

Program Overview

Monday, 24 July 2023

Time (h)	Centro Cultural e de Congressos de Aveiro				
9:00-10:30	Registration – Foyer de entrada				
Room	Grande Auditório				
10:30-10:50	Artur Silva - Vice-Rector of the University of Aveiro - Chair of the XXVIII Encontro Nacional da SPQ João Rocha - Department of Chemistry, University of Aveiro – Vice-Chair of the XXVIII Encontro Nacional da SPQ Joaquim Faria – Faculty of Engineering, University of Porto, President of the Sociedade Portuguesa de Química Armando Silvestre - Director of the Department of Chemistry, University of Aveiro				
CHAIRS:	Artur Silva, Univ. Aveiro and Joaquim Faria, Univ. Porto				
10:50-11:40	PL1 - <i>Embracing metals with proteins - a personal history</i> ; Ferreira da Silva Award José João Galhardas de Moura, New University of Lisbon, Portugal				
11:40-12:30	PL2 - <i>Lanthanide nuclear paramagnetic shift and relaxation in structural NMR and MRI - a personal experience</i> ; Fraústo da Silva Award Carlos Frederico de Gusmão Campos Geraldes, University of Coimbra, Portugal				
12:30-14:00	Lunch Break				
Room	Grande Auditório				
CHAIR:	Artur Silva, Univ. Aveiro				
14:00-14:50	PL3 - <i>Transition metal catalysis in biological habitats</i> Jose Luis Mascareñas, Universidade de Santiago, Spain				
Room Grande Auditório	Chair: Fernanda Proença, Univ. Minho	Room Pequeno Auditório	Chair: Mário Nuno Berberan e Santos, IST, Univ. Lisboa	Room 5	Chair: Diana Pinto, Univ. Aveiro
14:55-15:25	KN1 - <i>The physics and chemistry of directional freezing: implications in biofabrication and cryobiology</i> Francisco M. Fernandes, Sorbonne Université, France	14:55-15:25	KN2 - <i>Coordination polymers: From self-assembly to functional (bio)materials</i> Alexander Kirillov, Universidade de Lisboa, Portugal	14:55-15:25	KN3 - <i>Wine industry's untapped goldmine: Unlocking the potential of by-products in the Circular Economy</i> Ana Novo Barros, University of Trás-os-Montes e Alto Douro, Portugal
15:25-15:40	OC1 - <i>Enhanced biomass processing using a ternary deep eutectic solvent</i> André M. da Costa Lopes, University of Aveiro, Portugal	15:25-15:40	OC3 - <i>DPA fluorescent sensors: "walking" towards the NIR</i> Artur J. Moro, Universidade NOVA de Lisboa, Portugal	15:25-15:40	OC5 - <i>Improved functional excipients for high value pharmaceuticals</i> Cláudia Bento, Hovione Farmacêcia S.A., Portugal
15:40-15:55	OC2 - <i>Understanding the chemistry behind the Kigali Amendment to the Montreal Protocol: an accurate computational protocol</i> Luís P. Viegas, University of Coimbra, Portugal	15:40-15:55	OC4 - <i>Addressing drug resistance in methicillin-resistant Staphylococcus aureus through mass spectrometry multiple omics</i> Pedro C. Rosado, Instituto Superior Técnico, Universidade de Lisboa, Portugal	15:40-15:55	OC6 - <i>Nitro group-containing compounds as histone deacetylase inhibitors</i> Joana L. C. Sousa, University of Aveiro, Portugal

15:55-17:15	Coffee break & Poster discussion - CCA				
17:15-17:45	KN4 - <i>Manipulation of organic molecules by infrared vibrational excitation</i> Cláudio Manaia Nunes, University of Coimbra, Portugal	17:15-17:45	KN5 - <i>Photoresponsive host-guest systems with potential biological applications</i> Nuno Basilio, Universidade NOVA de Lisboa, Portugal	17:15-17:45	KN6 - <i>Semifluorinated soft-matter</i> Eduardo Filipe, Instituto Superior Técnico, Universidade Lisboa, Portugal
17:45-18:00	OC7 - <i>The extraction residues as a promising source of fiber and proteins</i> Tatiane C. G. Oliveira, Instituto Politécnico de Bragança, Portugal	17:45-18:00	OC9 - <i>Unlocking the potential of chromeno[3,4-b]xanthenes as multifunctional compounds for Alzheimer's disease</i> Daniela Malafaia, University of Aveiro, Portugal	17:45-18:00	OC11 - <i>Innovation in cork: A cork-Chemistry relationship</i> Raquel Nunes da Silva, Cork Technological Centre, Portugal
18:00-18:15	OC8 - <i>Electrostatics on biomolecules-based drug delivery systems</i> Sandra C. C. Nunes, University of Coimbra, Portugal	18:00-18:15	OC10 - <i>Recovery of palladium by solvent extraction – A contribution for the recycling of PGMs from end-of-life devices</i> Ana P. Paiva, Universidade de Lisboa, Portugal	18:00-18:15	OC12 - <i>Featuring hyperbaric storage for Clostridium perfringens endospores' inactivation – a novel breakthrough on food safety?</i> Carlos Pinto, University of Aveiro, Portugal
Room: Grande Auditório	Chair: Cláudia Lopes, Univ. Aveiro	Room: Pequeno Auditório	Chair: Eduarda Pereira, Univ. Aveiro	Room: 5	Chair: Vânia Calisto, Univ. Aveiro
18:15-19:00	Flash 1-7	18:15-19:00	Flash 8-14	18:15-19:00	Flash 15-21
19:00	Porto de Honra – CCA				
Tuesday, 25 July 2023					
Time (h)	Centro Cultural e de Congressos de Aveiro				
Room	Grande Auditório				
CHAIR:	João Rocha, Univ. Aveiro				
9:00-9:50	PL4 - <i>Catalytic amination of bio-based compounds</i> Karine de Oliveira Vigier, Institut de Chimie des Milieux et Matériaux de Poitiers (IC2MP), France				
Room: Grande Auditório	Chair: Victor de Freitas, Faculty of Sciences, Univ. Porto	Room: Pequeno Auditório	Chair: Verónica de Zea Bermudez, UTAD	Room: 5	Chair: Filipe Almeida-Paz, Univ. Aveiro
9:50-10:20	Ferreira da Silva - Tribute Session				
	OC13 - <i>O Laboratório Ferreira da Silva: crónica de uma reconstrução desejada</i> Marisa Monteiro, Museu de História Natural e da Ciência da Universidade do Porto, Portugal	9:50-10:20	KN7 - <i>Engineering of silk-based materials: a quest for eco-sustainable resources</i> Rui F.P. Pereira, University of Minho, Portugal	9:50-10:20	KN8 - <i>Exploring the use of metals and metallic salts in the synthesis of flavonoids</i> Raquel Soengas, University of Oviedo, Spain
10:20-10:50	OC14 - <i>Os zoilos e os templos das ciências</i> Manuel João Monte, Universidade do Porto, Portugal	10:20-10:35	OC15 - <i>Photoreduction of carbon dioxide using a novel Re(I) complex</i> Marcos A. Bento, University of Aveiro, Portugal	10:20-10:35	OC17 - <i>Effect of alkylsilane and alkylsiloxane chains on the thermophysical properties of ionic liquids</i> Rodrigo M. A. Silva, University of Porto, Portugal
		10:35-10:50	OC16 - <i>Hydrogen production via electrocatalytic ammonia conversion using metal-organic frameworks films</i> Duarte Borralho, Universidade de Lisboa, Portugal	10:35-10:50	OC18 - <i>New 4-(N-cinnamoylbutyl)amino-acridines as potential multi-stage antiparasitic leads</i> Mélanie Fonte, University of Porto, Portugal
10:50-11:15	Coffee break - CCA				

11:15-11:30	OC19 - <i>Os alcalóides de Ferreira da Silva: Evolução do conhecimento da sua toxicologia</i> Fernando Remião, Universidade do Porto, Portugal	11:15-11:45	KN9 - <i>Theoretical insight into hole-transporting materials for perovskite solar cells</i> Enrique Orti, Universidad de Valencia, Spain	11:15-11:45	KN10 - <i>Computing your way out of experimental problems, from nanocarbon to covalent organic frameworks and beyond</i> Manuel Melle-Franco, University of Aveiro, Portugal
11:30-11:45	OC20 - <i>Carbon materials for advanced water treatment</i> Vânia Calisto, University of Aveiro, Portugal				
11:45-12:00	OC21 - <i>Qualidade, autenticidade e segurança alimentar: o valioso contributo do Professor Ferreira da Silva</i> Isabel M.P.L.V.O. Ferreira, Universidade do Porto, Portugal	11:45-12:00	OC24 - <i>Development of new analogs with anticancer activity from metabolic products of marine bioluminescent reactions</i> Luís Pinto da Silva, University of Porto, Portugal	11:45-12:00	OC27 - <i>Pharmaceuticals detection by LC-MS/MS to test materials for (bio)sensors</i> M ^a João Nunes, Nova University Lisbon, Portugal
12:00-12:15	OC22 - <i>A avaliação da autenticidade do Vinho do Porto ao longo dos tempos</i> Manuel Lima Ferreira, Instituto dos Vinhos do Douro e do Porto, Portugal	12:00-12:15	OC25 - <i>Development and evaluation of o-nitrophenethylphotocaged prodrugs for glioblastoma</i> João Vaz, Universidade de Lisboa, Portugal	12:00-12:15	OC28 - <i>Ionic systems as additives for energy applications</i> Luis C. Branco, LAQV-REQUIMTE, NOVA School of Science and Technology, Portugal
12:15-12:30	OC23 - <i>O passado como conhecimento para o futuro</i> Vicente Ferreira da Silva	12:15-12:30	OC26 - <i>Indicator displacement assays using water-soluble deep cavity cavitands for the detection of benzodiazepines</i> Beatriz Raimundo, Universidade Nova de Lisboa, Portugal	12:15-12:30	OC29 - <i>Pharmaceutical organic salts and ionic liquids based on Streptomycin and Cefuroxime antibiotics</i> Francisco Faisca, Nova University Lisbon, Portugal
12:30-14:00	Lunch Break				
Room	Grande Auditório				
CHAIR:	Luís Belchior Santos, Faculty of Sciences, Univ. Porto				
14:00-14:50	PL5 - <i>Tormented polycyclic aromatic compounds</i> Robert Pascal, Bernard Villars Baus Chair in Chemistry, School of Science & Engineering, Tulane University, New Orleans, LA, USA				
Room: Grande Auditório	Chair: Amparo Faustino, Univ. Aveiro	Room: Pequeno Auditório	Chair: Pedro Carvalho, Univ. Aveiro	Room: 5	Chair: Jorge Saraiva, Univ. Aveiro
14:55-15:25	KN11 - <i>Metalloprotein chaperones: regulating protein aggregation and metal ion dyshomeostasis in Alzheimer's disease</i> Cláudio M. Gomes, Universidade de Lisboa, Portugal	14:55-15:25	KN12 - <i>Insights on the design of highly stable noble metal-free carbon electrocatalysts for oxygen reduction reaction</i> Rui S. Ribeiro, University of Porto, Portugal	14:55-15:25	KN13 - <i>The whereabouts of iron in the human body: insights from blood serum chemistry</i> André M.N. Silva, Universidade do Porto, Portugal
15:25-15:40	OC30 - <i>Host-guest complexes based on p-sulfonatocalix[n]arenes and a pyranoflavylum-type dye for dynamic capture of biogenic amines</i> Ana Sofia Pires, Nova University Lisbon, Portugal	15:25-15:40	OC32 - <i>Realizing the machine learning power for catalysis: the role of small open data</i> Pedro S. F. Mendes, Instituto Superior Técnico, Portugal	15:25-15:40	OC34 - <i>Dynamic G-quadruplex based perfusable supramolecular hydrogels embedded in photo-cross-linkable matrices for bioapplications</i> João Borges, University of Aveiro, Portugal
15:40-15:55	OC31 - <i>Exploring photocatalytic properties of titanate hybrid nanotubular materials for sustainable applications</i> Olinda C. Monteiro, University Lisbon, Portugal	15:40-15:55	OC33 - <i>Extraction, identification, and antioxidant potential of phenolic compounds from stone pine cone</i> Cláudia M. B. Neves, Polytechnic Institute of Viseu, Portugal	15:40-15:55	OC35 - <i>BASHY platform: Bioimaging and therapeutics</i> Fábio M. F. Santos, Universidade de Lisboa, Portugal
15:55-17:30	Coffee break & Poster discussion - CCA				
17:30-18:00	KN14 - <i>Near infrared light absorbing nanomaterials for cancer photothermal therapy</i> Ilídio J. Correia, Universidade de Coimbra, Portugal	17:30-18:00	KN15 - <i>Advanced treatment technologies for wastewater resources recovery</i> Vitor Vilar, University of Porto, Portugal	17:30-18:00	KN16 - <i>Rethinking C-N and S-N bond formation</i> M ^a Manuel B. Marques, Universidade Nova de Lisboa, Portugal
18:00-18:15	OC36 - <i>New chitin derived furanic platforms as bio-based synthons</i> Rafael F. A. Gomes, Universidade de Lisboa, Portugal	18:00-18:15	OC37 - <i>C₂ Hydrocarbons production via oxidative coupling of methane over ABO₃ perovskites (A = La, Pr, Sm, Dy, Yb and B = Mo, Mn, Ga and In)</i> Joana F. Martinho, IST, Portugal	18:00-18:15	OC38 - <i>Extracting zeolite preparation data from scientific papers in PDF automatically</i> Daniel P. Costa, Instituto Superior Técnico, Portugal

Room	Grande Auditório				
CHAIR:	António Jorge Parola, Univ. Nova de Lisboa				
18:15-19:05	PL6 - <i>New directions for artificial molecular machines and motors</i> Alberto Credi, Department of Industrial Chemistry, Università di Bologna, Bologna, Italy				
19:30	Congress Dinner – Restaurante Universitário, Univ. Aveiro				
Wednesday, 26 July 2023					
Time (h)	Centro Cultural e de Congressos de Aveiro				
Room	Grande Auditório				
CHAIRS:	Artur Silva, Univ. Aveiro and Joaquim Faria, Univ. Porto				
9:00-9:50	PL7 - <i>From anisotropic to asymmetric nanoparticle growth, Portuguese-Spanish award "Madinaveitia-Lourenço"</i> Luis Manuel Liz-Marzan, Bionanoplasmonics Lab, CIC biomaGUNE, Donostia/San Sebastián, Spain				
Room: Grande Auditório	Chairs: Armando Pombeiro, IST, Univ. Lisboa and José Moura, Univ. Nova de Lisboa	Room: Pequeno Auditório	Chair: Armando Silvestre, Univ Aveiro	Room: 5	Chair: Manuel Coimbra, Univ. Aveiro
9:50-10:05	<i>Fraúst da Silva - Tribute Session</i> OC39 - <i>Fraúst da Silva and the two Cultures: Biographic note</i> Armando Pombeiro, Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa	9:50-10:20	KN17 - <i>Molecular design of nitroprusside-based hybrid functional materials</i> Wei-Jian XU, University of Aveiro, Portugal	9:50-10:20	KN18 - <i>Augmenting the reactions' portfolio of quinic acid</i> Nuno R. Candeias, University of Aveiro, Portugal
10:05-10:20	OC40 - <i>Remembering Fraúst da Silva</i> José J. G. Moura, Departamento de Química, FCT, Universidade Nova de Lisboa				
10:20-10:35	OC41 - <i>Metal complexes in biological media. Relevance of assessing their speciation</i> João Pessoa & Isabel Correia, Centro de Química Estrutural, Institute of Molecular Sciences and Departamento de Engenharia Química, Instituto Superior Técnico, Universidade de Lisboa	10:20-10:35	OC43 - <i>Natural deep eutectic solvents from fundamentals to applications</i> Andreia S. F. Farinha, King Abdullah University of Science and Technology, Saudi Arabia	10:20-10:35	OC45 - <i>Titanium-catalysed synthesis of imineureas</i> César P. Reis, Instituto Superior Técnico, Portugal
10:35-10:50	OC42 - <i>O Sudário de Turim, fonte de extraordinária informação científica</i> Victor M. M. Lobo, Departamento de Química, FCT, Universidade de Coimbra	10:35-10:50	OC44 - <i>Biorecovery of critical elements from fluorescent lamp wastes using the marine macroalga Ulva sp.</i> João Pinto, University of Aveiro, Portugal	10:35-10:50	OC46 - <i>The meso-tetrakis(pentafluorophenyl)-porphyrin: a platform for heterogeneous catalysts</i> Mário M. Q. Simões, University of Aveiro, Portugal
10:50-11:15	Coffee break - CCA				
11:15-11:30	OC47 - <i>The undiscovered world of Werner complexes</i> Maria José Calhorda & Nuno A.G. Bandeira, Departamento de Química e Bioquímica, Faculdade de Ciências, Universidade de Lisboa	11:15-11:45	KN19 - <i>The 12 Labours of HERCULES...or from mythology to the frontiers of Chemistry and Art...or chronicle of a ready-made</i> António Candeias, City University of Macau Chair in Sustainable Heritage, Portugal	11:15-11:45	KN20 - <i>Endoperoxide-based hybrids as tools to fight infectious diseases; synthesis, structure and properties.</i> Maria L. S. Cristiano, University of Algarve, Portugal
11:30-11:45	OC48 - <i>A praise for denitrification</i> Isabel Moura, Departamento de Química, FCT, Universidade Nova de Lisboa				
11:45-12:00	OC49 - <i>O Triunfo do azul na Natureza e no antropoceno. Sobre a evolução (Química) dos sistemas de cor nas plantas. O Caso das hortênsias</i> Fernando Pina, Departamento de Química, FCT, Universidade Nova de Lisboa	11:45-12:00	OC52 - <i>meso-Aryl-1,3,5,7-tetramethyl BODIPY dyes revisited: A systematic approach for synthetic optimization</i> Alexandre P. Felgueiras, University of Coimbra, Portugal	11:45-12:00	OC55 - <i>Detection of mutations in epidermal growth factor receptor using gold nanoparticle aggregation</i> Anupong Nuekaew, Universidade do Porto, Portugal

12:00-12:15	OC50 - <i>Ligações de hidrogénio e outras interações não-covalentes em química de coordenação</i> M. Fátima Guedes da Silva, Departamento de Eng. Química, IST, Universidade de Lisboa	12:00-12:15	OC53 - <i>Influence of proton transfer on the luminescence of organic dyes</i> Samuel Guieu, University of Aveiro, Portugal	12:00-12:15	OC56 - <i>How to reduce the problematic CO₂? Lessons from Biology</i> Luisa Maia, Universidade Nova de Lisboa, Portugal
12:15-12:30	OC51 - <i>Living with Chemistry in a virtual world-“A Química na era da desmaterialização do conhecimento”</i> Clementina Teixeira, Departamento de Eng. Química, IST, Universidade de Lisboa	12:15-12:30	OC54 - <i>Metalloproteins from pathogenic bacteria - targets for new antibiotics</i> Sofia Pauleta, Universidade Nova de Lisboa, Portugal	12:15-12:30	OC57 - <i>Contribution of non-ionic interactions on bile salt binding by chitoooligosaccharides: potential hypocholesterolemic activity</i> Filipe Coreta-Gomes, University of Aveiro, Portugal
12:30-14:00	Lunch Break				
Room	Grande Auditório				
CHAIR:	Baltazar de Castro, Faculty of Sciences, Univ. Porto				
14:00-14:50	PL8 - <i>Development of solar photoreactors for water treatment</i> Sixto Malato, Water Solar Treatment Unit, Plataforma Solar de Almería, Almería, Spain				
Room: Grande Auditório	Chair: Mário Simões, Univ. Aveiro	Room: Pequeno Auditório	Chair: Rita Ferreira, Univ. Aveiro	Room: 5	Chair: Anabela Valente, Univ. Aveiro
14:55-15:25	KN21 - <i>Synthesis and end-of-life tailoring of furan-based polymers: in the pathway to sustainable polymers</i> Andreia F. Sousa, University of Coimbra, Portugal	14:55-15:25	KN22 - <i>Brown algae metabolites: the catalysts for biomass valuing</i> Susana M. Cardoso, University of Aveiro, Portugal	14:55-15:25	KN23 - <i>Discovery of dual inhibitors of PD-L1 and TGF-β1 leveraged by in silico methods</i> Rita Guedes, Universidade de Lisboa, Portugal
15:25-15:40	OC58 - <i>Red color stabilization of anthocyanins with lignosulfonates from the pulp industry</i> Joana Oliveira, Universidade do Porto, Portugal	15:25-15:40	OC60 - <i>Hafnium-containing modified zeolites or silicates for catalytic transfer hydrogenation of furfural to useful bioproducts</i> M ^a Margarida Antunes, University of Aveiro, Portugal	15:25-15:40	OC62 - <i>Synthesis of β-functionalized porphyrin-Ir(III) complexes as photosensitizer agents towards cancer cells</i> Nuno M. M. Moura, University of Aveiro, Portugal
15:40-15:55	OC59 - <i>Self-assembled binary structures of Mn(III), Fe(III) and metal-free porphyrins in catalytic hydrogenation assisted by sunlight</i> Gabriela A. Corrêa, Universidade do Porto, Portugal	15:40-15:55	OC61 - <i>(Photo)Oxidative transformation of biomass derived molecules into valuable products</i> Iwona Kuzniarska-Biernacka, Universidade do Porto, Portugal	15:40-15:55	OC63 - <i>Validation of a methodology to quantify several elements in fruits according to ISO 17025</i> M ^a Eduarda Pereira, University of Aveiro, Portugal
15:55-16:15	Coffee break - CCA				
16:15-16:45	KN24 - <i>Analytical challenges in the detection of plant food supplements adulteration</i> Joana S. Amaral, Instituto Politécnico de Bragança, Portugal	16:15-16:45	KN25 - <i>Automation of molecular recognition strategies for enhanced analytical methods</i> Marcela A. Segundo, University of Porto, Portugal	16:15-16:45	KN26 - <i>Building chemical strategies to expand flavylum-based dyes applications</i> Luís Cruz, University of Porto, Portugal
16:45-17:00	OC64 - <i>Exploiting the versatility of electroactive organic building blocks for the construction of functional framework materials</i> Manuel Souto, University of Aveiro, Portugal	16:45-17:00	OC65 - <i>All-solid-state thermally-chargeable textile supercapacitors based on CNTs and PEDOT:PSS-doped PVA/H₃PO₄ electrolyte</i> Joana S. Teixeira, University of Porto Portugal	16:45-17:00	OC66 - <i>Prediction of molecular properties of metal-containing drugs using machine learning models</i> Vincenzo Vigna, University of Calabria, Italy
Room	Grande Auditório				
CHAIRS:	Artur Silva, Univ. Aveiro and Joaquim Faria, Univ. Porto				
17:00-17:35	<i>Machine learning tools to accelerate the chemical sciences; Vicente de Seabra medal</i> Tiago Correia de Oliveira Rodrigues, Faculty of Pharmacy, University of Lisbon				
17:35	Closing Ceremony / Poster awards Artur Silva - Vice-Rector of the University of Aveiro - Chair of the XXVIII Encontro Nacional da SPQ João Rocha - Department of Chemistry, University of Aveiro – Vice-Chair of the XXVIII Encontro Nacional da SPQ Joaquim Faria – Faculty of Engineering, University of Porto, President of the Sociedade Portuguesa de Química				

