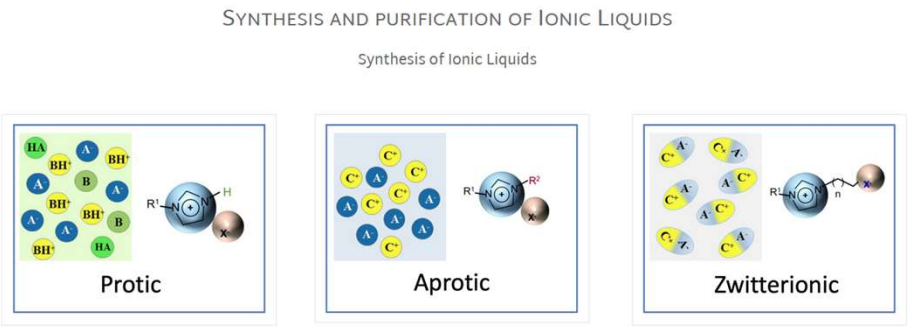
WG3

Main outcomes:

Development of methodologies for thermodynamic studies of non-aqueous solutions:

- Online release of guidelines on the synthesis of ionic liquids.





https://www.cost-nectar.eu/pages/wg3_ion_liq.html

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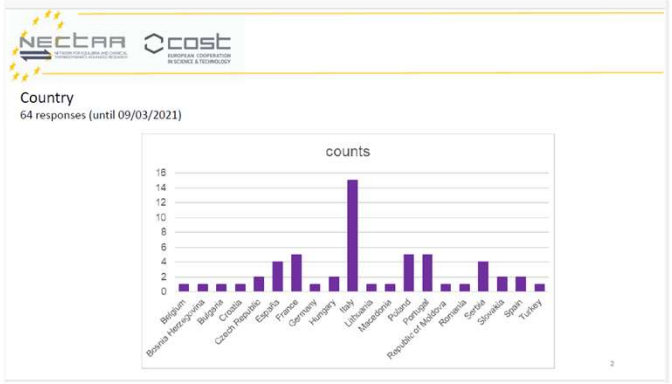
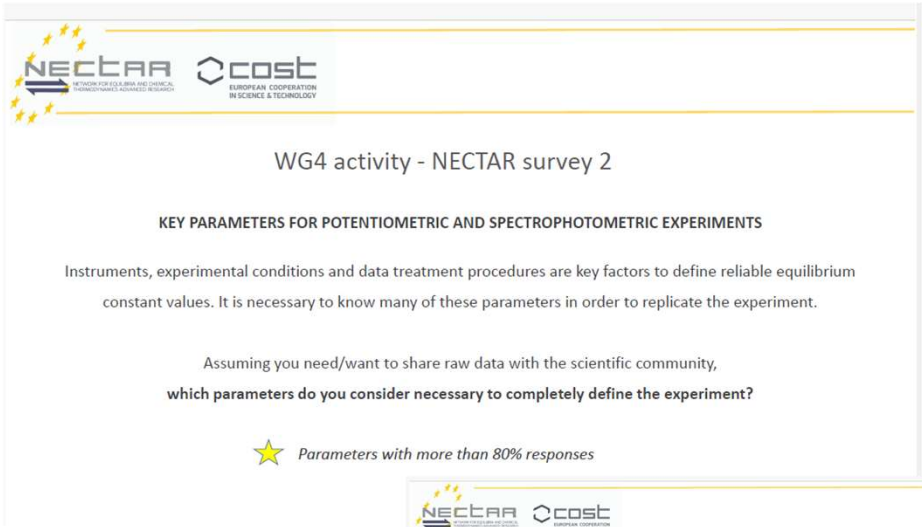
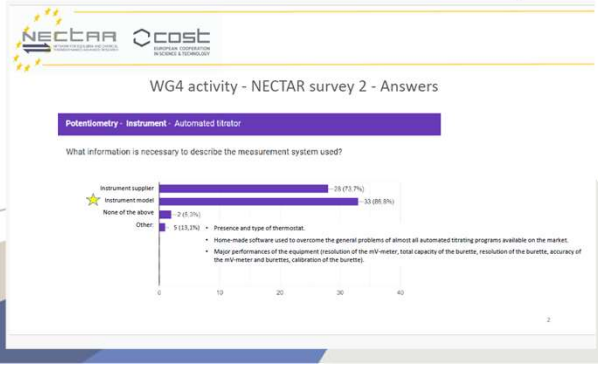
WG4

Main outcomes:

Dedicated surveys comparisons and release of new software:







https://www.cost-nectar.eu/pages/guides.html

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WG4

Main outcomes:

Release/publication of a critical comparison between available software for potentiometric data analysis.

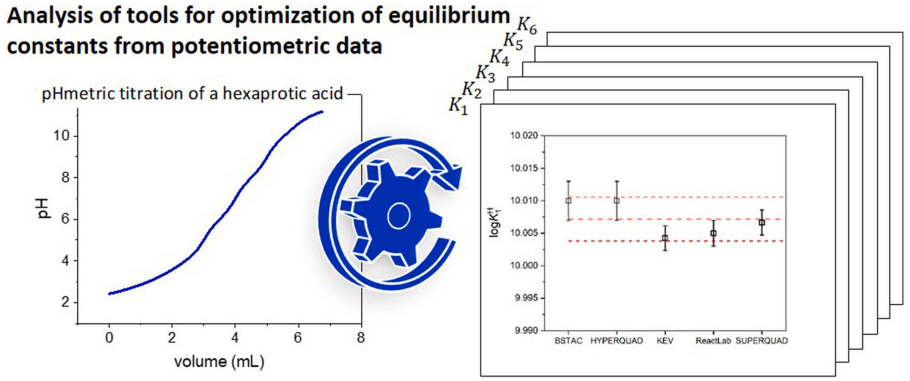
ELSEVIER

Analytica Chimica Acta
Volume 1303, 15 May 2024, 342476

A tutorial on potentiometric data processing. Analysis of software for optimization of protonation constants

Silvia Berto [a], Salvador Blasco [b], Lorenzo Castellino [a], Aleksandar Cvetkovski [c], Concetta De Stefano [d], Sofia Gama [e], Enrique García-España [b], Petr Hermann [f], Gabriele Lando [d], Matteo Marafante [a], Michel Meyer [g], Winfried Plass [h], Lauryn Quinodoz [g i], Demetrio Milea [d]

https://doi.org/10.1016/j.aca.2024.342476



https://doi.org/10.1016/j.aca.2024.342476

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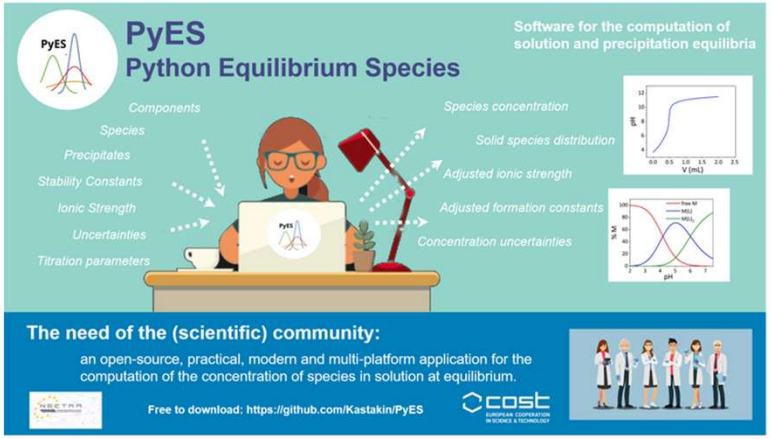
WG4

Main outcomes:

Dedicated surveys comparisons and release of new software:

PyES, an open-source software for the computation of in solution and precipitation equilibria



GEMS - The GEneral Microspeciation Solver
A program aimed at solving acid-base microspeciation equilibria from NMR and spectroscopic data.

SpectrApp, a one-stop solution for small to mid-sized soft modeling problems.
It provides tools for loading, cleaning and manipulating datasets coming from different sources

https://www.cost-nectar.eu/pages/software.html

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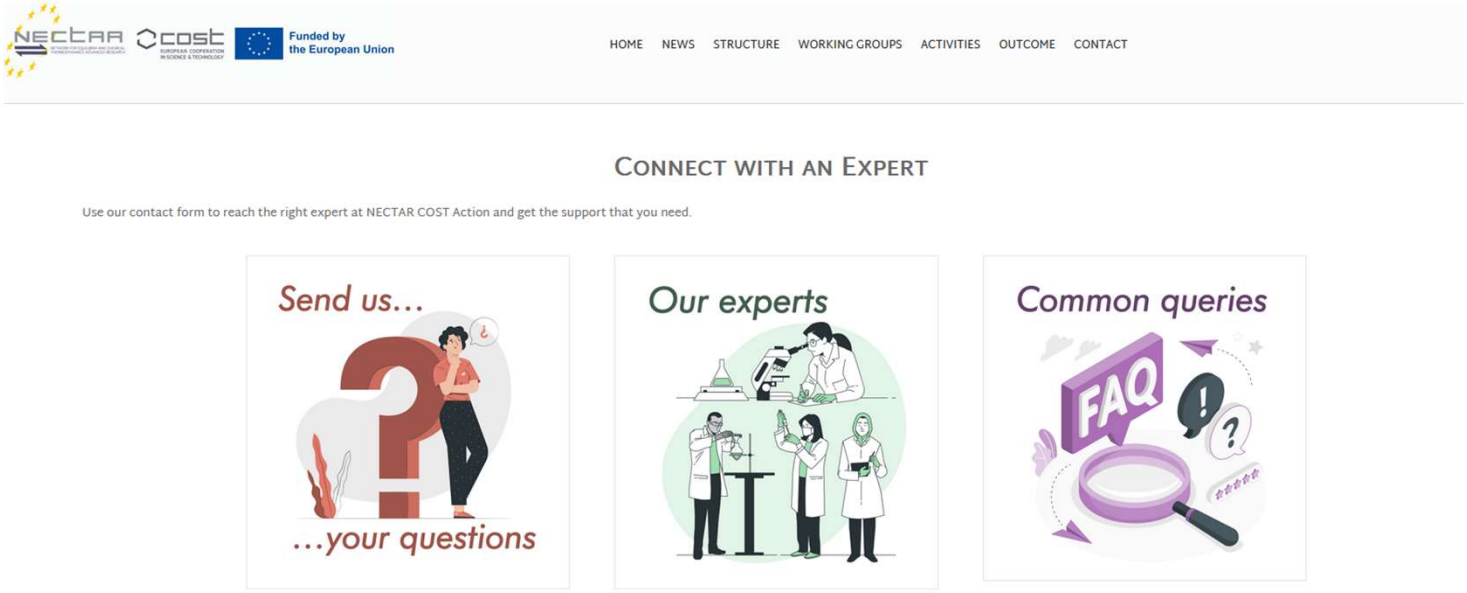
WG4

Main outcomes:

NECTAR Q/A solution environment for enterprises and other stakeholders: “Connect with an Expert”



https://www.cost-nectar.eu/pages/expert.html

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WG5

Communication and dissemination:

- www.cost-nectar.eu

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WG5

Communication and dissemination:

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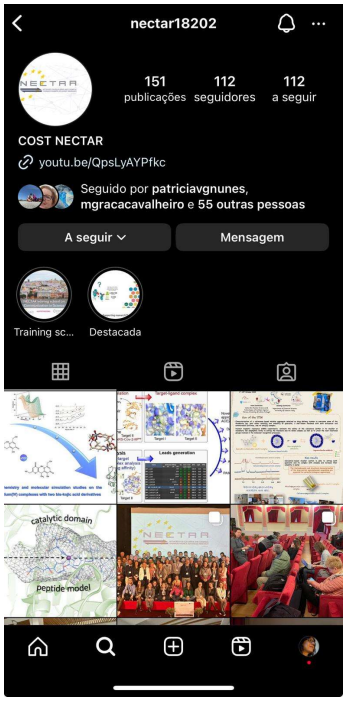

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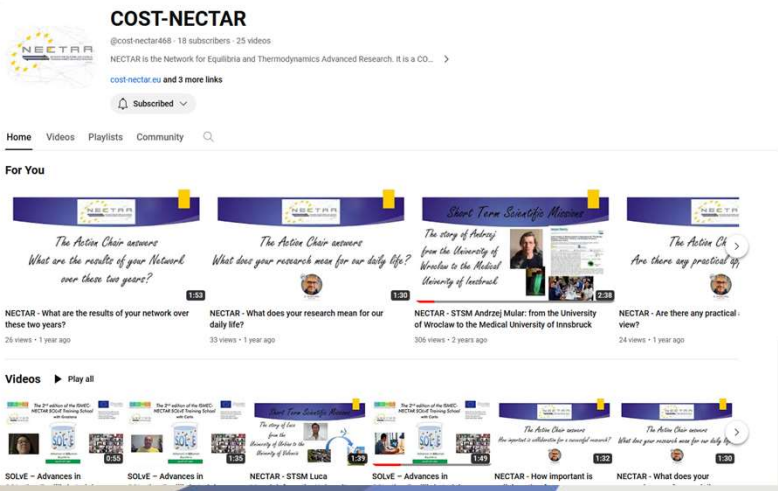

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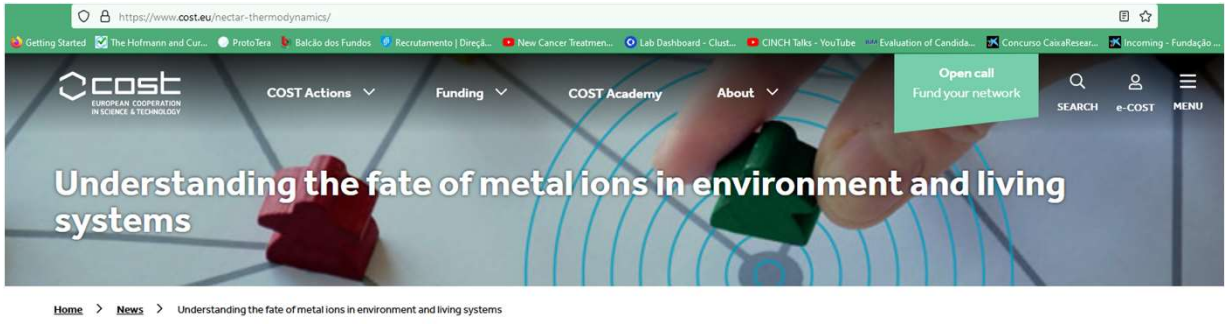
WG5

Communication and dissemination:

- www.cost-nectar.eu

- https://www.cost.eu/nectar-thermodynamics/



03/10/2022

NECTAR COST Action investigates potential solutions

The thermodynamic study of chemical equilibria embraces all areas of chemical sciences. Chemical compounds are present in different environments. The fundamental knowledge of the thermodynamics of chemical processes has a tremendous impact on many disciplines such as biology, medicine, environmental sciences, agriculture, and engineering.

Speciation modelling based on chemical equilibrium data allows us to identify these forms and is commonly used as a predictive tool for the behaviour of compounds in different environments. This improves commercial products' performance, discloses the mobility of pollutants and toxicants in the environment, optimises industrial processes, and explains the mode of action of biologically active substances. Furthermore, advanced thermodynamic studies yield deeper insights into the mechanisms of these interactions.

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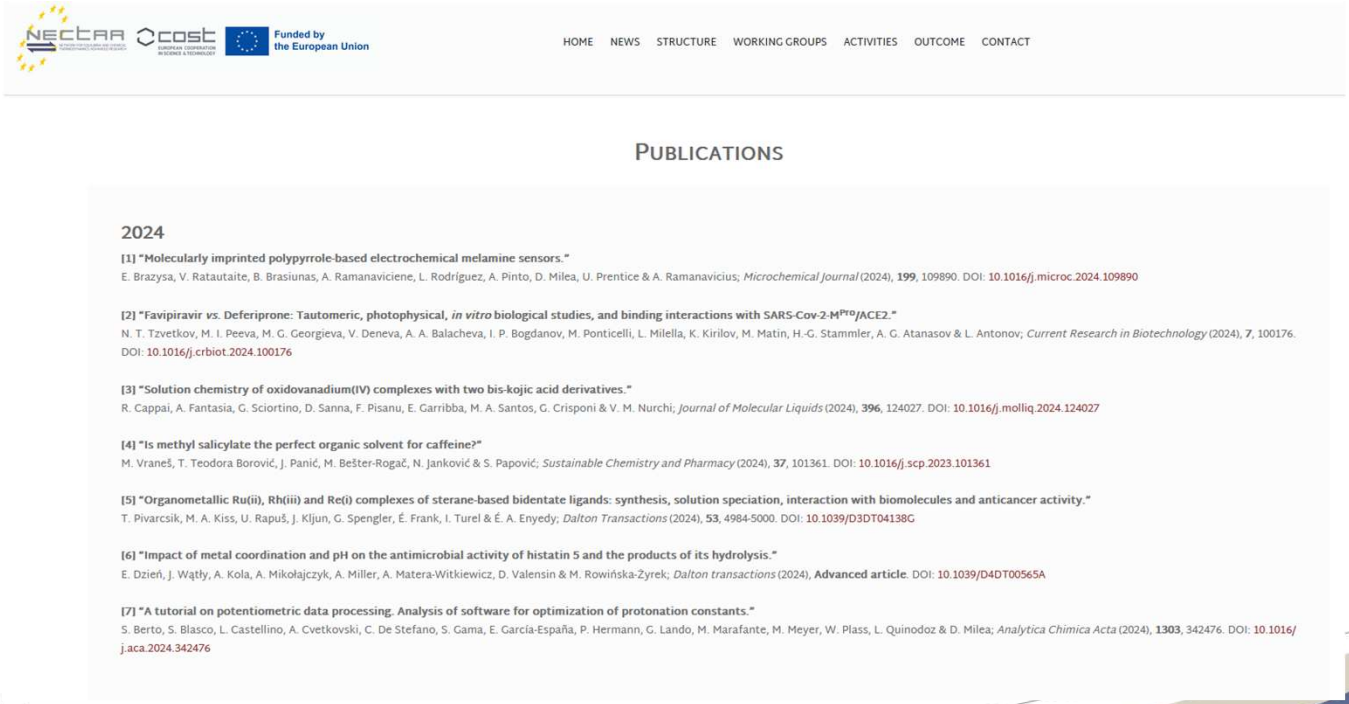
Communication and dissemination:

83 papers from collaborations among NECTAR members, some as OA.



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HOME NEWS STRUCTURE WORKING GROUPS ACTIVITIES OUTCOME CONTACT

PUBLICATIONS

2024

[1] "Molecularly imprinted polypyrrole-based electrochemical melamine sensors."
E. Brazysa, V. Ratautaite, B. Brasiunas, A. Ramanaviciene, L. Rodríguez, A. Pinto, D. Milea, U. Prentice & A. Ramanavicius; *Microchemical Journal* (2024), **199**, 109890. DOI: 10.1016/j.microc.2024.109890

[2] "Favipiravir *vs.* Deferiprone: Tautomeric, photophysical, *in vitro* biological studies, and binding interactions with SARS-Cov-2-M^{pro}/ACE2."
N. T. Tzvetkov, M. I. Peeva, M. G. Georgieva, V. Deneva, A. A. Balacheva, I. P. Bogdanov, M. Ponticelli, L. Milella, K. Kirilov, M. Matin, H.-G. Stammler, A. G. Atanasov & L. Antonov; *Current Research in Biotechnology* (2024), **7**, 100176. DOI: 10.1016/j.crbiot.2024.100176

[3] "Solution chemistry of oxidovanadium(IV) complexes with two bis-kojic acid derivatives."
R. Cappai, A. Fantasia, G. Sciortino, D. Sanna, F. Pisanu, E. Garribba, M. A. Santos, G. Crisponi & V. M. Nurchi; *Journal of Molecular Liquids* (2024), **396**, 124027. DOI: 10.1016/j.molliq.2024.124027

[4] "Is methyl salicylate the perfect organic solvent for caffeine?"
M. Vraneš, T. Teodora Borović, J. Panić, M. Bešter-Rogač, N. Janković & S. Papović; *Sustainable Chemistry and Pharmacy* (2024), **37**, 101361. DOI: 10.1016/j.scp.2023.101361

[5] "Organometallic Ru(ii), Rh(iii) and Re(i) complexes of sterane-based bidentate ligands: synthesis, solution speciation, interaction with biomolecules and anticancer activity."
T. Pivarcsik, M. A. Kiss, U. Rapuš, J. Kljun, G. Spengler, É. Frank, I. Turel & É. A. Enyedy; *Dalton Transactions* (2024), **53**, 4984-5000. DOI: 10.1039/D3DT04138G

[6] "Impact of metal coordination and pH on the antimicrobial activity of histatin 5 and the products of its hydrolysis."
E. Dzień, J. Wątły, A. Kola, A. Mikołajczyk, A. Miller, A. Matera-Witkiewicz, D. Valensin & M. Rowińska-Żyrek; *Dalton transactions* (2024), **Advanced article**. DOI: 10.1039/D4DT00565A

[7] "A tutorial on potentiometric data processing. Analysis of software for optimization of protonation constants."
S. Berto, S. Blasco, L. Castellino, A. Cvetkovski, C. De Stefano, S. Gama, E. García-España, P. Hermann, G. Lando, M. Marafante, M. Meyer, W. Plass, L. Quinodoz & D. Milea; *Analytica Chimica Acta* (2024), **1303**, 342476. DOI: 10.1016/j.aca.2024.342476

https://www.cost-nectar.eu/pages/publications.html

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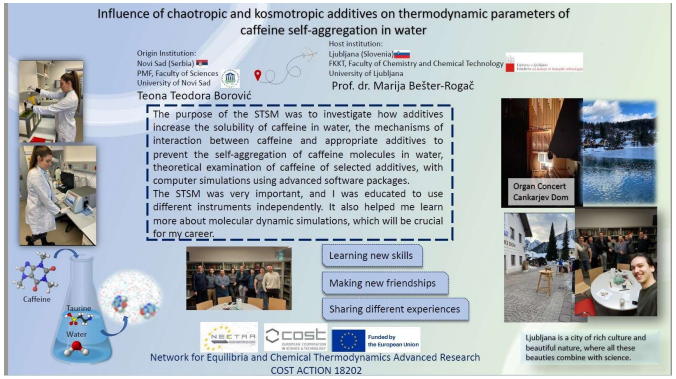
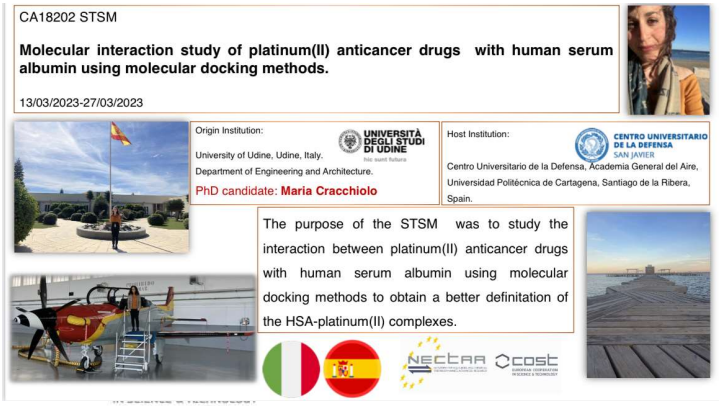
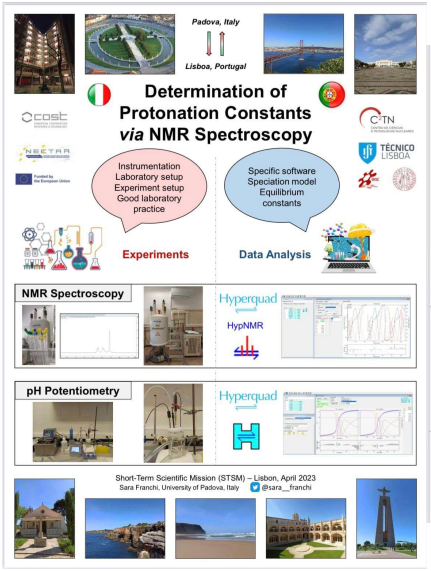
Grants:

- 66 STSMs and 2 ITCGs



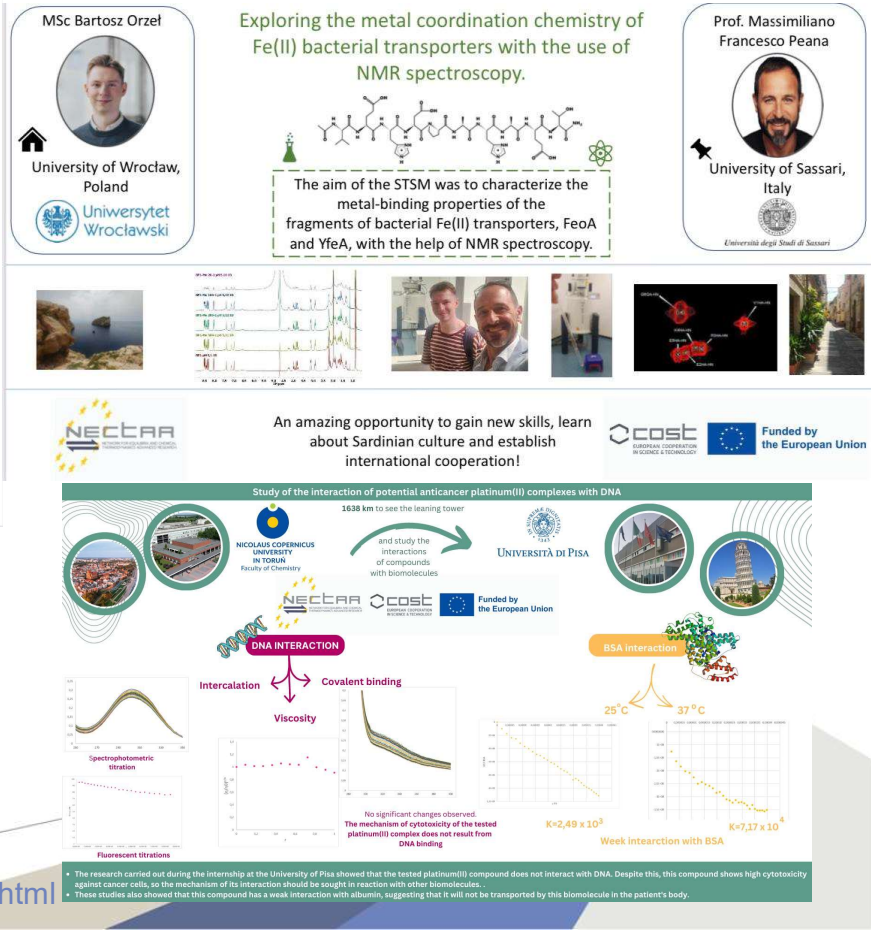


https://www.cost-nectar.eu/pages/stsm.html



https://www.cost-nectar.eu/pages/itc.html

"Thermodynamic Minds"



NECTAR CA18202

Network for Equilibria and Chemical Thermodynamics Advanced Research
COST ACTION 18202

Meetings:

https://www.cost-nectar.eu/pages/meetings.html

- 1st European NECTAR Conference, Belgrade, 5-6/Mar/2020
- NECTAR Spring Web-Meeting, 25-26/Mar/2021
- 2nd European NECTAR Conference, Lisbon, 25-27/Aug/2021
- WG1 NECTAR Workshop, Orsay, 31Mar-01Apr/2022
- WG2 and WG4 joint NECTAR Workshop, Valência, 9-10/Jun/2022
- 3rd European NECTAR Conference, Ljubljana, 24-26/Aug/2022
- WG5 NECTAR Workshop, Cagliari, 30/May/2023
- WG2 and WG4 joint NECTAR Workshop, Urbino, 14-15/Jun/2023
- NECTAR WG3 Workshop, Chișinău, 29-30/Aug/2023
- 4th European NECTAR Conference and Final Action Meeting, Milazzo, 26-27/Feb/2024
- Regular (monthly) virtual MC/CG/WG meetings

NECTAR CA18202

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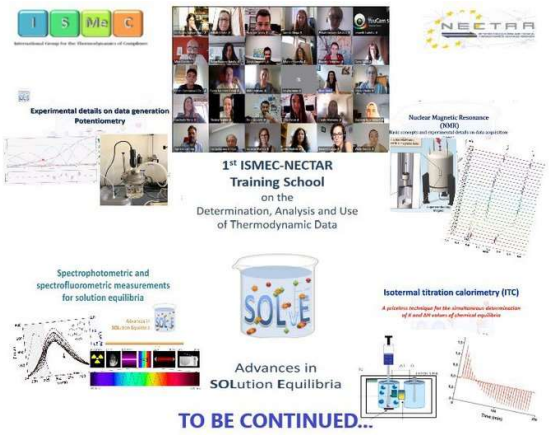
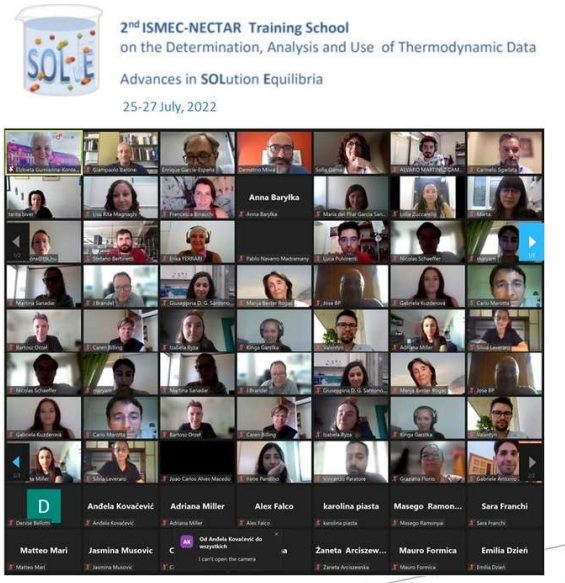
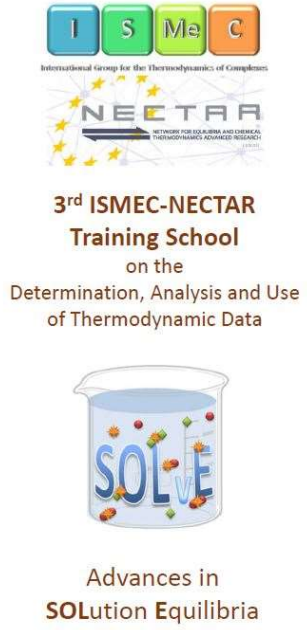
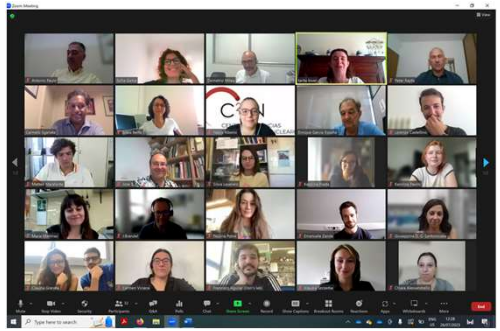
Training Schools: https://www.cost-nectar.eu/pages/1st_ts.html **"Thermodynamic Minds"**

- 3 SOLvE - ISMEC-NECTAR TS on the Determination, Analysis and Use of Thermodynamic Data (1st: 26–28/Jul/2021, 2nd: 25–27/Jul/2022, 3rd: 24-26/Jul/2023).









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"Thermodynamic Minds"

- 3 SOLvE - ISMEC-NECTAR TS on the Determination, Analysis and Use of Thermodynamic Data (1st: 26–28/Jul/2021, 2nd: 25–27/Jul/2022, 3rd: 24-26/Jul/2023).
- NECTAR TS on Calorimetry, Ljubljana, 27/Aug/2022.

- NECTAR TS on Communication in Science (NECTAR-SciComm), Cagliari, 29/May/2023.

- NECTAR Advanced school on aqua ions and hydrolysis-related equilibria, Zagreb, 29/Sep/2023.

Sustaining the network beyond the Action

There are many ongoing projects and collaborations ongoing.

A CIG (*SOFTSTAC – SOFTware for STAbility Constants determination*) has also been submitted.

The training of ECIs and the new "thermodynamic minds" will ensure a high standard for future research in the field of chemical thermodynamics.

Dissemination and communication activities are already promoting public awareness of the importance of this field in daily life, ensuring a high interest for NECTAR activities even beyond the Action end.