

Preliminary poster presentations

Physical Foundations of Organic Reactivity

- PP1 - **Abdelkrim Touabet**, Analysis of Natural Substances Using a New Liquid Crystal as Stationary Phase.
- PP2 - **Aicha Hassani**, BIOLOGICAL ACTIVITIES AND PHYTOCHEMICAL STUDY OF CISTUS SALVIIFOLIUS
- PP3 - **Ana Rosa Garcia**, Chemistry of Model Catalytic Systems at Very Low Pressure: Studies by RAIRS
- PP4 - **André K. Eckhardt**, Spectroscopic Evidence for Aminomethylene (H-C-NH₂) – The Simplest Amino Carbene
- PP5 - **Amin Ismael**, Insights into the photochemistry of 5-aminotetrazole derivatives; effect of the saccharyl moiety on the photostability
- PP6 - **Bernard Denegri**, Different Solvolytic Behavior of Aryl/Alkyl Carbonates, Carboxylates and Phenolates
- PP7 - **Carolina Rio**, The termolecular reaction $H + O_2 + M \rightarrow HO_2 + M$
- PP8 - **Charles Perrin**, Polynomial Coefficients. Application to Spin-Spin Splitting by N Equivalent Nuclei of Spin $I > 1/2$
- PP9 - **Cláudio Nunes**, Cyclization of triplet 2-formyl-phenylnitrene to 2,1-benzisoxazole: A new heavy-atom tunneling event?
- PP10 - **Davide Corinti**, Structural insights into non-covalent halide adducts with tyrosine and 3-nitrotyrosine using ion-spectroscopy
- PP11 - **Elisa M. Brás**, The Structure and Properties of a Novel Sulphonyl-Bridged Thiadiazolyl-Saccharinate Ligand
- PP12- **Ephrath Solel**, Fulvalene: Computationally Tuning Aromaticity and Tunneling
- PP13 - **Fynn Röhricht**, Anisotropy of the Current Induced Density (ACID)- A new Method for Prediction and Explanation of Diels-Alder Reactions
- PP14 - **James Scotson**, Effects of Binary Solvent Mixtures on Reactivity
- PP15 - **Jan M. Schümann**, A synthetical approach to 1,4-di-substituted-cyclooctatetraene based dispersion balances
- PP16 - **Jesús Sanjosé-Orduna**, Road to a full understanding of the C-H Activation using Cp*Co(III) metal complexes
- PP17 - **Jin-Dong Yang**, iBonD: a Databank of Measured pKa and BDE Values
- PP18 - **Kazuhide Nakata**, Computational Study of the Through-Resonance Effect Operating on (Phenylamino)methyl Cations
- PP19 - **Lijuan Song**, Understanding and Utilizing the Role of London Dispersion Interactions in Catalysis

- PP20 - **Luuk Kortekaas**, Protonation of Spiropyrans: Revising Acidochromism and Electrochromism
- PP21 - **Mika Maehara**, Interaction of 3,6-Dimethylfluorenylidene with Ammonia and Water at Cryogenic Temperatures
- PP22 - **Mirela Matic**, Solvolytic Reactivity of Organophosphates and Organophosphinates
- PP23 - **Moisés Canle**, Photochemistry of thiazolidines in solution
- PP24 - **Morten Peters**, Development of a contrast agent based on FeIII-Recordplayer
- PP25 - **Nadezhda Danilenko**, Quantum chemical calculation of SuFEx reaction thermodynamics
- PP26 - **Neshat Rozatian**, Kinetics of Fluorination of 1,3-Dicarbonyls
- PP27 - **OUASSILA FERROUKHI**, Influence of Alkyl Spacer on the Physical Behaviors of Novel Mesogenic Bioactive Phases for GC
- PP28 - **Pengju Ji**, Homolytic Bond Dissociation Enthalpies in Room Temperature Ionic Liquids
- PP29 - **Potlaki TSEKI**, The chemical behaviour of nitromethane in inert solvents examined through spectroscopic techniques
- PP30 - **Rikuo Akisaka**, Kinetic stabilization of singlet-2,2-dialkoxy-1,3-diradical by introducing bulky substituents
- PP31 - **Rui M. Borges dos Santos**, Thermochemistry of peroxy radicals: a combined photoacoustic calorimetry, quantum chemistry, and molecular dynamics study.
- PP32 - **Said Sebih**, Application of a New Liquid Crystal as Stationary Phases for the Separation of Some Volatile Aroma Compounds
- PP33 - **Sayaka Hatano**, Development of a Photo-Induced Fast Spin-State Switching Molecule
- PP34 - **Soulimane Boudah**, Synthesis, Characterization and Analytical Study of Salicylidene Imine Liquid Crystals Used as Stationary Phase in CPG
- PP35 - **Zoe Dominguez**, Chiroptical Properties of Azabora[5]helicene Architectures
- PP36 - **Yusuke Inagaki**, Rotation of the pi-System Rotor in Crystalline Molecular Gyrotops
- PP37 - **Zoran Glasovac**, The Role of Intramolecular Hydrogen Bonds in Construction of Model Donor-Acceptor Salt Bridged Crystals
- PP38 - **Jorn D. Steen**, Proton dependent redox chemistry of spiropyrans
- PP39 - **Gulce Ogruç-Ildiz**, Structural Aspects and Reactivity of 5-Methylhydantoin

Reaction mechanisms and Catalysis

- PP40 - **Alba Pereira Vilar**, Formation of pillar[5]arene based stable rotaxane with azobenzene
- PP41 - **Alyssa Gilbert**, Investigation of the effects of ionic liquids as solvents on a unimolecular substitution process
- PP42 - **Anastasiia Kovrizhina**, Methods for the preparation of new 11H-indeno[1,2-b]quinoxalin-11-one oxime analogs as promising JNK inhibitors
- PP43 - **André D. Lopes**, Catalytic Performance of Pyridyl-Benzimidazole Oxidomolybdenum(VI) Complex in Olefin Epoxidation
- PP44 - **Anna Rovaletti**, Theoretical investigation on the effect of ligand bulkiness on the reactivity of organometallic complexes.
- PP45 - **Basim Asghar**, Assessment of the nucleophilic reactivity of some heterocyclic amines with superelectrophilic 4,6-dinitrobenzofuroxan
- PP46 - **Barbara Ticconi**, Oxidation of aliphatic and aromatic amino acids with H₂O₂ catalyzed by a nonheme imine based iron complex
- PP47 - **Christina McCulley**, A Mechanistic Examination of the Influence of Alkene Substitution on Rates of Biomimetic Pt-Promoted Polyene Polycyclization
- PP48 - **Christof Jaeger**, Thermodynamic Reaction Control in Radical Enzymes and the Role of Orientated Electric Fields
- PP49 - **Elisa M. Brás**, UV-induced photolysis of a dispiro-1,2,4-trioxolane with antiparasitic activity
- PP50 - **Gabriel J. Reyes-Rodríguez**, Evans Enolates: Lithium Hexamethyldisilazide-Mediated Enolization of Acylated Oxazolidinones
- PP51 - **Hidetoshi Noda**, On the Mechanism of Direct Amidation Catalyzed by the B₃NO₂ Heterocycle
- PP52 - **Inmaculada Moreno**, Oxidation of Desmetryn by Peroxynitrous Acid
- PP53 - **Ivana Biljan**, Self-Assembly and Dimerization of Aromatic Dinitroso Derivatives on Gold Surface
- PP54 - **JESSICA JAZMIN SANCHEZ GARCIA**, Bis-cations with two (2,3-diferrocenylcyclopropenium) fragments stabilized with diaminoalkanes: synthesis and reactivity
- PP55 - **Jiayun Zhu**, Towards an Organocatalytic Route for the d¹-Deuterated of Aldehydes
- PP56 - **Jiri Hanusek**, Kinetics and Mechanism of Cu(I)-catalyzed [3+2]cycloaddition between phenyl sydnone and phenylacetylenes
- PP57 - **João Lourenço**, Catalytic Conversion of Glycerol to Value-Added Products
- PP58 - **Joel Le Bars**, Kinetic investigation of methyl bromide reaction with ethanolamine

- PP59 - **Julian Helberg**, The Phosphane-Catalyzed Oligomerization of Isocyanates – Mechanistic Study and Identification of a Transient Intermediate
- PP60 - **Karin Schaffarczyk** McHale, Interactions of the components of ionic liquids with species along the reaction coordinate of substitution processes
- PP61 - **Kevin O. Maduka**, Synthetic and Kinetic Evaluation of Triazolyl Mimics of Thiamine Pyrophosphate (TPP) for Biocatalysis
- PP62 - **Lidia Cavaca**, Oleuropein: a valuable chiral building block
- PP63 - **Long Zhang**, The enantiocontrol in Primary amine Catalysis
- PP64 - **Patrick Jüstel**, Concurrent SN1 and SN2 Mechanisms in Solvolysis Reactions
- PP65 - **Paulina Pavez**, Dual function of Amino Acids Ionic Liquids (AAILs) on the Degradation of Organophosphate Pesticide, Paraoxón®
- PP66 - **Pedro Horta**, Synthesis and Structure of a Novel O-linked Diazirine-Quinolone Conjugate
- PP67 - **Markus Schauer**mann, NMR evidence for the aromatic, thiamine-like Breslow-Intermediate
- PP68 - **Miroslav Ludwig**, Push-Pull Dicyanoimidazoles in Photoredox Catalysis
- PP69 - **Nelaine Mora-Diez**, Modelling the Repair of Damaged Proteins by Antioxidants
- PP70 - **Rafael Gomes**, Mechanistic studies on the Formation of Novel Cyclopentenones from Activated Furans
- PP71 - **Raquel Fernandes**, Photocatalytic synthesis of benzaldehyde derivatives
- PP72 - **Rebecca Hawker**, Rational selection of the components of an ionic liquid solvent to control the reaction outcome of some organic processes
- PP73 - **Roberto Colunga**, A Radical Twist In The Mechanism Of Lithium-Halogen Exchange
- PP74 - **Roberto Figueroa**, Synthesis of amino acid ionic liquids (AAILs) and their effect in the reactivity of Thiol-Michael addition reaction.
- PP75 - **Rodrigo Montecinos**, Synthesis and Characterization of Pillar[5]Arene functionalized with Hydroxy-L-proline. Searching an Asymmetric Organocatalyst
- PP76 - **Ricardo Ferreira Affeldt**, Experimental and Theoretical Evidence of Intramolecular Bifunctional Catalysis in Amide Cleavage
- PP77 - **Roland Löw**, Relaxation Time Measurements of Azo Functionalized TATA Platforms
- PP78 - **Romain Lepage**, Computational study of the mechanism of glycosylation of L-idose derivatives

- PP79 - **Tainah Dorina Marforio**, A Mechanistic Insight into CNT-Catalyzed Oxidative Dehydrogenation of Ethylbenzene to Styrene. A DFT Computational Study
- PP80 - **Tatiana Nekipelova**, Mechanism of the Annulation of 4-Ethynylanisole with Mixed Phosphonium-Iodonium Ylide
- PP81 - **Thomas Dent**, Investigation of the caesium effect in palladium catalysed coupling reactions
- PP82 - **Uta Wille**, Decoding the mechanism of environmental radical polyester degradation
- PP83 - **Xiuling Cui**, Alkynone-Based Synthesis of Heterocycles

Supramolecular and Systems Chemistry

- PP84 - **Agustin Morales**, Use of Photolabile Ru(II) Complexes for Supramolecular Release
- PP85 - **Alexandra Filipe**, A brief survey on diffusion wave spectroscopy in soft matter systems
- PP86 - **Alexandre Miranda**, Synthesis and Anion Recognition by Dinitrophenylurea-Dihomooxalix[4]arene Receptor
- PP87 - **Alvaro Cañete**, Synthesis and spectroscopic characterization of 4-(diethylamino)salicylaldehyde bearing at coumarin derivative. Effect of Cucurbit[7]uril encapsulation on its spectral properties.
- PP88 - **Andreas H. Heindl**, Tuning the Switching Properties of Macrocyclic Azobenzenes by Ring Strain
- PP89 - **Angel Acuña Barros**, Nitric Oxide release from a cucurbituril encapsulated NO-donor
- PP90 - **Baya Berka-Zougali**, COMPARISON OF THE CHEMICAL COMPOSITION AND BIOLOGICAL ACTIVITIES OF ESSENTIAL OILS OBTAINED BY CLASSICAL STEAM DISTILLATION (SD)
- PP91 - **Davor Margetic**, Self-Assembly of Aromatic Donor-Acceptor Systems by Guanidine-Carboxylate Binding
- PP92 - **Filip Ulatowski**, Dynamic combinatorial libraries that can classify molecules according to their structural features
- PP93 - **Guntram Schwarz**, Electrochromic properties of Metallo-supramolecular Polymers
- PP94 - **Joana Cristo**, How does cholesterol affect the fluidity of model lipid bilayers at the molecular level?
- PP95 - **João Ravasco**, New double functionalizable trans-cyclooctenes for enhanced spatial and temporal resolution study of biological systems
- PP96 - **Jackson Jose Alcazar Jimenez**, Reactivity of carbonates and thiocarbonates derivatives toward hydrolysis reaction in the presence of calixarene

- PP97 - **J.C. Mejuto**, STABILITY OF IPRODIONE IN AOT-BASED REVERSE MICELLES UNDER ALKALINE CONDITIONS
- PP98 - **Jorge Martins**, Measuring dielectric constants of lipid bilayers: excluding experimental artifacts from pyrene fluorescence in liposomes
- PP99 - **José G. Santos**, Hydrolysis reactions of carbonates and thiocarbonates derivatives. Supramolecular Catalysis by Cucurbit[7]uril.
- PP100 - **Kajetan Dąbrowa**, Dynamic control of ion-pair binding by photo-tunable azobenzene-derived hosts
- PP101 - **Koki Ikemoto**, Synthesis and Structures of Nanometer-sized Geodesic Phenylene Bowl
- PP102 - **Leandro Scorsin**, A Kinetic Study With Neutral and Cationic Dioxolanes Catalyzed by CB7
- PP103 - **Marcella de Sá Haddad Queiroz**, Study of phase solubility of bioactive naphthoquinones
- PP104 - **Margarita E. Aliaga**, Cucurbit[7]uril encapsulation effect on tautomerism equilibrium in aza-coumarin and quinoxalinone scaffolds.
- PP105 - **Matthew Watson**, Predicting Reactivity in Binary Solvent Mixtures Using a Supramolecular Solvation Model
- PP106 - **Miguel Ángel Romero Carrasco**, Binding of Terpenes by Cucurbituril Macrocycles
- PP107 - **Nelaine Mora-Diez**, Macroscopic pKa prediction of polyprotic acids from DFT calculations: the case of acetohydroxamic acid
- PP108 - **Niklaas Jan Buurma**, I2CITC : Modular Deconvolution of ITC Data for Complex Equilibrium Systems
- PP109- **Olimpo García-Beltrán**, Synthesis and characterization of a new coumarin-derivative chemosensor to detect mercuric ions
- PP110 - **Orlando Oliveira**, Towards Catalytic Metalated Covalent Organic Frameworks through Supramolecular Strategies
- PP111 - **Patricia Remón**, Chemical Communication in a Supramolecular Cascade
- PP112 - **Pravat Mondal**, Thio-Bambusurils
- PP113 - **Rubén Martín**, Encryption of Chemical Information in a Supramolecular Assembly
- PP114 - **Sebastian Hamer**, Dipolar Molecular Rotors in Surface-anchored Metal Organic Frameworks
- PP115 - **Silvia Hristova**, Theoretical design and spectral investigations of tautomeric rotary switches
- PP116 - **Rui Fausto**, The Role of Perchlorate Anion on Dimerization of a Macroacyclic Binuclear Cu(II) Complex: Comparison with a Mononuclear Ni(II) Macrocylic Complex

PP117 - **Rubén Martín**, Encryption of Chemical Information in a Supramolecular Assembly