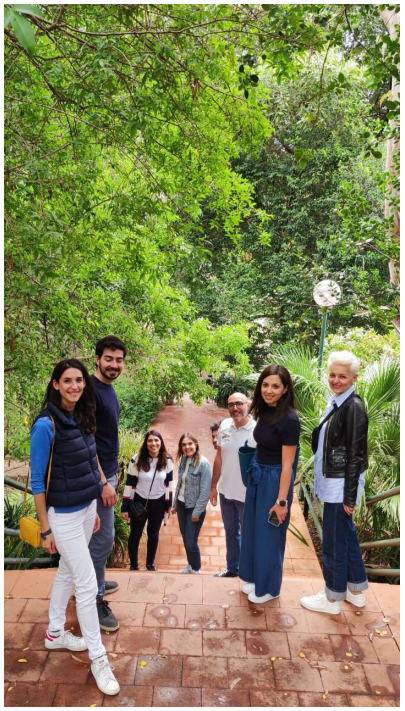
NECTAR
NETWORK FOR EQUILIBRIA AND CHEMICAL THERMODYNAMICS ADVANCED RESEARCH
CA18202

cost
EUROPEAN COOPERATION IN SCIENCE & TECHNOLOGY

Funded by the European Union

WG-5 SUMMARY

NECTAR for the future: new trends and exploitation of results



STVDIORVM VNIVERSITAS MESSANAE A.D.1548

4th European NECTAR Conference and Final Action Meeting

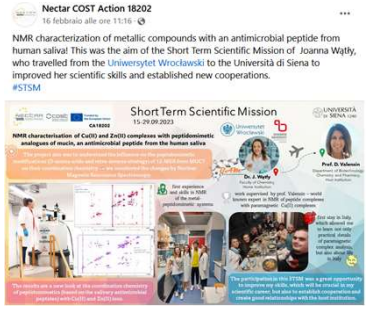
Milazzo, February 26th – 27th, 2024

THE AIM

- Transfer of the network's activities and results to NECTAR members and to society
- Promotion on social media
- Management of the website
- Communication between WGs and members

SOCIAL MEDIA PROMOTION

- Papers
- Short Term Scientific Missions
- Training schools
- Meetings



@CostNectar
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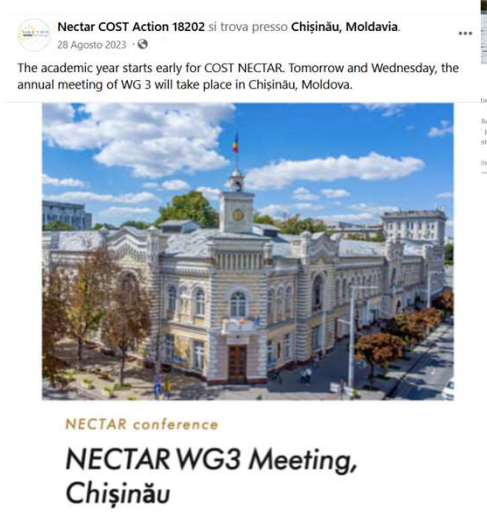
@nectar18202
COST-NECTAR
NECTAR COST Action

CONFERENCES, MEETINGS, SEMINARS…

- Communication by email
- Publication on website
- Promotion on social media



NECTAR Training School on Communication in Science (NECTAR-SciComm)

- **About:** Don't you want to get your colleagues and the public excited about science –about your science–; about COST NECTAR science? If your answer is yes, this training is for you!
- **Date:** May 29th, 2023.
- **Place:** Botanic garden of Cagliari, Cagliari, Italy.

1st NECTAR Training School
on
Communication in Science
(NECTAR-SciComm)

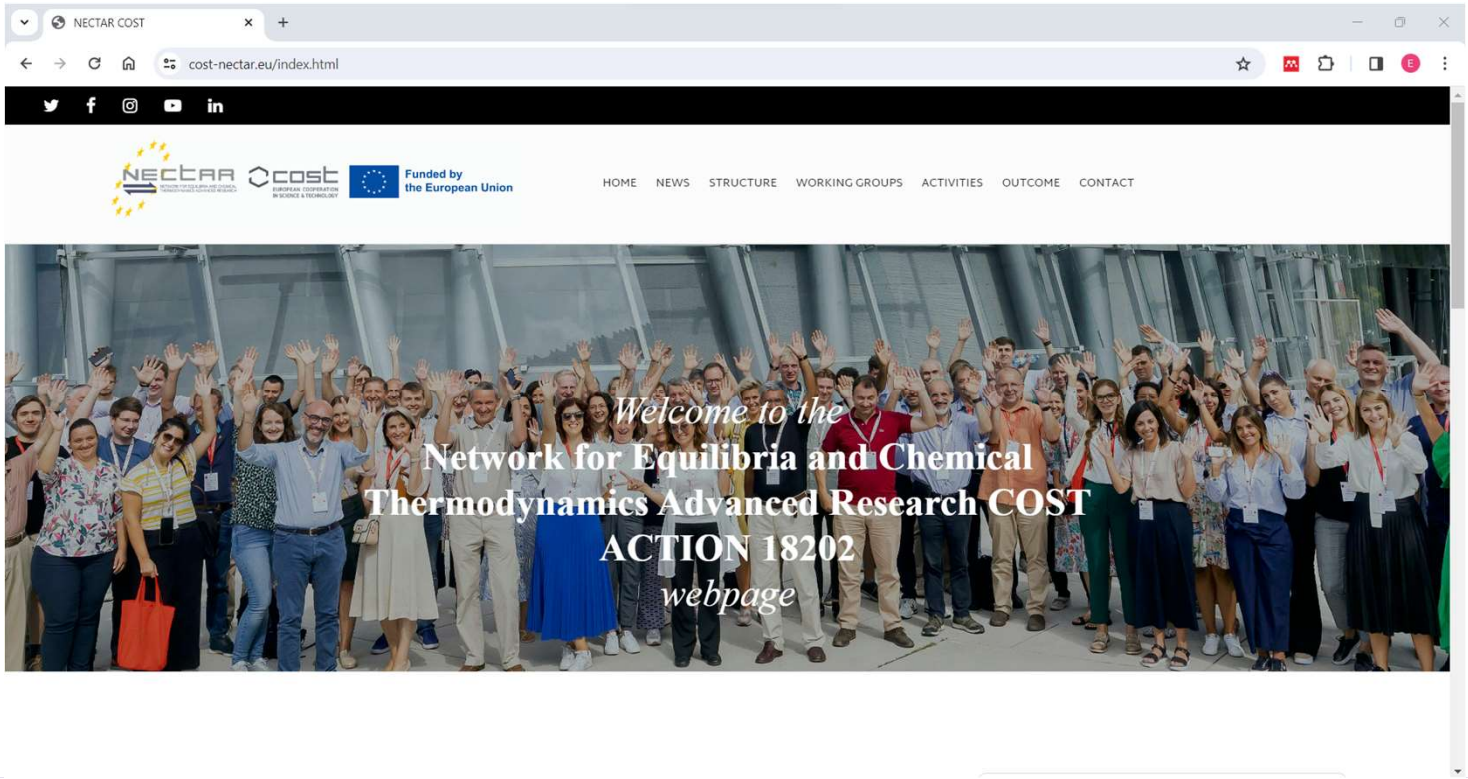
NECTAR-SciComm

Science communication – from the theory to the practice

5 invited speakers and 16 participants

- **Science Communication within and outside NECTAR** (**Elzbieta GUMIENNA-KONTECKA (SCM)** University of Wroclaw, Poland)
- **Introduction to Science Communication** (**Empar VENGUT CLIMENT** University of València, Spain)
- **From theory to practice: can an efficient communication contribute to the prevention, monitoring and management of invasive alien species?** (**Michela MARIGNANI** University of Cagliari, Italy)
- **Video editing tools accessible to everyone** (**Emanuele ZANDA** University Paris-Saclay, France)
- **Unravelling your jargon: How to better communicate science to the media.** (**Adriano CERQUEIRA** NOVA University of Lisbon, Portugal)

WEBSITE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Network for Equilibria and Chemical Thermodynamics Advanced Research COST ACTION 18202
webpage

NECTAR - News

cost-nectar.eu/pages/news.html

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HOME NEWS STRUCTURE WORKING GROUPS ACTIVITIES OUTCOME CONTACT

News

NECTAR conference

4th European NECTAR Conference and Final Action Meeting, Milazzo

The 4th European NECTAR Conference will take place in Milazzo on 26-27th February

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NECTAR STSMs

10th NECTAR CA18202 Call for Short Term Scientific Missions (STSM) Applications

The application period for the STSM is open until 5th Nov. Read here the details.

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NECTAR conference

NECTAR WG3 Meeting, Chişinău

The NECTAR WG3 meeting will take place in Chişinău, from August 29th to 30th 2023

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

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ACTION MEETINGS
STSM
TRAINING SCHOOL
ITC CONFERENCE GRANTS

UPCOMING MEETINGS

DOCUMENTATION OF OTHER MEETINGS

FIRST (KICK-OFF) MC MEETING

FIRST CG/WG AND SECOND MC MEETING

SECOND CG MEETING

THIRD (ONLINE) MC MEETING

SECOND WG MEETING

Here the important downloable documentation relative to the second WG meeting can be found. In particular, the Agenda, Minutes, Book of abstracts and Meeting programme.

THIRD WG MEETING

Here the important downloable documentation relative to the third WG meeting. In particular, the COST-NECTAR 2nd meeting circular, Program, Book of abstracts, Agenda and Minutes.

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

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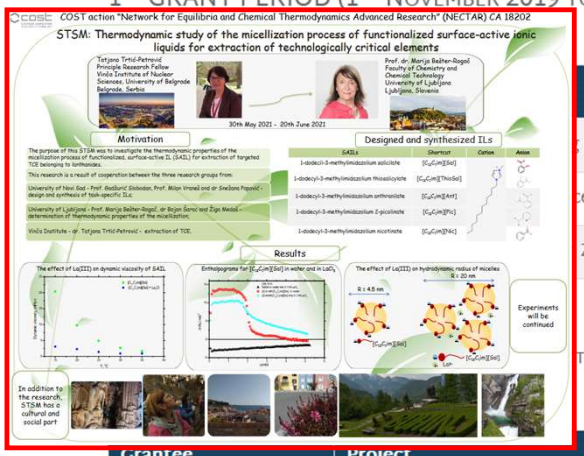
ACTIVITIES
- ACTION MEETINGS
- STSM
- TRAINING SCHOOL

GRANTEES OF THE CALLS

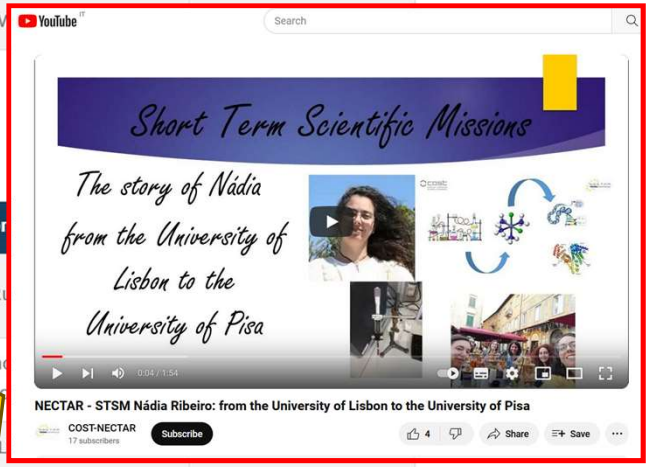
1ST GRANT PERIOD (1ST NOVEMBER 2019 TO 30TH APRIL 2020)



	Home institution	Host institution
peptides for oxidation catalysis in presence of Cu	U. Parma, IT	U. Aix-Marseille, FR
ces/carriers	U.A. Barcelona, ES	U. Udine, IT
Zr-89 radiometal: design, synthesis and thermodynamic properties	U. V	

T OCTOBER 2021)

Grantee	Project	Hor
Lucija Knežević	tudying Vanadium-organic ligand complexation toward better understanding of Vanadium biogeochemical behaviour	I. Ru
Tatjana Trtic-Petrovic	Thermodynamic study of the micellization process of functionalized surface-active ionic liquids for extraction of technologically critical elements	Vinc
Nádia Ribeiro	Evaluation of the DNA affinity of metal complexes derived from 8-hydroxyquinoline ligands	



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

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PUBLICATIONS

ACKNOWLEDGEMENT GUIDELINES

OTHER PAPERS OF PARTICIPANTS

Papers with NECTAR Aknowldgements

2024

[1] "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

(collaboration: University of Novi Sad and University of Kragujevac, Serbia + University of Ljubljana, Slovenia)

2023

[1] "Fe(II), Mn(II), and Zn(II) Binding to the C-Terminal Region of FeoB Protein: An Insight into the Coordination Chemistry and Specificity of the Escherichia coli Fe(II) Transporter."

B. Orzel, A. Pelucelli, M. Ostrowska, S. Potocki, H. Kozlowski, M. Peana & E. Gumienna-Kontecka; *Inorganic Chemistry* (2023), **62**, 18607–18624. DOI: 10.1021/acs.inorgchem.3c02910

(collaboration: University of Wrocław and University of Opole, Poland + University of Sassari, Italy)

2022

[1] "Noncovalent Assembly and Catalytic Activity of Hybrid Materials Based on Pd Complexes Adsorbed on Multiwalled Carbon Nanotubes, Graphene, and Graphene Nanoplatelets."

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

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HOME NEWS STRUCTURE WORKING GROUPS ACTIVITIES OUTCOME CONTACT

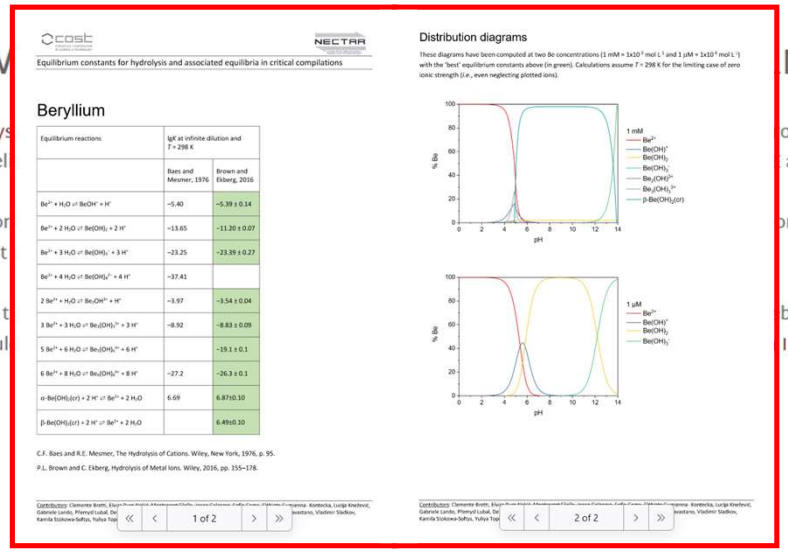
- PUBLICATIONS
- ACKNOWLEDGEMENT GUIDES
- WG1 PERIODIC TABLE
- WG3 PROPERTIES OF SOLVENTS
- WG3 SYNTHESIS AND PURIFICATION OF IONIC LIQUIDS
- WG4 TOOLS
- WG5 COMMUN. GUIDE

W …IBRIA) C…

WG1 - NECTAR for highly hydrolys… …olysis constants o… …periodic table. This work is related to its task of providing rel… …and LVC.

You can find the result of the wor… …ontaining its hydrc… …lues) at infinite dilution and T = 298 K gathered from the most…

Various approaches can be used t… …bye-Hückel, Speci… …ory (SIT) and Pitzer models). The final selection criterion shoul… …l. (eds.), Modelling… OECD: Paris, 1997.



1																	2
H																	He
3	4											5	6	7	8	9	10
Li	Be											B	C	N	O	F	Ne
11	12											13	14	15	16	17	18
Na	Mg											Al	Si	P	S	Cl	Ar
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe

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

Definition of Donor Number (DN):

A donor number (DN) is a quantitative measure of Lewis basicity. Victor Gutmann [V. Gutmann, Electrochim. Acta, 1976, 21, 661–670, 21] defined DN (also referred to as "donicity"), as a quantitative measure for the tendency to donate electron pairs to acceptors. The DN-scale is determined by the value of the reaction enthalpy between the Lewis acid $SbCl_5$ and chemical compound dissolved in 1,2-dichloroethane.

List of Solvents

Find the solvent...

- Acetone
- Acetonitrile
- Benzene
- 1-Butanol
- γ-Butyrolactone
- Carbon tetrachloride
- Chloroform
- Cyclohexane
- Diethylene glycol
- Diethyl carbonate
- Dimethyl sulfoxide
- 1,4-Dioxane
- Ethanol
- Ethyl acetate
- Formamide
- Glycerol
- Methanol
- N-methyl formamide
- 1-Propanol
- Propylene carbonate
- Pyridine
- Tetrahydrofuran
- Toluene
- Water

Ethan

Melting po 1 atm) = **-114.15 °C**

Boiling poin atm) = **78.293 °C**

Dielectric co nt (25 °C) = **24.35**

Dynamic visc y (25 °C) = **1.087 mPa·s**

Density (25 °C **.7850 kg·dm^{-3}**

Dipole momen the gas phase) = **1.66 D**

Donor number (+info)= **(32) kcal·mol^{-1}**

Acceptor number (+info)= **37.9**

$E_T(30)$ (+info)= **51.9 kcal·mol^{-1}**

E_T^N (+info)= **0.65**

(Click to clear)

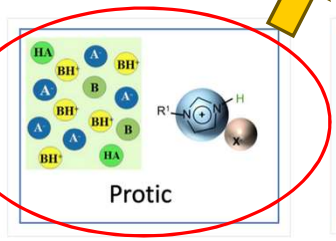
Protic Ionic Liquids (PILs)

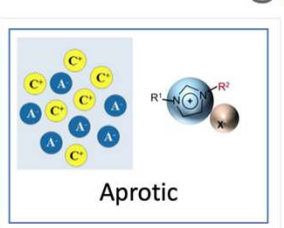
Protic ionic liquid (PIL) is a subclass of ionic liquid that has a protonated cation and can be synthesized through a neutralization reaction which involves transferring proton from a Brønsted acid to a Brønsted base.

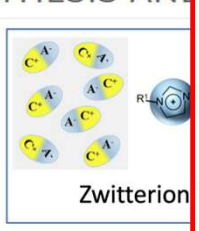
$$B + A \rightarrow HB^+ + A^-$$

- PILs are a good conductor of protons and ions.
  - Water may be used as a solvents or titration can be performed without any solvent. Example
- Complete proton transfer between the acid and base must occur for optimal production.
- The cation on which the proton resides determines the proton activity of the IL.
  - To achieve this, there must be **a high pKa difference** between the acid and bas
- In aqueous solutions, **a difference greater than 10** is sufficient for more than **99% proton transfer**.
- Various factors, such as the physical and chemical properties of the base and acid determine the extent of proton transfer and ionicity of the IL.
- A highly recommended procedure is to determine an acid-base titration curve for the two components dissolved in water.
- The equivalence point and pH at the end point confirm the purity of the IL after synthesis and any subsequent handling procedures.
- Diluting an IL sample in water to the standard concentration confirms the previously determined equivalence point pH.

SYNTHESIS AND



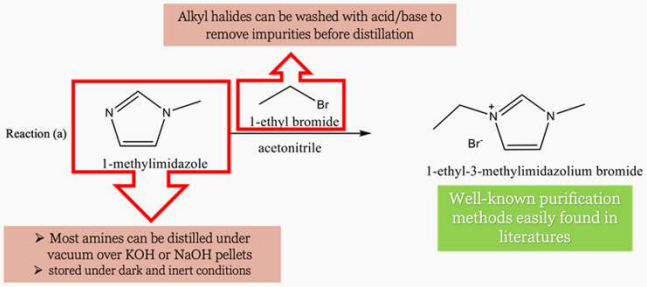




Synthesis of Ionic Liquids

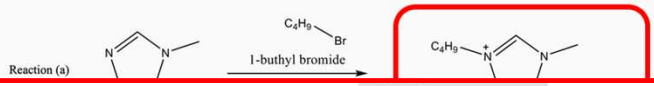
Purification

Starting compounds should be purified to prevent the formation of byproducts during the metathesis reaction.



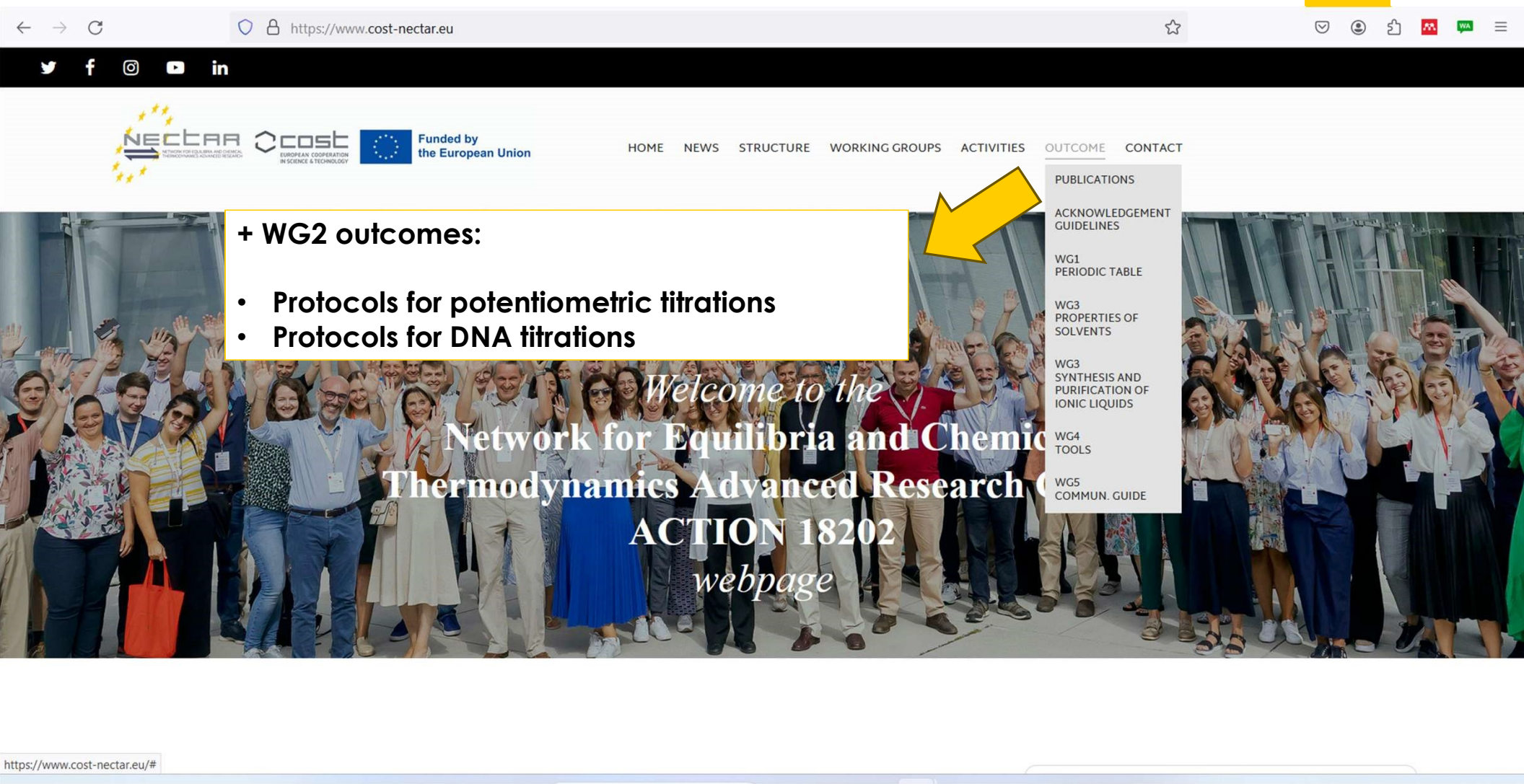
It is recommended to carry out the quaternization step right after purifying the starting compounds, as prolonged exposure to light or moisture can generate new impurities. Alternatively, starting compounds like amines can be stored under dark and inert conditions until needed.

Dry solvents and inert conditions must also be used during the generation of the quaternized salt. Precautions may vary depending on the alkyl halide used. For example, the synthesis of $[C_2mim]I$ requires the reaction to be carried out in the dark to avoid photo-oxidation of the iodide, compared to [C2mim]Br synthesis. In general, it is recommended to purify the quaternized salt before using it in the metathesis reaction.



WG5
COMMUN. GUI

Purification and Challenges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WG5 COMMUN. GUIDE
+ WG2 outcomes:
• Protocols for potentiometric titrations
• Protocols for DNA titrations
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webpage
https://www.cost-nectar.eu/#

https://www.cost-nectar.eu/pages/wg4_tools.html

GEMS - The GEneral Microspeciation Solver

A program aimed at solving acid-base microspeciation equilibria from NMR and spectroscopic data. It is maintained by Dr. Salvador Blasco (University of Valencia, Spain).
The source code and executables can be downloaded free of charge: Click here to go to the download page
Publication: Click here to go to the article

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. It is available both as a web application, hosted on a UniTO server accessible free of charge, and as an installable application that can be run locally on the user's machine.
It was developed by Dr. Eugenio Alladio and Dr. Lorenzo Castellino (University of Turin, Italy).
Click here to launch the spectra application

OTHER USEFUL TOOLS FOR THE NECTAR COMMUNITY

Stability Constant Explorer, a search program for NIST SRD 46 "Critically Selected Stability Constants of Metal Complexes" database for Microsoft Windows 7 or later (64 bit)
Click here to go to the Stability Constant Explorer page

Author: Naoyuki Hatada, Ph.D. Department of Materials Science and Engineering, Kyoto University.
The accompanying database file (NIST_SRD_46_ported.db) is based on the following dataset which is distributed at the NIST website: Donald R. Burgess (2004), NIST SRD 46. Critically Selected Stability Constants of Metal Complexes: Version 8.0 for Windows, National Institute of Standards and Technology

How may I correctly prepare a titration to improve my skills on absorbance/fluorescence titrations?

Where can I find reliable stability constants?

The stability constants can be found in the scientific literature or in databases. The databases can be compiled with or without a critical evaluation of the stability constants collected values. Below you can find some links to databases:

- IUPAC Chemical Data Series
- NEA - Electronic database of the TDB Project
- NIST Critically Selected Stability Constants of Metal Complexes
- Stability Constant Explorer - Database of Stability Constants of Metal Complexes
- JESS Thermodynamic database of chemical reactions

Before using a stability constant to draw a species distribution diagram, it is essential to verify the chemical equilibrium to which it refers and ensure that it is compatible with the equilibrium formulation used by the software employed to calculate the concentration of the species.

How can I draw a species distribution diagram for a water solution?

Why should a PhD student participate to the NECTAR COST ACTION?

Why use a multi-technique approach to the speciation study of metal-ligand system in solution?

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