



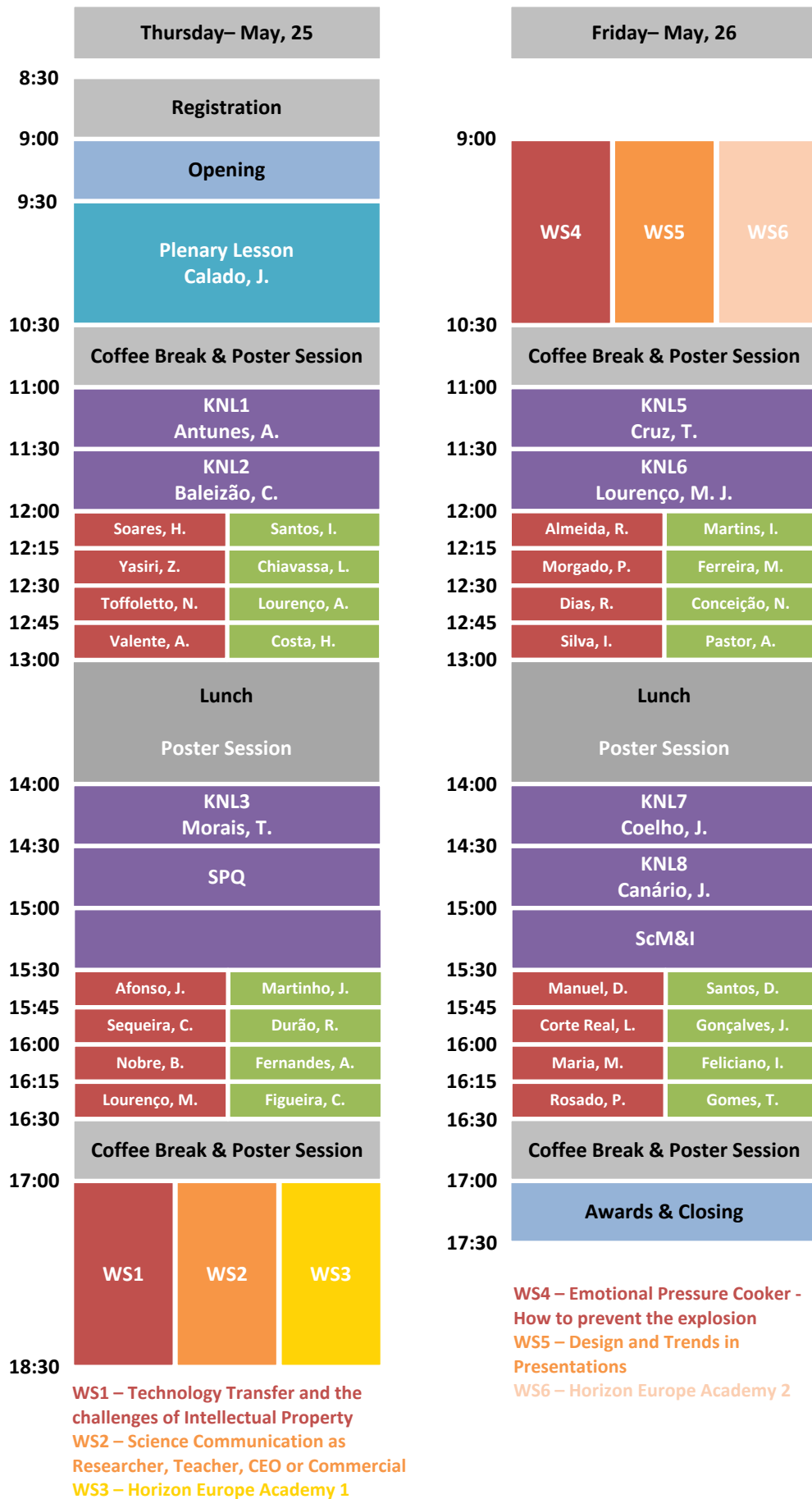
**CQE Days**  
**May 25<sup>th</sup> and 26<sup>th</sup>**

Programme Booklet

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# Overall Programme – Presentations



## Welcome to the 5<sup>th</sup> edition of CQE Days!

In 2019 CQE Days went live at Academia das Ciências de Lisboa. The following two editions were online due to the pandemic restrictions, and in 2022 CQE Days returned to a presential format at Faculdade de Ciências.

This year we are going back to the original venue, Academia das Ciências de Lisboa. As the CQE Days aim to share the research of all CQE members, all keynote lectures and all oral communications are from CQE members. We are also pleased to announce that we have a Plenary Lesson that will be given by Prof. Jorge Calado, one of the founding members of CQE.

Trying to supplant previous editions, this year we also bring you a few workshops. For the younger members we have sessions to help their development of communication and other soft skills; for more senior members, we have sessions directed at explaining/improving applications in European calls.

In this year's gathering we have circa 300 participants and about 200 communications, distributed by the four thematic lines (SYNCat, MATSoft, SUSChem, and MEDLife) that showcase CQE's contribution and commitment to research and the advancement of the field of chemistry. We hope this year's CQE Days will kindle interactions between group members and promote more than ever the establishment of stronger internal synergies between the four thematic lines.

Lisbon, May 25, 2023  
The Organising Committee

# Committees

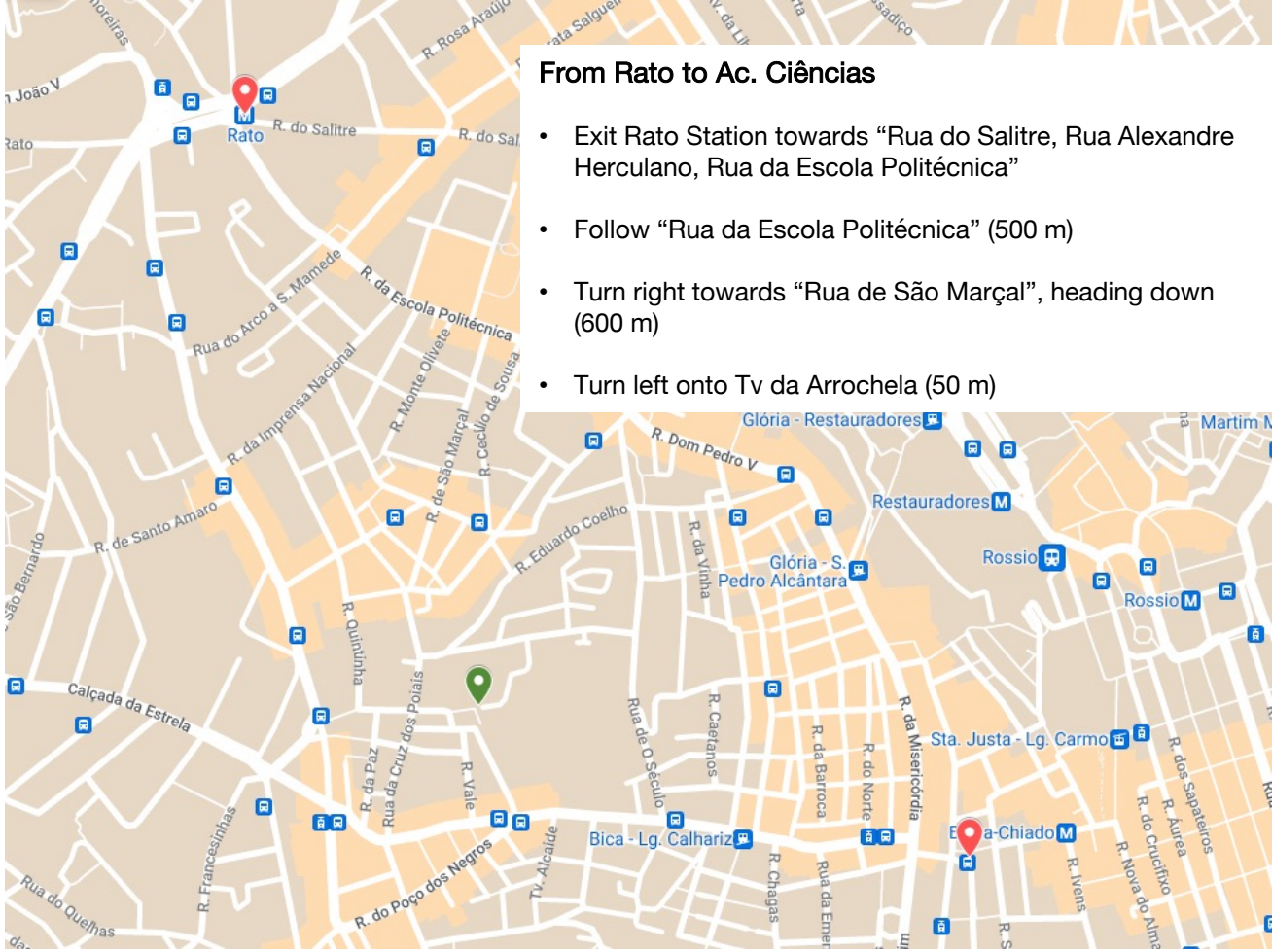
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## Organising Committee

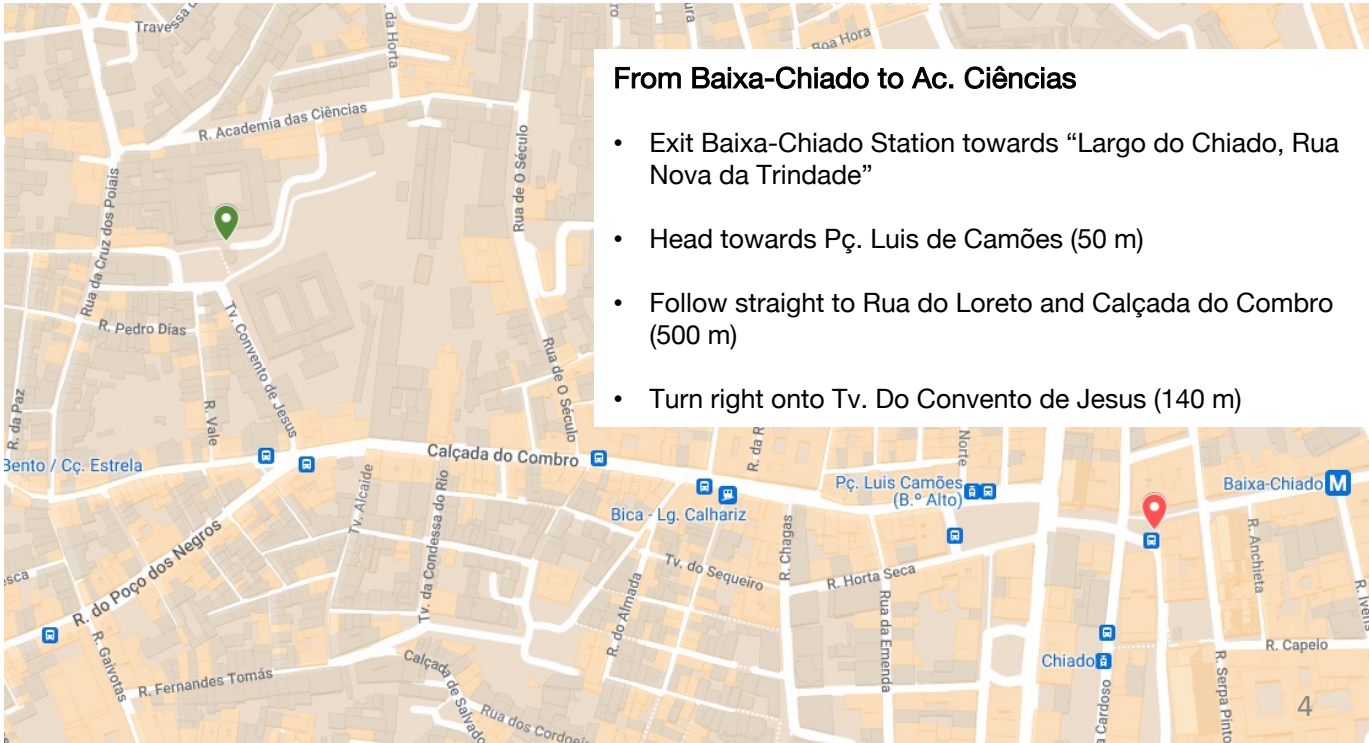
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**Academia das Ciências**  
Largo de Jesus  
1200-474 Lisboa



### From Rato to Ac. Ciências

- Exit Rato Station towards “Rua do Salitre, Rua Alexandre Herculano, Rua da Escola Politécnica”
- Follow “Rua da Escola Politécnica” (500 m)
- Turn right towards “Rua de São Marçal”, heading down (600 m)
- Turn left onto Tv da Arrochela (50 m)



### From Baixa-Chiado to Ac. Ciências

- Exit Baixa-Chiado Station towards “Largo do Chiado, Rua Nova da Trindade”
- Head towards Pç. Luis de Camões (50 m)
- Follow straight to Rua do Loreto and Calçada do Combro (500 m)
- Turn right onto Tv. Do Convento de Jesus (140 m)

# Oral Presentations

## Thursday Morning – May, 25

9:00	Opening Ceremony	(Salão Nobre, JN Canongia Lopes)
9:30	Plenary Lesson: PL1 Calado	(Salão Nobre, chair: G Justino)
9:30	<b>On Being a Scientist</b>	
	Jorge Calado	PL1
10:30		
	Keynote Session 1 <span style="float: right;">(Salão Nobre, chair: G Justino)</span>	
11:00	<b>Chemical Toxicology: from the minimization of chemically induced adverse effects to the development of diagnostic tools</b>	
	Alexandra Antunes	KNL1
11:30	<b>Smart hybrid polymer@silica nanocarriers for control release</b>	
	Carlos Baleizão	KNL2
12:00		
	Parallel Sessions	
	Oral Session 1 <span style="float: right;">(Salão Nobre, chair: G Justino)</span>	
12:00	<b>Cell adhesion and associated functions are dependent on a strict regulation of TBCCD1 levels</b>	
	Helena Soares	O1
12:15	<b>Repurposing montelukast for Alzheimer's – a proteomics assessment of a new in vitro neuron model</b>	
	Zainab Al-Yasiri	O2
12:30	<b>Peptide-eluting contact lenses enhance topical drug delivery across the ocular barriers</b>	
	Nadia Toffoletto	O3
12:45	<b>A new ruthenium-cyclopentadienyl compound as a promising cancer MDR reversing agent</b>	
	Andreia Valente	O4
13:00		
	Oral Session 2 <span style="float: right;">(Aula Maynense, chair: V André, MJ Ferreira)</span>	
12:00	<b>Stimuli responsive surfactants: towards smart templates for mesoporous silica nanoparticles</b>	
	Inês Santos	O5
12:15	<b>Smart self-healing polymer materials for supercapacitors</b>	
	Luisa Chiavassa	O6
12:30	<b>CO<sub>2</sub> mineralization using industrial solid wastes</b>	
	António Lourenço	O7
12:45	<b>Assessment of biomass-derived GACs for point-of-use water filters</b>	
	Henrique Costa	O8
13:00		



## Thursday Afternoon – May, 25

### Keynote Session 2

(Salão Nobre, chair: A Mestre, C Bacariza)

14:00

#### **Novel approaches to fight metastatic cancer: the journey from small molecules to smart metallodrugs**

Tânia Morais

KNL3

14:30

#### **SPQ**

João Paulo Leal

15:00

### Parallel Sessions

### Oral Session 3

(Salão Nobre, chair: A Mestre, C Bacariza)

15:30

#### **Fatty acids-based Eutectic Solvents Liquid Membranes for Removal of Micropollutants from Water**

João Afonso

O9

15:45

#### **On Capillary Viscosity Measurements: How Far do Surface Tension Effects go?**

Carolina Sequeira

O10

16:00

#### **Pressurized liquids to obtain DHA enrich extracts from microalga *Cryptocodinium cohnii***

Beatriz Nobre

O11

16:15

#### **Validation of physical-chemical tests of solid biofuels for the international accreditation of analytical capabilities**

Marta Lourenço

O12

16:30

### Oral Session 4

(Aula Maynense, chair: MJ Ferreira, T Cruz)

15:30

#### **Nanofibers of LnInO<sub>3</sub> perovskites (Ln= La, Pr, Sm, Dy and Yb) as catalysts for the Oxidative Coupling of Methane**

Joana Martinho

O13

15:45

#### **Electrochemical Functionalization of Quinolizidine Alkaloid**

Raquel Durão

O14

16:00

#### **Thermo- and Photo-responsive Spin Labile Fe(III) complexes**

André Fernandes

O15

16:15

#### **Methyl- and phenylnickel complexes with triazole-tethered phenoxyimine ligands for the catalytic hydrosilylation of olefins**

Cláudia Figueira

O16

16:30

## Thursday Afternoon – May, 25

### Parallel Sessions

#### Workshop 1

(Salão Nobre)

17:00

#### **Technology Transfer and the challenges of Intellectual Property**

Patrícia Lima and Carla Patrocínio

WS1

18:30

#### Workshop 2

(Salão das Reuniões Internacionais)

17:00

#### **Science Communication as Researcher, Teacher, CEO or Commercial**

Alexandra Antunes, Zita Martins and Tiago Silva

WS2

18:30

#### Workshop 3

(Aula Maynense)

17:00

#### **Horizon Europe Academy 1**

Ana Espada and Patrícia Guerreiro

WS3

18:30

## Friday Morning – May, 26

### Parallel Sessions

#### Workshop 4

(Salão Nobre)

9:00

#### **Emotional Pressure Cooker – How to prevent the explosion**

Sofia Knittel

WS4

10:30

#### Workshop 5

(Salão das Reuniões Internacionais)

9:00

#### **Design and Trends in Presentations**

Marta Daniela Santos and Patrícia Guerreiro

WS5

10:30

#### Workshop 6

(Sala das Sessões)

9:00

#### **Horizon Europe Academy 2**

Ana Espada and Patrícia Guerreiro

WS6

10:30

## Friday Morning – May, 26

### Keynote Session 3

(Salão Nobre, chair: K Shimizu, M Andrade)

11:00

**Exploring the potential of late transition metal complexes toward olefin, carbonyl, and carbon dioxide reduction**

Tiago Cruz

KNL5

11:30

**Marine resources: discoveries and alternatives with future in Technological Chemistry**

Maria José Lourenço

KNL6

12:00

### Parallel Sessions

### Oral Session 5

(Salão Nobre, chair: K Shimizu, M Andrade)

12:00

**Understanding the Thermal Conductivity of Ionic Liquids: A Direction to Select New Heat Transfer Fluids**

Rafael Almeida

O17

12:15

**Perfluorinated (PFAS) Pollutants – Molecular Modelling and Simulation for Environmental Remediation**

Pedro Morgado

O18

12:30

**Sustainability analysis and decision making of a Ca- Looping plant using water as fluidisation fluid for calcination**

Ricardo Dias

O19

12:45

**Sodium Salt with Fatty Acids Eutectic mixtures as Electrolytes for Supercapacitors**

Inês Silva

O20

13:00

### Oral Session 6

(Aula Maynense, chair: S Realista, N Xavier)

12:00

**Continuous-Flow Electrochemical Oxidation of Abietanes**

Inês Martins

O21

12:15

**The unexpected reactivity of Ruthenium hydrides supported by di-tert-butylpyridylphosphine**

Maria João Ferreira

O22

12:30

**Peroxidative oxidation of cyclohexane in aqueous CH<sub>3</sub>CN medium using Cu(II or I) complexes bearing hydrazone or 1,3,5-triaza-7-phosphaadamantane-derived ligands**

Nuno Conceição

O23

12:45

**Study of new Ni-based coordination polymers as promising De-NO<sub>x</sub> photocatalysts**

Adrián Pastor

O24

13:00

## Friday Afternoon – May, 26

	Keynote Session 4 <span style="float: right;">(Salão Nobre, chair: P Pinheiro, G Justino)</span>	
14:00	<b>Data-Driven Prediction of Bioorthogonal Reactions</b>	
	Jaime Coelho	KNL7
14:30	<b>Climate change in the Arctic: Chemistry as a crucial tool to measure, understand and mitigate</b>	
	João Canário	KNL8
15:00	<b>ScM&amp;I</b>	
	Ana Espada and Patrícia Guerreiro	
15:30		
	<b>Parallel Sessions</b>	
	Oral Session 7 <span style="float: right;">(Salão Nobre, chair: P Pinheiro, G Justino)</span>	
15:30	<b>Synthesis of novel D-glucopyranuronamide-based nucleoside analogs of potential anticancer interest</b>	
	Domingos Manuel	O25
15:45	<b>Exploring the anticancer potential of novel Cu(II) and Zn(II) complexes of 8-hydroxyquinoline Schiff bases</b>	
	Leonor Corte-Real	O26
16:00	<b>Determination of six PEth homologues in whole blood by liquid-liquid extraction and UHPLC-MS/MS</b>	
	Marisa Maria	O27
16:15	<b>Targeting PBP2a to overcome <math>\beta</math>-lactam resistance in methicillin-resistant <i>Staphylococcus aureus</i></b>	
	Pedro Rosado	O28
16:30		
	Oral Session 8 <span style="float: right;">(Aula Maynense, chair: A Mestre, V Ferreira)</span>	
15:30	<b>Exploring the Temperature Effect on Potentiostatically Synthesized PEDOT:PSS films: Electrochemical and Mass Flow Characterization</b>	
	Daniel Santos	O29
15:45	<b>Stimuli-Triggered Activated Nanoparticles to Eliminate Formaldehyde Emission</b>	
	José Gonçalves	O30
16:00	<b>Thermodynamic and Kinetic approach of the Formation of Multicomponent-Crystals with Different Stoichiometries: Maleic Acid and Phenylalanine</b>	
	Inês Feliciano	O31
16:15	<b>Studying shifts in the magnetic behaviour of iron complexes via ligand and counterion modifications</b>	
	Tiago Gomes	O32
16:30		
17:00		
	Awards & Closing <span style="float: right;">(JN Canongia Lopes)</span>	
17:30		

# CQE | Infrastructure & Facilities

## Thursday and Friday Coffee Break and Lunchtime – May, 25 and 26

CQE   Infrastructure & Facilities	(Claustro)
<b>CQE-Ciências: Lab &amp; Computer Infrastructures facility</b> Bárbara Velasco Anes	IF1
<b>biobank   CQE: a powerful tool for medicinal chemistry</b> Pedro F. Pinheiro, Gonçalo C. Justino and M. Matilde Marques	IF2
<b>NMR: a support technique at CQE</b> Maria João Ferreira, José Ascenso, Pedro Pinheiro and Gonçalo Justino	IF3
<b>Mass Spectrometry Facility at Instituto Superior Técnico</b> Maria Conceição Oliveira and João Paulo Leal	IF4

# Poster Presentations



## Thursday and Friday Coffee Break and Lunchtime – May, 25 and 26

Poster Sessions	(Claustro)
<b>Functionalization of Natural Bisquinolizidine Alkaloids</b> Abdullahi Muiz, Jaime Coelho and Raquel Durão	P1
<b>Green metrics for the production of methanol</b> Goi Alessandra, Roberta Bertani, Luísa M. D. R. S. Martins and Ana P. C. Ribeiro	P2
<b>HBpin/MoO<sub>2</sub>Cl<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub> as an efficient catalytic system for the reduction of esters, lactones and polyester plastic waste</b> A. C. Fernandes and Daniel L. Lourenço	P3
<b>Valorization of polyester and polycarbonate plastic waste catalyzed by zinc compounds</b> T. A. H. Branco and A. C. Fernandes	P4
<b>Enantioselective Epoxidation of Styrene Derivatives with Fe<sub>3</sub>O<sub>4</sub> Magnetic Nanoparticles Functionalized with Mo</b> Ana C. Henriques and Carla D. Nunes	P5
<b>Synthesis of ultra-high molecular weight polyethylenes catalyzed by vanadium aroylhydrazine-arylolates</b> A. M. Faisca Phillips, H. Suo, M. Satrudhar, L. M. D. R. S. Martins, M. F. G. da Silva, A. J. L. Pombeiro, M. Han and W.-H. Sun	P6
<b>IPaintS – Intelligent Coating Sensors for Treating Concrete Structures</b> C. S. G. P. Queirós, R. Galhano, C.V. Esteves, O. Ferreira, J. Lopreto, C. Gonçalves and A. F. Cristino	P7
<b>Cooperation of coordination and halogen bonds in capture of Pd(0)</b> Atash V. Gurbanov, Rosa M. Gomila, Antonio Frontera, Namiq Q. Shikhaliyev, Nazrin R. Zeynalli, Kamran T. Mahmudov and Armando J. L. Pombeiro	P8
<b>Extraction and characterization of chitin extracted from Black Soldier Fly exuviae and synthesis of bioplastics</b> Beatriz Abreu, Ana Maria Ferraria and Ana Paula Ribeiro	P9
<b>Software tools for a Sustainable Chemistry</b> Beatriz Afonso, Ana Ribeiro and Luísa Martins	P10
<b>Application of continuous flow chemistry in the synthesis of agrochemical active ingredient metabolites</b> Carlota P. Ferreira, Duarte B. Clemente, Carlos M. Monteiro and Jaime A. S. Coelho	P11
<b>Ni-based activated carbons for CO<sub>2</sub> methanation: On the role of the activation method and ceria incorporation</b> Vittorio Vitacchione, Paula Teixeira, José M. Lopes, Carlos Henriques, Stefania Specchia and Carmen Bacariza	P12
<b>Concrete cracking inhibitory agents using pH-sensitive macrocyclic amines</b> Catarina V. Esteves, Diogo S. Baptista, Olga Ferreira, Rui G. Santos and Ana F. Cristino	P13
<b>Imineureas production via catalytic synthesis using Titanium(IV) ketimide complexes</b> César P. Reis, Vânia André, Ana M. Martins and Maria João Ferreira	P14
<b>Crystallographic Studies to Direct the Self-Assembly Synthesis of Bioactive Coordination Polymers</b> Chris H. J. Franco, Rafaela G. Cabral, Tiago A. Fernandes, Ana C. Sousa and Alexander M. Kirillov	P15

## Thursday and Friday Coffee Break and Lunchtime – May, 25 and 26

Poster Sessions	(Claustro)
<b>Metal-organic frameworks films for ammonia conversion</b> Duarte Borralho, Paulo N. Martinho, Maria E. Melo Jorge and Sara Realista	P16
<b>Electrochemical cyanation of sparteine</b> Duarte B. Clemente, Sara Lima, Carlos A. M. Afonso and Jaime A. S. Coelho	P17
<b>Co(II) and Co(III) coordination compounds for CO<sub>2</sub> photoreduction</b> Eduardo Paes, Rafaela T. Marques, Marcos Bento and Paulo N. Martinho	P18
<b>Isomerization of limonene to high added value products over optimized sulfonated carbons</b> Gabrielle Mathias Reis, Renan S. Nunes, Dalmo Mandelli and Wagner Alves Carvalho	P19
<b>CO<sub>2</sub> methanation in cement sector: Assessing catalysts performance under oxygen and steam-containing feeds</b> Gilda Carvalho, Daniela Spataru, José M. Lopes, Carlos Henriques and Carmen Bacariza	P20
<b>Heterometallic Cyanometallate-driven Coordination Polymers: Self-assembly, Structural Features, and Magnetic Properties</b> Inês Costa, Chris Franco, Vânia André, Laura Pereira and Alexander Kirillov	P21
<b>Reaction of bis(2,4-bis(trichloromethyl)-1,3,5-triazapenta-dienato)-Zn(II) with pyrazole, 4,4'-bipyridine and Cu(acac)<sub>2</sub></b> Ismayil M. Garazade, Atash V. Gurbanov, Ana V. M. Nunes, Kamran T. Mahmudov and Armando J. L. Pombeiro	P22
<b>Highly Efficient Mechanochemical Synthesis of Metal-Free and Hybrid Perovskites</b> Katherine Bettencourt, Inês Feliciano O and M.Fátima M. Piedade	P23
<b>Nanocomposites used as catalysts in ultrasound-assisted peroxidative oxidation of primary and secondary alcohols</b> Luís Correia, Maxim Kuznetsov and Elisabete Alegria	P24
<b>Modeling preferential solvation in aqueous binary mixtures using 2-chloro-2-methylpropane as a kinetic probe</b> A. Pinção, L. Moreira, R. Elvas-Leitão and F. Martins	P25
<b>CO<sub>2</sub> reduction using Fe(II) complexes</b> Marcos Bento, Edwin Devid, João Rocha, Michael Gleeson and Paulo Martinho	P26
<b>Revisiting solvent effects on the solution enthalpies of 3-methylimidazolium tetrafluoroborates: a QSPR comparative study</b> M. Reis, L. Moreira, N. Nunes, R. Elvas-Leitão and F. Martins	P27
<b>Synthesis of C-glycoside Analogues with Potential against Carbapenem-resistant Gram-negative Bacteria</b> Mónica Miranda, Rita Almeida and Ana Marta Matos	P28
<b>Synthesis and characterization of magnetic MOFs</b> Nuria Mulero, Marta M. Alves and Ana Paula C. Ribeiro	P29
<b>Sol-gel-Derived Synthetic CaO-Based Materials for Thermochemical Energy Storage</b> David Piqué, Paula Teixeira and Carla I. C. Pinheiro	P30
<b>Oxidative desulfurization of sulfur compounds with Molybdenum supported catalysts</b> Pedro Moreira and Carla Nunes	P31

## Thursday and Friday Coffee Break and Lunchtime – May, 25 and 26

Poster Sessions	(Claustro)
<b>Water-soluble mixed-valence cobalt(II,III) complex as a homogeneous catalyst for the mild peroxidative oxidation of toluene</b> Peixi Liu, Kamran Mahmudov, Zihua Wang, Elisabete Alegria Armando Pombeiro	P32
<b>CO<sub>2</sub> valorisation with earth abundant metals and cryptates</b> Rafaela T. Marques, Sara Realista, Rui Santos and Paulo N. Martinho	P33
<b>Effect of substituents on the chalcogen bonding in 5-substituted benzo[c][1,2,5]selenadiazoles and their copper(II) complexes</b> Vusala A. Aliyeva, Atash V. Gurbanov, M. Fátima C. Guedes da Silva, Kamran T. Mahmudov and Armando J. L. Pombeiro	P34
<b>Glycerol Mixtures</b> Luis Juan, Ana Paula Ribeiro and Ana Cristino	P35
<b>Polyaromatic Group Containing Cd(II)-based Coordination Polymers for Adsorption and Catalytic applications</b> Anirban Karmakar, Anup Paul and Armando J. L. Pombeiro	P36
<b>Ethylene photooxidation using BEA zeolite based TiO<sub>2</sub> composites</b> Ricardo Ferreira, Auguste Fernandes, João Lourenço, João Silva, Isabel João, Sérgio Morales-Torres, Luísa Pastrana-Martinez, Francisco Maldonado-Hódar and Filipa Ribeiro	P37
<b>Light propelled nanovehicles for drug delivery</b> Ana Marta Cabral, Carlos Baleizão and José Paulo Farinha	P38
<b>Advanced High Strength Steel in sodium chloride media: corrosion characterization</b> Afonso Cruz, Maryna Taryba and Fátima Montemor	P39
<b>Pollutant Recycling and Remediation using High-Performance Carbon-based Composite Materials</b> Beatriz M. Rodrigues, Maria J.G. Ferreira, Alexander M. Kirillov and Tiago A. Fernandes	P40
<b>9-Borafluoren-9-yl and diphenylboron tetracoordinate complexes of 8-quinolinato ligands with heavy atom substituents: synthesis, fluorescence and application in OLED devices</b> Carina Fialho, Tiago F. C. Cruz, Maria José Calhorda, Luís F. Vieira Ferreira, Piotr Pander, Fernando B. Dias, António L. Maçanita and Pedro T. Gomes	P41
<b>Triamcinolone acetone delivery from cyclodextrin-containing contact lenses to treat diabetic retinopathy</b> Carolina Marto-Costa, Carlos Pinto, Jorge Saraiva, Madalena Salema-Oom, Ana Silva-Herdade, Carmen Alvarez-Lorenzo and Ana Paula Serro	P42
<b>On the Stability of Celecoxibe-Tramadol-HCl: Co-crystal versus Amorphous Nanoparticles</b> Daniel Valente-Matias, Aaron O'Sullivan, Carlos Bernardes, Luis Padrela and Manuel Minas da Piedade	P43
<b>Polydopamine/polypyrrole co-polymers for amperometric biosensors</b> Diana M. Carneiro, Jorge F. Zeferino, Luís C. Almeida, Jorge P. Correia and Ana S. Viana	P44
<b>Niacin Crystal Nucleation from Ethanol Solutions</b> Diogo S. Baptista and Carlos E. S. Bernardes	P45
<b>Removal of Dyes from Aqueous Solutions using Poly(ionic liquid)s</b> Gabriela Caetano, Bruna Soares, Maria Manuela Correia and Isabel Marrucho	P46

## Thursday and Friday Coffee Break and Lunchtime – May, 25 and 26

Poster Sessions	(Claustro)
<b>Revisiting the vapor liquid equilibria of water+methanol and ethanol+n-butanol binary mixtures</b> Inês Sacristão, Beatriz Nobre, António Palavra and Ana F. Cristino	P47
<b>On the Hydrophobicity of Hydrophobic Eutectic Solvents</b> João Afonso, Line Marschal, Carlos Conceição de Souza, Bernardo Dias Ribeiro and Isabel Marrucho	P48
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Cátia F. Marques, Pedro F. Pinheiro and Gonçalo C. Justino

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