Minutes of the Management Committee Meeting of the COST Action

CA18202 - Network for Equilibria and Chemical Thermodynamics Advanced Research

COST Action CA18202: "Network for Equilibria and Chemical Thermodynamics Advanced Research"
Management Committee Meeting
27/02/2024 at 16:00:00 (CET)
Face to Face
Teatro Trifiletti, Via Cumbo Borgia, 98057 Milazzo (ME, Italy)
Zoom Platform
https://videoconf-colibri.zoom.us/j/95549949594?pwd=dGk0UFI0NWhnVHVRVVVURVU0ZEJjUT09

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ACTION Status at date:

- Action parties: 31 COST countries
- CSO approval: 04/06/2019
- Start date: 02/10/2019

i. Agenda and Materials

The MC meeting agenda is in Annex 1. The MC meeting was organised to take some necessary decisions and indications following previous MC meeting.

ii. Participants and Hosting Team

Meeting was hosted in Milazzo (IT). Participants are listed in attendance list (attached online by GHM who was present at meeting).

iii. Pre-requisites for the Decision Making

During the meeting, the participants acknowledged and agreed to comply with the Rules of Procedure for the MC from Annex I COST Action Management, Monitoring and Final Assessment (COST 134/14: https://www.cost.eu/uploads/2019/11/COST-134-14-REV-4-Action-management-monit-and-final-assess.pdf)

Before any decision was taken, the Action Chair (AC) verified that the minimum of 2/3 (21) of the parties present; the necessary quorum to approve decisions was achieved (21 members present and/or connected online through ZOOM platform) allowing the MC meeting to officially take place in accordance with Article 9 of the Rules of Procedure for the MC (see https://www.cost.eu/uploads/2019/11/COST-134-14-REV-4-Action-management-monit-and-final-assess.pdf).

1) Welcome to participants, verification of the quorum and adoption of agenda

MC meeting started on time. The AC (Demetrio Milea) welcomed the participants, including those who connected online at link sent via email to MC parties not physically present in Milazzo.

According to Pre-requisites of point iii., 31 Member Countries are parties of the Action. Quorum is represented by 21 Members

Member		Member		Member	
Albania (AL)	A	France (FR)	P	North Macedonia (MK)	P
Austria (AT)	A	Germany (DE)	P	Poland (PL)	P
Belgium (BE)	A	Greece (EL)	P	Portugal (PT)	P
Bosnia and Herzegovina (BA)	P	Hungary (HU)	P	Romania (RO)	A
Bulgaria (BG)	P	Iceland (IS)	A	Serbia (RS)	P
Croatia (HR)	P	Ireland (IE)	P	Slovakia (SK)	P
Czech Republic (CZ)	P	Italy (IT)	P	Slovenia (SI)	P
Denmark (DK)	A	Lithuania (LT)	A	Spain (ES)	P
Estonia (EE)	A	Malta (MT)	A	Switzerland (CH)	P
Finland (FI)	P	Moldova (MD)	A	Turkey (TR)	P
				United Kingdom (UK)	P

P = Present; A = Absent

Members present were: 21

Members absent were: 10

AC announced that quorum was reached to have a regular meeting, and for approving decisions. As such, AC declared that MC Meeting could officially take place and that all votes and decisions taken will be approved instantly.

AC acknowledged all MC Member Representatives who were present, either physically or online, for their great efforts in support of the Action and for their sense of responsibility.

Concerning absent members, AC informed that he received explanations from some members, who could not attend either for serious institutional and/or personal issues, while some other members were not able to connect to the platform to attend online.

Nevertheless, AC could not avoid to mention the absence and/or lack of interest of some Member Representatives, which causes systematic difficulties in Action Management, in relation to delays in approving decisions that cannot be done instantly, but need time because of the e-vote required timing.

AC reads the Agenda (Annex 1), previously sent by email to all MC Members.

AC launched the vote for the Adoption of Agenda.

Agenda was unanimously adopted.

2) Information to the MC

a. Recap of the minutes of the last meeting, e-votes and matters arising since the last meeting

Last MC meeting was held online on 25/09/2023 minutes are shown and submitted for approval.

Minutes were unanimously approved.

AC recalled that an Explicit MC vote was launched about the approval of a COST Innovators Grant (CIG) application – IG18202 on 26/01/2024 (SOFTSTAC - SOFTware for STAbility Constants determination), submitted by NECTAR. Results: Approved: 28 Abstension: 3

Any matter was bringed to discussing by any of the participants.

b. Core Croup: report from the Core Group, including delegated decisions

CG meeting was held immediately before MC meeting. Main topics were related to the management and results of the Action, especially in relation to deliverables from various WGs for current and entire Action, networking activities. WGs and Managers reports are reported as Annexes 2-10.

c. Action Membership: New Specific Organisations and COST Members represented in the MC

At present time, no requests for new MC memberships were received.

d. Action Participation: WG membership and applications, New MC members/Observers and provisional substitution.

AC reminded MC about new WG membership and application procedures since last meeting, reporting that, actually, NECTAR consists of 294 registered participants.

AC informed MC that, due to their impossibility to attend MC meeting, the following members were provisionally substituted, just for the present meeting:

1) Dijana Jelic, Bosnia and Herzegovina, substituted by Mersiha Suljkanovic
2) Matteo Tegoni, ITALY, substituted by Carmelo Sgarlata

e. Budget status: summary from the Grant Holder.

GH informed MC that almost all budget allocated for GP5 will be spent for planned activities.

GH informed that some unspent money from some Networking Activities could be spent for "last minute" STSMs. AC asks mandate to MC to take decision on budget changes to allow those STSMs.

AC launched the vote for this mandate.

Proposal was unanimously approved by MC.

f. Update from the COST Association.

NO COST representatives were present at meeting.

However, AC informed MC that annotated rules were changed again, especially in relation to reimbursements.

3) Follow up and discussion on the

a. Action management: structure, leadership positions and other supporting roles. Mandates to the Core Group (if applicable)

AC informed participants that all leadership positions are now reported on COST official CA18202 webpage (https://www.cost.eu/actions/CA18202/) as well as in NECTAR official webpage (https://cost-nectar.eu/).

Considering the end of the Action, no further changes are necessary.

b. Implementation of the COST Excellence and Inclusiveness Policy

COST Excellence and Inclusiveness Policy is very well implemented by NECTAR CA18202 Action.

c. Grant Awarding by the Action

AC informed MC that Grant Awarding process is going on in a very positive and fruitful way. For the present GP5, 10 STSMs have been completed/assigned.

d. Progress of each working group

WG leaders/co-leaders of each of the 5 Action's WGs informed MC about their activities for GP3. Particular attention was given to the progress of deliverables expected for the end of GP5 for each WGs, as well as the end of the Action. All planned deliverables will be provided within the end of Action. MC gave mandate to AC to collect from WG leaders/coleaders the expected deliverables and WGs planned activities, and to report them. WG leaders/co-leaders agreed to provide those data in written form ASAP, and not after the end of Action, in order to allow AC to prepare all required documents and final report in due time.

e. Science Communication Plan

AC invited SCM and WG5 leader to refer about the Science Communication Plan and Dissemination activities. Scientific results obtained within the Action have been published in peer reviewed and high

impact journals, both regular and open access, properly acknowledging COST Association and NECTAR CA18202. An updated list is reported in Action webpage (www.cost-nectar.eu). Overall, Science Communication Plan, as well as Dissemination Activities, are well implemented and no particular changes were suggested. SCM and WG5 leader just underlined again the importance of collaborations and "publications" within Action's aims and between at least three Action's members (i.e. 3 Countries), with the aim of strenghtening the network, as well as the importance of Dissemination Activities.

f. Progress on MoU Objectives, WG tasks, deliverables, and Goals for the current GP

AC remembered MC what are MoU general objectives, as well as the GP5 goals and deliverables. On the basis of reports provided by WG leaders and Coordinators/Managers about the status of the Action, the progress of the Action in terms of fulfillment of on MoU Objectives, WG tasks, deliverables, and Goals for the current GP can be considered as highly satisfactory. A final report will be due till the 1st of May.

4) Planning

a. Revision of Work and Budget Plan of the current GP

AC informed MC that, for current GP, almost all planned activities have been completed, and the allocated budget almost entirely spent according to WBP for GP5.

b. Draft plans for the following GP and Action extension

Being the end of the Action, no plans were setup. As action extension, NECTAR recently submitted a COST Innovators Grant (CIG) application – IG18202 on 26/01/2024 (SOFTSTAC - SOFTware for STAbility Constants determination).

c. Upcoming activities

All Action activities will be finalised within the end of the Action.

5) Monitoring and Reporting to the COST Association

The Final Action Report will be prepared by the end of April.

6) AOB

No other point was found to be relevant to be further discussed.

7) Summary of MC decisions

From the 31 COST Member Countries of the Action, 21 (twenty one) were present and represented by their corresponding MC members. MC meeting was valid to make proposals and take and approve decisions, summarized as follows:

- **Decision 1:** Agenda of the meeting was adopted.
- **Decision 2:** The minutes of MC meeting 25/09/2023 were approved.
- **Decision 3:** AC received mandate for last-minute budget changes.

8) Closing

In conlusion, AC thanked all people present for their active participation to the meeting and to the Action, acknowledging the excellent work done by everybody during the years.

Meeting was officially closed.

List of Annexes

- Annex 1 – Agenda
- Annex 2-10 – WGs and Managers Final reports.

Minutes prepared by:

- *Action Chair*
- *Action Vice-Chair*

ANNEX 1

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3. Follow up and discussion on the
   a) Action management: structure, leadership positions and other supporting roles. Mandates to the Core Group (if applicable)
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ANNEX 2 – 10

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

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, Universitý of Strasbourg, **France**, 2022.

NECTAR COST Action 18202
WG1

STSMs

Bartosz Orzeł (Biological Inorganic Chemistry Group, University of Wroclaw, **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 Dzyhovskyi, (Biological Inorganic Chemistry Group, University of Wroclaw, **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: MatteoTegoni, 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, Grabriele 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

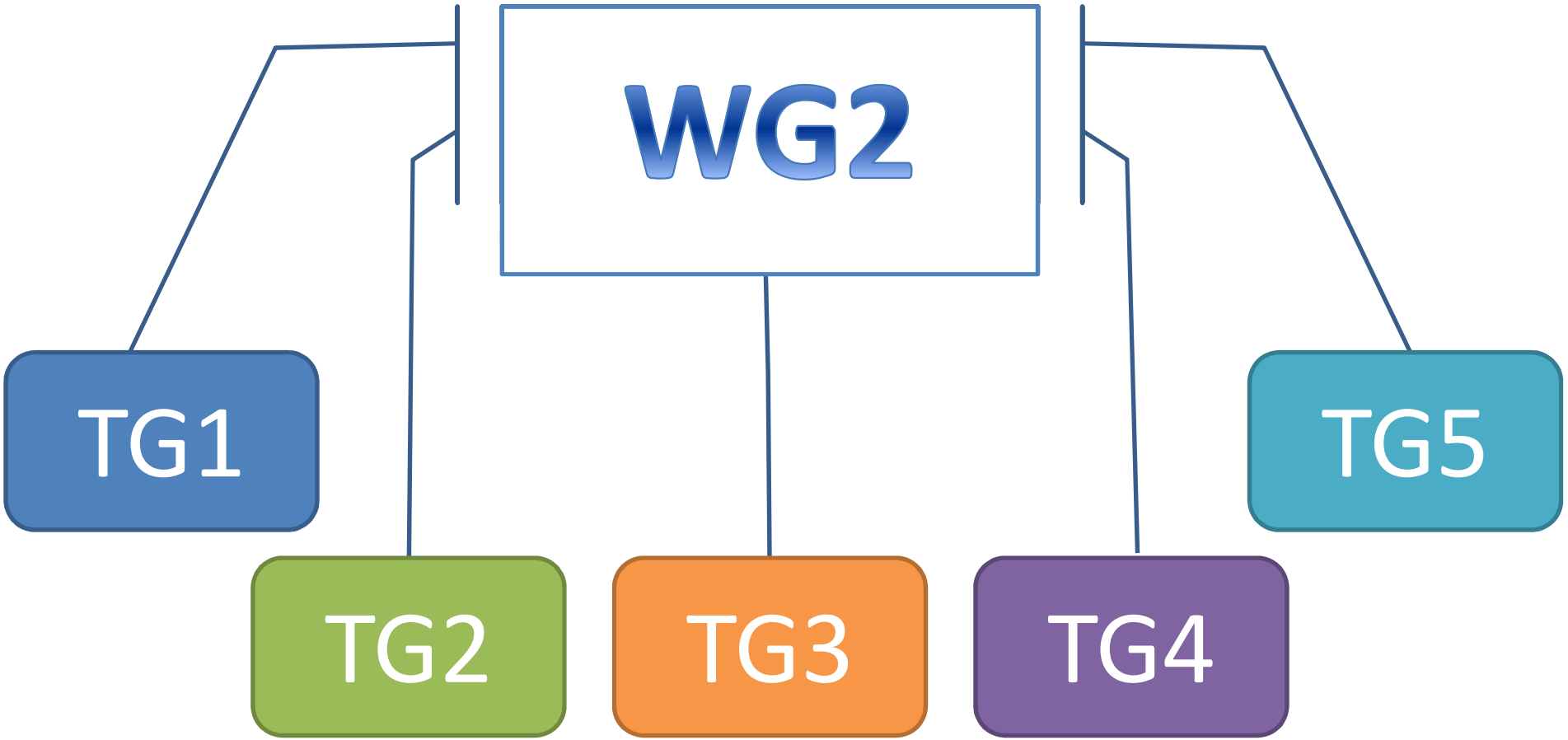
- "New insights on U(IV) hydrolysis studies"
  In charge: Vladimir

- "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

WG2

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


WG2
TG1
TG2
TG3
TG4
TG5

TG1

Task Group 1

Complexes of polydentate ligands

Working Group 2

TASK GROUP 1

Complexes of polydentate ligands

How to deal with complexones and macrocycles ?

Potentiometric „good laboratory practice“ for titrations of polydentate ligand systems

What was taken into account

1. Materials and stock solutions:

- strong acid & base stock solutions
- ligand & metal ion purity and stock solutions
- choice of background electrolyte

2. Electrode system calibration:

- pH range of calibration titration and calibration parameters
- data at high & low pH

3. Titrations:

- detailed experimental set-up (suitable pH ranges / concentrations, M:L ratios)
- calibration-titration relations

4. Data treatment:

- data precision & titration reproducibility, a number of titration & data points
- programs for data treatment & statistical parameters
- choice of chemical model

Test systems: EDTA and EDTA-Zn^{2+}

- EDTA chosen as suitable ligand – easily available, no problems with reaction kinetics, suitable necessary titration pH range, easy to deal with …

- Chemical model with H^+/Zn^{2+} is reasonably educative => several protonations in acid solution, protonated complexes & hydroxido species

- Conditions tested: pH ranges 1.5-11.8 & 1.8-12, EDTA concentrations 0.001-0.005 M, hydroxide concentrations, 0.1 & 0.2 M, ionic strength 0.1 & 0.2 M

- Conditions chosen: pH range at least 1.7 to at least 11.5, *c*(EDTA) 0.002 & 0.003 M, *I* = 0.1 M KCl, *c*(KOH) 0.1–0.2 M, Zn:L ratio 0.95–0.98:1, *t* = 25 °C

- Other recommended conditions: in –log[H^+], four-parameter electrode calibration, calibration followed by titration, at least 3+3 titration for each EDTA concentration, 50–60 points per titration

Data obtained & evaluation

- Four labs participated – Debrecen Messina, Prague, Turin.

- Different programs used for data treatment : BSTAC, OPIUM, PSEQUAD

- Global fitting done by each group, detailed statistical analysis of all data done by Matteo Marafante (Torino).

- Reasonable agreement between data obtained by the groups.

- Results in agreement with published data & procedure can be recommended as "good laboratory practice".

- **However…** The most acidic EDTA protonation constant ($\log K_5$ ~1.2) should be determined – thus, titration should start from acidic solutions (pH 1.5–1.7). Otherwise, $\log K_4$ value is not fully correct.

- **However…** The highest attention should be paid to a correct calibration of electrode systems, four-parameter calibration is highly recommended.

Final values

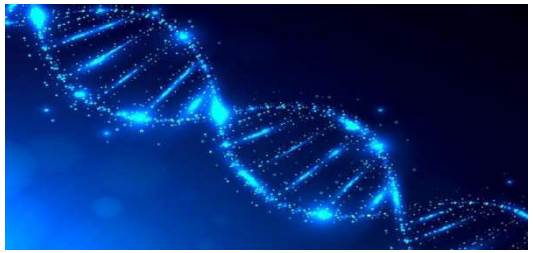
From detailed statistical analysis of all data done by Matteo Marafante (Torino).

Constant	Values Interval (this work)	Average (this work)	Confidence Interval (C.I.)	NIST database	IUPAC database
$\log K_1$	10.15–10.18	10.17	± 0.08	10.19	10.12
$\log K_2$	6.12–6.23	6.17	± 0.07	6.13	6.13
$\log K_3$	2.66–2.87	2.75	± 0.14	2.69	2.77
$\log K_4$	2.02–2.25	2.11	± 0.17	2.0	2.01
$\log K_5$	(0.9–1.34)	1.15	± 0.57	1.5	(1.4)
$\log K_6$	–	–	–	–	(0.1)

- **But missing…** How to deal with systems where complexation kinetics is slow

  => “batch” / “out-of-cell” titrations.

TG2

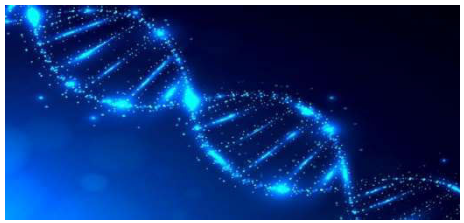


Task Group 2
BIOSUBSTRATES BINDING

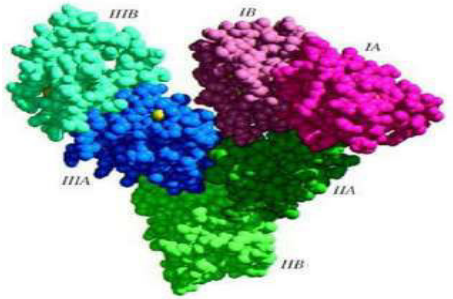
Our task

Identify target systems for studies on biosubstrates binding to be used as validation standard. Development and testing of recommended procedures.

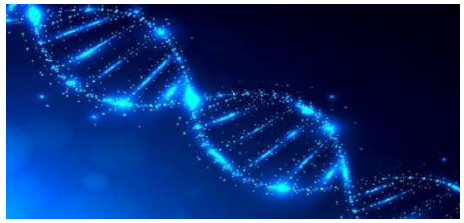
First step: dye/DNA intercalation



A target (“golden standard”) system is chosen on the basis of reactants stability and cost, availability and ease of handling. The different research groups will perform tests on the evaluation of binding constant for the target system. Results will be checked to perform intercalibration exercises between laboratories.



Paper work - Deliverables



The report was refined and split into 2 deliverables:

(i) best practices/purity issues/experimental aspects

(ii) data treatment/equations&software comparisons

Submitted on October 2022

JOB DONE

The people working on this part is quite ready to submit a paper on this part.

DREAMS…

Demetrio proposed to produce a deliverable where the different buffers are listed with pros and cons (in particular given the differences we noticed at the beginning).

CALIXARENE SYSTEM to test data fitting

NEW CALIXARENE SYSTEM to test data fitting

Everybody of us was asked to fit a simple 1:1 titration data kindly shared by Nuno Basilio. We have used whatever equation and software and compare the logK number we get.

We demonstrated what we wanted (🎉 👌): now, different people, using different data fit, obtained LogK numbers with little dispersion (+/- 0.1 Log units, ca. 1% error on Log K value, ca. 20% error on K value).

These data/thresholds can be used as a "general check" as for what is acceptable as an error on fluorescence titrations on more simple 1:1 systems. For DNA the error is (much) higher due to complexity of the system and use of simplified models.

PROTEIN BINDING: INTER-LABORATORY EXERCISES

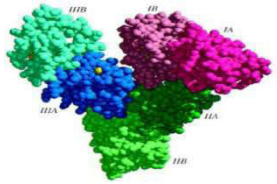
ONGOING EFFORTS

- **We have evaluated different systems and finally chosen ibuprofen/bovine serum albumin (IBU/BSA) and defined exactely the phosphate buffer to be used in our tests**

- **We have faced problems to define IBU molar extinction coefficient, but finally solved this point trough literature/measurements in different labs**

- **We have prepared a NEW PROTOCOL for BSA TITRATIONS**

- **Different groups have performed titrations**



- **We are now at the stage of fitting these titrations to compare our numbers on binding constant….**

TG3

Task Group 3
Peptides

COST Action CA18202
NECTAR
Network for Equilibria and Chemical Thermodynamics Advanced Research

4th European NECTAR Conference
and Final Action Meeting

Milazzo, February 26th-27th, 2024

University of Wroclaw, Poland
Universitat Autoǹoma de Barcelona, Spain
University of Siena, Italy
University of Balearic Islands, Spain
University of Opole, Poland
University of Ferrara, Italy
University of Sassari, Italy
University of Granada, Spain

NECTAR for strong and/or multifunctional ligands, macromolecules

Sławomir Potocki
University of Wrocław

Funded by the European Union

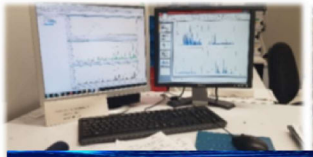
Histidine–rich C–terminal (HRCT) tail of GroEL1 chaperonins as a potential regulator of metal ions concentration in *Mycobacterium tuberculosis* – study on stoichiometry of metal-HRCT complexes

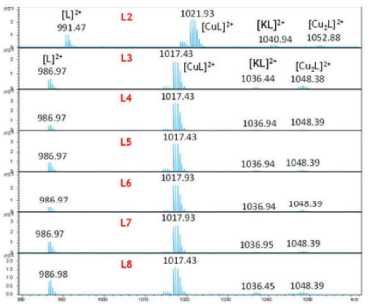
MSc Anna Rola
Origin Institution:
Faculty of Chemistry
University of Wroclaw

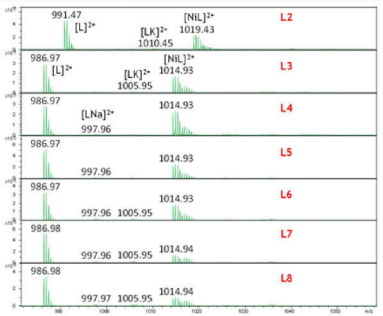
The main aim of this **STMS** was to characterize the stoichiometry and prefered metal-binding sites of model peptides Cu(II)/Ni(II)-complexes in the presence of equimolar amount, as well as an excess of metal ions. For this purpose, **high-resolution mass spectrometry** was used.

Prof. Oscar Palacios Bonilla
Host Institution:
Department of Chemistry
Universitat Autònoma de Barcelona

It was a great opportunity to learn new scientific skills, make international friendships and explore the catalan culture!







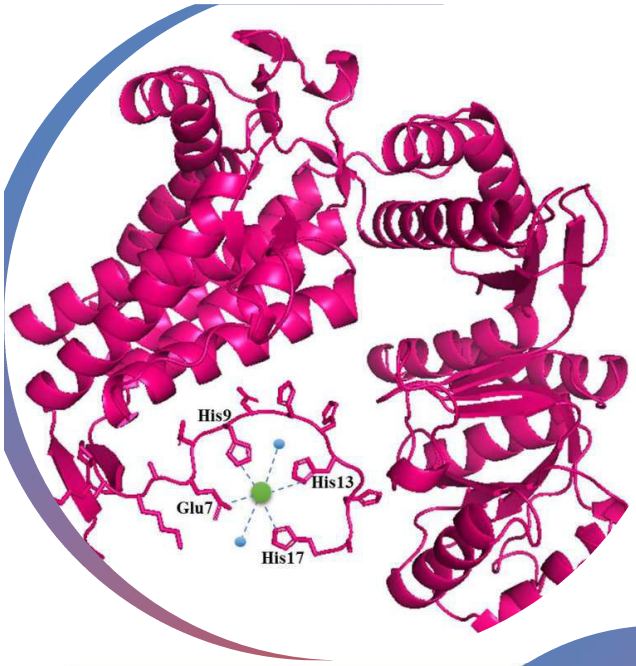
L2: Ac-DKPAKAEDHDHHHGHAH, L3: Ac-DKPAKAEDQDHHHGHAH, L4: Ac-DKPAKAEDHDQHHGHAH
L5: Ac-DKPAKAEDHDHQHGHAH, L6: Ac-DKPAKAEDHDHHQGHAH, L7: Ac-DKPAKAEDHDHHHGQAH
L8: Ac-DKPAKAEDHDHHHGHAQ

MILAZZO February 2024

Histidine-Rich C-Terminal Tail of Mycobacterial GroEL1 and Its Copper Complex—The Impact of Point Mutations

Anna Rola*, Oscar Palacios, Merce Capdevila, Daniela Valensin, Elżbieta Gumienna-Kontecka, and Sławomir Potocki*

Cite this: *Inorg. Chem.* 2023, 62, 18, 6893–6908
Publication Date: April 24, 2023
https://doi.org/10.1021/acs.inorgchem.2c04486



Coordination sphere for a Ni(II)-L2 (L2: Ac- DKPAKAEDHDHHHGHAH) complex at pH around 7.1.

+

Dalton Transactions

ɣyond Copper: Examining the Significance of His-Mutations in Mycobacterial GroEL1 HRCT for Ni(II) Complex Stability and Formation

Journal:	*Dalton Transactions*
Manuscript ID	DT-ART-01-2024-000011
Article Type:	Paper
Date Submitted by the Author:	02-Jan-2024
ɔmplete List of Authors:	Rola, Anna; University of Wrocław, Faculty of Chemistry Kola, Arian; University of Siena, Department of Biotechnology, Chemistry and Pharmacy Valensin, Daniela; University of Siena, Department of Chemistry Palacios, Oscar; Universitat Autonoma de Barcelona, Chemistry Capdevila, Mercè; Universitat Aut&#65533;noma de Barcelona, Departament Química Gumienna-Kontecka, Elzbieta; University of Wroclaw, Faculty of Chemistry Potocki, Slawomir; University of Wroclaw, Department of Chem

The presence of Lys5 residue significantly increases the stability of the system. His9 and His13 are the crucial residues for Ni(II) binding, whereas His12 has minimal relevance in complex formation.

STSM COST Nectar -
Exploiting NMR spectroscopy to determine coordination mode of the Zn(II), Ni(II), and Cu(II) complexes with metallopeptidases.

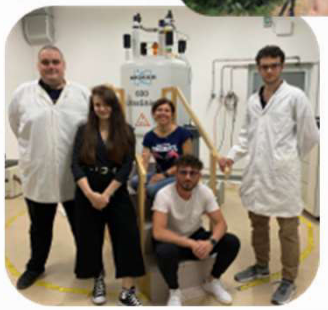
Origin Institution: University of Wrocław, Poland, Department of Chemistry
MSc Paulina Potok

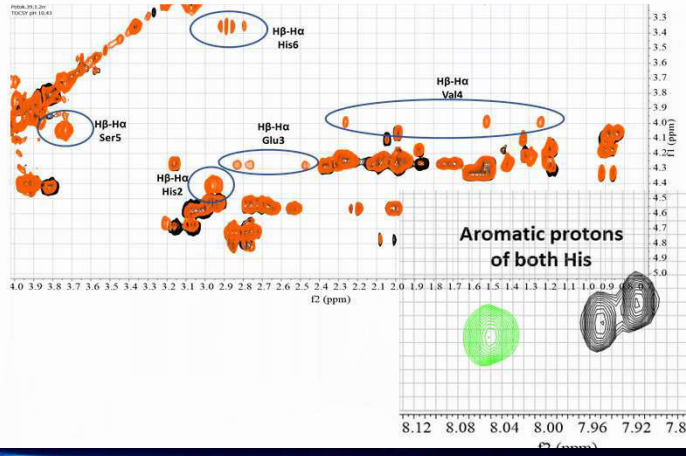
CA18202 STSM
31 days

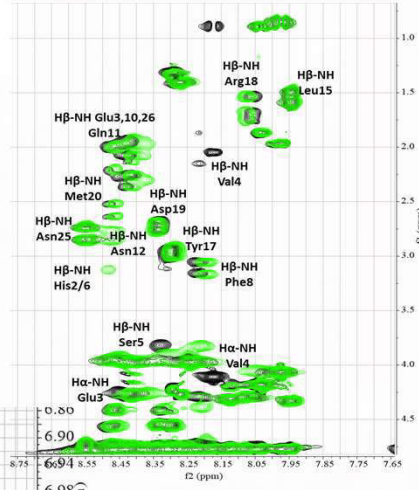
Host Institution: University of Siena, Italy Department of Biotechnology, Chemistry and Pharmacy
Prof. Daniela Valensin

DIPARTIMENTO DI BIOTECNOLOGIE, CHIMICA E FARMACIA

The main goal of the proposed **STSM project** was to characterize the coordination mode of metallopeptidases from pathogenic bacteria with transition metal ions Zn(II), Ni(II), and Cu(II) by **Nuclear Magnetic Resonance Spectroscopy.**





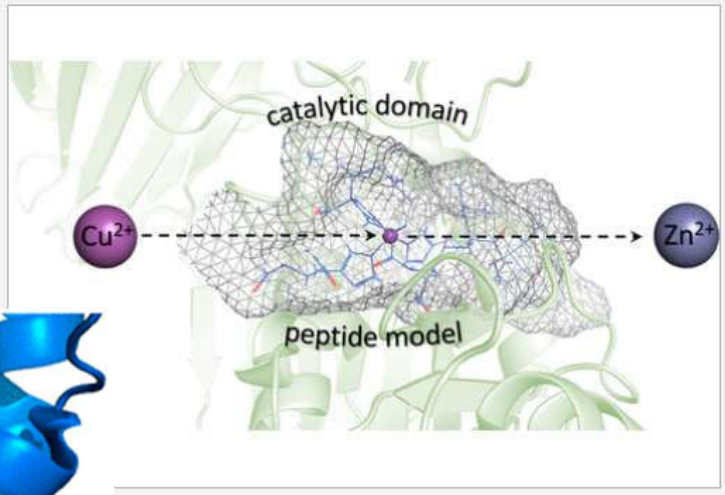


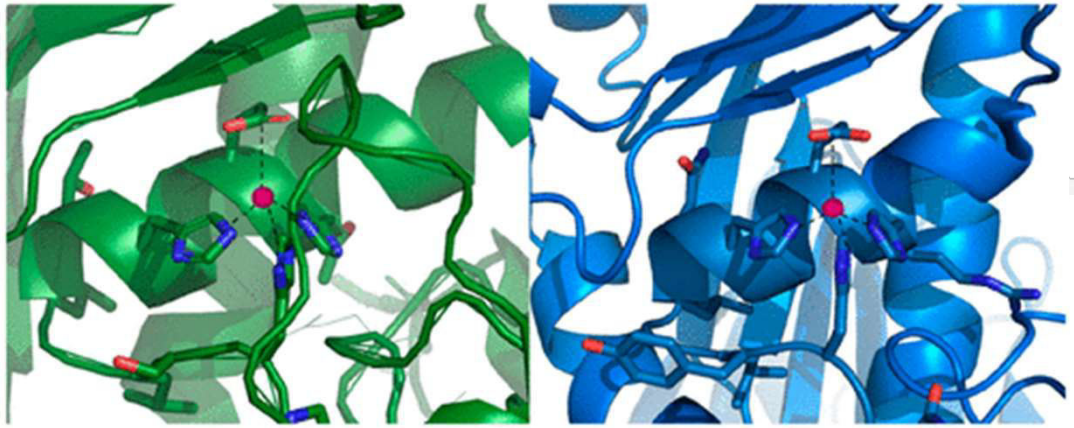
MILAZZO February 2024

Copper Forms a PPII Helix-Like Structure with the Catalytic Domains of Bacterial Zinc Metalloproteases

Paulina Potok, Arian Kola, Daniela Valensin, Merce Capdevila, and Sławomir Potocki*

Cite this: *Inorg. Chem.* 2023, 62, 45, 18425−18439
Publication Date: November 1, 2023
https://doi.org/10.1021/acs.inorgchem.3c02391





CH vs. HC-Promiscuous Metal Sponges in Antimicrobial Peptides and Metallophores

Garstka Kinga

Dzyhovskyi Valentyn

Wątły Joanna

University of Wrocław

Świątek-Kozłowska Jolanta

Kozłowski Henryk

Stokowa-Sołtys Kamila

University of Ferrara

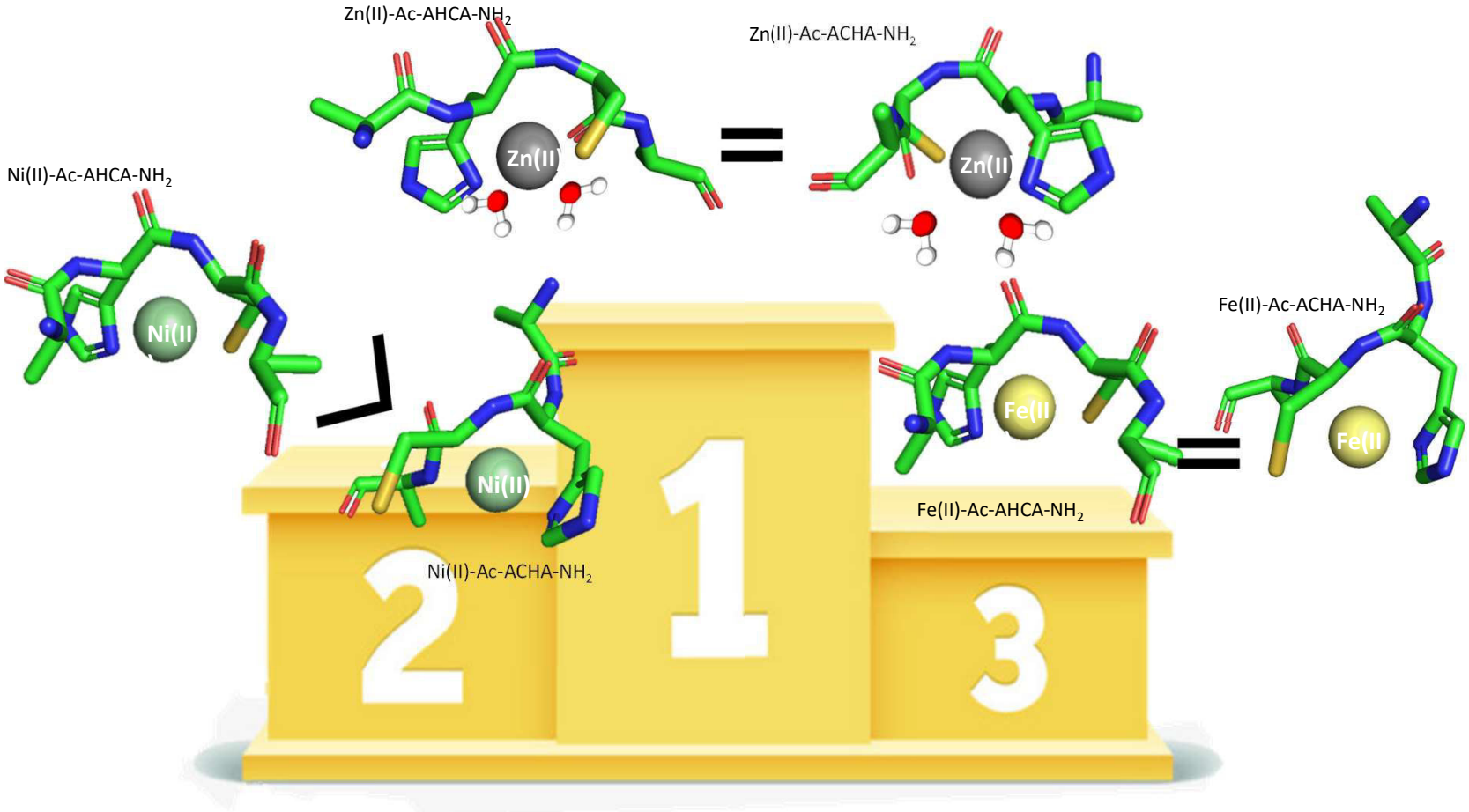
University of the Balearic Islands

Rowińska-Żyrek Magdalena

Barceló-Oliver Miquel

Bellotti Denise

Molecules, 2023, **28**, 3985/1-3985/14
DOI:10.3390/molecules28103985

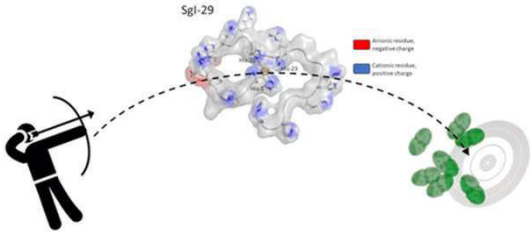


Garstka, K.; Dzyhovskyi, V.; Wątły, J.; Stokowa-Sołtys, K.; Świątek-Kozłowska, J.; Kozłowski, H.; Barceló-Oliver, M.; Bellotti, D.; Rowińska-Żyrek, M.
CH vs. HC—Promiscuous Metal Sponges in Antimicrobial Peptides and Metallophores, Molecules, 2023, **28**, 3985/1-3985/14, DOI:10.3390/molecules28103985

Semenogelins Armed in Zn(II) and Cu(II): May Bioinorganic Chemistry Help Nature to Cope with *Enterococcus faecalis*?

Dorota Dudek, Adriana Miller, Aleksandra Hecel, Arian Kola, Daniela Valensin, Aleksandra Mikołajczyk, Miquel Barcelo-Oliver, Agnieszka Matera-Witkiewicz, and Magdalena Rowińska-Żyrek*

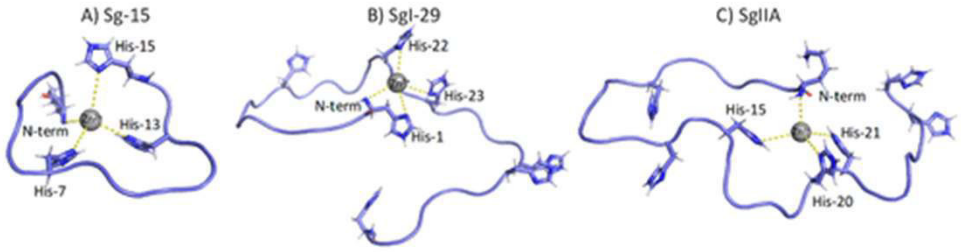
Cite this: *Inorg. Chem.* 2023, 62, 34, 14103−14115
Publication Date: August 15, 2023
https://doi.org/10.1021/acs.inorgchem.3c02390



The Cu(II)-induced antimicrobial activity of Sg-15 against *Enterococcus faecalis* is shown.

The most abundant proteins from human semen, results in the formation of 26- and 29-[illegible] respectively), which share a common 15

Sgl-29	HNKQEGRDHDKSKGHFHRVVIHHKGGKAH
SgIIA	KQEGRDHDKSKGHFHMIVIHHKGGQAHHG
Sg15 (common region)	KQEGRDHDKSKGHFH



MILAZZO February 2024

Joint work on the characterization of Fe(II) bacterial transporters

Bartosz Orzeł MSc

Prof. Elżbieta Gumienna-Kontecka

Uniwersytet Wrocławski

Prof. Massimiliano Francesco Peana

Università degli Studi di Sassari

Inorganic Chemistry

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pubs.acs.org/IC

Article

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

Bartosz Orzel, Alessio Pelucelli, Malgorzata Ostrowska, Sławomir Potocki, Henryk Kozlowski, Massimiliano Peana, and Elzbieta Gumienna-Kontecka*

Cite This: *Inorg. Chem.* 2023, 62, 18607−18624

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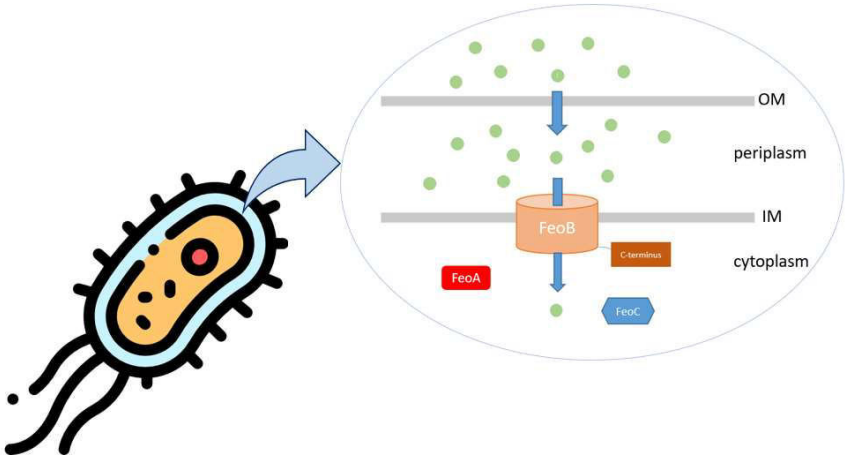
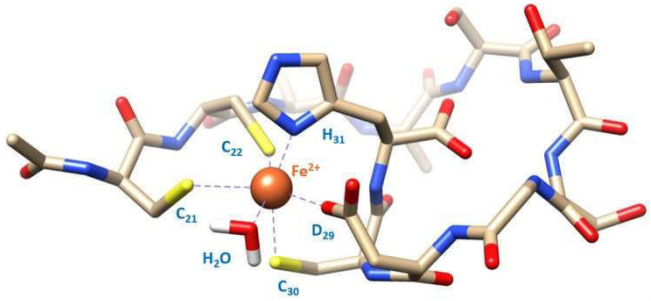
Iron(II) bacterial transporters, such as **Feo system**, are crucial for bacterial survival and pathogenicity.

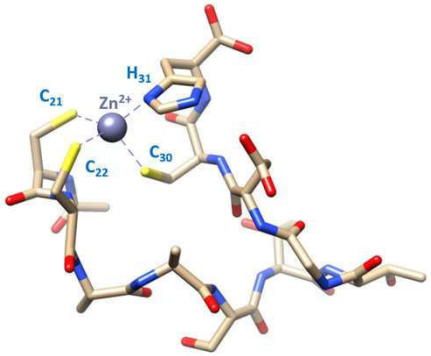


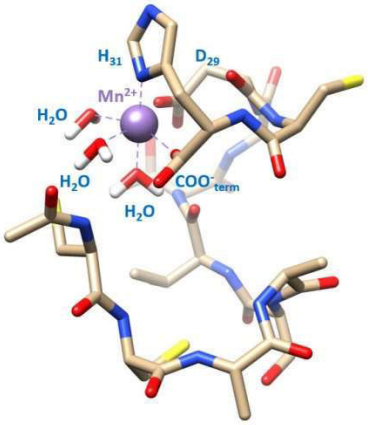
B. Orzeł, A. Pelucelli, M. Ostrowska, S. Potocki, H. Kozłowski, M. Peana, E. Gumienna-Kontecka, *Inorganic Chemistry* **2023**, 62(45), 18607–18624.

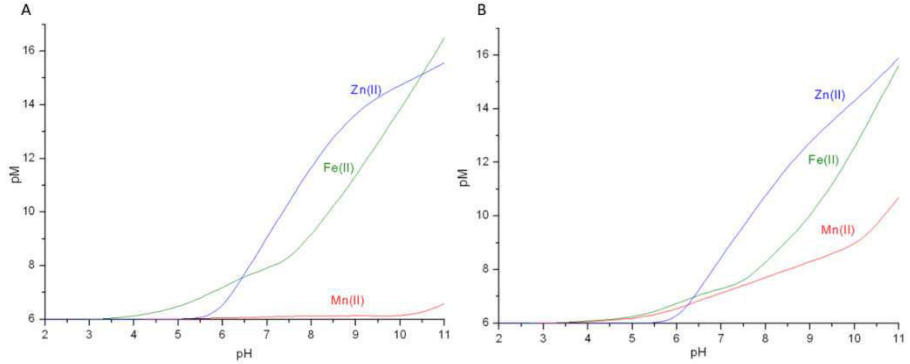
Ac- $C_{21}C_{22}A_{23}A_{24}S_{25}T_{26}T_{27}G_{28}D_{29}C_{30}H_{31}$ P1

Ac- $R_1R_2A_3R_4S_5R_6V_7D_8I_9E_{10}L_{11}L_{12}A_{13}T_{14}R_{15}K_{16}S_{17}V_{18}S_{19}S_{20}C_{21}C_{22}A_{23}A_{24}S_{25}T_{26}T_{27}G_{28}D_{29}C_{30}H_{31}$ P2









Comparison of K_d values for studied and biological ligands for Fe(II), Zn(II) and Mn(II).[a]

Ligand	Fe(II)	Mn(II)	Zn(II)	Ref.
P2	$4.75\cdot10^{-7}$	$7.02\cdot10^{-7}$	$6.31\cdot10^{-8}$	This work
E.coli Fur	$1.2\cdot10^{-6}$	$2.4\cdot10^{-5}$	$1.4\cdot10^{-10}$	78
S.pyogenes MtsA	$4.3\cdot10^{-6}$	-	-	79
B.subtilis MntR	-	$0.2\cdot10^{-6}$-$2\cdot10^{-6}$	-	80
Y.pestis YfeA	-	$1.78\cdot10^{-8}$	$6.6\cdot10^{-9}$	81
T.pallidum TroA	-	$7.1\cdot10^{-9}$	$2.25\cdot10^{-8}$	82
D.radiodurans MntH	-	$1.9\cdot10^{-4}$	-	83
Synechocystis ZnuA	-	-	$7.3\cdot10^{-9}$	84

[a] K_d values calculated for our systems as: $Kd = \frac{[M][L]}{[ML]}$ at pH=7.0.

"Histidine-Rich C-Terminal Tail of Mycobacterial GroEL1 and Its Copper Complex–The Impact of Point Mutations."
A. Rola, O. Palacios, M. Capdevila, D. Valensin, E. Gumienna-Kontecka & S. Potocki; *Inorganic Chemistry* (2023), **62**, 6893–6908. DOI: 10.1021/acs.inorgchem.2c04486
(collaboration: University of Wroclaw, Poland + Universitat Autònoma de Barcelona, Spain + University of Siena, Italy)

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DOI: 10.1021/acs.inorgchem.3c02390
(collaboration: University of Wroclaw and Wrocław Medical University, Poland + University of Siena, Italy + University of Balearic Islands, Spain)

"CH vs. HC—Promiscuous Metal Sponges in Antimicrobial Peptides and Metallophores."
K. Garstka, V. Dzyhovskyi, J. Wątły, K. Stokowa-Sołtys, J. Świątek-Kozłowska, H. Kozłowski, M. Barceló-Oliver, D. Bellotti & M. Rowińska-Żyrek; *Molecules* (2023), **28**, 3985/1-3985/14.
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(collaboration: University of Wroclaw and University or Opole, Poland + University of Balearic Islands, Spain + University of Ferrara, Italy)

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P. Potok, A. Kola, D. Valensin, M. Capdevila & S. Potocki; *Inorganic Chemistry* (2023), **62**, 18425–18439. DOI: 10.1021/acs.inorgchem.3c02391
(collaboration: University of Wroclaw, Poland + University of Siena, Italy + Universitat Autònoma de Barcelona, Spain)

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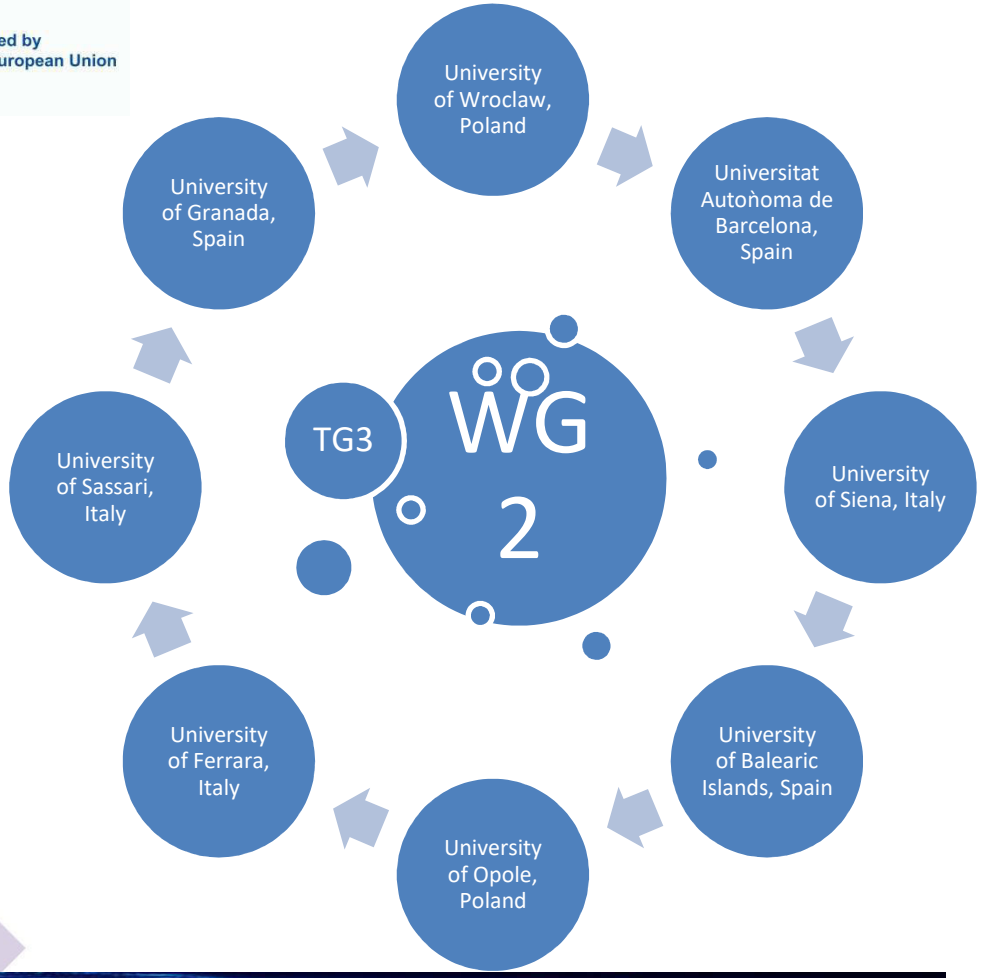
(collaboration: University of Wrocław and University of Opole, Poland + University of Sassari, Italy)

"The N-terminal domain of Helicobacter Pylori's Hpn protein: the role of multiple histidine residues."
D. Bellotti, A. Sinigaglia, R. Guerrini, E. Marzola, M. Rowińska-Żyrek, M. Remelli; *J. Inorg. Biochem.* (2021), **214**, 111304. DOI: 10.1016/j.jinorgbio.2020.111304
(collaboration: University of Ferrara, Italy + University of Wroclaw, Poland)

"Novel insights into the metal binding ability of ZinT periplasmic protein from Escherichia coli and Salmonella enterica."
D. Bellotti, M. Rowińska-Żyrek, M. Remelli; *Dalton Trans.* (2020), **49**, 9393–9403. DOI: 10.1039/D0DT01626H
(collaboration: University of Ferrara, Italy + University of Wroclaw, Poland)

"Exploring the specificity of rationally designed peptides reconstituted from the cell-free extract of Deinococcus radiodurans toward Mn(II) and Cu(II)."
M. Peana, E. Gumienna-Kontecka, F. Piras, M. Ostrowska, K. Piasta, K. Krzywoszyńska, S. Medici, M. A. Zoroddu; *Inorg. Chem.* (2020), **59**, 4661–4684. DOI: 10.1021/acs.inorgchem.9b03737
(collaboration: University of Wroclaw, Poland + University of Sassari, Italy + Public Higher Medical Professional School, Poland)

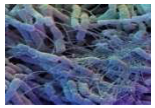
"Zinc(II) – the overlooked éminence grise of chloroquine's fight against COVID-19?"
A. Hecel, M. Ostrowska, K. Stokowa-Sołtys, J. Watły, D. Dudek, A. Miller, S. Potocki, A. Matera-Witkiewicz, A. Domínguez-Martin, H. Kozłowski, M. Rowinska-Zyrek; *Pharmaceuticals* (2020), **13**, 228.
DOI: 10.3390/ph13090228
(collaboration: University of Granada, Spain + University of Wroclaw, Poland + Public Higher Medical Professional School, Poland)


University of Wroclaw, Poland
Universitat Autònoma de Barcelona, Spain
University of Siena, Italy
University of Balearic Islands, Spain
University of Opole, Poland
University of Ferrara, Italy
University of Sassari, Italy
University of Granada, Spain
TG3
WG 2

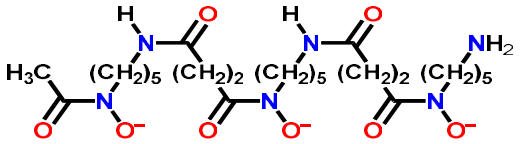
TG4

Task Group 4
Metallophores

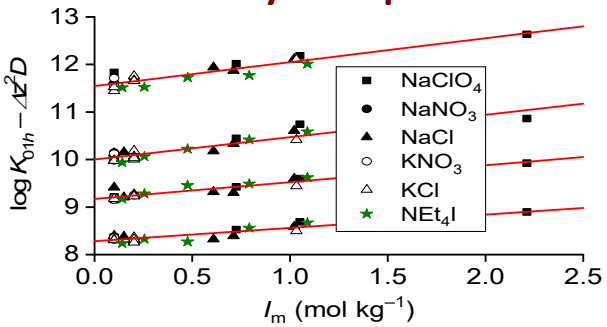
New Insights into the Acid-Base Properties of DFO



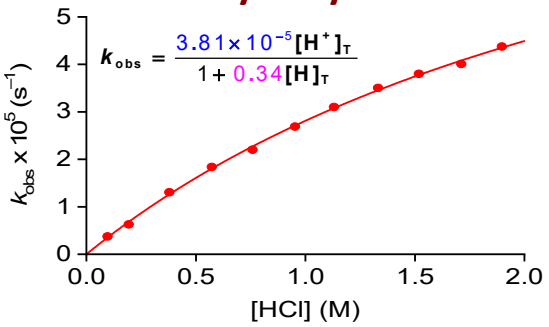
Streptomyces sp.



SIT analysis of pKa's



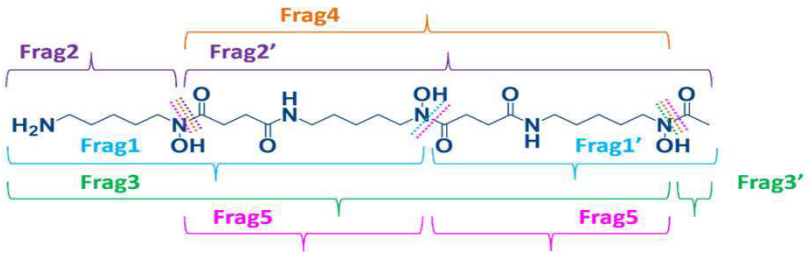
H$^+$-assisted hydrolysis kinetics



New pKa measurements in NEt$_4$I

I (M)	log $K_1 \pm 2\sigma$	log $K_2 \pm 2\sigma$	log $K_3 \pm 2\sigma$	log $K_4 \pm 2\sigma$
0.138	10.79 ± 0.03	9.46 ± 0.02	8.94 ± 0.02	8.25 ± 0.03
0.243	10.67 ± 0.02	9.50 ± 0.02	9.01 ± 0.02	8.35 ± 0.02
0.436	10.73 ± 0.02	9.57 ± 0.01	9.15 ± 0.01	8.31 ± 0.02
0.689	10.67 ± 0.03	9.70 ± 0.01	9.16 ± 0.01	8.62 ± 0.02
0.905	10.85 ± 0.04	9.84 ± 0.01	9.29 ± 0.02	8.75 ± 0.03

LCMS analysis of the fragmentation pattern



In collaboration with C. Bretti

In collaboration with S. Gama

Metal-complexes as Potential drugs

Journal of Molecular Liquids 396 (2024) 124027

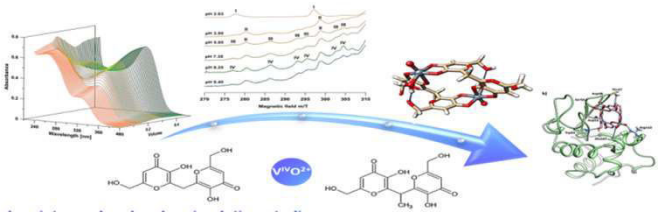
Contents lists available at ScienceDirect

Journal of Molecular Liquids

journal homepage: www.elsevier.com/locate/molliq

Solution chemistry of oxidovanadium(IV) complexes with two bis-kojic acid derivatives

Rosita Cappai [a,b,*], Alessandra Fantasia [b], Giuseppe Sciortino [c], Daniele Sanna [d], Federico Pisanu [e], Eugenio Garribba [e], M. Amélia Santos [f], Guido Crisponi [b], Valeria M. Nurchi [b]



molecules

MDPI

Article

A Multi-Technique Investigation of the Complex Formation Equilibria between Bis-Deferiprone Derivatives and Oxidovanadium (IV)

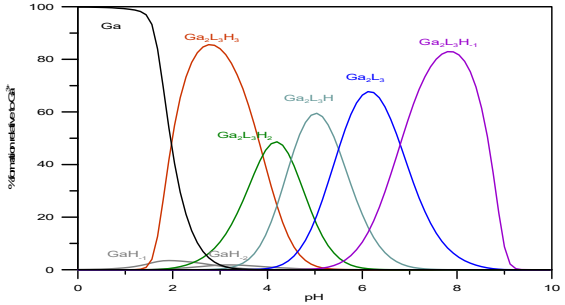
Rosita Cappai [1], Alessandra Fantasia [1], Guido Crisponi [1], Eugenio Garribba [2], M. Amélia Santos [3] and Valeria Marina Nurchi [1,*]

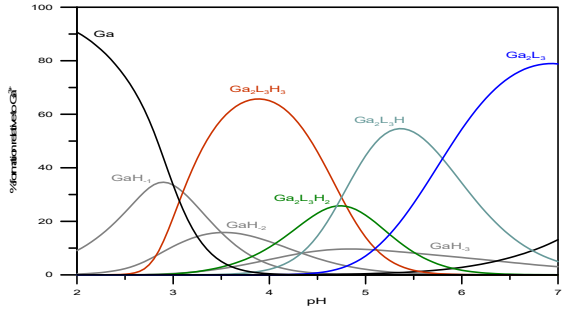
Metal-complexes as Potential drugs

Gd(III) and Ga(III) complexes with a new tris-3,4-HOPO ligand as new imaging probes: complex stability, magnetic properties and biodistribution

S. Chaves, K. Gwizdała, K. Chand, a L.Gano, A Pallier, É. Tóth, M. A. Santos, | *Dalton Trans*., 2022, 51, 6436–6447, https://doi.org/10.1039/D2DT00066K (*coll*. **Portugal, France , Poland**)

Ga(III) complexes with biskojic acids as new metallophoress: complex stability, and biological properties. D. Griffith, R. Cappai , M.A.Santos *et al*. (work in progress) (*coll*. **Ireland , Italy , Portugal**)

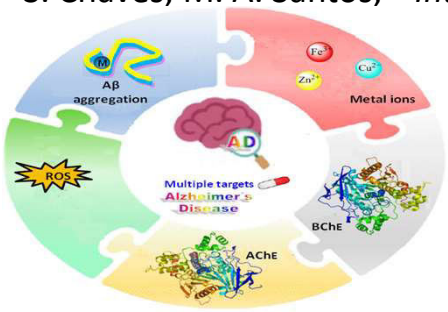


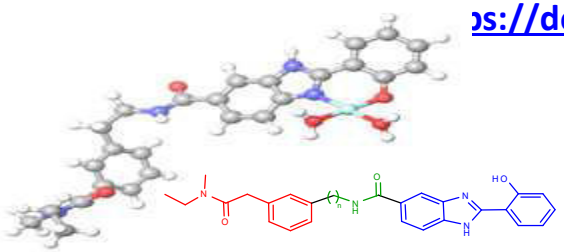


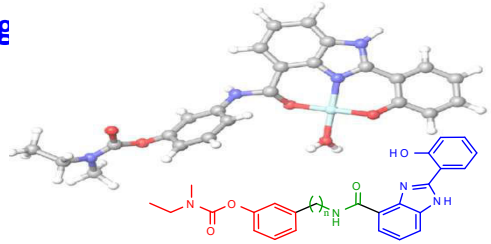
Multitarget metal chelators for potential therapy of Alzheimer´s Disease (AD)

Rivastigmine–Benzimidazole Hybrids as Promising Multitarget Metal-Modulating Compounds for Potential Treatment of Neurodegenerative Diseases" ,

D. Vicente-Zurdo, L. Brunetti, L. Piemontese, B. Guedes, S.M Cardoso, D. Chavarria, F. Borges , Y. Madrid, Y. Madrid, S. Chaves, M. A. Santos, " *Int. J.* https://doi.org

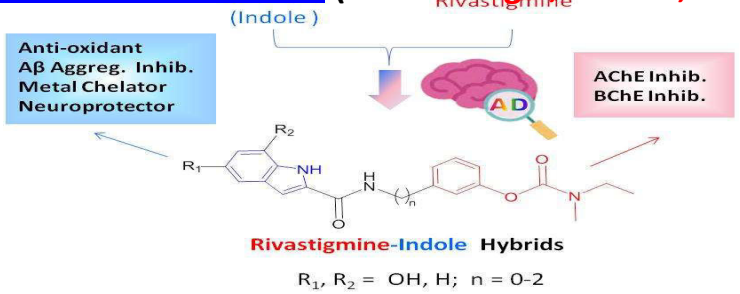






New Multitarget Rivastigmine-Indole Hybrids as Potential Drug Candidates for Alzheimer´s Disease",

L. Bon , A. Banás , I. Dias , I Melo-Marques , S. M. Cardoso, S. Chaves, M. A. Santos, *Pharmaceutics* **2024**, *16*(2), 281; https://doi.org/10.3390/pharmaceutics16020281 (*coll.* Portugal, France , Poland)



TG5

Task Group 5
Calorimetry

Milazzo, Feb
26-27 2024

WG2
Task Group n.5 on Calorimetry

ITC study of multiple host-guest complex formation: an interlaboratory exercise

Research groups from:

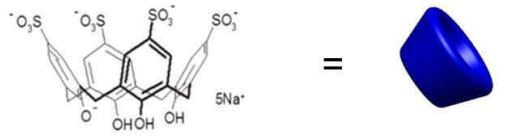
Catania, Ferrara, Firenze, Ljubljana,
Messina, Strasbourg, Udine, Wroclaw

Main goals of WG2 - TG5

- Experimental design/conditions for the analysis of multiple equilibria
- Data refinement: use proper chemical models and software
- Critical comparison of data/results obtained by different labs, instruments, software
- Guidelines on the correct use of ITC data for the study of solution equilibria
- Training people: invite researchers to deal/interact with trained people, STSM

inter-laboratory exercise → «best practices» protocol

ITC titration for a host-guest 1:1 complex in buffered aqueous solution



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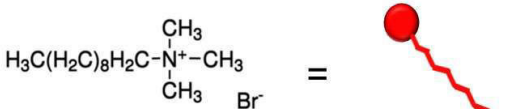

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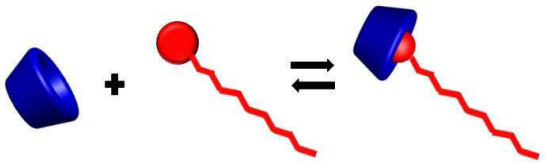
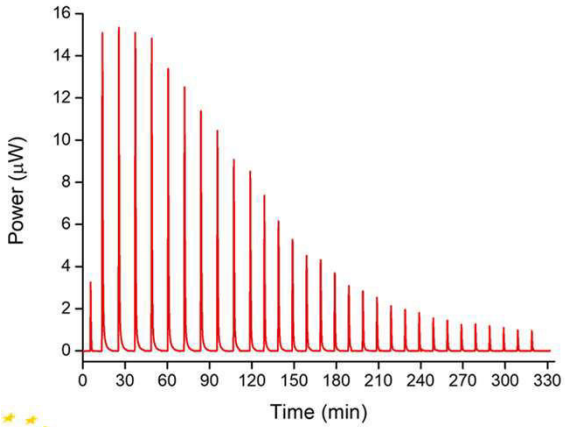
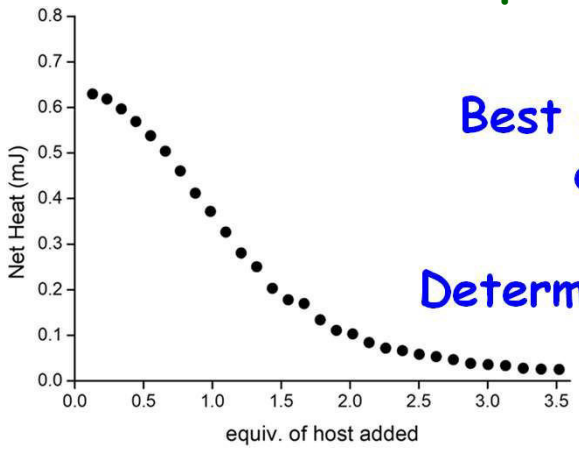


Simple host-guest equilibrium

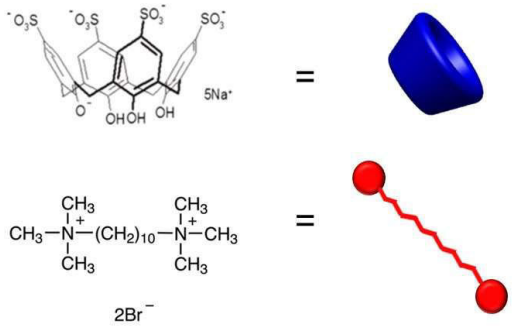


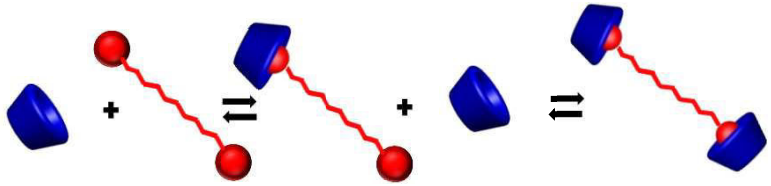


Best experimental design and data analysis model

Determination of accurate K and ΔH values

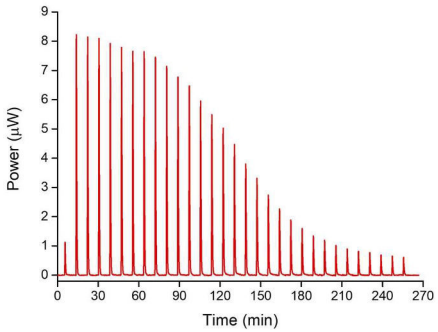
ITC titrations for host-guest 1:1 and 2:1 complexes in buffered aqueous solution

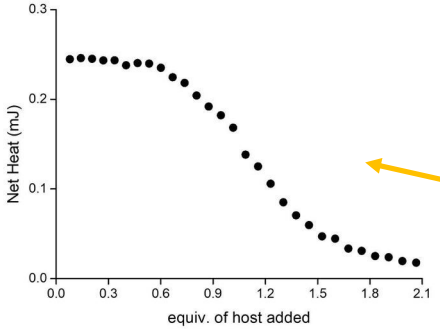


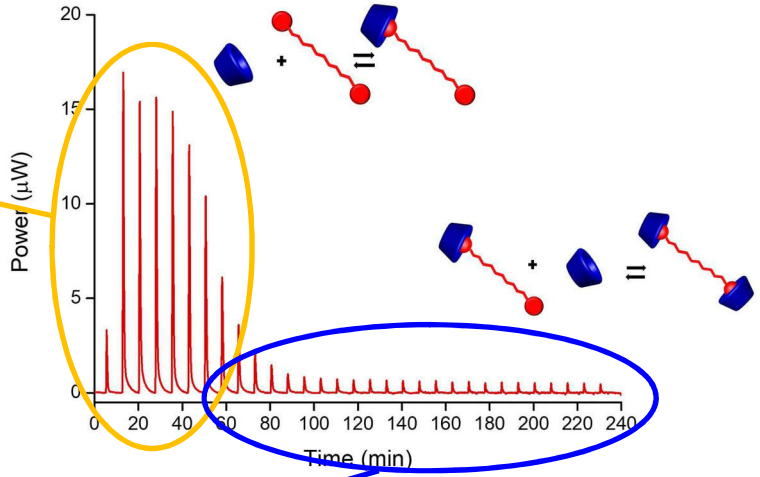


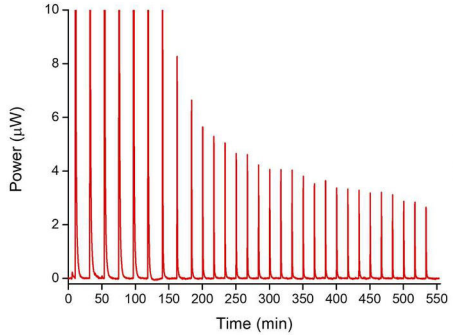
Multiple host-guest equilibria

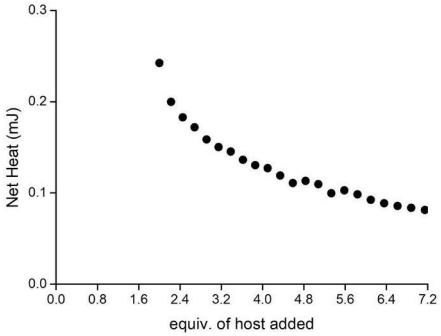
ITC titration for host-guest 1:1 and 2:1 complexes in buffered aqueous solution











Issues in the heat measurement!!

Careful <u>experimental design</u> needed for the determination of accurate K and ΔH values

WG2
Task Group n.5 on Calorimetry

- Proper design of ITC experiments to measure reliable heat values for the different complexation steps of multiple equilibria.

- The appropriate data refinement should include all the equilibria occurring in solution and the exact stoichiometry of the species rather than "obscure" binding models used by most software.

- The results from this excercise will contribute to prepare new guidelines on correct experimental design and data analysis in ITC titrations.

THANK YOU FOR THE GREAT TIME!!
LET'S KEEP IN TOUCH

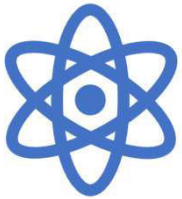
WG3 meeting

Tuesday, 27 February 2024

Milazzo, Italy

WG3: NECTAR for multicomponent solutions and complex matrices

Thermodynamic and chemical equilibrium data and speciation studies of real systems (e.g. natural waters, biological fluids, commercial products).



Classical procedures for the study of the equilibria in multicomponent systems (e.g. ionic liquids, mixed solvents, heterogeneous systems, etc.) are often inadequate when a high number of components is present in the matrix.

In this respect, there is an urgent need to update and adapt experimental procedures and computational approaches.

WG3 report

Oct 2019 – Feb 2024	
Collaborations activities	Around 15 active participants.
Networking activities:	2 NECTAR conferences organized by WG3 members; 10 STSMs by WG3 members; TS in calorimetry organized in Ljubljana
Dissemination and communication activities	8 with COST acknowledgement and 1 with „3 countries rule“ Two guidelines given at NECTAR web page
Participation at all NECTAR meetings	15 posters 20 oral presentations

WG3: NECTAR for multicomponent solutions and complex matrices defined in Brussels

Complex materices	Speciation studies	Heterogeneous systems
• Task specific ionic liquids • Ionic liquids + molecular solvent	• Sulphur speciation • Critical elements • 3D metallacage complexes	• Sorbent materials • Nanoscale systems

• Task Specific ILs: Chelating ILs, Pharmaceutically Active ILs, Zwitterionic ILs, Surface Active ILs (RS, SI, CZ)

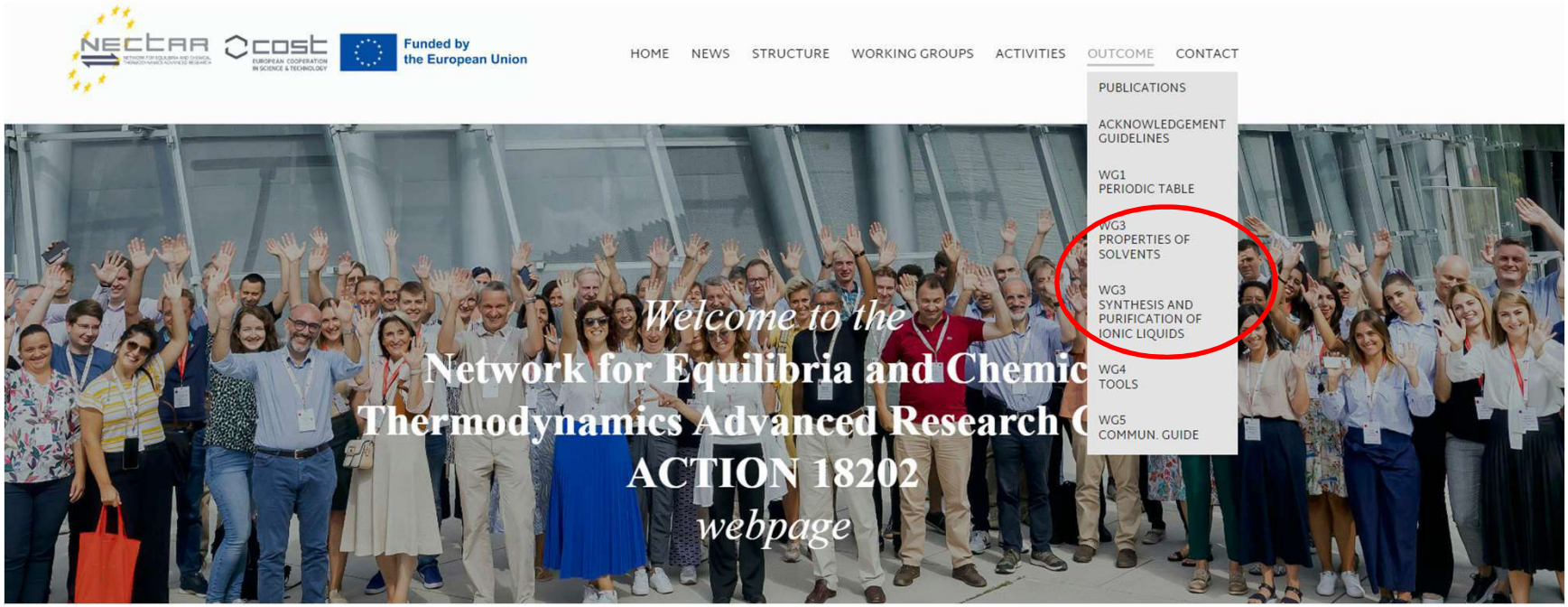
• Mixtures of ILs and MS (aqueous solutions): determination of the thermodynamic parameters, equilibrium constants, evaluation of the interactions experimentally and using MD especially NCI, interactions of drugs or biologically active substances (RS, SI)

• Speciation studies: Sulphur speciation of free and incapsulated drugs Raloxifene and Tizanidine and method developing (DK), speciation of supramolecular self-assembled 3D metallacage complexes (DE), extraction of critical elements using ionic liquids (RS), heterogeneous equilibria (MD)

Task

- Defining recommended experimental and data analysis procedures and guidelines for an accurate speciation of systems in complex matrices such as ionic liquids, mixed solvents, systems containing surfactants or sorbent materials.
- Release first guidelines on interactions in non-aqueous systems

Guidelines


NECTAR
cost
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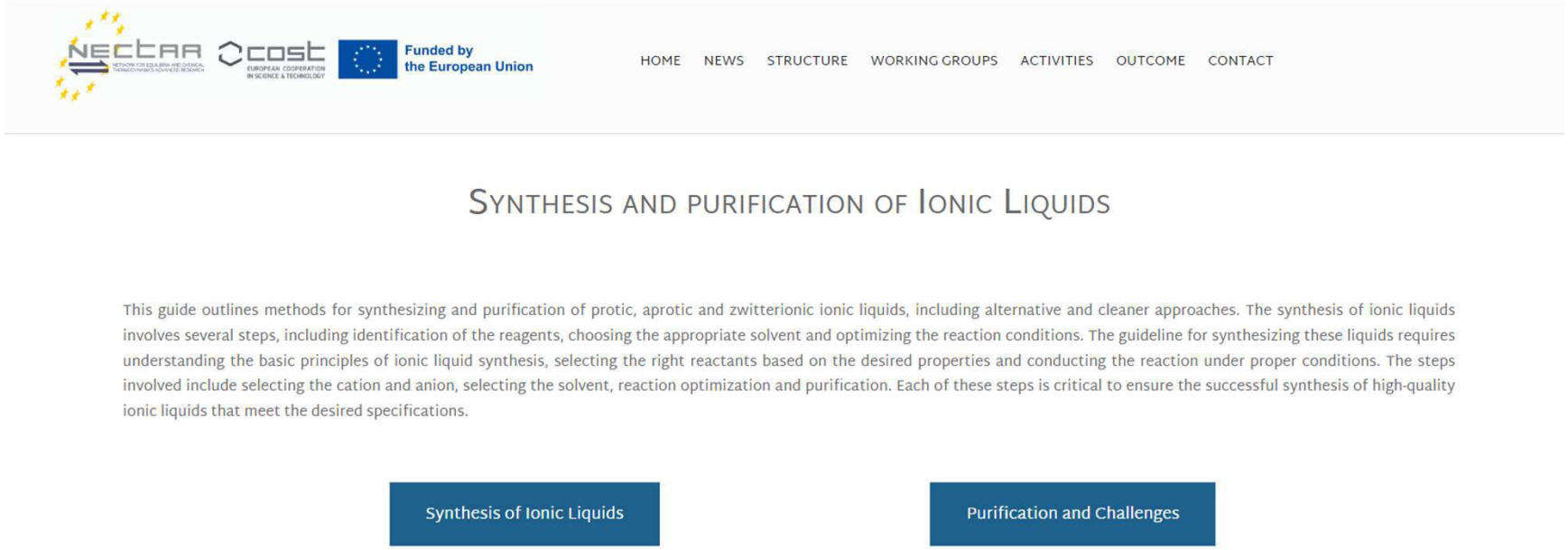
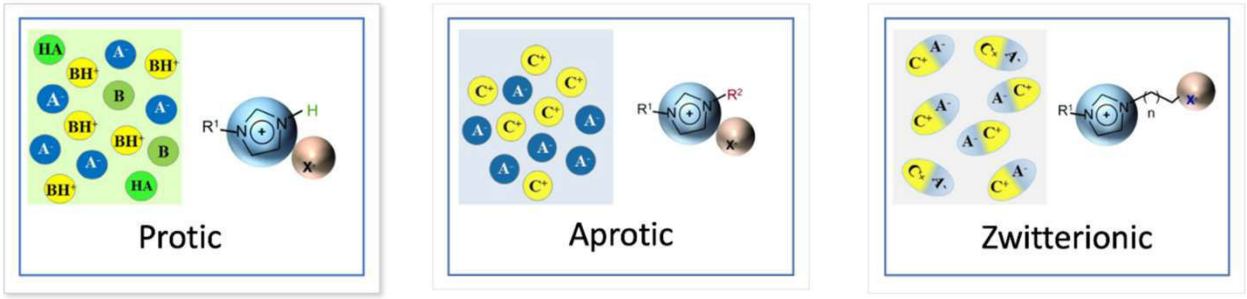
HOME
NEWS
STRUCTURE
WORKING GROUPS
ACTIVITIES
OUTCOME
CONTACT
PUBLICATIONS
ACKNOWLEDGEMENT GUIDELINES
WG1 PERIODIC TABLE
WG3 PROPERTIES OF SOLVENTS
WG3 SYNTHESIS AND PURIFICATION OF IONIC LIQUIDS
WG4 TOOLS
WG5 COMMUN. GUIDE
Welcome to the
Network for Equilibria and Chemic
Thermodynamics Advanced Research C
ACTION 18202
webpage

Ionic liquids – guidelines for synthesis and purification



Synthesis and purification of Ionic Liquids

Synthesis of Ionic Liquids



Synthesis and purification of Ionic Liquids

Synthesis of Ionic Liquids

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 a proton from a Brønsted acid to a Brønsted base.

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

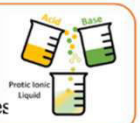
- PILs are a good conductor of protons and ions.
- Water may be used as a solvents or titration can be performed without any solvent. Example
- Complete proton transfer between the acid and base must occur for optimal production.
- The cation on which the proton resides determines the proton activity of the IL.
- To achieve this, there must be **a high pKa difference** between the acid and base.
- 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.

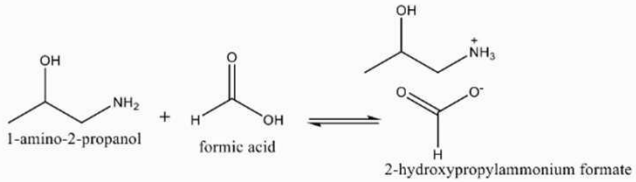
Synthesis and purification of Ionic Liquids

Synthesis of Ionic Liquids

Example:

Without solvent:
Cheap,
no waste,
takes only 10 minutes



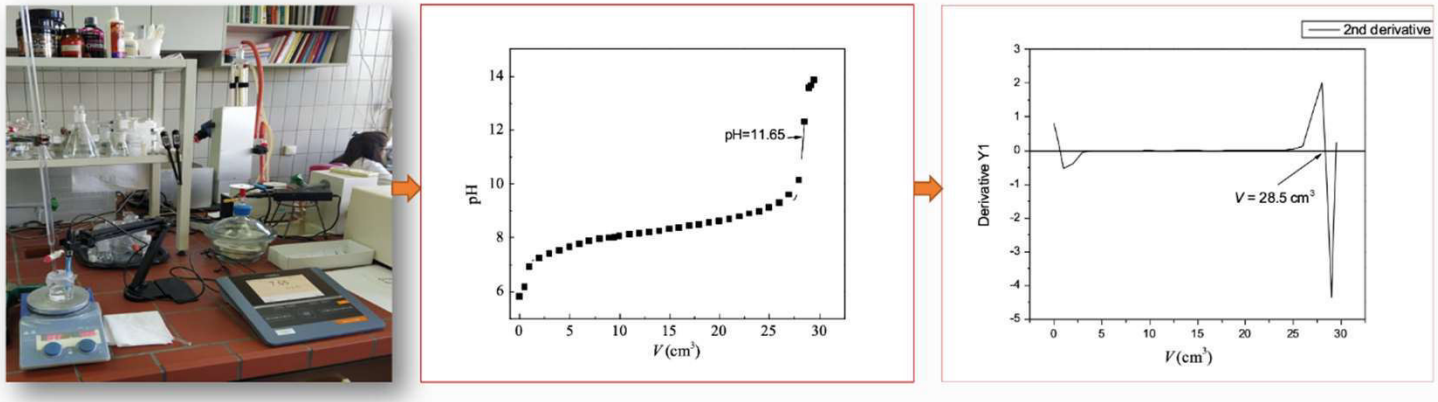


Tips:
During the reaction cooling is necessary since this reaction is exothermic

(Click to close)

- 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 base.

Titration curve:



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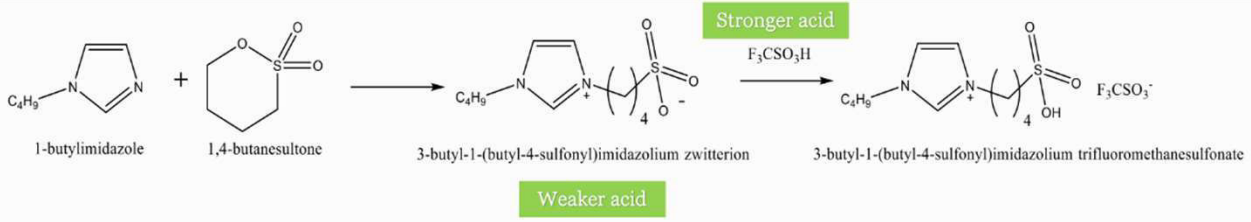
- The equivalence point and pH at the end point confirm the purity of the IL after synthesis and any subsequent handling procedures.
- Diluting an IL sample in water to the standard concentration confirms the previously determined equivalence point pH.

Example:

- the Bronsted acidic IL, 3-butyl-1-(butyl-4-sulfonyl)imidazolium trifluoromethanesulfonate, can be synthesized over two steps.
- First, 1-butylimidazole reacts with 1,4-butanesultone to generate the zwitterion.
- Second, the zwitterion is acidified by adding trifluoromethanesulfonic acid, which protonates the zwitterion to form the trifluoromethanesulfonate anion.
- The low pKa of the acid helps to transform the sulfonate group into a sulfonic acid, making the reaction successful.



1-butylimidazole + 1,4-butanesultone → 3-butyl-1-(butyl-4-sulfonyl)imidazolium zwitterion → 3-butyl-1-(butyl-4-sulfonyl)imidazolium trifluoromethanesulfonate

(Click to close)

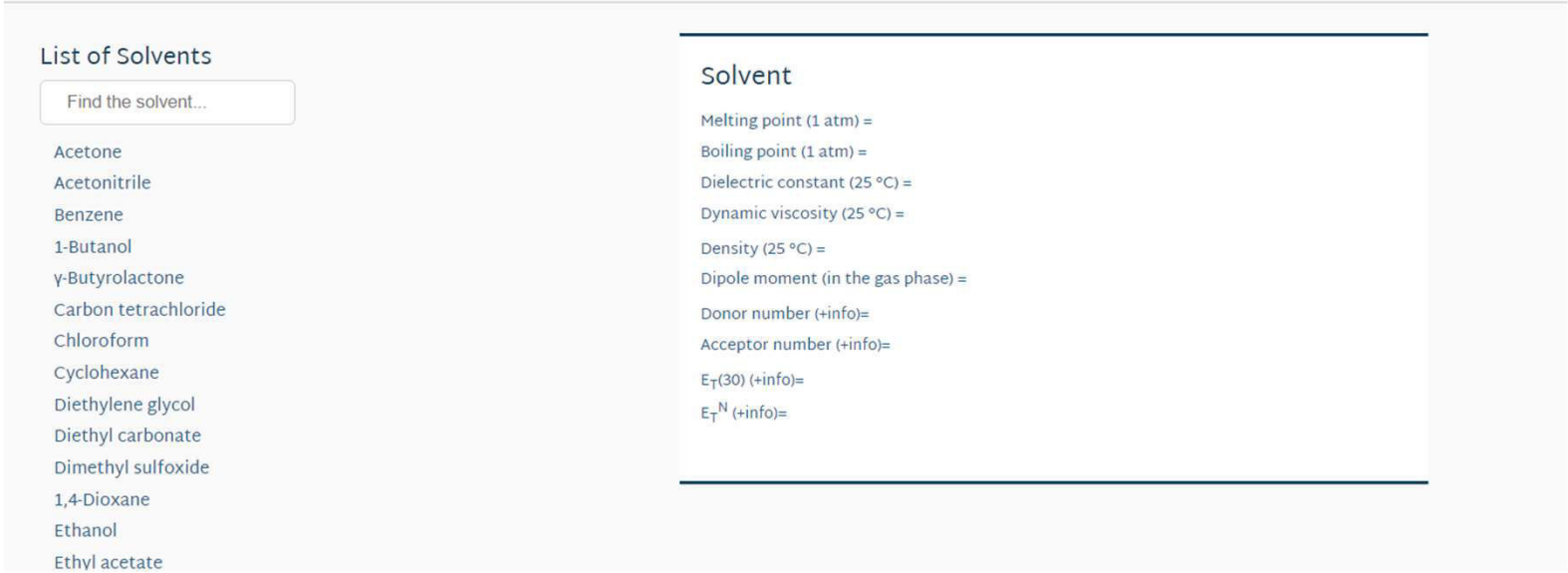
These zwitterionic liquids are similar to ILs but cannot migrate in an electric field. They help ensure that the Li^+ ions can transport smoothly in the electrolyte.
The reaction involves the nucleophile 1-methylimidazole reacting with 1,3-propanesultone. The sultone undergoes ring opening at the α-carbon to produce the zwitterion with >98% yield. Zwitterionic ILs can act as Bronsted acids. This property makes them useful as catalysts and solvents. Example.

II. Properties of solvent

PROPERTIES OF SOLVENTS

Below is a list of some of the most commonly used solvents. Clicking on each of them will take you to a list with the following properties: melting point, boiling point, dielectric constant, dynamic viscosity, dipole moment, donor number, acceptor number, empirical solvent polarity parameter (E_T), and normalized E_T^N.

If not denoted differently, data are taken from the book J. M. G. Barthel, H. Krienke, W. Kunz, Physical Chemistry of Electrolyte Solutions, Modern Aspects, Springer, 1998.



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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

Acetone

Melting point (1 atm) = **-94.7 °C**
Boiling point (1 atm) = **56.29 °C**
Dielectric constant (25 °C) = **20.56**
Dynamic viscosity (25 °C) = **0.303 mPa·s**
Density (25 °C) = **0.7844 kg·dm^{-3}**
Dipole moment (in the gas phase) = **2.69 D**
Donor number (+info)= **17.0 kcal·mol^{-1}**
Acceptor number (+info)= **12.5**
$E_T(30)$ (+info)= **42.2 kcal·mol^{-1}**
E_T^N (+info)= **0.35**

(Click to clear)

WG4 DEVELOPMENT OF TOOLS, SERVICES AND FACILITIES FOR THE NECTAR COMMUNITY

TASK: PROVIDING UPDATED GUIDELINES, SOFTWARE AND SERVICES TO ENHANCE THE EFFECTIVENESS OF OUR RESEARCH INTO EQUILIBRIUM THERMODYNAMICS AND THE APPLICATION OF THE OUTCOMES

ONCE UPON A TIME;

Turin:
Master thesis on the development of a new version of ES4 software

Valencia:
Development of software for microspeciation analysis from NMR data fitting

Project start
02/10/2019

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Task Group – Software Development
September 2020

Project start
02/10/2019

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Task Group – Software Development
September 2020

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On-line Meeting of WG4
Task Group – Software Development
17/02/2021

- ✓ SpectrApp v.0 presentation
- ✓ Agreement to:
  - prepare survey on current software
  - test the available software on a dataset
  - develop software for potentiometric data analysis

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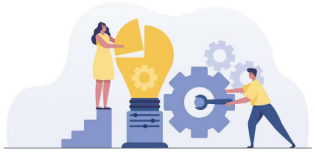

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- ✓ Survey results

NECTAR Spring Web-Meeting
25-26/03/2021

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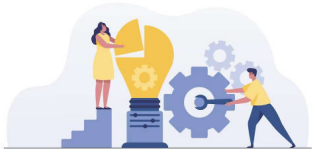

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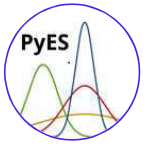
NECTAR Spring Web-Meeting
25-26/03/2021

WG2 - WG4 meeting, Valencia
9-10/06/2022

- ✓ Presentation of 1st version of PyES



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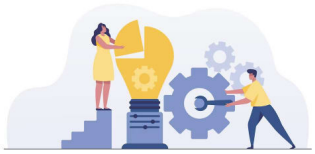

On-line Meeting of WG4
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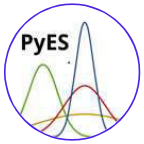

- ✓ Presentation of preliminary results of a comparative study on the current tools for optimization of stability constants from potentiometric data

3rd European NECTAR Conference
Ljubljana, 24-26/10/2022

https://www.uv.es/supramol/pages/software.html


Chemometrics and Intelligent Laboratory Systems 231 (2022) 104672

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journal homepage: www.elsevier.com/locate/chemometrics

GEMS, a tool for microspeciation analysis from NMR data fitting☆

Salvador Blasco[a,*], Mario Inclán[a,b], Begoña Verdejo[a], Enrique García-España[a]

[a] Institute of Molecular Science, University of Valencia, c/Catedrático José Beltrán Martínez 2, 46980, Paterna, Valencia, Spain
[b] Escuela Superior de Ingeniería, Ciencia y Tecnología, Universidad Internacional de Valencia - VIU, Valencia, Spain

GEMS publication
15 December 2022

https://www.uv.es/supramol/pages/software.html


Chemometrics and Intelligent Laboratory Systems 231 (2022) 104672

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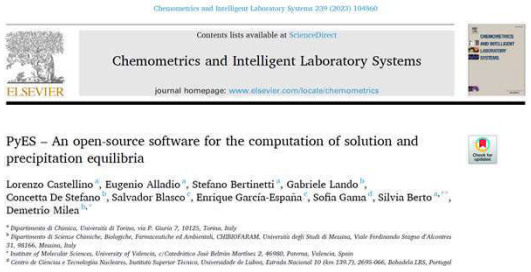
Chemometrics and Intelligent Laboratory Systems 239 (2023) 104860

Contents lists available at ScienceDirect

Chemometrics and Intelligent Laboratory Systems

journal homepage: www.elsevier.com/locate/chemometrics

PyES – An open-source software for the computation of solution and precipitation equilibria

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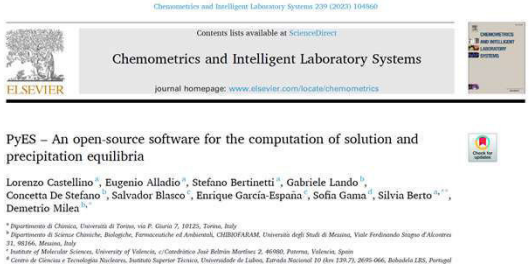
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Currently under second revision for publication in Analytical Chimica Acta

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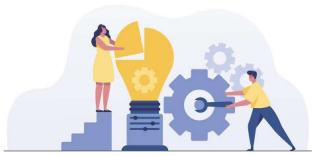

NECTAR WG1 meeting, Zagreb
28–29/09/2023

- ✓ Agreement to:
  - develop database searching software
  - apply FAIR principles to equilibrium data

https://www.uv.es/supramol/pages/software.html

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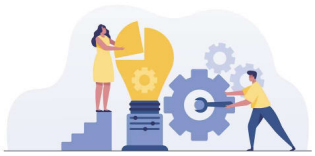

NECTAR WG1 meeting, Zagreb
28–29/09/2023

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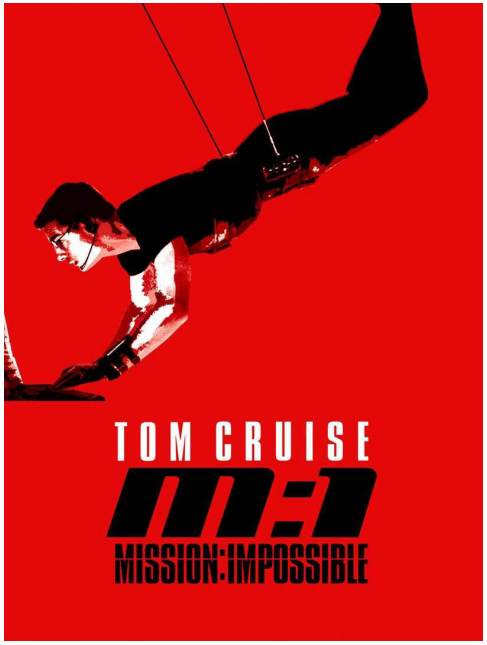
  - apply FAIR principles to equilibrium data

4th European NECTAR Conference and Final Action Meeting,
Milazzo, 26-27/02/2024

We feel like Ethan Hunt at the end of his first mission



We still have many more missions to solve

1. **SpectrAPP development**
   - Insertion of MCR-ALS
2. **Database searching software**
3. **PyES development and integration with related software:**
   - Follow up and application of the (solved) **issues and guidelines** coming from the different **interlab experiments** carried out within NECTAR
   - Implementing the **experimental design** function by suitably tuning the concentration of the reactants and the observable to be measured
   - Multiple species and stoichiometry, no binding models
   - Integration of PyES with related software for the analysis of potentiometric, UV-vis/fluo and calorimetric data also as a function of ionic strength and temperature

We still have many more missions to solve

4 **Survey**

What data do you consider necessary to completely define the experimental conditions?

How to compile metadata files

Potentiometry and UV-vis experiments

Deadline: May 2024

5 Analysis of the current tools for optimization of **formation constants** from potentiometric data on a more complex system.

Acknowledgments


Prof. Demetrio Milea


Dr. Sofia Gama

Prof. Winfried Plass


Prof. Aleksandar Cvetkovski

and all the colleagues who actively collaborated to achieve these outcomes;

by measurements, tests, discussions, revisions and much food for thought!

Acknowledgments

Department Chemistry
2023 - 2027 DEPARTMENT OF EXCELLENCE
Ministero dell'Università e della Ricerca
UNIVERSITÀ DI TORINO


Dr. Eugenio Alladio


Dr. Stefano Bertinetti


Dr. Lorenzo Castellino


Dr. Matteo Marafante

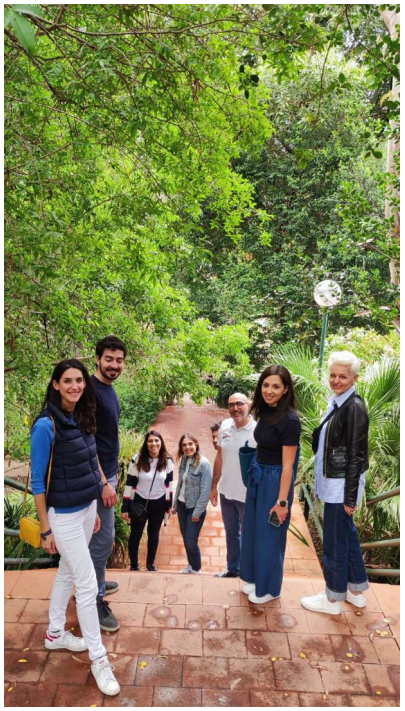
NECTAR
NETWORK FOR EQUILIBRIA AND CHEMICAL THERMODYNAMICS ADVANCED RESEARCH
CA18202

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

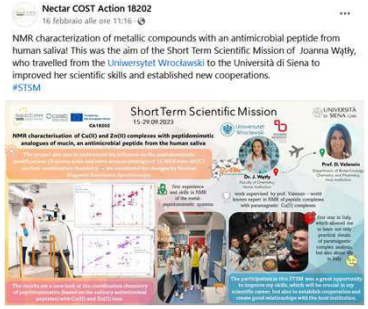
Milazzo, February 26th – 27th, 2024

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

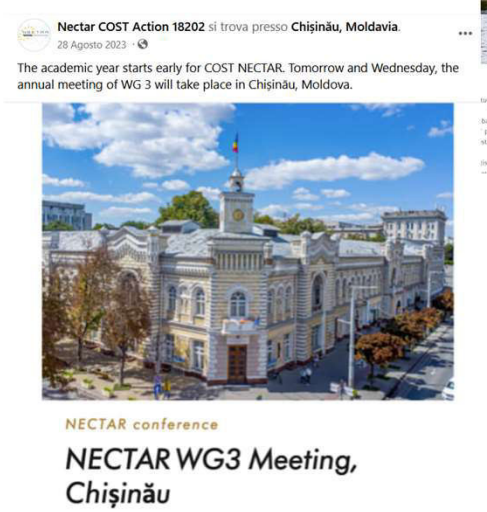
- Papers
- Short Term Scientific Missions
- Training schools
- Meetings



@CostNectar
@CostNectar
@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)

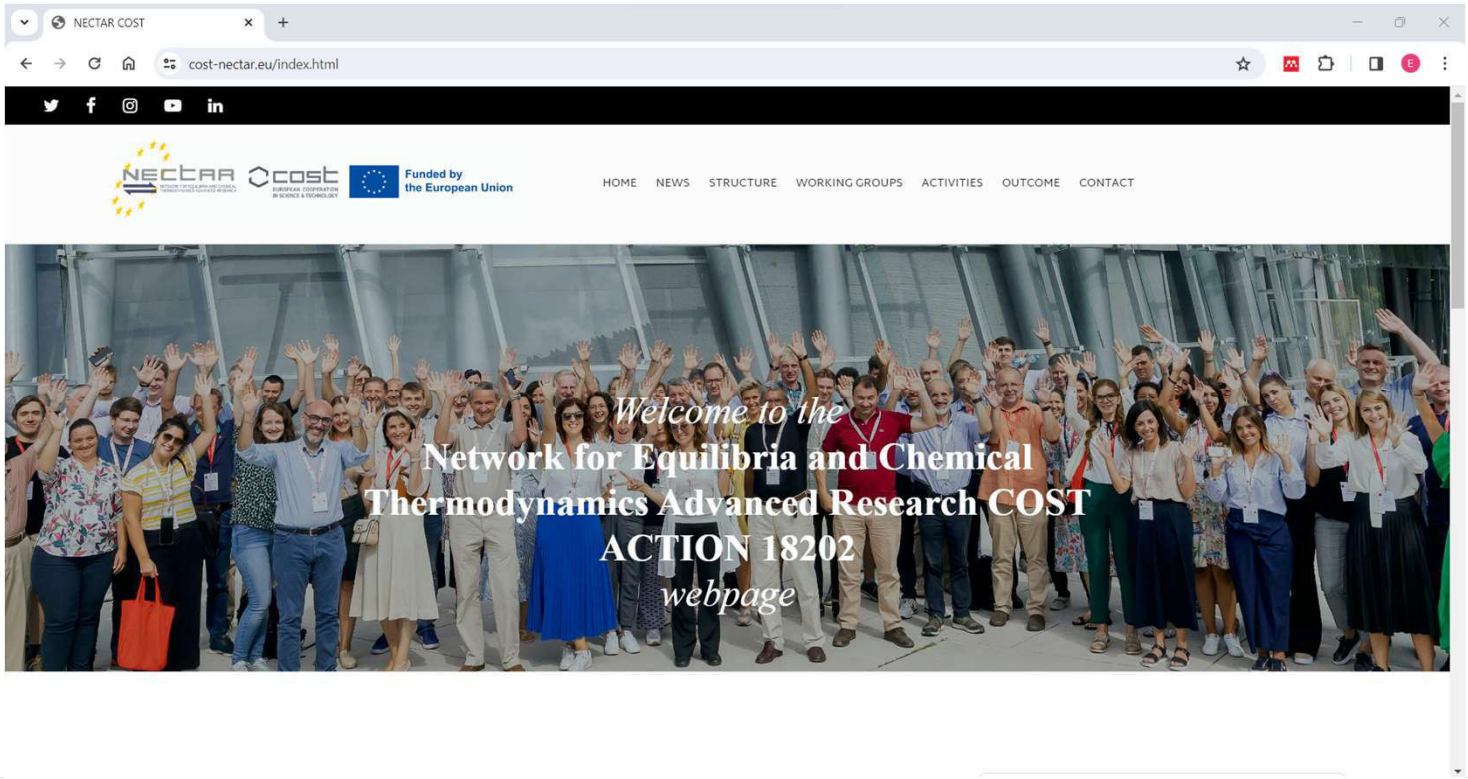
NECTAR-SciComm

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


NECTAR COST
cost-nectar.eu/index.html
Funded by the European Union
HOME
NEWS
STRUCTURE
WORKING GROUPS
ACTIVITIES
OUTCOME
CONTACT
Welcome to the
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

Network for Equilibria and Chemical Thermodynamics Advanced Research
COST ACTION 18202

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.

Network for Equilibria and Chemical Thermodynamics Advanced Research
COST ACTION 18202

NECTAR conference

NECTAR WG3 Meeting, Chişinău

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

Network for Equilibria and Chemical Thermodynamics Advanced Research
COST ACTION 18202

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

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HOME NEWS STRUCTURE WORKING GROUPS ACTIVITIES OUTCOME CONTACT

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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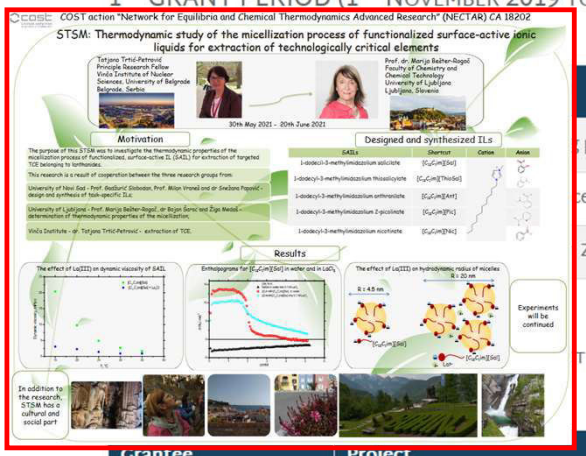
HOME NEWS STRUCTURE WORKING GROUPS ACTIVITIES OUTCOME CONTACT

ACTION MEETINGS
STSM
TRAINING SCHOOL

GRANTEES OF THE CALLS

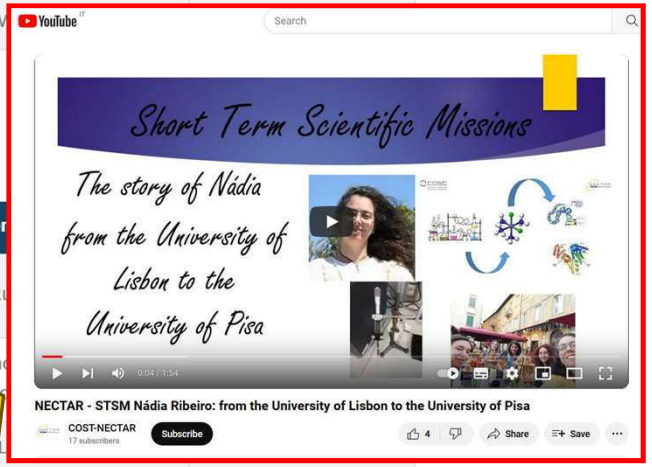
1ST GRANT PERIOD (1ST NOVEMBER 2019 TO 30TH APRIL 2020)



	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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HOME NEWS STRUCTURE WORKING GROUPS ACTIVITIES OUTCOME CONTACT

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

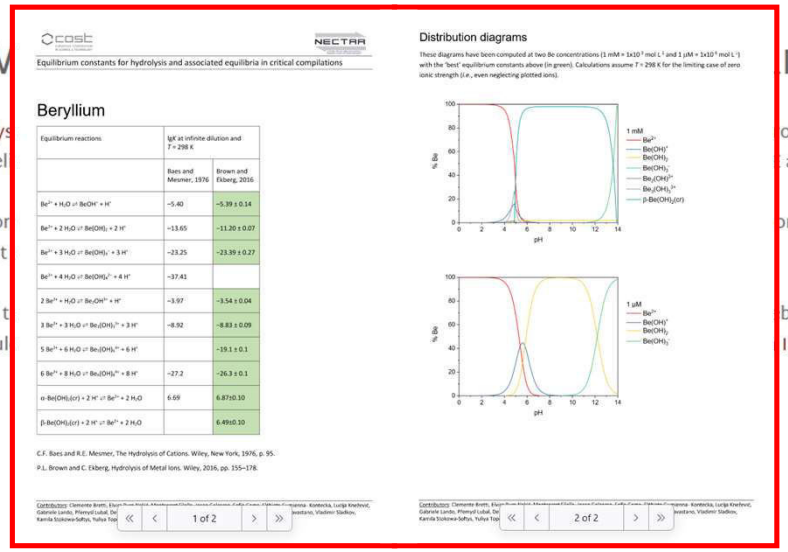
- PUBLICATIONS
- ACKNOWLEDGEMENT GUIDES
- WG1 PERIODIC TABLE
- WG3 PROPERTIES OF SOLVENTS
- WG3 SYNTHESIS AND PURIFICATION OF IONIC LIQUIDS
- WG4 TOOLS
- WG5 COMMUN. GUIDE

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.

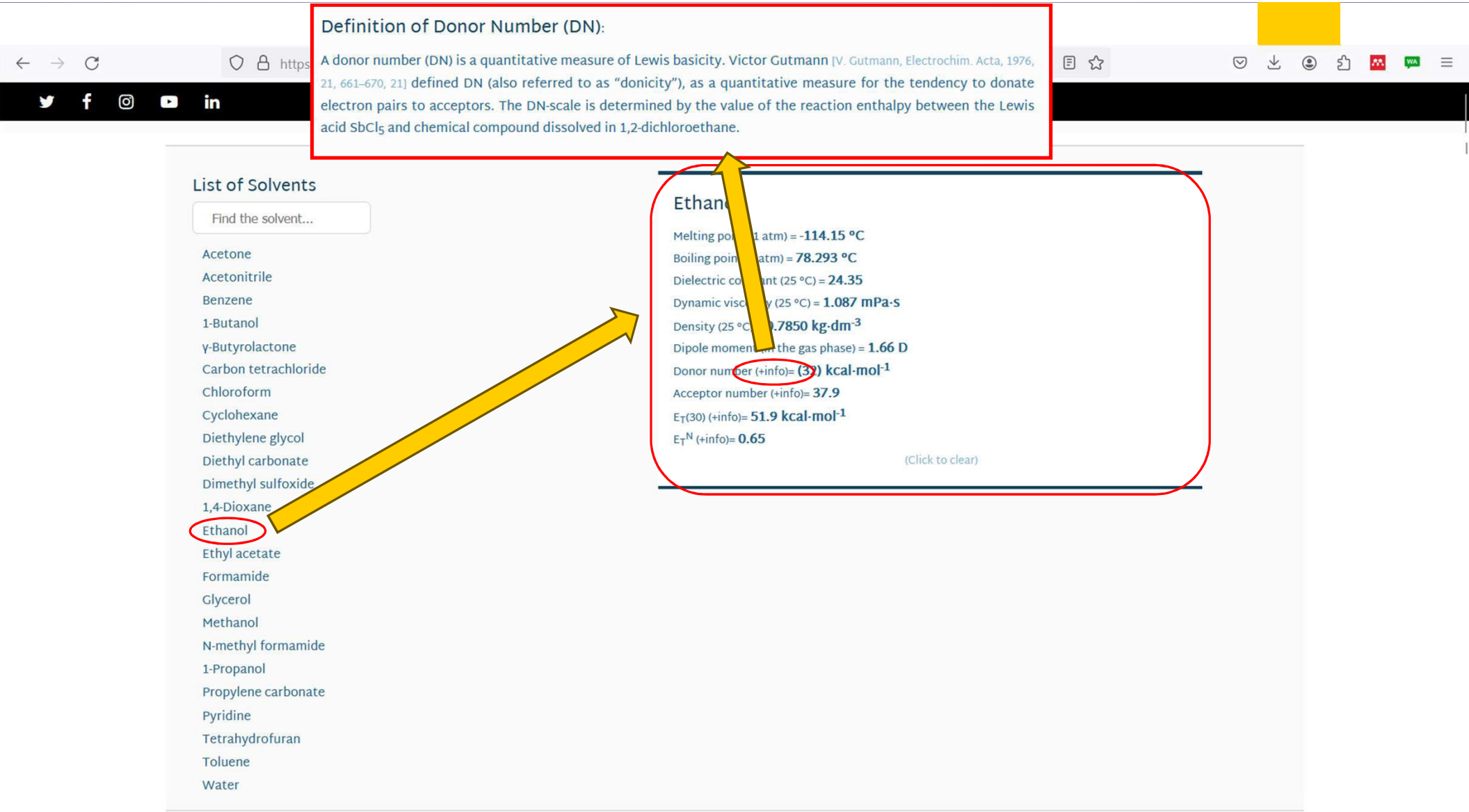
You can find the result of the wor… …ontaining its hydrc… …lues) at infinite dilution and T = 298 K gathered from the most…

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 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 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 ant (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
ET(30) (+info)= 51.9 kcal·mol-1
ETN (+info)= 0.65
(Click to clear)

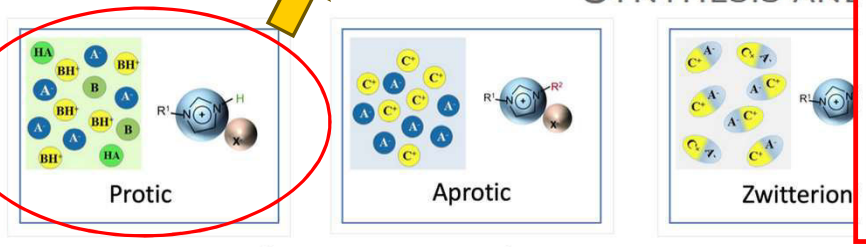
Protic Ionic Liquids (PILs)

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.

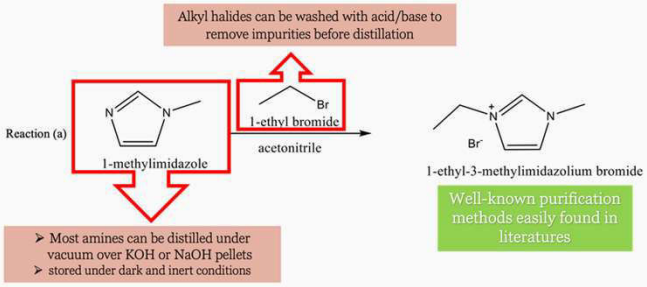
SYNTHESIS AND



Synthesis of Ionic Liquids

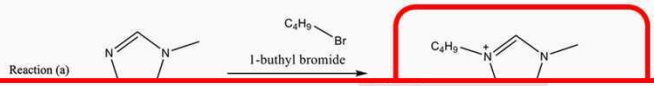
Purification

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



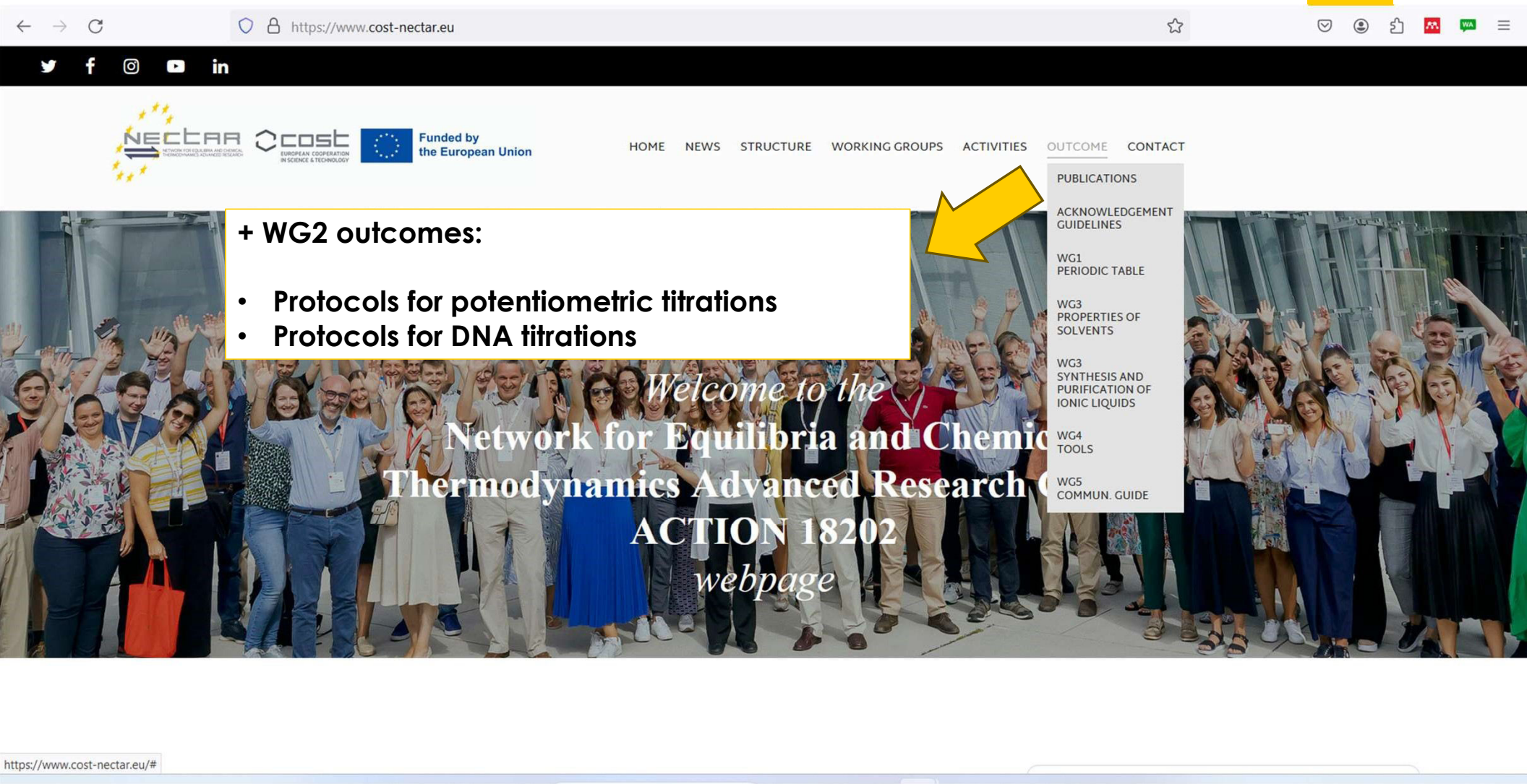
It is recommended to carry out the quaternization step right after purifying the starting compounds, as prolonged exposure to light or moisture can generate new impurities. Alternatively, starting compounds like amines can be stored under dark and inert conditions until needed.

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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HOME
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WG1 PERIODIC TABLE
WG3 PROPERTIES OF SOLVENTS
WG3 SYNTHESIS AND PURIFICATION OF IONIC LIQUIDS
WG4 TOOLS
WG5 COMMUN. GUIDE
+ WG2 outcomes:
• Protocols for potentiometric titrations
• Protocols for DNA titrations
Welcome to the
Network for Equilibria and Chemic
Thermodynamics Advanced Research
ACTION 18202
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

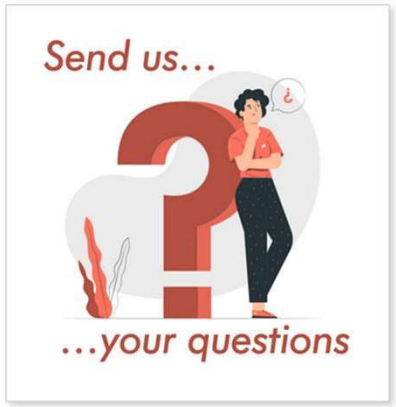
SpectrApp, a one-stop solution for small to mid-sized soft modeling problems.

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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NECTAR COST Action

SHORT TERM SCIENTIFIC MISSIONS

(STSM)

Final meeting, Milazzo - February 2024

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EUROPEAN COOPERATION
IN SCIENCE & TECHNOLOGY

Funded by the Horizon 2020 Framework Programme
of the European Union

NECTAR
NETWORK FOR EQUILIBRIA AND CHEMICAL
THERMODYNAMICS ADVANCED RESEARCH

SHORT TERM SCIENTIFIC MISSION (STSM)

CALL #	Countries (Home)
Call 1 (November 2019)	Italy (3), France
Call 2 (July 2020)	Italy (2), Poland, Croatia, Hungary, Slovakia, Republic of Serbia
Call 3 (October 2020)	Italy (2), Poland (3), Spain
Call 4 (February 2021)	Spain, Poland (2), Italy (2)
Call 5 (August 2021)	Italy (2), Poland (2)
Call 6 (January 2022)	Poland (3), Spain, Germany, Italy, Czech Republic, Republic of Serbia, Bosnia and Herzegovina, Hungary
Call 7 (June 2022)	Poland (3), Spain, Italy (2), Republic of Serbia, North Macedonia
Call 8 (November 2022)	Poland (3), Italy (4), Hungary, Republic of Serbia (2), France
Call 9 (June 2023)	Poland (2), Republic of Serbia (3), Italy
Call 10 (November 2023)	Republic of Serbia (2), Italy, Slovenia, Poland (2), Slovak Republic, Spain, Hungary, Moldova

SHORT TERM SCIENTIFIC MISSION (STSM)

	Grants	Budget
GP1	3	3 600 €
GP2	17	23 050 €
GP3	21	26 400 €
GP4	18	24 400 €
GP5	10	14 100 €

COST training school

Call Open for 1st SOLvE Training School!

1st ISMEC - NECTAR Training School on the Determination, Analysis and Use of Thermodynamic Data.
Deadline for applications: ***June 15th, 2021***

Network for Equilibria and Chemical Thermodynamics Advanced Research
COST ACTION 18202

COST training school

Call Open for 2nd SOLvE Training School!

2nd ISMEC - NECTAR Training School on the Determination, Analysis and Use of Thermodynamic Data.
Deadline for applications: ***June 24th, 2022***

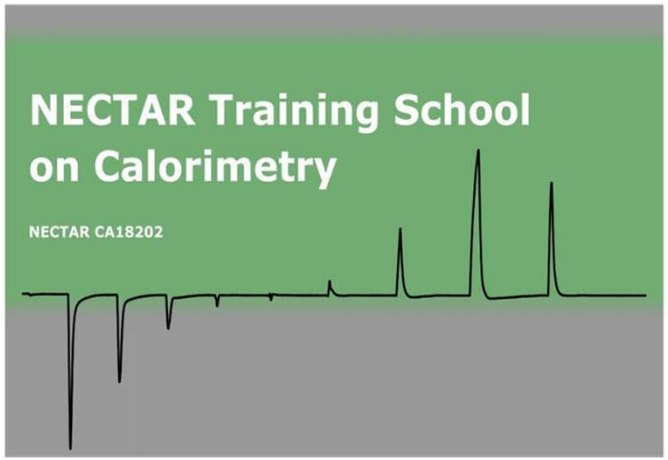
Network for Equilibria and Chemical Thermodynamics Advanced Research
COST ACTION 18202

COST training school

Call Open for 3rd SOLvE Training School!

3rd ISMEC - NECTAR Training School on the Determination, Analysis and Use of Thermodynamic Data.
Deadline for applications: ***July 7th, 2023***

Network for Equilibria and Chemical Thermodynamics Advanced Research
COST ACTION 18202



COST training school

NECTAR training school on Calorimetry

Date: August 27th, 2022
Place: University of Ljubljana, Slovenia
Deadline for applications: ***July 22nd, 2022***

Network for Equilibria and Chemical Thermodynamics Advanced Research
COST ACTION 18202

COST training school

NECTAR training school on Communication in Science

Date: May 29th, 2023
Place: Botanic Garden, Cagliari (Italy)
Deadline for applications: ***April 23rd, 2023***

Network for Equilibria and Chemical Thermodynamics Advanced Research
COST ACTION 18202

COST advanced school

NECTAR Advanced school on aqua ions and hydrolysis-related equilibria

Date: September 29th, 2023
Place: Ruđer Bošković Institute, Zagreb (HR)
Deadline for applications: ***July 17th, 2022***

Network for Equilibria and Chemical Thermodynamics Advanced Research
COST ACTION 18202

cost
EUROPEAN COOPERATION IN SCIENCE & TECHNOLOGY

Dedicated to:

....students (MSc, PhD), post docs or professionals involved in the study of solution equilibria and the analysis of relevant thermodynamic parameters.

The well-known computer science motto of "garbage-in garbage-out" perfectly holds also for chemical thermodynamics.

Researchers working in this field need high-quality data to obtain high-quality results. Analogously, any subject dealing with chemical thermodynamics need high-quality data and models to ensure their robustness for high-quality applications.

SOLvE in an **online** training school which will help people dealing with solution equilibria in promoting good laboratory practices. Experienced professors will provide focused theoretical background, practical aspects and tips for high-quality experimental data collection and clues for robust data analysis through different models and protocols (ranging from Excel to more specialised software). The main experimental approaches for solution equilibria will be presented and discussed. Applications of each technique to cutting-edge research will be also highlighted.

www.cost-nectar.eu
www.ismecgroup.org

Organized by:

Chairs:

Tarita Biver	University of Pisa (IT)
Sofia Gama	University of Białystok (PL)
Demetrio Milea	University of Messina (IT)
Carmelo Sgarlata	University of Catania (IT)

NECTAR Supervision:

Enrique García-España	University of Valencia (ES) TS Coordinator

Important info:

Deadline: 15th June 2021

Registration fee: 30 €
15 NECTAR free slots available

Registration fee includes:
- 12 + 1 topic lectures
- Training material

Min number of participants required: 10

Contact – Info – Registration:

solve@uwb.edu.pl

International Group for the Thermodynamics of Complexes

1st ISMEC-NECTAR Training School

on the
Determination, Analysis and Use
of Thermodynamic Data

Advances in SOLution Equilibria

July 26th-28th, 2021

1st ISMEC-NECTAR Training School

on the

Determination, Analysis and Use of Thermodynamic Data

Advances in SOLution Equilibria

July 26th-28th, 2021

Credits: Sofia Gama

2.5 DAYS ⇒ INTRODUCTION TO SOLUTION EQUILIBRIA + 4 FOCUSED TOPICS

A **plenary lecture** will introduce the theoretical background for a correct approach to solution equilibria.

Each session of the school (half a day) will be focused on a specific technique

- Potentiometry & Electrochemical techniques
- Spectrophotometry & Spectrofluorimetry
- NMR
- Calorimetry

At the end of each session, an experienced researcher will present the applications of each technique in nowadays research.

www.cost-nectar.eu
www.ismecgroup.org

PROGRAMME (CET time)

July 26th	July 27th	July 28th
	9:30-10:20 TOPIC 2 Theory	9:30-10:20 TOPIC 4 Theory
10:00-10:20 Opening	10:30-11:20 Data treatment	10:30-11:20 Data treatment
10:20-12:00 *Introduction to solution equilibria*	11:30-12:20 Application	11:30-12:30 Application
	12:20-13:00 Open discussion	12:20-13:00 Open discussion
Lunch Break	Lunch Break	Closing remarks
15:00-15:50 TOPIC 1 Theory	15:00-15:50 TOPIC 3 Theory	
16:00-16:50 Data treatment	16:00-16:50 Data treatment	
17:00-17:50 Application	17:00-17:50 Application	
17:50-18:30 Open discussion	17:50-18:30 Open discussion	

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EUROPEAN COOPERATION IN SCIENCE & TECHNOLOGY

Dedicated to:

....students (MSc, PhD), post docs or professionals involved in the study of solution equilibria and the analysis of relevant thermodynamic parameters.

The well-known computer science motto of "garbage-in garbage-out" perfectly holds also for chemical thermodynamics.

Researchers working in this field need high-quality data to obtain high-quality results. Analogously, any subject dealing with chemical thermodynamics needs high-quality data and models to ensure their robustness for high-quality applications.

SOLvE in an **online** training school which will help people dealing with solution equilibria in promoting good laboratory practices. Experienced professors will provide focused theoretical background, practical aspects and tips for high-quality experimental data collection and clues for robust data analysis through different models and protocols (ranging from Excel to more specialised software). The main experimental approaches for solution equilibria will be presented and discussed. Applications of each technique to cutting-edge research will be also highlighted.

www.cost-nectar.eu

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Chairs:

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Sofia Gama	University of Bialystok (PL)
Demetrio Milea	University of Messina (IT)
Carmelo Sgarlata	University of Catania (IT)

NECTAR CA18202 Supervision:

Enrique García-España	University of Valencia (ES) TS Coordinator

Important info:

Deadline: 24th June 2022

Registration fee: 30 €
15 NECTAR CA18202 free slots available

Registration fee includes:
- Topic lectures
- Training material

Min number of participants required: 10

Contact – Info – Registration:

solve@uwb.edu.pl

International Group for the Thermodynamics of Complexes

2nd ISMEC-NECTAR Training School

on the
Determination, Analysis and Use
of Thermodynamic Data

Advances in SOLution Equilibria

July 25th-27th, 2022

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International Group for the Thermodynamics of Complexes

NECTAR

NETWORK FOR EQUILIBRIA AND CHEMICAL THERMODYNAMICS ADVANCED RESEARCH

2nd ISMEC-NECTAR Training School

on the

Determination, Analysis and Use of Thermodynamic Data

Advances in **SOL**ution **E**quilibria

July 25th-27th, 2022

cost EUROPEAN COOPERATION IN SCIENCE & TECHNOLOGY

- ✓ **INTRODUCTION TO EQUILIBRIA**
- ✓ **FOCUSED TOPICS**
- ✓ **THEORY & PRACTICE**
- ✓ **APPLICATIONS**

A lecture will introduce the framework for a correct approach to chemical speciation in solution

Then, the school will focus on the theoretical background and practical information for the study of solution equilibria by using:

- **electrochemical techniques**
- **spectroscopic/spectrometric techniques**
- **calorimetric techniques**

Also, experienced researchers will present their applications in nowadays research

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PROGRAMME (CET time)

July 25th	July 26th	July 27th
10:00-10:10 Opening	9:30-10:50 EXAFS Theory, Applications & Software	9:30-10:20 Calorimetry Instrumentation & Data Analysis
10:20-11:20 Introduction to Solution Equilibria		10:30-11:20 Calorimetry Main Issues & Case Studies
Coffee Break		
11:40-12:40 Theoretical Calculations for Speciation	11:10-12:30 Fluorescence Theory, Applications & Software	11:40-12:30 Calorimetry Applications
12:40-13:00 Q&A	12:40-13:00 Q&A	12:30-13:00 Q&A/Closing
Lunch Break		
15:00-16:20 Voltammetry & Potentiometry Theory	15:00-16:20 EPR Theory, Applications & Software	
Coffee Break		
16:40-18:00 Voltammetry & Potentiometry Applications	16:40-18:00 EPR Applications & Software	
18:00-18:30 Q&A	18:00-18:30 Q&A	

solve@uwb.edu.pl

2nd ISMEC-NECTAR Training School
on the Determination, Analysis and Use of Thermodynamic Data

Advances in **SOL**ution **E**quilibria

DETAILED PROGRAMME (CET)

2nd ISMEC-NECTAR Training School Programme

Monday, July 25th		Tuesday, July 26th		Wednesday, July 27th	
09:30 - 09:40	Opening Ceremony	9:30 - 10:50	Maria Rosa Beccia (Univ of Nice, France)	9:30 - 10:20	Bojan Šarac / Žiga Medoš (Univ of Ljubljana, Slovenia)
09:40 -10:40	Enrique Garcia-España (Univ of Valencia, Spain)			10:30 - 11:20	Matteo Savastano (Univ of Florence, Italy)
10:40 - 11:00	Coffee Break	10:40 - 11:00	Coffee Break	11:20 - 11:40	Coffee Break
11:00 - 12:00	Giampaolo Barone (Univ of Palermo, Italy)	11:10 - 12:30	Mauro Formica (Univ of Urbino, Italy)	11:40 - 12:30	Marija Bešter Rogač (Univ of Ljubljana, Slovenia)
12:00 - 12:30	Elżbieta Gumienna-Kontecka (Univ of Wroclaw, Poland)				
12:40 - 13:00	Q & A	12:40 - 13:00	Q & A	12:40 - 13:00	Q & A
13:00 - 15:00	Lunch Break	13:00 - 15:00	Lunch Break		
15:00 - 16:20	Caren Billing (Univ of Witwatersrand, South Africa)	15:00 - 16:20	Oluseun Akintola (Univ of Jena, Germany)		
16:20 - 16:40	Coffee Break	16:20 - 16:40	Coffee Break		
16:40 - 18:00	Gabriele Lando (Univ of Messina, Italy)	16:40 - 18:00	Nóra V. May (Research Centre for Natural Sciences, Hungary)		
18:00 - 18:30	Q & A	18:00 - 18:30	Q & A		

Monday, July 25th

9:30 – 9:40 **Opening**

9:40 – 10:40 **"Supramolecular Chemistry in water. Case reports"**
Enrique Garcia-España (University of Valencia, Spain)

10:40 – 11:00 ***Coffee Break***

11:00 – 12:00 **"Structure, stability and metal coordination of ligands in solution investigated by DFT calculations"**
Giampaolo Barone (University of Palermo, Italy)

12:00 – 12:30 **"How to present your research with impact"**
Elżbieta Gumienna-Kontecka (University of Wroclaw, Poland)

12:40 – 13:00 **Q&A**

Dedicated to:

....students (MSc, PhD), post docs or professionals involved in the study of solution equilibria and the analysis of relevant thermodynamic parameters.

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Sofia Gama	Univ Bialystok (PL) / Univ Lisbon (PT)
Demetrio Milea	University of Messina (IT)
Carmelo Sgarlata	University of Catania (IT)

NECTAR CA18202 Supervision:

Enrique García-España University of Valencia (ES)
TS Coordinator

Important info:

Deadline: 7th July 2023

Registration fee: 30 €
15 NECTAR CA18202 free slots available

Registration fee includes:
- Topic lectures
- Training material

Min number of participants required: 10

Contact – Info – Registration:

solve@cost-nectar.eu

3rd ISMEC-NECTAR Training School

on the
Determination, Analysis and Use
of Thermodynamic Data

Advances in
SOLution **E**quilibria

July 24th-26th, 2023

3rd ISMEC-NECTAR Training School

on the

Determination, Analysis and Use of Thermodynamic Data

Advances in **SOL**ution **E**quilibria

July 24th-26th, 2023

The school contains both

- ✓ **THEORY & PRACTICE**
- ✓ **FOCUSED TOPICS**

Two opening lectures will introduce the framework for a correct approach to chemical speciation in solution and multivariate tools.

Then, the school will focus on the theoretical background and practical information for the study of solution equilibria by using:

- **spectroscopic/spectrometric techniques**
- **electrochemical techniques**
- **calorimetric techniques**

Practical examples will show how to extract a robust binding constant value from the experiments.
Two plenary lectures will present further points of view on solution equilibria.

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PROGRAMME/MAIN TOPICS (CET time)

July 24th	July 25th	July 26th
9:00-9:20 **Opening**	9:10-10:10 **T. Biver** How to design spectroscopic experiments	9:10-10:10 **C. Sgarlata** How to design calorimetric experiments
9:20-10:50 **S. Berto** Speciation and use of databases	10:10-11:20 Spectroscopy: a practical test	10:10-11:20 Calorimetry: a practical test
Coffee Break	*Coffee Break*	
11:10-12:40 **R. Biesuz** Multivariate tools	11:40-12:40 **P. Rapta** Spectro-electrochemistry	11:40-12:40 **A. Paulo** Metal-Based Radio-pharmaceuticals
12:40-13:00 **Q&A**	12:40-13:00 **Q&A**	12:40-13:00 **Q&A/Closing**
Lunch Break		
15:00-16:20 **S. Gama** How to design NMR experiments	15:00-16:20 **D. Milea** How to design potentiometric experiments	
Coffee Break		
16:40-18:00 NMR: a practical test	16:40-18:00 Potentiometry: a practical test	
18:00-18:30 **Q&A**	18:00-18:30 **Q&A**	

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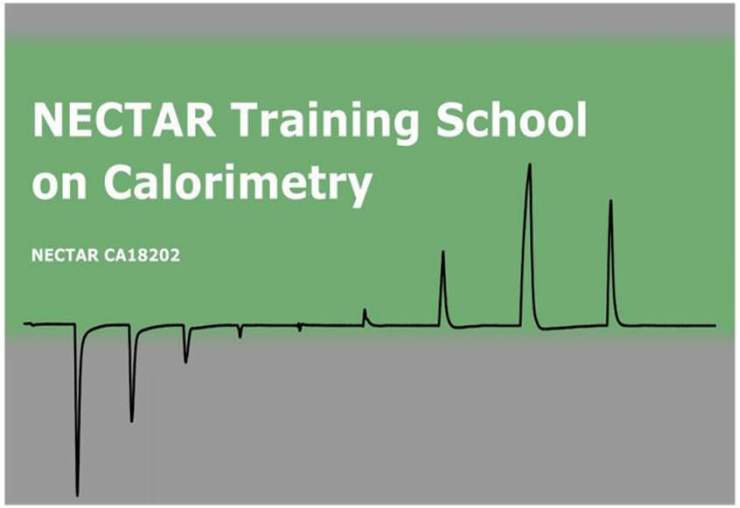

COST training school

NECTAR training school on Calorimetry

Date: August 27th, 2022
Place: University of Ljubljana, Slovenia
Deadline for applications: *July 22nd, 2022*

Network for Equilibria and Chemical Thermodynamics Advanced Research
COST ACTION 18202

Application Deadline: **July 22nd, 2022**
Registration: **cost.nectar@fkkt.uni-lj.si**
Max. Number of Participants (NECTAR CA18202 trainees): **15**

Programme:

08:45 **Opening**

09:00-10:00 **Peter VIKEGARD Waters Sverige AB**
Isothermal calorimetry: A discussion on measuring principles, systematic/random error, and experimental problems

10:00-11:00 **Carmelo SGARLATA University of Catania**
ITC for the study of host-guest systems: Issues related to multiple equilibria data fitting

---BREAK---

11:30-12:30 **Žiga MEDOŠ University of Ljubljana**
Detailed overview of using ITC to study micellization

12:30-13:30 **San HADŽI University of Ljubljana**
ITC with biomolecules: Successes and failures

---LUNCH---

15:00-16:00 **Andrea MELCHIOR University of Udine**
Titration calorimetry applied to the study of complex formation in solution and on surfaces

16:00-17:00 **Joel TELLINGHUISEN Vanderbilt University**
Better ITC by avoiding common pitfalls and misconceptions

---Q&A session---

17:30 **Practical demonstration in LAB**

Scientific Commitee:
Marija BEŠTER-ROGAČ University of Ljubljana (Chair)
Carmelo SGARLATA University of Catania (Chair)
Demetrio MILEA University of Messina (NECTAR CA18202 Action Chair)
Sofia GAMA University of Bialystok (NECTAR CA18202 Vice Chair)
Enrique GARCÍA-ESPAÑA University of Valencia (NECTAR CA18202 TS Coordinator)

COST training school

NECTAR training school on Communication in Science

Date: May 29th, 2023
Place: Botanic Garden, Cagliari (Italy)
Deadline for applications: *April 23rd, 2023*

Network for Equilibria and Chemical Thermodynamics Advanced Research
COST ACTION 18202

NECTAR-SciComm program

Monday, 29th May

9:00 – 9:15	**Registration**
9:15 – 9:30	**Opening ceremony**
9:30 – 10:30	**Science Communication within and outside NECTAR** Elzbieta GUMIENNA-KONTECKA (SCM) - *University of Wroclaw, Poland*
10:30 – 11:00	*Coffee break*
11:00 – 11:45	**Introduction to Science Communication** Empar VENGUT CLIMENT – *University of València, Spain*
11:45 – 12:15	**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*
12:15 – 12:45	**Video editing tools accessible to everyone** Emanuele ZANDA – *University Paris-Saclay, France*
12:45 – 14:30	*Lunch break*
14:30 – 16:15	**Unravelling your jargon: How to better communicate science to the media. Part 1** Adriano CERQUEIRA – *NOVA University of Lisbon, Portugal*
16:15 – 17:45	*Coffee break*
16:45 – 17:45	**Unravelling your jargon: How to better communicate science to the media. Part 2** Adriano CERQUEIRA – *NOVA University of Lisbon, Portugal*
17:45 – 18:00	**Closing ceremony**

Funded by the European Union

COST advanced school

NECTAR Advanced school on aqua ions and hydrolysis-related equilibria

Date: September 29th, 2023
Place: Ruđer Bošković Institute, Zagreb (HR)
Deadline for applications: *July 17th, 2022*

Network for Equilibria and Chemical Thermodynamics Advanced Research
COST ACTION 18202

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

THANKS TO

Tarita Biver	University of Pisa (IT)
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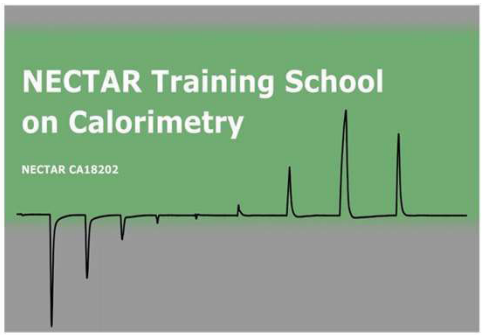

Scientific Commitee:
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Carmelo SGARLATA University of Catania (Chair)
Demetrio MILEA University of Messina (NECTAR CA18202 Action Chair)
Sofia GAMA University of Bialystok (NECTAR CA18202 Vice Chair)

COST training school

NECTAR training school on Communication in Science

COST advanced school

NECTAR Advanced school on aqua ions and hydrolysis-related equilibria

THANKS TO

Demetrio Milea (Action Chair)	U. Messina
Sofia Gama (Action vice-Chair)	U. Białystok
Alvaro Martinez (WG5 Leader)	U . Valencia
Emanuele Zanda (WG5 co-Leader)	U. Paris-S.
Elzbieta Kontecka (Sc. Comm. Manager)	U. Wrocław
Rosita Cappai	U. Sassari

Prof. Elvira Bura Nakić Ruđer Bošković Institut , Zagreb
Dr. Dario Omanović Ruđer Bošković Institut , Zagreb
Dr. Saša Marcinek Ruđer Bošković Institut , Zagreb
Dr. Lucija Knežević University of Zagreb
Dr. Olga Iranzo (leader WG1) Institut des Sciences Moléculaires de Marseille
Prof. Montserrat Filella (co-leader WG1) University of Geneva

all the coaches and trainees that have participated in the schools

SPECIAL THANKS AND CONGRATULATIONS TO

4TH EUROPEAN NECTAR CONFERENCE
MILAZZO, FEBRUARY 26TH-27TH 2024

ITC-CA18202
NETWORK FOR EQUILIBRIA AND CHEMICAL THERMODYNAMICS ADVANCED RESEARCH

Prof.Dr. Emel YILDIZ
ITC Coordinator

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CA18202 NECTAR

NECTAR involves; European Scientists Working in The Field of Chemical Equilibrium Thermodynamics and Technology-oriented Partners and Enterprises

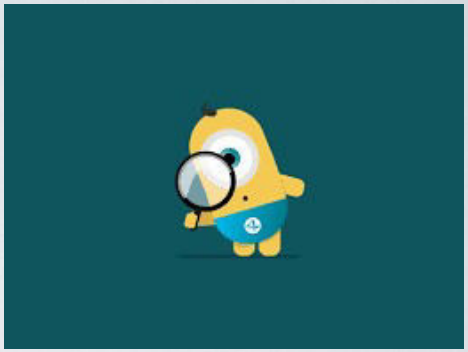
10/02/2019- 04/01/2024

- Number of parties : **31**
- Number of ITC: **19**

NECTAR...

In the field of chemical thermodynamics:

- Bringing together professionals at all levels and in different sectors
- Fostering innovations and knowledge exchange
- Leveraging complementary skills
- Keeping abreast of the latest findings and developments
- Creating a valuable platform for content sharing



- Coordination and promotion of ITCs' participation (increasing the number of partners),
- Participation of non-academic organizations and companies

Current situation (ITC)

Albania	Moldova
Bosnia & Herzegovina	North Macedonia
Bulgaria	Serbia
Croatia Greece	Slovakia
Czech Republic	Slovenia
Estonia	Poland
Hungary	Portugal
Lithuania	Romania
Malta	Turkiye

Other ITCs

- Cyprus,
- Latvia,
- Luxembourg,
- Montenegro,

COST Near Neighbor Country

Institution Name	Country
Enamine Limited Liability Company (Enamine LLC)	Ukraine
Taras Shevchenko National University of Kyiv	Ukraine

INTEGRATION

- IPC (from USA and Australia) and two NNC (both from Ukraine) partners
- NNCs (Near Neighbor Countries, Russia, Egypt, Tunisia, Algeria) and Israel

ITC'S CALLS

COST Action CA18202
NECTAR – Network for Equilibria and Chemical Thermodynamics Advanced Research

Inclusiveness Target Countries (ITC) Conference Grants (CG)

Call for ITC Conference Grant Applications

Fourth Grant Period, 1 November 2022- 31 October 2023

COST Action NECTAR opens a call for applications to ITC Conference to be developed under the scope of the referredAction, in the terms described in this document.
The main procedures/regulations concerning ITC Conferences are governed by the Rules and Principles for COST activities (level A) and the Rules for COST Actions (level B), from which the Annotated Rules for COST Actions (level C) result, https://www.cost.eu/uploads/2021/07/COST-088-21-Level-A-Rules-and-Principles-for-COST-Activities.pdf). COST Grant Awarding User Guide (https://www.cost.eu/uploads/2021/12/Grant-Awarding-userguide.pdf, Page 7), Please read this section prior to preparing your ITC Conference application.

Thermodynamic protonation parameters of a tryptophan metabolite (8-hydroxyquinoline-2-carboxylic acid, 8-HQA)

VALÈNCIA, 5th - 8th June 2022

[a] University of Bialyst
[b] University of Bialystok, Fa
[c] Università degli Studi di Messina, Dipartim

Tryptophan (Trp) is an essential exogenous amino ac
and the central nervous systems, with a significant
(8-HQ) metabolites, reported as anti-microbial, an
solutions seems to be a crucial aspect to access the
298.15 K are not sufficient. For that purpose, the de
present some preliminary results on the thermodyn
aqueous solution determined by ISE-H+ (glass electro

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Report on the outcomes of a presentation and participation in a ITC Conference[1]

Action number: CA18202

Grantee name: Anna Baryłka

Conference Details

Conference title: ISMEC 2022 International Symposium on Metal Complexes

Conference web-page: https://www.ismec2022.org/index.html

Conference venue[2]: Organized by the Institute of Molecular Science, Faculty of Chemistry, University of Valencia, will take place in the auditorium of the Valencia's Botanic Garden

Conference start and end date: 05/06/2022 to 08/06/2022

Accepted contribution details

Title of the presentation: Thermodynamic protonation parameters of a tryptophan metabolite (8-hydroxyquinoline-2-carboxilic acid) and its molecular precursors: a potentiometric study at different temperatures

Type of the presentation: poster

Co-authors: Aneta Bagińska, Beata Godlewska-Żyłkiewicz, Demetrio Milea, Sofia Gama

ITC Conference Grant
- APPLICATION FORM[1] -

Action number: CA18202

Applicant name: Valentyn Dzyhovskyi

Conference Details

Conference title: 16th European Biologic Inorganic Chemistry Conference (EuroBIC-16)

Conference web-page: https://eurobic16.sciencesconf.org/

Conference venue[2]: face to face

Conference start and end date: 17/07/2022 to 21/07/2022

Accepted contribution details

Title of the presentation: Coordination properties of ligands constituting fragments of FeoB from *Staphylococcus aureus*

Type of the presentation: poster

Co-authors: Kamila Stokowa-Sołtys

Other details of the presentation: specify here any additional details related to the contribution (e.g. title of the session / track of the conference programme in which the contribution is accepted)

CONCLUSION

- Two ITC's conference grant announced
- Two applicants awarded
- Early-stage researchers as MC substituted and companies added to NECTAR from ITCs
- Third ITC's conference grant call was prepared but not announced

and

Facebook @CostNectar,

Instagram @nectar18202,

X @CostNectar,

Linked in Nectar Cost Action!

With the hope of being together in a new COST Action…

for your attention!

cost
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IN SCIENCE & TECHNOLOGY

NECTAR
NETWORK FOR EQUILIBRIA AND CHEMICAL THERMODYNAMICS ADVANCED RESEARCH

Memorandum of Understanding for the implementation of the COST Action "Network for Equilibria and Chemical Thermodynamics Advanced Research" (NECTAR) CA18202

Equal Opportunities Manager

responsible for fulfilling the requirements of

i) involvement of **I**nclusiveness **T**arget **C**ountries

ii) gender balance

iii) involvement of **E**arly **C**areer **I**nvestigators

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Involvement of **I**nclusiveness **T**arget **C**ountries

Starting: 64 people from 19 coutries

Now: **293** people from **32** countries

Albania: 2
Bosnia and Herzegovina: 3
Bulgaria: 2
Czech Republic: 14
Estonia: 1
Croatia: 14
Greece: 2
Hungary: 8
Lithuania: 2
Malta: 1
Moldova: 18
Poland: 18
Portugal: 13
Romania: 3
Slovenia: 20
Slovakia: 3
North Macedonia: 2
Serbia: 15
Turkey: 4

19 ITC countries
145 people (**49%**)

ITC countries:
Albania, Armenia, **Bosnia and Herzegovina**, **Bulgaria**, Cyprus, **Czech Republic**, **Estonia**, **Croatia**, Georgia, **Greece**, **Hungary**, **Lithuania**, Latvia, **Malta**, **Moldova**, Montenegro, **Poland**, **Portugal**, **Romania**, **Slovenia**, **Slovakia**, **North Macedonia**, **Serbia**, **Turkey**, Ukraine

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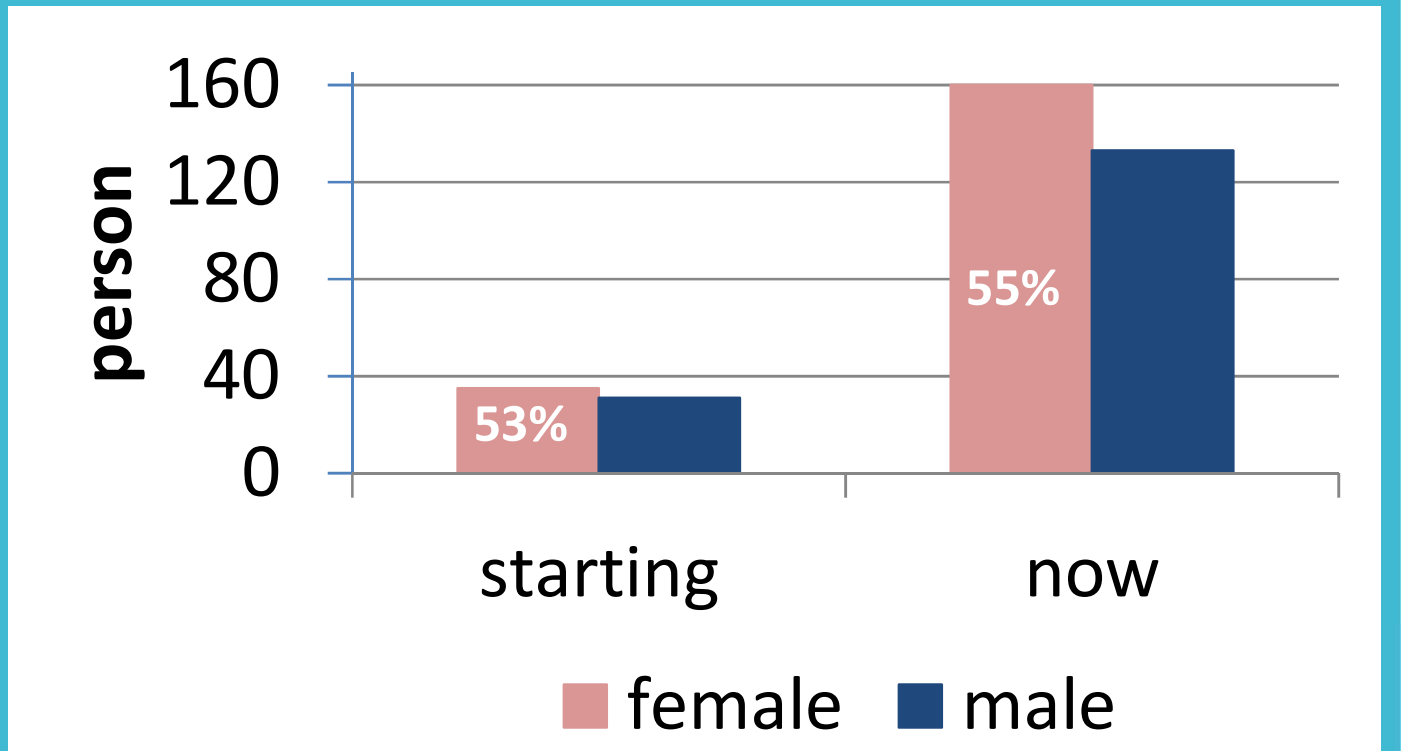
Gender balance



Starting:

35 female

31 male

Now:

160 female

133 male

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Early Career Investigators

to encourage and suppoort them

- to actively take part in all levels

- to interact with and learn from more experienced researchers

- to take the short term missions

Starting:
10 ECI
(16%)

Now:
80 ECI
(27%)

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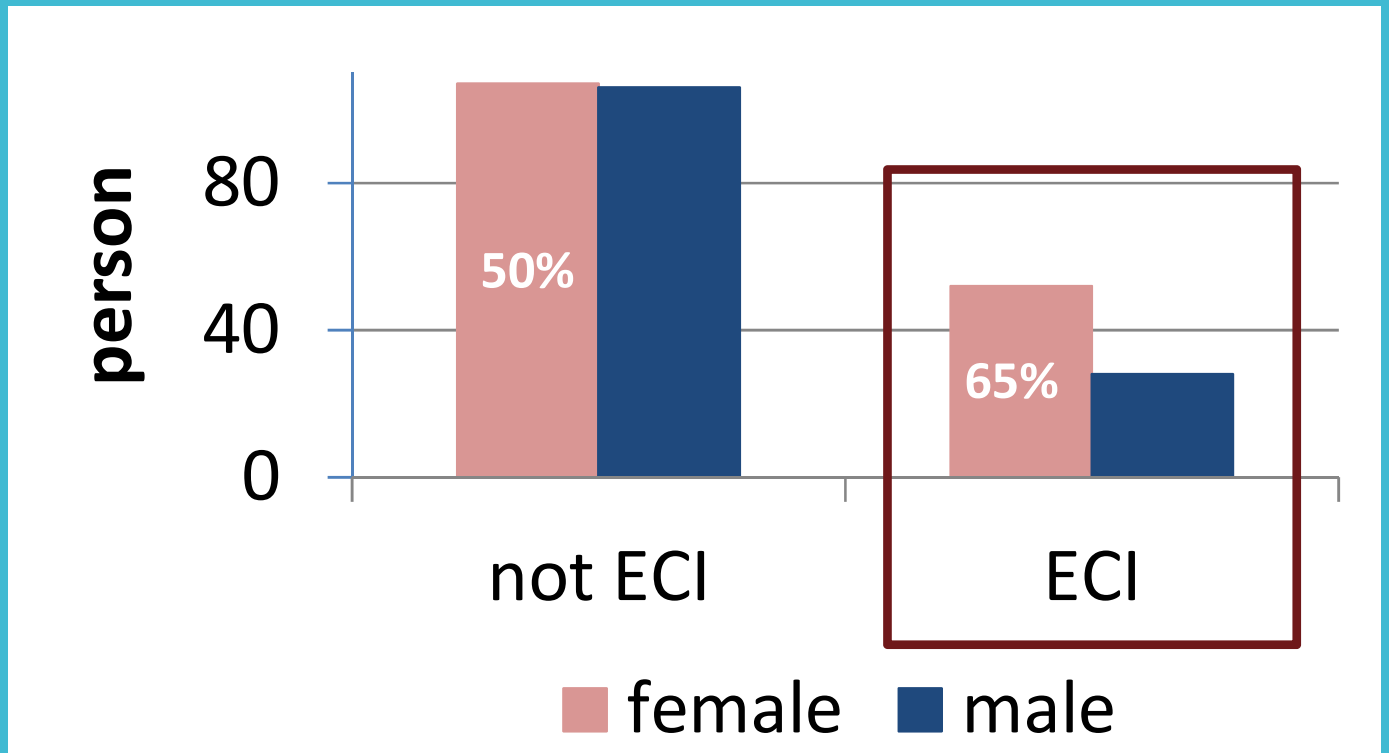
NETWORK FOR EQUILIBRIA AND CHEMICAL THERMODYNAMICS ADVANCED RESEARCH

Early Career Investigators



Starting:

10 ECI

(16%)

<u>Now</u>:

80 ECI

(27%)

52 female

28 male

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