



73rd Southeastern Regional ACS Meeting

Chemistry transcending boundaries for a sustainable future

TECHNICAL PROGRAM

Oct. 19, 2022

PUERTO RICO CONVENTION CENTER, SAN JUAN, PUERTO RICO
Hosted by the ACS-Puerto Rico Section



WENESDAY MORNING

WEDNESDAY MORNING

Puerto Rico Convention Center 202 A

Biochemistry I Structure / Dynamics

E. I. Pares-Matos, *Organizer*

X. Liu, *Presiding*

8:30 Introductory Remarks.

8:40 20. Structural Characterization of Superoxide Dismutase Amyloid Fibrils in the Presence of H₂S.

P.M. Miranda-Castrodad, T. Victor, R. Pietri

9:00 21. Importance of Hsp60's C-terminal tail in refolding of misfolded substrates. **D.H. von Salzen**

9:20 22. Withdrawn

9:40 23. Molecular docking studies between Ras2p,

the cytoplasmic domain of three members of the Wsc-family and several therapeutic drugs. **E.I.**

Pares-Matos, K. Carrasquillo-Carrión, A. Roche

Lima, J. Rodríguez Medina

10:00 Coffee Break.

10:25 24. Withdrawn

10:45 25. Disease-associated non-coding variants alter NKX2-5 DNA binding affinity. **E.G.**

Peñalva-Martínez, D.A. Pomales-

Matos, A. Rivera-Madera, L. Sanabria, B.M.

Rosario, J.A. López Gonzales

11:05 26. The role of flanking residues on AT hook motif activity. **K.L. Buchmueller**

11:25 27. Beyond the End Replication Problem:

Using smFRET to investigate the formation and dynamics between G Quadruplexes and T-Loops in Human Telomeres. **A. Lacen**, H. Lee

Puerto Rico Convention Center 104 A

Advances in Nanomaterials for Biomedical and Biomedical Applications

M. Nurunnabi, *Organizer*

M. Narayan, *Presiding*

8:30 Introductory Remarks.

8:40 1. Nanoprobe mediated non-invasive imaging of cardiotoxicity induced by chemotherapeutic. **M.**

Nurunnabi

9:00 2. An electrochemical biosensing strip for

telomerase activity detection: as a translational research alternative in oncology. **R. Diaz-Ayala**, L.

Cunci, C.I. González, C.R. Cabrera

9:20 3. Withdrawn

9:40 4. Withdrawn

10:00 Coffee Break.

Our deepest gratitude goes to our Diamond Sponsor Oakwood Chemical

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WENESDAY MORNING

10:25 5. Advancing Carbon Nano Materials to intervene in the structural-drivers of neurodegenerative onset and progress. **M. Narayan**

10:45 6. Bioactive electrospun cellulose acetate scaffolds for bone tissue engineering applications. **S.A. Bello**, O.A. Rodriguez-Rivera, E. Nicolau

11:05 7. Combining Bioorthogonal Chemistry with Fluorescent Silica Nanoparticles for the Ultrasensitive Detection of HIV-1 p24 Antigen. **S.S. Iyer**, T. jia, V. Saikam, Y. Luo, X. Sheng, J. Fang, J. Natekar, M. Kumar

11:25 8. Nanomaterials dynamics in Soil-plant continuum. **M. Shrivastava**

11:45 9. Synthesis and characterization of different morphologies of iron oxide nanoparticles for biomedical applications. **A. Lavin**, **G. Morell**, W.S. Pantoja Romero, N. Medina, B. Weiner

12:00 10. Bioconjugation of enveloped viruses as nanovectors for immunotherapy applications. M. Kingsak, K. Metavarayuth, **Q. Wang**

Puerto Rico Convention Center 201 A

Analytical Chemistry I – Remediation

L. Cunci, *Organizer*

L. V. Fernandez-Vega, *Presiding*

8:30 Introductory Remarks.

8:40 11. Electrochemical Bioremediation of Uranium (VI) Using *Geobacter sulfurreducens* on Boron-Doped Diamond Electrode Surface. **A.J. Acevedo**, E.G. Rosario-Cruz, J.R. Caicedo-Villamil, G.A. Toranzos-Soria, C.R. Cabrera

9:00 12. Chronoamperometric detection of glutathione using copper nanoparticle electrodeposition at graphene oxide modified electrode. **M.B. Wayu**

9:20 13. Assessing and rationalizing the electrocatalytic activity of bimetallic nanocarbides towards the oxygen evolution reaction. **R. Lazenby**, A. Ritz, I.A. Bertini, E.T. Nguyen, G.F. Strouse

9:40 14. Deciphering Aggregation Induced Electrogenerated Chemiluminescence Mechanism of

9,10-Diphenylanthracene Derivatives. **J.A. MOTCHAALANGARAM**, K. Aumick, W. Miao

10:00 Coffee Break.

10:25 15. Naproxen removal from water using Ca-Fe(III) alginate beads. **D. Sanchez**

10:45 16. Withdrawn

11:05 17. Multicomponent deoxyribozymes for identification of pathogenic mycobacteria. R. Connelly, K. Rodriguez, J. Ahn, A. Fergus, K. Rohde, **Y. Gerasimova**

11:25 18. Effect of gamma irradiation on Vitamin D stability in salmon. **P.R. Calvo**, J.S. Brown

11:45 19. Historical variation of trace metals in sediments from Deering Bay waterways (South Florida). **M. Ceccopieri**, P.R. Gardinali

Puerto Rico Convention Center 201 B

Inorganic Chemistry I - Inorganic materials

M. B. Santiago-Berrios, *Organizer*

E. Melendez, *Presiding*

8:30 Welcoming remarks.

8:40 28. Valence-to-core x-ray emission spectroscopy as a probe of platinum catalysis. **C.J. Pollock**, L.M. Debeve

9:00 29. The class of sulvanites Cu_3MX_4 (M = V, Nb, Ta; X = S, Se, Te) at the nanoscale: Synthesis and applications. **D.R. Radu**, C. Lai

9:20 30. The Influence of Covalency on Magnetic Exchange in Manganese Monochalcogenides. J.K. Clark, V. Garlea, **M. Shatruk**

9:40 31. Understanding Phase Control in the synthesis of Iron Sulfides. **J. Espano**, J. Macdonald

10:00 Coffee Break.

10:25 32. Reorganization Energy and Charge Transfer from Quantum Dots. M.J. Fort, S.M. Click, E.H. Robinson, F. He, P.V. Bernhardt, S.J. Rosenthal, **J. Macdonald**

WENESDAY MORNING

10:45 33. Withdrawn

11:05 34. The advantages of passivation layer on the top of perovskite layer by organic molecules. **M.H. Alotaibi**, h. alhajri, e. alharbi, F. Alasmari, M. Ajarim, H. Albrithin, S. Zakeeruddin, M. Graetzel

11:25 35. Withdrawn

11:45 36. Automated generation and theoretical predictions for dye sensitized solar cell dyes. **T. Santaloci**, A. Wallace, J.H. Delcamp, R.C. Fortenberry

Puerto Rico Convention Center 204

Inorganic Porous and Layered Materials Symposium I

M. Pica, M. Ramos-Garcés, L. Sun, *Organizers*
J. L. Colon, *Presiding*

8:30 Opening remarks.

8:40 37. Resilience of inorganic layered materials: the case of nanocrystalline zirconium phosphate and its use for the synthesis of functional derivatives. **M. Pica**, A. Donnadio, M. Nocchetti, R. Vivani, M. Casciola

9:00 38. Surface modification of layered structured nanomaterials for drug delivery. **J. González-Villegas**, K. Salazar-Ayala, A. Velázquez-Matos, J.L. Colon

9:20 39. Multitechnique insight into an unusual cooperative CO₂ absorption mechanism in a perfluorinated CeIV MOF. **F. Costantino**, M. Taddei, D. Morelli Venturi, V. Crocellà, M. Signorile, C. Atzori, L. Calucci, M. Cavallo, M. Geppi

9:40 40. Designing Electrocatalytic MOFs: Considerations from Redox Hopping Electron and Ion Transport. **A.J. Morris**

10:00 Coffee Break.

10:25 41. Hierarchically Porous Metal–Organic Frameworks: Preparation, Properties, and catalytic Performance. **Q. Zhang**

10:45 42. Metal-modified zirconium phosphate electrocatalysts for the oxygen evolution reaction. **M.V. Ramos-Garcés**, J. Sanchez, T.F. Jaramillo, J.L. Colon

11:05 43. Design of processable polymeric carbon nitride for a range of photo(electro)catalytic applications. **S. Garcia-Granda**, I. Krivtsov, C. Adler, A. Vazirani, D. Mitoraj, R. Beranek

11:25 44. A Hierarchical Activated Carbon – Silicoaluminophosphate Composite Prepared via Confined Space Synthesis for the Deep Removal of Carbon Dioxide from Humid Gas Phase. **G. del Valle Perez**, J.C. Muñoz-Senmache, P.E. Cruz Tato, E. Nicolau, A.J. Hernandez

11:45 45. Withdrawn

Puerto Rico Convention Center Ball Room A

Nanotechnology Approaches to Biology and Medicine

P. S. Weiss, *Organizer, Presiding*

8:30 Opening Remarks.

8:40 46. Nanotechnology Approaches to Biology and Medicine. **P.S. Weiss**

9:20 47. Withdrawn

9:40 48. Targeted ligand design of N-heterocyclic carbenes for biological applications on gold surfaces. I.M. Jensen, G. Kaur, J.P. Camden, **D.M. Jenkins**

10:00 49. Ionic Liquid-Coated Polymeric Nanoparticles for Targeted in situ Hitchhiking on Blood Components. **E.E. Tanner**

10:20 Coffee Break.

10:45 50. Choline carboxylic ionic liquid-based gold nanoparticles for biomedical applications. **P. Vashisth**, E.E. Tanner, C. Smith

11:05 51. Application of DMPO-nitrone adduct aided nano-bioassay for quantifying Particulate Matter (PM)-induced oligomerization process of Amyloid Beta proteins. **J. Bang**, J. Wei, K. Omar, R. Hawkins, D.K. Taylor, B.K. Dey

WENESDAY MORNING

11:25 52. EPR Spectroscopy in Studies of Nanomaterials. **A.I. Smirnov**

11:45 53. Ionic liquid to invade skin barriers to improve topical drug delivery. **M. Nurunnabi, M. Huda**

Puerto Rico Convention Center 202 B

Organic Chemistry I Organic Reagents

D. J. Sanabria-Rios, *Organizer*

J. A. Prieto, *Presiding*

8:30 Opening Remarks.

8:40 54. Overriding Embedded Heteroatoms: A Gateway to Alternate Selectivity in Lithiation Reactions. **A.A. Thomas**

9:00 55. Synthesis and Application of Organic Ferrocene Derivatives in Perovskite Solar Cells. **A. Burgos Suazo, E. Ortiz Muñoz, I. Montes, D.M. Pinero Cruz, J.L. Colon**

9:20 56. Selective microwave heating of homogeneous organic reaction mixtures. **G.B. Dudley**

9:40 57. Withdrawn

10:00 Coffee Break.

10:25 58. Design and Optimization of Potent Cereblon-Recruiting HaloPROTACs. **S. Nelson, B. Ody, R. Liu, S. Whitzel, C. Dodd, L. Williams, J. Yin, M.L. Turlington**

10:45 59. Styrene synthesis via crossed aldehyde-aldehyde aldol coupling promoted by trimethylsilyl trifluoromethanesulfonate. **C.W. Downey**

11:05 60. Dipyrindinium thiazolothiazoles photochemical sensors. **T.J. Adams, M. Acharya, Q. Nguyen, M.G. Walter**

11:25 61. Cycloaddition Reactions with Organocobaloximes. **O. Ahrens, D.M. Diaz, J. Lagana, K. Cartwright**

11:45 62. Using Cobaloximes as “Directing Groups” for Chiral Ligands. **J. Lagana, K. Cartwright**

12:05 End of Session.

Puerto Rico Convention Center 203

Surface Chemistry: Polymer Science, Self-Assembly, and Bio interfaces

R. Quiñones, *Organizer, Presiding*

8:30 Opening remarks.

8:40 63. Synthesis of metal-binding polymers for water purification. **P.R. Calvo**

9:00 64. Withdrawn

9:20 65. Biomolecular Attachment Yield Analysis on Surface Structurally Diverse Microgel Particles. **M. Gaines, J. Kamuche, L. Norris, I. Page, S. Oliveros Gomez, M. Grover**

9:40 66. Surface enhanced self-limiting growth of one-dimensional arrays of DNA Origami dimers. **N. Shin, D.P. Neff, M.L. Norton**

10:00 Coffee Break.

10:25 67. DNA aptamers for material targets. **V. Milam, M. Tapp, P. Dennis, R. Naik**

10:45 68. Protein Stability on Nanoparticle Surfaces: A Material Difference. **N.C. Fitzkee, R. Somarathne, C. Kariyawasam, R. Yadav**

11:05 69. Zinc triggered release of encapsulated cargo from liposomes via a synthetic lipid switch. **R. Sagar, J. Lou, A. Watson, M. Best**

11:25 70. Friction of fatty acids at different sliding speeds. **R. Cui, G. Diaz De la Cruz, M. Ruths**

11:45 71. High-temperature fluoropolymers, aromatic networks, and carbon therefrom for advanced composites & energy applications. **D.W. Smith, G. Munoz, E. Borrego, S. Athukorale, K.M. Mukeba, C.U. Pittman**

Puerto Rico Convention Center 208 A

Trends in Chemistry Education

D. Cruz-Ramirez de Arellano, *Organizer*

M. Oliver-Hoyo, *Presiding*

WENESDAY MORNING

8:30 Introductory Remarks.

8:30 72. Analysis of representations in chemistry textbooks: A literature review. **B. Thompson**, Z. Bunch, M. Popova

8:30 73. Reconceptualizing representational competence through the analysis of student reasoning about representations of molecular structure. **M. Popova**

8:30 74. Embedding Team Science in Course-based Undergraduate Research Experiences. **J.P. Walker**, C.I. Andersen

8:30 75. Withdrawn

8:30 Coffee Break.

8:30 76. Withdrawn

8:30 77. Development of interactive pre-laboratory assignments and their impact on the laboratory experience. **L.L. Serbulea**, N. Jannatifar, S. Stegner

8:30 78. Infusion of Organic Synthesis Research into Organic Chemistry I lab at WSSU. **F. Guo**

8:30 79. Incorporating proteomics into introductory analytical laboratories during COVID-19. **S. Verberne-Sutton**, K. Stepler, K. Kapp, R.A. Robinson

8:30 80. Design and implementation of an interdisciplinary course in chemical biology. **A. Fikes**, M.C. Srougi



WEDNESDAY AFTERNOON

WEDNESDAY AFTERNOON



Puerto Rico Convention Center 203

3rd Users' Meeting of the UPR MSRC X-Ray Diffraction Facility

D. M. Piñero Cruz, *Organizer, Presiding*

1:25 Introductory remarks.

1:35 **81.** Recognizing Synthetic Pathways with the use of Crystallography: Crystal Structures of 4-methylbenzene-1,2-dithiol derivatives. **V.Y. Soto-Diaz**, D.M. Pinero Cruz

1:55 **82.** Synthesis, characterization, and Hirshfeld surface analysis of dithiolene systems as potential chelating ligands. **K.T. Cordero-Gimenez**, D.M. Pinero Cruz

2:15 **83.** Crystallographic and computational calculations of Pd and Pt non-innocent salen-like complexes. **J.O. Rivera**, J. Jones, D.M. Pinero Cruz

2:35 **84.** Crystal structure of novel ferrocenyl-urea-chalcones. **J.A. Mendez Roman**, D.M. Pinero Cruz, I. Montes

2:55 **85.** Structural Modification Phenomena in Bromine Substituted Ferrocenyl Chalcones. **A. Burgos Suazo**, E. Ortiz Muñoz, I. Montes, D.M. Pinero Cruz

3:15 Intermission.

3:40 **86.** Polymorphism and chemical properties in Ferrocenyl Furan Chalcones isomers. **A.S. Rodriguez Rolon**, S. Delgado, J.J. Soto Perez, D.M. Pinero Cruz, C.R. Cabrera, I. Montes

4:00 **87.** Crystal structure and Hirshfeld surface analysis of three novel substituted phthalonitriles. **J.A. Cruz-Lozada**, D.M. Pinero Cruz

4:20 **88.** X-Ray crystallography of heterocyclic ferrocenyl chalcones. **A.M. Sanchez**, P.M. Bonilla Crespo, D.M. Pinero Cruz, I. Montes

4:40 Concluding remarks.

Puerto Rico Convention Center 104 B

ACS Chemistry Festivals, Non-formal Chemistry Education around the World

S. Sandi-Ureña, *Organizer*

I. F. Cespedes-Camacho, *Presiding*



1:25 Introductory remarks.

1:35 **89.** "Festival de Química" a model to globally communicate the value of chemistry in our daily lives: history and impact. **I. Montes**, L. Raines

2:15 **90.** Improving All People's Lives through the Transforming Power of Chemistry Outreach. **L. Raines**, P. Galvan, N. Bakowski, T.M. Chambers

2:35 **91.** The first ACS Chemistry Festival in Costa Rica: a general overview. **I.F. Cespedes-Camacho**

2:55 **92.** Chemistry outreach initiatives and student engagement in Jamaica. **A. Goldson-Barnaby**

3:15 Coffee Break.

3:40 **93.** Earth Week during the pandemic: An international collaboration. **B.C. Galarreta**, C.V. Gauthier

4:00 **94.** Girls in science day. **C. Guzman-Quilo**, G. Monzón

4:20 **95.** More chemistry, better life - Festival - Más Química, Mejor vida: A Festival for the student volunteers! **S. Sandi-Ureña**

4:40 Final remarks.

Puerto Rico Convention Center 201 A

Analytical Chemistry II - Sensors

L. Cunci, *Organizer, Presiding*

1:25 Introductory Remarks.

WEDNESDAY AFTERNOON

1:35 96. Mycotoxin screen test using aptameric plasmonic nanosensors. **B.C. Galarreta**, Y. Hernández, A. Saldaña, S. Córdova, M. Licuona Puma

1:55 97. Chemical fingerprinting sensors in aqueous and environmentally relevant media. **M. Bonizzoni**, X. Yao, Y. Xu, M. Ihde

2:15 98. Electrochemical aptamer-based sensor for the measurement of Neuropeptide Y using methylene blue as a label redox probe. **L.F. Lopez**, L. Martinez, L. Cunci

2:35 99. Simultaneous Electrochemical Detection of Multiple Neurotransmitters. **K. Xu**, E.S. McClain, D.R. Miller, D.E. Cliffler

2:55 100. Enhancement of paper-based biosensors for sweat with guanosine-based supramolecular particles. **D.L. Rodriguez Ayala**, J.M. Rivera

3:15 Coffee Break.

3:40 101. Electrochemical flexible biosensor development for neuropeptides and neurotransmitters detection in sweat. **A. Espinosa Vazquez**, E. Vazquez, L. Acosta, J. Diaz, K. Vicente Ramos, L. Cunci

4:00 102. DNA based microparticle molecular tension sensors for mapping cell mechanics in non-planar geometries and for high-throughput quantification. **Y. Hu**, V. Ma, R. Ma, W. Chen, Y. Duan, R. Glazier, B. Petrich, R. Li, K. Salaita

4:20 103. Novel screening method for fish exposed to Perfluoroalkyl substances (PFAS): Raman spectroscopy of blood plasma and machine learning. **L. Pérez Almodovar**, I.K. Lednev

Puerto Rico Convention Center 202 A

Biochemistry II Biosensors / Signaling

E. I. Pares-Matos, *Organizer*
A. Baerga-Ortiz, *Presiding*

1:25 Introductory Remarks.

1:35 104. Bacterial Glycan Enrichment and Immobilization for Glycan Interacting Partner Analysis. **A. Murray**, J.M. Troutman

1:55 105. Withdrawn

2:15 106. In-cell mixture synthesis for profiling lipid metabolism and signaling. Q. Zhang, Y. Zhang, Z. Han, **Q. Zhang**

2:35 107. Linearly polarized and integrating sphere-assisted resonance synchronous spectroscopies as bioscience tools: An example application with protein and silver nanoparticle interactions. **K.R. Carter**, M. Wamsley, J. Emerson, D. Zhang

2:55 108. Withdrawn

3:15 Coffee Break.

3:40 109. The release of the sulfonamide Toll-Like Receptor-4 inhibitor TAK-242 from surface modified cell surfaces attenuates allogenic immune responses in a in vitro co-culture model. **J. Mattke**, S. Vasu, C. Darden, M.A. Plunk, M.C. Lawrence, R.R. Kane, B. Naziruddin

Puerto Rico Convention Center 202 C

Discovery and Production of Bioactive Marine Natural Products

Y. Ding, *Organizer, Presiding*

1:25 Introduction.

1:35 110. What have we learned in the Caribbean about marine α -methoxylated fatty acids. **N.M. Carballeira**

1:55 111. Friomaramides. J. Bracegirdle, D. Casandra, P. Subramani, J. Rocca, J. Adams, N. Wilson, **B. Baker**

2:15 112. Bioactive marine algae natural and pseudo-natural products. M.L. Matos-Hernandez, W.O. Mendoza-Morales, G. Dyer, J. Cassel, I. Tietjen, T. Messick, **E.J. Caro-Diaz**

2:35 113. Discovery and production of bioactive marine natural products through genome-based and synthetic biology approaches. **Y. Ding**

2:55 114. Biosynthetic diversification of diketopiperazine natural products. **A.L. Lane**

3:15 Coffee Break.

WEDNESDAY AFTERNOON

3:40 115. Under the hood: surprises in biosynthesis of pyrrolic polyketides. **V. Agarwal**

4:00 116. Investigating the Effects of Heterologous Expression on Folding and Function of Actinomycetal Megasyntases. **T. Sword**

Puerto Rico Convention Center 209 C

Enabling Technologies in Drug Discovery and Development

A. Christian, *Organizer, Presiding*
T. J. Henderson, *Presiding*



1:25 Introduction.

1:35 117. Withdrawn

1:55 118. Withdrawn

2:15 119. Manufacturing Process Development of Nembrotinib (MK-1026). **N.R. Deprez**

2:35 120. Procedures and Concerns for the Industrial Synthesis of Isocyanates and Isothiocyanates. **T.T. Romoff**, B.J. Marchyshyn, A. Smith, G. Butler

2:55 121. Novel antibiotics target BamA lateral gate opening as mechanism of action. **K.M. Kuo**, J. Liu, A. Pavlova, J. Gumbart

3:15 Coffee Break.

3:40 122. Molecular hybridization: An effective and potential tool for the development of therapeutic agents. **S.S. Panda**

4:00 123. Structure-based approaches to inhibit *Streptococcus mutans* cariogenic virulence. **S.E. Velu**

4:20 124. Betulinic Acid Derivatives as Potential Anti-Cancer Agents. **S.C. Jonnalagadda**

Puerto Rico Convention Center 208 A

Evaluation and Assessment in Chemistry Education

M. Oliver-Hoyo, *Organizer*
D. Cruz-Ramirez de Arellano, *Presiding*

1:25 Introductory remarks.

1:35 125. Reflections on using a Specifications Grading approach for organic chemistry I & II courses at Georgia Gwinnett College. **M.S. Morton**, M. Anzovino, o. Villanueva

1:55 126. Exploring student engagement in self-assessment through a two-tiered general chemistry instrument. **M. Balabanoff**

2:15 127. Fundamentals of chemistry: course impact and retention. **P.A. Shelton**, A.H. Shelton

2:35 128. Decoupling upper level labs from lecture courses in favor of a course-based research model. **L.B. Thompson**, S. Frey

2:55 129. Design and assessment of virtual cell culture laboratory training experiences for undergraduate and graduate students. D. Tredwell, D. Spencer, C. McKeown, B. Huckaby, A. Wiedner, J. Dums, N. Sudduth, E. Brown, P. Albright, A. Jhala, **M.C. Srougi**

3:15 Coffee Break.

3:40 130. Withdrawn

4:00 131. Key Stakeholders' Interpretations of Scientific Information Literacy: A Survey of Orange and Seminole County K-16 Educators. **M. Lam**, **C. Randles**

4:20 132. Creating a culture of assessment within the university and chemistry department. **H.V. Clontz**

Puerto Rico Convention Center 204

Inorganic Porous and Layered Materials Symposium II

J. L. Colon, M. Ramos-Garcés, L. Sun, *Organizers*
M. Pica, *Presiding*

1:25 Opening remarks.

WEDNESDAY AFTERNOON

1:35 142. Imaging and Dynamics of 2-Dimensional H-BN Nanosheets in Aqueous Solution. U. Umezaki, A. Smith McWilliams, Z. Tang, A. Kolomeisky, M. Pasquali, **A.A. Marti-Arbona**

1:55 143. Controlling the formation of 2D MOFs versus 1D metal organic nanotubes (MONTs). J.A. Barrett, P. Nalaoh, **D.M. Jenkins**

2:15 144. Multivariate metal-organic frameworks as organic based solid-solution crystals with predictable structure, variable composition, and tunable fluorescent, redox, and photoredox properties. **F.J. Uribe-Romo**

2:35 145. Synthesis and Characterization of Zeolite-Encapsulated Organometallic Complexes for Oxidation Chemistries. E. Iaiia, A. Shrestha, A. Soyemi, J.L. Groeber, G.R. Rana, A. Chowdhury, C.R. Diemer, T. Szilvasi, M.G. Bakker, **J.W. Harris**

2:55 146. Withdrawn

3:15 Coffee Break.

3:40 147. Modulation of Ruthenium (II) Tris-(2,2'-bipyridine) Photophysics through Cavity Size in Zn (II) and Zr (IV) Metal Organic Frameworks. **R.W. Larsen**, J.M. Mayers

4:00 148. Nanoconfined catalytic sites in 2D layered metal oxides for the electrocatalytic oxygen evolution reaction. **D.R. Strongin**, U. Kakati, J. Ning, B. Roe, J. Sun

4:20 149. Andrographolide encapsulation in metal-organic frameworks as a drug delivery system for cancer applications. **W.S. Pantoja Romero**, Y. Aysa, A. Lavin Flores, N. Medina, G. Morell, B. Weiner, J. Coronas

Puerto Rico Convention Center 202 B

Organic Chemistry II Synthesis

D. J. Sanabria-Rios, *Organizer, Presiding*

1:25 Opening Remarks.

1:35 150. Synthetic efforts towards the total synthesis of Balgacyclamide's A & B. **S.M. Rivera Gotay**, A. Torres Hernandez, P.K. Desman, R. Rafferty

1:55 151. Enantioselective Synthesis of Triarylmethanes via Dirhodium Diaryl Carbene Compounds. **M. Lee**, H.M. Davies

2:15 152. Synthesis of Flavonoid 7-O-Glycosides. **L. Cai**

2:35 153. Design and synthesis of potential drug candidates for SARS-CoV-2. **L. Brown**, **S.S. Panda**

2:55 154. Synthesis and characterization of a Triapine azo compound as a potential anti-cancer drug. **A.E. Cardona Rivera**, N.K. García, R. Rodriguez, A.D. Tinoco

3:15 Coffee Break.

3:40 155. Discovery and Development of a Scalable Asymmetric Synthesis of Complex Cyclopropyl Boronates. **A. Gutierrez Bonet**

4:00 156. Ferrocenyl-urea-chalcones as potential anticancer agents. **J.A. Mendez Roman**, E. Peterson-Peguero, I. Montes

4:20 157. Building a toolkit of catechols to probe dioxygenase activity. **L.W. Peterson**, J. Steiner, E.G. Gruss, G. Xhafkollari, K.L. Nyamkondiwa, T.R. Squires, D. Strzeminski, S. Leyes-Porello, H. Caplan, K.L. Colabroy

4:40 End of Session.

Puerto Rico Convention Center 104 A

Sustainable Nanotechnology

C. L. Haynes, R. Hernandez, S. E.

Mason, *Organizers*

L. Echegoyen, *Presiding*

1:25 Opening remarks.

1:35 159. Exohedral and endohedral fullerene derivatives for applications in perovskite solar cells and as electrocatalysts for the Hydrogen evolution Reaction (HER) and Oxygen Reduction Reaction (ORR). **L. Echegoyen**

2:15 160. Density Functional Theory Simulation of Metal-Supported Metal Nanoparticles. **J.A. Santana**

WEDNESDAY AFTERNOON

2:35 161. Functional Nanocomposites for Energy Applications. **X. Zhang**, S. Sarwar, H. Du, Y. Liang, H. Wang, M. Flores

2:55 162. Green Molecular-Microwave Synthesis of Oxidation-Resistant Copper Nanoparticles for Air-Stable Printed Electronics. **L.J. Treadwell**, H. Lee

3:15 Coffee break.

3:40 163. Removal of arsenic, vanadium, and emerging organic pollutants (triclosan, organic dyes, benzene and derivatives, polyaromatic hydrocarbons) from water using nanomaterials, bio-nano composites, bio-beads, and recycled crumb rubber. **F.R. Roman**

4:00 164. Rational Design of Zeolites to Remove Siloxanes with High Adsorption Loading and Enhanced Adsorption Energy. **B. Liu**, Z. Chen

4:20 165. Withdrawn

Puerto Rico Convention Center Ball Room A

The Chemistry of Solar Fuels I

J. L. Dempsey, J. Velazquez, J. Y. Yang, *Organizers*
J. L. Colon, *Presiding*

1:25 Opening remarks.

1:35 166. The LiSA Roadmap: Routes to selective synthesis of liquid solar fuels via coupled microenvironments. **H. Atwater**

1:55 167. CO₂ electrochemical reduction mechanism on copper electrodes: Intrinsic kinetics and the role of mass transport. J. Jang, **C.G. Morales-Guio**

2:15 168. Chemical challenges facing scalable hydrogen production with alkaline membrane electrolyzers. **S.W. Boettcher**

2:35 169. On the mechanism of water oxidation in nickel-iron layered double hydroxides. **B.M. Hunter**

2:55 170. Earth-abundant electrocatalysts for the oxygen evolution reaction of water splitting using nanostructured layered inorganic materials. **J.L. Colon**, M. Ramos-Garcés, J. Sanchez, K. La Luz-Rivera, A. Cortés-Ortiz, V.M. Figueroa-Lozada, Y. Serrano-Rosario, Y. Wu, I. Barraza-Alvarez, D. Villagran, T.F. Jaramillo

3:15 Coffee Break.

3:40 171. Aqueous interfaces and energy transformations: first principles studies. **G.A. Galli**

4:00 172. Contactless Measurement of the quasi Fermi levels in illuminated Films of BiVO₄, GaP, and CuGa₃Se₅ in Contact with Aqueous Electrolytes. **F.E. Osterloh**, K. Becker, A.C. Kundmann, S. Daemi, Y. Cheng

4:20 173. How the Surface Chemistry of Tungsten Oxide Influences its Activity for the Oxygen-Evolution and Chlorine-Evolution Reactions. **B.M. Bartlett**

Puerto Rico Convention Center 201 B

Inorganic Chemistry II -Synthesis

M. B. Santiago-Berrios, *Organizer*
J. Roque, *Presiding*

1:25 Welcoming Remarks.

1:35 133. Designing stable and efficient hydrogen evolution catalysts. **C.A. Mebi**

1:55 134. Accessing new quaternary Chevrel phase compositions (AxByMo6S8) via electrochemical intercalation. **K. Ritter**, E. Cortez, J. Velazquez

2:15 135. Ferrocenyl diphosphine nickel and platinum carbonyls: a comparative study. **A. Z. Leal**, **S. Schreiner**

2:35 136. Nickel Complexes with Redox Active and Pendant Bases for Light-Driven Hydrogen Production. **W.T. Eckenhoff**

2:55 137. Graphene composite materials to enhance photoelectrochemical performance for water splitting. **G.K. WATIRO**

3:15 Coffee Break.

3:40 138. Synthesis and Analysis of Chromium (III) Phosphate. **J.W. Hall**, S.K. Hutchison, M. Subramaniam

4:00 139. The mechanism to metastability in copper selenides. **A. Koziel**, R.B. Goldfarb, E.J. Endres, J. Macdonald

WEDNESDAY AFTERNOON

4:20 140. Simulating photophysical properties of d6 and d8 organometallic qubits candidates using ORCA, DFT and Post-Hartree-Fock methods, at a high-performance computing environment. **D.C. Alamo**, D.A. Hrovat, T.R. Cundari

4:40 141. When congeners are not comparable: The case of the bulky tetra(allyl) germanium, [Ge{1,3-(SiMe₃)₂C₃H₃}₄]. **L. Wenger**, T.P. Hanusa

Puerto Rico Convention Center Ball Room B

6:30 - 8:30 Sci-Mix Poster Session I

N. M. Carballeira, *Organizer*

M. J. Bayro, D. Cruz-Ramirez de Arellano, R. Quinones, B. J. Ramos-Santana, M. B. Santiago-Berrios, *Presiding*

6:30 - 8:30

Chemical Education.

179. Creating Community and Encouraging Professional Development in Undergraduate Research Programs. **V.P. McCaffrey**

180. Withdrawn

181. Withdrawn

182. Empowering students to take ownership of learning: Impact of algorithmic questions and re-takes in general chemistry assessments. **M. Mendez Polanco**

183. Withdrawn

184. Helping students bridge the gap between general chemistry and organic chemistry: Introduction of mindful doodling into organic chemistry I courses at Georgia Gwinnett College. **M.S. Morton**

185. EPRI|U: A Snapshot of the Education and Training Continuum in the Energy Sector. **B.A. Maynard**, P. Schwenk, T. Green, T.E. Slayton, K. Hallman, C. Fitzsimmons, C. Lease

186. Career Soft Skills Workshop Targeted for STEM Majors. **N.O. Flynn**

187. Professional STEM Identity: Exploring how students identify within their profession and factors

that impact it. C. Bechard, A. Castillo, T. Legron-Rodriguez, **N. Lapeyrouse**

188. Connecting the Community to the Chemistry of Fashion: A Conversation Grounded in Diversity, Equity, and Inclusion. **P.M. Leggett Robinson**, L.A. Royer, T. Blue, M. Kelley, J. Robinson, N.L. Powell, F. Doxie

189. ACS resources for risk- based safety education. **M. Gmurczyk**

190. Withdrawn

191. Get involved with the ACS Division of Chemical Education. **D. Cruz-Ramirez de Arellano**

192. Comics and Superpowers: A Hook for Student Engagement in a General Chemistry Course. **A.L. Patrick**

193. Molecules that changed the world: Enhancing chemical literacy through a first-year seminar course for all majors. **A.C. Gaquere**

194. Development and application of a threshold concept scoring rubric. **A. Bly**, S. Nkomo

195. C.H.E.M. Leaders: Soft skills and leadership training program outside a chemistry curriculum. **B.L. Butler**

196. William Kelly pneumatic iron process-revisited. **B.G. Loganathan**

197. Development of Modern Virtual Scientific Instruments for use in Chemical Education. **L. Slaber**, R. Gomez, B. Sermania, S. Shamloo, N. VanFossen, M. Stewart, P. Raston

198. Relationship of Fatty Acid Structure and Soap Properties: Inquiry Based Lab Experiment for Undergraduate Chemistry. **F.F. Marques Burke**, A. Klazinga

199. Development of new laboratory practices for the organic chemistry course focused on the synthesis of ferrocenyl derivatives using Friedel-Craft and esterification reactions. **U. Maldonado**, **R. Perez-Martinez**, G. Narvaez, R.R. Rodriguez Berrios

WEDNESDAY AFTERNOON

200. Progress Towards an Aqueous Thermally Regenerative Electrochemical Cycle (TREC) Cell.

R.A. Girgis, R.J. Noll

201. Withdrawn

202. Promoting -inclusion- through active learning to improve students' performance and perception of the General Chemistry course.

B. Castillo, R. Tremont, J. Vedrine-Pauleus, L. Casillas-Martinez

203. Quantitative look at how students fared in two chemistry classes during COVID-19 hybrid instruction.

D.R. Zuidema

204. Creating successful student chapters workshop.

S. Hutchison, **L. Woods**, J.M. Hanna, W. Case, J.L. Brumaghim, J.G. Kaup

205. Hypervalent iodine mediated 6-endo alkoxyamination.

J. Carter, D. Liskin

206. "Chemistry in your life": non-formal educational experiences designed for community outreach activities.

M.H. Moreno, **E. Duclos Polanco**, **Y. Ortega Avilés**, **A. Llanos De Jesus**, I. Montes Gonzalez

207. Design of an inclusive Pre-semester STEM bootcamp experience for Latinxs.

I.I. Rodriguez-Velez, **S.I. Rodriguez-Maldonado**, P.X. Rosario-Nieves, K.M. Alicea-Torres, M. Morales-Burgos, L. Casillas-Martinez

208. Development of selective oxidation of primary and secondary alcohols in undergraduate organic chemistry laboratory.

M. Long, R.A. Quinlan, D.V. Liskin

209. Overcoming the challenges of virtuality to impact our members and community through the transforming power of chemistry.

E. Almanzar, G. Bosques, A. Conde, **O.A. Conde**, C. Cruz, C. Cruz, N. Lebron Acosta, **A. Llanos De Jesus**, U. Maldonado, **M. Rodríguez**, J. Rosa, Y. Vélez, I. Montes Gonzalez

210. The Transformation of the General Chemistry Course in the University of Puerto Rico, Río Piedras Campus from Face-to-face to an Online Course.

K. Davila-Diaz

211. Lewis-Acid controlled endo hydroxyamination of tethered aminoalkenes.

S. Stock, D. Liskin

212. Buffer-free Quantification of Iron in Ferrous Sulfate Supplements Using Cyclic Voltammetry.

L. Eubanks, **I. Agyekum**

213. Withdrawn

214. Research for improved student experiences in Science Technology Engineering and Math (RISE in STEM).

M.P. Alvarez, D.I. Torres-Padilla, G. Haynes

215. Withdrawn

216. Multi-step synthesis of phenylalanine and related amino acids for the organic chemistry laboratory.

K. Shehata, **C. Clinger**

217. Withdrawn

Surface Chemistry.

218. Studying the ecotoxicity of algal polysaccharide-gold nanoparticles in marine ecosystems.

M. Torres, L.M. Diaz

219. Molecular Dynamics Simulation of Poloxamer 188 and POPC Membranes.

M. Turnipseed

220. Sargassum sp., Jania sp., and Ulva sp.- based fashion nanostructured textiles.

J. Luciano, L.M. Diaz

221. Engineering a new class of structurally and electronically robust supramolecular-based light-harvesting materials with optimized charge carrier mobilities through covalent confinement of non-equilibrium self-assemblies.

V.A. Paulino, O. Jean-Hubert

222. Tuning the structure-function properties of chromophoric states of an NDI-based redox probe to dictate the potentiometric properties of n-type hybrid Si interfaces.

I. Tsironi, A. Mukhopadhyay, O. Jean-Hubert

223. Withdrawn

224. Rylene dye-based out-of-equilibrium semiconducting transient self-assemblies driven by

WEDNESDAY AFTERNOON

the consumption of carbodiimide fuels. **I. Tsironi, J. Maleszka**, R. Wilson, O. Acevedo, O. Jean-Hubert

225. Compilation and update of scientific articles focused on nanostructured materials for hydrogen production. **E. RODRIGUEZ-HERNANDEZ**, J. MENDOZA NIETO

226. Dicyclopentadiene Aerogels via Chemically Induced Phase Separation (CIPS). **Z.J. Fossitt**, K.E. Johnson, R.M. Mayville, H.J. Schanz

227. Cyclic disulfide liposomes for membrane functionalization and cellular delivery. **M. Qualls**, J. Lou, D. McBee, J.A. Baccile, M. Best

228. Dynamic cell adhesion studies on novel touch spun nanofibers. **V.N. Mohakar**, V. Reukov, S. Minko

229. Analyzing Growth of B35 Neuroblastoma Cells on Nitinol Nanoparticles Modified with Antibiotics. **A. Damai**, R. Quinones, N. Spitzer, B. Crockett

230. Morphological and Physiochemical Effect of Cellulose Polymerized Ionic Liquid as a function of Alky Chain Length. **K. Nguyen**, L. Freeman, T. Summers-James, K.M. Miller, D. Salas-De la Cruz

231. Evaluation of Halogen Macroinitiators using Atom Transfer Radical Polymerization (ATRP) to Develop Zwitterionic Membranes. **A.S. Rodriguez Rolon**, E. Nicolau

232. 3D printed sound absorber panels. **N. Gama**, G. Pinheiro, I. Cardoso, R. Ribeiro, P. Pinto, V. Freitas, A. Ferrira

233. Preparation and characterization of chitosan-coffee silverskin composites. **Y. Cortes Rosario**, O.M. Suárez

234. Machine-learning enabled design of polyolefin deconstruction processes. **P. Gonzalez**

235. Novel Dual Drug Loaded Chitosan - Graphene Quantum Dots Composite for Therapeutic Delivery and Tracking Through Enzymatic Stimuli Response. **K. B N**, R. Shambu, S. k

236. Mechanically Active Depolymerizable Polymer. **J. Rivera**, H. Tze-Gang, J. Wang

237. Withdrawn

238. Withdrawn

Biochemistry

239. Backbone Functionalization and Morphology of HEC in response to Ionic Liquids. **T. Summers-James**, K. Nguyen, K.M. Miller, D. Salas-de la Cruz

240. Effect of silver nanoparticles on migratory properties of cultured fibroblasts. **B. Sharma**

241. Development of DNA aptamers against structural proteins of SARS-CoV-2. **R. Velazquez Roig**, J.A. López Gonzales

242. Structural heterogeneity in the HIV-1 capsid: Microcrystallization and NMR analysis. Guivert Michel, Raixie Melendez, Jeremy Gonzalez, Marvin J. Bayro. **G. Michel**

243. Isolation and characterization of protein complexes of overexpressed Human Serum Amyloid A from cytokines-induced HepG2 cells. **C.G. Garcia-Cortes**

244. Use of biocompatible and antimicrobial superficial coating using a peptide polymer conjugate to combat biofilm formation. **V. Ortiz Gomez**, A. Gomez Cardona, R. Maldonado Hernandez, E. Nicolau

Inorganic Chemistry

245. Crystal Structure, Hirshfeld Analysis, and DFT calculations of Ferromagnetically-Coupled CuII3-Pyrazolato Polymorphs. **K. Rue**, G. Mezei, L. Mathivathanan, A.M. Mebel, R. Raptis

246. Synthesis, Characterization, and Reactivity of New Pincer Ligands for Forming Ruthenium Catalysts for Carbon Dioxide Reduction. **W. Silprakob**, S. Das, d. nugegoda, J.H. Delcamp, E.T. Papish

247. Stilbene-based metal-organic frameworks: synthesis, structure carbon dioxide adsorption properties. **C. Ingram**, **S. Golafale**, **D. Veazie**

248. Halogen Bonding of Triiodide Anions with Organoiodine Molecules. **M.M. Bandara**, K. Kobra, A. Peloquin, R. Dean, S.R. Watts, B. Sebastian-

WEDNESDAY AFTERNOON

Olazabal, E. Haines, A. Cobb, A. Miller, C.D. McMillen, W.T. Pennington

249. Novel two-dimensional metal metalloporphyrin framework films for the photocatalytic degradation of mustard simulant via singlet oxygen generation. **Z.L. Magnuson**, R.W. Larsen

250. Metal binding properties and cytotoxic activity of a potential inhibitor of ribonucleotide reductase. **I. Rodriguez**, C. Nieves, E. Almanzar, A. Soto-Millan, E. Strangmark, A.D. Tinoco

251. Withdrawn

252. Solution based synthesis of black indium oxide nanoparticles. **C.S. Armstrong**, K. Otero, E.A. Hernandez-Pagan

253. Withdrawn

254. Room Temperature Gas Sensor Based on Peripheral Tetrasubstituted Cobalt Phthalocyanines for the Detection of ppm Levels of Nitrogen Dioxide. **J.A. Cruz-Lozada**, D.M. Pinero Cruz, S. Flores

Undergraduates.

255. Lunar Basil: An Analysis of Basil by Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES) and Solid-Phase Microextraction (SPME) to Gas Chromatography Mass Spectrometry (GC-MS). **K. Harper**, N. Kriegel, F. Miccolis, G. Young, K.W. Barnes

256. Pedagogical approach to the simultaneous analysis of acetaminophen and caffeine in analgesics. **F. Pereira**, A. Ross, K.W. Barnes

257. Diffusion studies of liquid state quinidine compounds. **W.L. Collier**, T.D. Robertson, O.A. Cojocar

258. MALDI mass spectrometric approach for understanding metal speciation. **A. Vargas Figueroa**, A.D. Tinoco

259. Atomic and Molecular Investigation of Corrosion Using Handheld Instrumentation After Accelerated Weathering of Steel and Aluminum Substrates. **L. Kogan**, K.M. Bucholtz, J.D. Keene

260. Optimization of SPME Arrow Sampling for In-Situ Floral Scent Analysis. L. Melton, C. Grabbe, **B.O. Obi-Johnson**

261. What's the 4-1-1 on 4:20? Comparison of analysis methods for THC and CBD quantitation in hemp hearts and other products derived from cannabis. A. Brown, L. Reynolds, **M.J. Vergne**

262. Withdrawn

263. Identification of Heroin, Morphine, and Novel Synthetic Opioids using Thin Layer Chromatography for a Presumptive Field Test Kit. **C. McDavid**, J.O. Boles

264. Withdrawn

265. Efficiency of Solid Phase Extraction for the Quantitative Analysis of Poison Frog Alkaloids. **S. Moreau**, R.W. Fitch

266. Thermodynamic analyses of papGII, an E. coli adhesin. **S.A. Hinson**, M.T. Regaa, A.C. Sarcona, A.T. Mikaeel, T.B. Cavitt

267. Thermodynamic analyses of fimH, an E. coli adhesin. **A.C. Sarcona**, A.T. Mikaeel, S.A. Hinson, M.T. Regaa, T.B. Cavitt

268. Withdrawn

269. Testing the model of Nur function using non-standard amino acids. **V. Lightfoot**, N.E. Grosseohme

270. Extraction and in vitro evaluation of proteins obtained from endemic Puerto Rican flora for the treatment of Alzheimer's disease. D.J. Sanchez Rodriguez, M.P. Alvarez, **M. Sosa-Sanchez, I. Gonzalez Figueroa**

271. Determining the optimal nanodisc lipid to protein ratio for lipid mixes of varying lipid head groups and tail features. **K. Nguyen, K. Nguyen, K. Strickland**

272. Isolation of soil microbes and screening for antimicrobial activity against ESKAPE pathogens. **J. Miller**, E. Kim, J.D. Dattelbaum

273. How is the enolase enzyme capable of deprotonating 2-phosphoglycerate in the glycolysis

WEDNESDAY AFTERNOON

pathway? Contributions by resonance and inductive effects. **C. Urquhart**, A. Weinberg, J.M. Karty

274. Quantification of Bromotyrosine as a Biomarker for Pediatric Eosinophilic Esophagitis. **M.E. Thomas**, J.M. Woollery, W.M. Gilliland

275. ZCZ011 binding to the CB1 Receptor and G protein stabilization. J. Shim, **A. Hernandez**, F. Goodman

276. 2D-NMR Characterization of liquid state thioridazine drugs. **C.E. Rust**, O.A. Cojocaru

277. Transition state calculations for the possible synthesis of 10,11-diphenylcyclobuta[5,6]pyrazino[2,3-f][1,10]phenanthroline. **J. Powell**, S. Nkomo

278. Efficient NiFe electrocatalysts for oxygen evolution reactions. R. Lange, **A. Snyder**, F. Zuo

279. Synthesis and Characterization of 9,10-Bis-(iodoethynyl)anthracene for 2D Molecular Crystals from Halogen-Bonding. **N. Antoine**, **M. James**, J.A. Pienkos, K. Dungey, C. McMillen

280. Iridium-diphosphine carbonyl and hydride complexes: synthesis and structure. **B. Wargo**, **S. Schreiner**

281. Determining how the N-oxide functional group impacts the properties of transition metal compounds. **M. Shevlin**, V. Goodwin, C. McMillen, J.A. Pienkos

282. Synthesis and characterization of new complexes of ruthenium (II) with chelating phosphine ligands: structures and cytotoxic studies. **I. McNulty**, S. Schreiner

283. Withdrawn

284. Computational Study of structure and reactivities of free Radicals in the presence of different organic moieties. **K. Ra**, B.K. Dey

285. Emissive platinum complexes and the photophysical impact of the trifluoropropynyl ligand. **M. Thomas**, J. McCarthy, P.S. Wagenknecht

286. (Diethylaminosulfur) trifluoride (DAST)-mediated sulfonation of carboxylic acids with dimethyl sulfoxide. **S. Hutchins**, T. Porter, M.A. Lnu

THURSDAY MORNING

THURSDAY MORNING

Puerto Rico Convention Center 201 A

Analytical Chemistry III - Optical

L. Cunci, *Organizer*

L. F. Lopez, *Presiding*

9:55 Introductory remarks.

10:05 287. Synthesis of an asymmetric thiazolo[5,4-d]thiazole fluorescent dye library: From molecular design to biosensing applications. **P. Chakraborti**, O. Mikula, N. Sayresmith, M. Walter

10:25 288. Fluorescent silica nanoparticles having variable surface and internal properties for bioanalytical applications. **G. Patonay**, M. Henary

10:45 289. De Novo Construction of Fluorophores: A Chemical Strategy Towards Highly Sensitive and Highly Selective Turn-on Fluorescent Probes for Carbon Monoxide. **X. Yang**

11:05 290. Investigating cellulose nanoresin for extracting drinking water contaminants of per- and polyfluoroalkyl substances at picomolar scale. **R. Dosi**, S. Schmal, J.C. Poler

11:25 291. Binding interactions between colorimetric indicators and metal ions. **A.D. Dukes**, W.R. Craig, A. Labra-Arteaga, R. McPherson

11:45 292. Chemical and physical properties of unmodified and modified ground peanut hulls and their relation to biosorption applications. **C.L. Huffman**, S.W. Huffman, C. Knobloch, H. Truluck, M.J. Sands, M. Glatte

12:05 293. Enhancing sensor selectivity using extracting agents. **M.J. González**, U. Rathnaweera, H. Sowell, N. Busschaert

Puerto Rico Convention Center 104 B

Chemical Business Best Practices

X. Simon, *Organizer, Presiding*

9:55 Introductory Remarks.



10:05 294. ACS Division of Small Chemical Businesses (SCHB) background, programming, and member benefits. **X. Simon**, J.E. Sabol

10:25 295. Healthcare sustainability, disposable vs reusable speculums for pelvic examinations: A case study using a life cycle assessment approach. **M.I. Rodriguez Morris**, A. Hicks

10:45 296. Entrepreneurial journey of a great idea that delivers a breakthrough platform technology to address unmet needs in biopharma. **B. Pastrana-Rios**

11:05 297. From discovery to the clinic: The pathway for MBQ Pharma. **C.P. Vlaar**

11:25 298. Electrochemical impedance spectroscopy as a tool for translational research in oncology and the seed for an SBIR grant. **R. Diaz-Ayala**, L. Cunci, C.I. González, C.R. Cabrera

11:45 299. Industry collaboration: Joint development agreements in startup companies. **X. Simon**

12:05 300. Regulation of unstable chemicals: What happens when commercial chemicals are generated on demand. **X. Simon**

Puerto Rico Convention Center Ball Room A

DEIR Symposium: Building Inclusive DEIR Communities through Societal Organizations

B. Shannon, *Organizer*

R. A. Robinson, *Presiding*



9:55 Introduction.

THURSDAY MORNING

10:05 301. The state of science and the need for STEM advocacy. **J. Seth**

10:45 302. Systematizing Change and Altruism through Ecosystems focused on Broaden Participation in STEM. **T. Williams**

11:05 303. What about persons with disabilities in the DEIR discussion? **M.R. Cummings**

11:25 304. Working from the bottom up: When the top is conflicted on DEI for LGBTQ+ individuals. **C.J. Bannochie**

11:45 305. Importance of affinity organizations in corporate environments for growth and retention of diverse talent. **S. Kennedy**

12:05 306. Professional societies: Paving pathways and empowering legacies, an IDEAL journey. **C. Grant**

Puerto Rico Convention Center 202 C

Innovative Ways to Communicate the Value of Chemistry to the Public

S. R. Goode, *Organizer, Presiding*

9:55 Introductory remarks.

10:05 307. Connecting chemistry to society and fostering community appreciation of science. **B.Z. Shakhashiri**

10:45 308. ACS resources for communicating science to the public. **S.R. Goode**

11:05 309. Experiential learning through service: how chemistry lessons to young children keep chemistry majors engaged. E. Carver, M. Griffey, J. Pelren, D. Sizemore, E. Tester, J.V. Glass, **A.H. Shelton**

11:25 310. Cowboy Chemistry: Using storytelling, comedy, and podcasting to increase chemistry literacy, relatability, and accessibility. **D. Gardner**

11:45 311. Chemists Should Write Like Journalists and Talk Like Cavemen. **R.C. Fortenberry**

12:05 312. Finding the bigger picture: Chemicals in a global supply chain. **S.M. De Carlo**

Puerto Rico Convention Center 204

Inorganic Porous and Layered Materials Symposium III

J. L. Colon, M. Pica, L. Sun, *Organizers*
M. Ramos-Garcés, *Presiding*

9:55 Opening remarks.

10:05 313. Reversible Structural Transformations in Layered Solids. E. Broker, C. Hernandez, **B.M. Mosby**

10:25 314. Nacre-like Polymer/Clay Nanocoatings with Exceptional Mechanical, Barrier, and Flame-Retardant Properties from One-Step Coassembly. A.M. LaChance, **L. Sun**

10:45 315. Zirconium phosphates and phosphonates: from solid-state proton conductors to nanofillers for PEMFC ionomers. **A. Donnadio**, M. Pica

11:05 316. Hydrophobic silica aerogel characterization through ^{129}Xe NMR and other spectroscopic techniques. **J. Barboza**, I.F. Cespedes-Camacho

11:25 317. LDH-based composites as multifunctional materials. **M. Nocchetti**, A. Donnadio, M. Pica, R. Vivani

11:45 318. Methodical investigation of cation exchange reactions in metal chalcogenide thin films. **H. Lacey**, P. Zaman, J. Routzahn, E.A. Hernandez-Pagan

12:05 319. Structure-reactivity relationships in molybdenum chalcogenide electrocatalysts: Evaluating the interplay between aqueous proton stabilization and carbon dioxide conversion selectivity. **J.C. Ortiz**, J. Velazquez

Puerto Rico Convention Center 208 B

Interdisciplinary Science for Arid Lands Energy and Water Sustainability I

V. Bermudez Benito, J. D. Kubicki, *Organizers*
C. R. Cabrera, *Presiding*

9:55 Introductory Remarks.

THURSDAY MORNING

10:05 320. An Overview of the Kay Bailey Hutchison Desalination Plant. **S. Reinert**

10:25 321. Advanced treatment of treated sewage effluent (TSE) for beneficial reuse applications in desert climates. **O.O. Ogunbiyi**

10:45 322. Characterization of metal hydride materials for thermal energy storage systems. **Z.A. Duca**, S. Hunyadi Murph, H.T. Sessions, P.A. Ward

11:05 323. Tandem Microbial and Alkaline Fuel Cell Systems for Urine Purification for Water Reclamation at Arid Environments. W.J. Cardona, G.A. Toranzos-Soria, **C.R. Cabrera**

11:25 324. Modeling and Applications of Hyperspectral Imaging. **M. Velez-Reyes**

11:45 325. Advanced High Temperature Thermochemical Energy Storage Materials for Concentrated Solar Power Applications. **P.A. Ward**, Z. Duca, R. Zidan

12:05 326. Spin-regulated Catalysis for Energy and Water Sustainability. **S. Sreenivasan**

Puerto Rico Convention Center 208 C

Symposium on Sustainable Green Chemistry I

H. Cheng, *Organizer*

J. C. Colberg, *Presiding*



9:55 Introductory Remarks.

10:05 327. Family environmental sustainability action plan to reduce household GHG emissions: Key component in community climate change mitigation action plan. **R.C. Wingfield**

10:25 328. Organic batteries: A metal-free design for sustainable and high-performance energy storage. **J. Asenbauer**, K. Shi, M. Erakca, S.P. Bautista, M. Weil, V. Gouget, L. Picard, S. Jestin, S. Bayle, D. Bresser

10:45 329. Identifying electrocatalysts for reactive CO₂ capture (RCC). **A.C. Matus**, J.Y. Yang

11:05 330. Utilization of Carbon Dioxide in Copper-Catalyzed Boracarboxylative Difunctionalization of Alkenes. **B.V. Popp**

11:25 331. Withdrawn

11:45 332. Bioremoval of sulfur impurities from synthetic fuels using agricultural wastes. **A.E. Navarro**, A.O. Efunnuga, S. Cime

12:05 333. Molecular dynamics-driven search for natural disinfectants that universally target Receptor-Binding Domain of spike glycoprotein in SARS-CoV-2 variants. O. Ovchynnykova, **K. Kapusta**, N. Sizochenko, K.M. Sukhyy, W. Kolodziejczyk, J.M. Saloni

Puerto Rico Convention Center 208 A

The Chemistry of Solar Fuels II

J. L. Colon, J. L. Dempsey, J. Velazquez, J. Y.

Yang, *Organizers*

K. Bren, *Presiding*

9:55 Opening remarks.

10:05 334. EPR Studies of the Enzymatic Synthesis of the Organometallic H-Cluster of [FeFe] Hydrogenase. **R.D. Britt**

10:25 335. Cytochrome catalysts for artificial photosynthesis. **K. Bren**

10:45 336. Mechanism of Hydrogen Evolution with [Cp*Rh] Complexes. **J.D. Blakemore**, W. Henke, D.C. Grills, D.E. Polyansky, E. Fujita

11:05 337. Kinetic Enhancement of Proton Transfer Reactions in Electrocatalysis Using Nanocluster structures. **L.A. Berben**

11:25 338. Breaking Molecular Scaling Relationships for CO₂ Reduction: Increasing

THURSDAY MORNING

Electrocatalytic Activity at Decreased Effective Overpotentials with Molecular Catalysts. **C.C. McCrory**

11:45 339. Selective and efficient conversion of CO to methanol: Towards cascade strategies for CO₂ reduction to liquid fuels. A.V. Mueller, M. Ertem, D.E. Polyansky, G.J. Meyer, D.C. Grills, R. Sampaio, **J.J. Concepcion**

Puerto Rico Convention Center 209 C

Unusual Structure and Reactivity of Inorganic Molecules I

S. Westcott, *Organizer*

C. Martin, *Organizer, Presiding*

9:55 Opening remarks.

10:05 340. Organometallic single-molecule magnets containing radicals and bismuth. F. Benner, P. Zhang, F. Delano IV, **S. Demir**

10:25 341. Comparing First Row to Heavier Metal Reactivity Through SNS Amido and Thiolate Ligands. S. Ataie, M. Lohar, **R. Baker**

10:45 342. Ru-catalyzed ammonia oxidation: Mechanistic insights from stoichiometric and electrocatalytic reactions. **M.R. Smith**, C. Chen, R. Ghazfar, T. Hamann

11:05 343. C-H Activation Reactions with Complexes of Boryl-Centered Pincers. **O. Ozerov**, Y. Cao, W. Shih, N. Bhuvanesh, J. Zhou

11:25 344. Ambiphilic ligands featuring a carbenium ion as the Lewis acidic functionality. **F.P. Gabbai**

11:45 345. Synthesis, structure, and reactivity of mono- and binuclear [Ni] complexes supported by multidentate tautomeric ligands. **C. Kennedy**

Puerto Rico Convention Center 104 C

WCC Symposium: Crossing boundaries: The Resilience of Women Chemists Acá y Allá I

K. C. Caflin, *Organizer*

L. Tribe, *Presiding*



9:55 Introduction.

10:05 346. Women Chemists Committee: Celebrating women's accomplishments and resilience. **A.M. Balija**

10:45 347. A "jump" from a Caribbean island to being a chemistry faculty in the Appalachian. **R. Quinones**

11:05 348. Learning Agility, Career Resilience and Success in the Chemical Enterprise. **D. Haase**

11:25 349. "We are the sum of our experiences" – a STEM perspective. **M. Ruths**

11:45 350. Culturally sensitive strategies to promote inclusion for Latinas in STEM. **L. Casillas-Martinez**

Puerto Rico Convention Center 203

XRD in the Southeast - Advances in X-Ray Crystallography in Research I

W. E. Lynch, C. W. Padgett, D. M. Pinero Cruz, *Organizers, Presiding*

9:55 Welcome - Opening Remarks.

10:05 351. XRD to the rescue: Case studies from the coordination chemistry of new chalcogenone ligands. A.O. Clinkscales, **D. Rabinovich**

10:25 352. The titanium (IV) transferrin complex as a case study for transferrin bioregulation of nonferrous metals. **A.D. Tinoco**, J.A. Benjamin-Rivera, M. Saxena, S. Sharma, N. Noinaj, A. Vazquez, N. Zambrana

10:45 353. Indirect Substituent Effects through an Oxide Moiety in Oxo-Bridged Heme/Copper Assemblies. **S. Hematian**, F. Khan, R. Li, M. Tapia

11:05 354. Crystallography of Ionic Liquids: Explaining the unexpected properties of thiazolium salts. **P.C. Hillesheim**, L. Teodoro, M. Zeller

THURSDAY MORNING

11:25 355. Predicting long-range electronic coupling between metal centers: the role of XRD in identifying electronically delocalized systems. **K.M. Clark**

11:45 356. Uses of X-ray powder diffraction in layered inorganic nanomaterials chemistry research. **J.L. Colón**

Puerto Rico Convention Center Ball Room B

10:00 - 12:00 Sci-Mix Poster Session II

N. M. Carballeira, *Organizer*

J. Almirall, M. J. Bayro, L. Cunci, M. B. Santiago-Berrios, *Presiding*

Forensic Chemistry

357. Comparison of Vapor Profiles of Fresh and Highly Weathered Crude Oil. **M. Karpinsky**, S. Vaughan, V.A. Gokool, L. DeGreeff

358. Surface-enhanced Raman Spectroscopy (SERS) as a Detection Tool for Synthetic Cathinones. **M.O. Vendrell-Dones**, B. McCord

359. Influence of Soil Composition on the Release of VOCs from Buried Explosives. **E. Calabrese**, S. Vaughan, L. DeGreeff

360. Effects of Degradative Stress on the Headspace Profile of Fentanyl. **L. Forte**, A. Fulton, S. Vaughn, L. DeGreeff, H. Holness, K.G. Furton

361. Novel universal method based on Raman Spectroscopy and Machine Learning for the identification of all main body fluids: Method validation vs. environmental interferences. **L. Perez Almodovar**, I.K. Lednev

362. Determination of the breakdown products of black tar and powder heroin: Method optimization via Ultra Performance Liquid Chromatography-Photo Diode Array (UPLC-PDA) detection. **A. Sanchez**, B. McCord, I. Lurie

363. Quantitative analysis of Δ^9 -tetrahydrocannabinol (Δ^9 -THC) and other cannabinoids with the Fast-Blue BB colorimetric test. **N.B. Valdes**, R. Gorziza, J. Almirall

364. Use of Capillary Microextraction of Volatiles (CMV) for the Characterization of Volatile Organic Compounds (VOCs) emitted from Hemp and Marijuana Plants. **J. Rodriguez**, J. Almirall

365. Differentiation of structurally similar fentanyl analogs with theoretical and experimental analysis by Surface-enhanced Raman Spectroscopy (SERS). **S. Dogruer Erkok**, E. Hernandez, B. McCord

366. Utility of gas chromatography vapor-phase infrared spectroscopy (GC-VIR) for the identification of positional isomers of fentanyl related substances (FRS) and cannabinoids. **K. Ferguson**, J. Almirall

Biochemistry

367. Synthesis of HIV-1 maturation inhibition derivatives to assess Gag assembly stabilization. **K. Reyes Colon**, C. Díaz-Corretjer, C.P. Vlaar, M.J. Bayro

368. Investigation of methyl coenzyme M reductase assembly, post-translational modifications, and coenzyme F430 delivery. **C. Rand**, S.O. Mansoorabadi

369. Tracking of endogenous PER2 circadian oscillations via split-luciferase reporters. **B. Kalyanaraman**, C. Dahlke, S. Lellupitiyage Don, M.E. Farkas

370. Understanding network compensation in cellular circadian machinery via inducible degron technology. **K. Chhe**, S. Lellupitiyage Don, M.E. Farkas

371. Detection of fecal contamination of strawberries by digital PCR (dPCR). **N. Fernandez Tejero**, A. Sanchez, B. McCord, G.T. Duncan, C. Bilodeau

372. Toward the discovery of biological functions associated with the mechanosensor Mtl1p of *Saccharomyces cerevisiae* via integrative proteomics and metabolomics analyses. **N. Chorna**, N. Martínez Matías, S. González Crespo, L. Villanueva, I. Montes Rodríguez, L. Melendez Aponte, A. Roche-Lima, E. Santiago-Cartagena, B. Rymond, M. Babu, I. Stagljar, J. Rodríguez Medina

THURSDAY MORNING

373. Enzymatic activity of novel six-coordinate globinX. **R. Farhana**, B. Sophie, D. Vallerie, J. Miksovska

374. Investigation of structural effects of incorporation of 6-oxo-M1dG, a major peroxidation-derived DNA adduct into DNA duplex. **Y. Fu**, M.P. Stone, L.J. Marnett, P. Kingsley, R. Richie-Jannetta

375. Investigation of non-structural protein 2 (nsp2) inhibitors as therapeutics for encephalitis and Chikungunya viral infections. **O. Adeyinka**, D. Metibemu, O. Crown, O. Ajayi, I.V. Ogungbe

376. Novel vinyl sulfone-based inhibitors of trypanosomes that have *in vivo* efficacy. **D. Metibemu**, O. Ajayi, O. Crown, O. Adeyinka, **I.V. Ogungbe**

377. Design and synthesis of dual-targeting deferiprone-based therapeutics for the treatment of triple-negative breast cancer. **A. Johnston**, A.K. Oyelere

378. Kalanchoe daigremontiana (Raym.-Hamet & H. Perrier): Su efecto en el proceso de apoptosis de células cancerosas de ratón *Mus musculus*. **R. Rivera**

379. Synthesis and Cytotoxic Evaluation of 15-deoxy-Prostamide J2 and Related Derivative 15-deoxy-Prostamide J2-Arvanil. **D.J. Halatek**, C. Burns, R. Van Dross

380. Nanobodies as novel tools to target and study protein-protein interactions of core circadian clock proteins. **E.F. Rivera Iglesias**, S.S. Lellupitiyage Don, M.E. Farkas

381. Investigating the anti-quorum sensing activity of novel N-acyl-homoserine lactones in *Chromobacterium violaceum*. **S. Bosh-Fonseca**, R. García Del Valle, K. Acevedo-Rosario, J. González-Pagán, A. Diaz-Rosa, D.J. Sanabria-Rios, N.M. Carballeira

Physical Chemistry

382. Withdrawn

383. Adventures in DFTB: Towards Rational Dye Response Prediction. **G.R. Jenness**, H.R.

McAlexander, R. Lamb, T. Schutt, C. Bresnahan, M. Shukla

384. Halide-driven crystal structure control in manganese chalcogenide nanoparticles. **D. Gendler**, J. Bi, D. Mekan, E.A. Hernandez-Pagan

385. Operando potential-modulated excitation X-ray absorption spectroscopy as a phase-sensitive detection method for the study of dilute active sites for CO₂ electroreduction. **A. Garcia-Esparza**, X. Li, F. Babbe, J. Yano, D. Sokaras

386. Decarboxylation of methyl palmitate over a nickel molybdate catalyst: A reactive molecular dynamics study. M. Nyepetsi, **F. Mbaiwa**, O.A. Oyetunji, N. de Leeuw

387. Microwave spectroscopic study of inductive effects on intramolecular hydrogen bond strength. **R. Lavrich**

388. Excited state chemistry: Measuring two-state reactivity in metal mediated reactions. **D.J. Bellert**, T.R. Lewis

389. Interaction of the huntingtin N-terminal sequence with model cell membranes. J. Markle, **S. Frey**

390. Influence of hydrogen and ammonia addition to natural gas mixtures ignition inside a shock tube. M. Pierro, R. Rahman, J. Urso, A. Masunov, **S. Vasu**

391. DFT vs post Hartree-Fock, ORCA ESD vs non ESD, organometallic photophysical calculations. **D.C. Alamo**, D.A. Hrovat, T.R. Cundari

392. Complex synchronization behaviors in simple Belousov-Zhabotinsky oscillator networks. **S. Nkomo**

393. Effects of cancer-associated mutations on activity and oligomerization in Protein Arginine Methyltransferase 1. O.M. Price, A. Thakur, A. Ortolano, A. Towne, **C. Velez**, S. Nielson, O. Acevedo, J.M. Hevel

394. Fluorescence and quantum yield studies of new swirl emitting rhodindolizine dyes. **A.K. Shaik**, S. Chatterjee, K. Wijesinghe, D. Ndaleh, A. Antonysamy, J.H. Delcamp, N. Hammer

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395. Vibrational Strong Coupling in Nanoscale Hyperbolic Phonon Polariton Cavities. **A. Shmidt**, S. Nandanwar, L.N. Miller, J.R. Matson, T.G. Folland, J. Caldwell, L.E. Buchanan

396. Application of computational chemistry to the formation of pre-nucleation complexes in the atmosphere. **G.C. Shields**

Inorganic Chemistry

397. Exploring the role of the complex of Fe(III) with serum transferrin in regulating the transport of titanium(IV). **J.A. Benjamin-Rivera**, A.D. Tinoco, A. Vazquez, N. Zambrana, A. Torres

398. Withdrawn

399. Synthesis, characterization and functionalization of gold nanoparticles with thiolated anticancer compounds for breast cancer therapy. **G. Lorenzana-Vazquez**, I.E. Pavel, E. Melendez

400. Development of graphene quantum dot-decorated Au-Ag nanoparticles as multi-functional anti-cancer agents. **N. Medina**, W.S. Pantoja Romero, A. Lavin Flores, S.C. Díaz Vélez, M.T. Torres Mulero, B. Weiner, G. Morell

401. Sensitized and Self-sensitized Photocatalytic CO₂ Reduction to CO under Visible Light with Nickel (II) CNC-Pincer Catalysts. **S.Y. Manafe**, d. nugegoda, S. Das, J.H. Delcamp, E.T. Papish

402. Cobalt Phthalocyanine-Acid Modified Multiwalled Carbon Nanotubes Hybrids: NO₂ Gas Sensing Properties and Characterization. **C. Otero Velez**, S. Flores, D. Fonseca, D.M. Pinero Cruz

403. Investigating the Effects of (de)Protonation on the Photophysical Properties of our Dihydroxybipyridine Ru(II) Polypyridyl Complexes. **O.E. Oladipupo**, I. Fedin, C.G. Cameron, S.A. McFarland, E.T. Papish

404. Optimization of catalyst deposition for enhanced electrochemical reduction of carbon dioxide. **J.D. Rivera**, J.C. Ortiz, J. Velazquez

405. Characterizing the Binding of Ca(II) and Cd(II) to EF-hand Peptide V of Calbindin D 28K and EF-hand Peptides III and IV of Human Cardiac

Troponin C Using CD, ITC, and Fluorescence Spectroscopy. **C. Taylor**, L. Harrison, A. Wilson, K. Byers, A.M. Spuches

406. Characterization of Multiple Phases of Cu-Sb-S Nanoparticles Synthesized by a Modified Polyol Process. **J. Daniel**, M.E. Anderson

407. Design of alkyne-modified redox-active ligands for applications in flow chemistry. A. Yu, J. Bacsa, S. Blakey, **C.E. MacBeth**

408. Disaggregation kinetics of isorecticular metal organic frameworks. **K. Williamson**, D. Herr, H.P. Rathnayake

409. Mesoporous Activated Carbon as a Novel Substrate for MnO₂. **M. Thompson**, B. Baruah

410. Synthesis of Egyptian Blue and Mechanisms. **A. Kiss**, H.A. Stretz

411. Revisited Relativistic Dirac-Hartree-Fock X-ray Scattering Factors. I. Neutral Atoms with Z= 2 – 118. **O.o. Shiroye**, A. Volkov, F.F. Charlotte

412. Activation of hydrosilanes by zerovalent platinum complexes. **S. Schreiner**, K. Rogers, M. Puglisi

413. Withdrawn

414. Preliminary copper(I/II) coordination by ferroptosis inducing agent FIN56 and analogues for insight into its mechanism of action. **A.M. Orta-Rivera**, J. Vega Díaz, A. Vargas Figueroa, R. Skouta, A.D. Tinoco

415. Withdrawn I

416. Withdrawn

417. Modifying and investigating the substrate-dependant Pd@Fe₂O₃ catalyst-support synergism with ZnO ALD. **L. Shultz**, F. Liu, P. Banerjee, X. Feng, T. Jurca

418. Computer simulation of x-ray diffuse scattering from size effects and metal oxygen bond anisotropy in V_{1-x}M_xO₂ (M = Mo, Nb). **J. Phillips**, T.B. Rawot Chhetri, T.C. Douglas, J.M. Allred, M. Krogstad, M.A. Davenport, L. Whitt

THURSDAY MORNING

419. Withdrawn

421. Redox-Active Heterobimetallic Catalysts for Polymerization of Polyolefins. **N. Taylor**, T. Brewster

422. Title: Designing a Cardiolipin- Based Nanocarrier for effective delivery of Cytochrome c in Cancer Cells. **J. Acosta Mercado**, A.D. Tinoco

423. Synthesis, Characterization and relaxometric studies of octanuclear iron cluster for applications in Magnetic Resonance Imaging. **R.A. Banner**, R. Raptis

424. Elucidation of a new pharmacological strategy against cancer through the inhibition of ribonucleotide reductase by titanium (IV) . **O. Claudio Ares**, O.O. Del Leon-Velez, C.A. Marra Nazario, L.J. Delinois, E.G. Peña-Martinez, J.A. Rodríguez-Martínez, A.D. Tinoco

425. Characterizing the Binding of Ca (II) and Pb (II) to EF-hand Peptide V of Calbindin D 28K and EF-hand Peptides III and IV of Human Cardiac Troponin C Using CD, ITC, and Fluorescence Spectroscopy. **L. Harrison**, C. Taylor, A. Wilson, K. Byers, A.M. Spuches

426. Withdrawn

427. Crystal structure and Hirschfeld surface analysis of a mercury (II) chloride complex of a symmetric N-O-N ligand. **D.C. Bebout**, J.J. Derringer

428. Affecting intracellular iron and copper via a transmetalative approach as an anticancer treatment strategy. **L.V. Fernandez-Vega**, A.D. Tinoco

429. Removal of ibuprofen using tin oxide nanoparticles. **c.a. castro**, L. Alamo-Nole

Analytical Chemistry

430. Probe of surface roughness and morphological effects on bacterial adhesion to Ag/polydimethylsiloxane nanocomposites. **C.H. Sotomayor Martinez**, A. Ayala Ponce, R.F. Suárez-García, M.A. De Jesus

431. Sorting antioxidants from over-the-counter products using FTIR-ATR, square-wave voltammetry, and multivariate statistics. **H.Z. Msimanga**

432. Withdrawn

433. Study of hydrogen-bonded complexes containing melamine by Raman microscopy, scanning electron microscopy with X-ray microanalysis, and X-ray diffraction. **N.S. Chong**, J. Watkins, B. Ooi

434. Direct Electroreduction of CO₂ to Oxalate Salts in Anhydrous Media. **R. Brower**, B. Wuille Bille, J. Velazquez

435. Optimizing biochar conditions for lead (Pb) sorption and desorption in contaminated soils. **E. Uriona**, V. Boschi

436. Development of Non-targeted Analysis for Nitro Derivative of Arylamine using LC-QTOF: Optimization, Characterization, and Quantification. **K. Chen**, A.S. Edgar, C.H. Wong, D. Yang

437. Photodegradation of organic UV filters oxybenzone and avobenzone. **S. Landeweer**, Y. Ferreira, K. Meerbott, P.R. Gardinali

438. Sustainable agriculture/ aflatoxin is neither risky,nor impossible at Liaqat corp ltd since 1975,by field-based mobile innovative chemistry industrialization by profit-loss/PPP/turn-key/tech transfer basis. **L. Ali**

439. Investigating the use of COVID-19 odor expression as a non-invasive diagnostic tool. **J. Crespo Cajigas**, V.A. Gokool, H. Holness, A.T. Johnson, K.G. Furton

440. Withdrawn

441. Complex Sugar: Analysis of West Tennessee Honeys. **A.H. Shelton**, E. Ahmed, K. Kaul

442. A Wearable Biosensor to Diagnose Staphylococcus aureus Skin Infections. L. Ayres, J. Brooks, K. Whitehead, **C.D. Garcia**

443. Development of high-efficiency osmotic membrane functionalized with WS₂ nanosheets to

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dye remotion in forward osmosis. **L.C. Bermúdez-Morales**, E. Nicolau

444. Evaluation of model enzyme in Lyotropic liquid crystals selective separation and degradation. **L.N. Santiago-Martoral**, A.M. Figueroa, E. Nicolau

445. Tuning the Microenvironment Geometry Promotes Phase Formation. **G. Colon**, K. Vannoy, S. Voci, C. Renault, J. Dick

446. Characterization of Multimetallic Nanostructures by Anodic Stripping Voltammetry. D.K. Pattadar, B. Mainali, **S. Karangiya**, F.P. Patrick

447. On-site Preparation of Natural Deep Eutectic Solvents Using Solar Energy. R. Dazat, E.M. Vidal, A. Lorenzetti, **C.D. Garcia**, C. Domini, M.F. Silva, F. Gomez

448. Simultaneous quantitative analyses of ATP, creatine and creatine phosphate in brain samples. W. Lu, C. Kuan, **S.L. Wang**

449. Withdrawn

450. Real-time monitoring of seasonal variations in unique tributaries of the Biscayne Bay watershed by water quality research buoys. **K. Troxell**, P.R. Gardinali

451. Electrospun fibers for improving the performance of implanted nitric oxide-releasing glucose sensors. **T. Bradshaw**, M. Malone-Povolny, E. Merricks, T. Nichols, M. Schoenfisch

452. Analytical characterization of nitric oxide release-based killing of pathogenic bacteria. **H. Nguyen**, S. Picciotti, M. Duke, M.H. Schoenfisch

453. Electroneutrality condition allows for the electrodeposition of gold nanoparticles from aqueous nanodroplets. **J. Reyes Morales**, M. Moazeb, G.S. Colon Quintana, J. Dick

454. Determination of Cholesterol and Triglyceride levels: An electrochemical approach to monitor the enzymatic by-product Hydrogen Peroxide. **N.G. Hernandez Santiago**, P.E. Cruz Tato, J. Pazol Ramos, E. Nicolau

455. Microplastic distribution in three beaches of western Puerto Rico. **L. Tubens-Rivera**, **A.M. Gonzalez**

456. Development of electrochemical impedance spectroscopy for Neuropeptide Y detection using aptamer-modified microelectrodes. **Y. Vazquez**, L. Cunci, L. Fernandez-Vega, L.F. Lopez, D.E. Melendez

457. Investigation of mycelial bioremediation of environmentally hazardous herbicides using ultra pressure liquid chromatography. **C.S. Webber**, A.C. Brooks, S.R. Gowen, J.F. Wheeler, S.K. Wheeler

458. Comparing the Kinetic Stability of Storage Proteins in Tree Nuts: Implications for Their Potential Allergenicity. **C.A. Franquiz Santos**, E. Grace Rugaber, K. Krois, J. Rubet, J. Thibeault, W. Colon

459. Gamma radiation-induced photoluminescence in calcium phosphate glass and inhibiting effect from copper. **C.L. Crawford**, J. Jimenez

460. Adsorption of dimethyl sulfone and organosilanol compounds in water by zeolite beta. **A. Aviles**, P.J. Tarafa

461. Bioremediation of soil using biochar to remove organic and metals pollutants. **R.M. De Jesus**, L.M. Diaz

1041. Advanced Fiber Reinforcements for Durable Industrial Plastics. **V. Vasnetsov**, C. Vasnetsov, D. Patel

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Puerto Rico Convention Center 204

Inorganic Porous and Layered Materials Symposium IV

J. L. Colon, M. Pica, L. Sun, *Organizers*
M. Ramos-Garcés, *Presiding*

1:25 Opening remarks.

1:35 476. Withdrawn

1:55 477. Introduction of highly redox-active atomic centers in metal oxide nanoparticles for high-performance alkali-ion batteries. **D. Bresser**

2:15 478. Magnetically-driven quantum phase transitions in a low-dimensional pyrazine-bridged Cu²⁺ chain magnet. **A. Blockmon**, J. Jo, K. Park, E. Kirkman-Davis, M.M. Turnbull, S. McGill, J.H. Lee, J. Musfeldt

2:35 479. Exploration of amine ligand reactivity at semiconductor quantum dot surfaces for surface defect control. **C.Y. Dones Lassalle**, J.L. Dempsey

2:55 480. A Porous Boron Nitride Monolayer with Very Small Band Gap: A Computational Prediction. **J.J. Chen**, L. Lu, Z. Chen

3:15 Coffee break.

Puerto Rico Convention Center 202 A

Biochemistry III Drug Discovery

E. I. Pares-Matos, *Organizer, Presiding*

1:25 Introductory Remarks.

1:35 462. Ending serendipity in prenylome discovery using a prodrug-like strategy for isoprenoid precursors. **J.A. Baccile**

1:55 463. Effect of 2-hexadecynoic acid on the methicillin-resistant *Staphylococcus aureus* plasma membrane. G. Casillas-Vargas, H. Rivera, K. Brundage, N. Chorna, **D.J. Sanabria-Rios**

2:15 464. In vitro high throughput screening for the inhibitory effect of anthraquinone derivatives against

SARS-CoV-2 proteolytic enzymes. **K. Chavada**, D. Lewis, A. Sharma, A. Kwall, S. Sood, S. Rayalam, S. Taval, V.V. Mody

2:35 465. Potent and selective covalent inhibitors of the papain-like protease from SARS-CoV-2. **B.C. Sanders**, J.M. Parks

2:55 466. Metabolic Labeling of the *Mycobacterium tuberculosis* model organism, *Mycolicibacterium smegmatis*, using the isoprenoid precursors isopentenyl pyrophosphate (IPP) and dimethylallyl pyrophosphate (DMAPP). **D. McBee**, J.A. Baccile

3:15 Coffee Break.

3:40 467. Biochemical and therapeutic actions of cathepsin 1 (cat1) inhibitors against hepatocellular carcinoma. **O. Crown**, B. Kolawole, F. Noubissi-Kamden, **I.V. Ogungbe**

4:00 468. Pleiotropic effects of antibiotic adjuvants on the MRSA transcriptome. **H.B. Miller**

4:20 469. Biomanufacturing of Glioblastoma Multiforme Organoids with Intratumoral Heterogeneity for Improved Drug Development. S. Park, A.D. Avera, **Y. Kim**

Puerto Rico Convention Center 104 B

Frontiers in Nucleic Acids

R. M. Wadkins, *Organizer, Presiding*
M. P. Stone, *Presiding*

1:25 Introductory remarks.

1:35 470. High molecular weight polymers to study the effects of crowding on DNA i-motif structures. **R.M. Wadkins**, L. Rutherford, C. Turner, K. Morgan, A. Rhoads

2:15 471. Dialing it in: how DNA sequence encodes discrete conformational ensembles of nucleoprotein complexes. J.R. Terrell, T.N. Vernon, **G.M. Poon**

2:35 472. An Endosomal Trojan Horse to Improve Cytosolic Delivery of Spherical Nucleic Acids. **S. Narum**, B. Deal, K. Salaita

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2:55 473. Discovery of Chemical Probes for Single-Stranded Nucleic Acids. **W. Yang**, L. Wise, M. Pfanner

3:15 Coffee break.

3:40 474. Identifying stable, yet selective particle-immobilized double-stranded probes for unlabeled RNA target detection and capture. **V. Milam**, M. Adams

4:00 475. Deciphering Mutagenic Signatures in DNA Caused by Exposures to Genotoxins. **M.P. Stone**, R. Tomar, I. Minko, Y. Fu, M. Egli, R.S. Lloyd

Puerto Rico Convention Center Ball Room A

Interdisciplinary Science for Arid Lands Energy and Water Sustainability II

V. Bermudez Benito, J. D. Kubicki, *Organizers*
C. R. Cabrera, *Presiding*

1:25 Opening Remarks.

1:35 481. Diversification of Water Supplies for Long-term Sustainability in El Paso. **S. Reinert**, I. Santiago

1:55 482. Removal of endocrine disruptors in wastewater treatment plants: a binational study along the US-Mexico border region. **W. Lee**, B. ROCHA-GUTIERRE, R. De La Torre-Roche

2:15 483. Nano-enabled composite materials for water treatment: adsorption, electrochemical degradation, and detection methods. **D. Villagran**, M. Marcos, S. Yin, N. Ocuane, A. Castillo, J. Calvillo, J.L. Gardea-Torresdey

2:35 484. Oil spill contaminate removal by novel nanofiber-based membranes. **Z. liu**, R. Al-rewaily

2:55 485. Phytoremediation using mangroves and iron-based nanomaterials for contaminated environments. **K. Soto-Hidalgo**

3:15 Coffee Break.

3:40 486. From Glow-Sticks to Sensors: Single-Electrode Electrochemical Detection for Paper-

Based Devices. E.M. Vidal, C. Domini, D.C. Whitehead, **C.D. Garcia**

4:00 487. Density Functional Theory computation of adsorption of H₂O and carbon bearing species to clay mineral surfaces. **L. Tribe**

4:20 488. Organic-mineral interactions at the molecular level: impacts and research needs. **J.D. Kubicki**

Puerto Rico Convention Center 208 C

Leveraging Diversity and inclusion for Educational Excellence

B. A. Garcia, R. Joseph, *Organizers, Presiding*

1:25 Welcome.

1:35 489. Diversity and inclusion as key tools to advance education and research: Personal experiences and challenges. **D. Rabinovich**

1:55 490. How imaginative excellence promotes DEI in STEM. **E.J. Caro-Diaz**

2:15 491. Quantitative Mass Spectrometry for Exploring Epigenetic Mechanisms: A Career Perspective on Mentoring and Training. **B.A. Garcia**

2:35 492. Unrealized Dreams & Wisdom on the way to becoming a Professor. **R.A. Robinson**

2:55 493. From Lares, Puerto Rico to Cleveland, Ohio: Using DNA and Light to promote diversity, equity, and inclusion. **C.E. Crespo-Hernandez**

3:15 Coffee Break.

3:40 494. Development of Scientific Enquiry: Teaching the history of chemistry to non-chemistry major honors students. **A.H. Shelton**, J.V. Glass

4:00 Panel Discussion.

Puerto Rico Convention Center 201 B

Photoinduced Processes in Macroscopic, Supramolecular and Nanoscale Inorganic Materials I

A. A. Marti-Arbona, *Organizer, Presiding*

THURSDAY AFTERNOON

1:25 Introductory Remarks.

1:35 495. Step-Changing Solar Energy Conversion Schemes at the Nanoscale. **D. Guldi**

1:55 496. Using quantum coherence as a roadmap for synthetic design in light-to-chemical energy conversion. **J.K. McCusker**

2:15 497. Single-molecule photocatalysts for hydrogen production with red light. **C. Turro**

2:35 498. Recent photochemical and photophysical advances of Pd decorated p-n heterojunction nanomaterial BiVO₄/BiOBr/Pd. **V. Zollo**, A.E. ElMetwally, L. Bachas, M.R. Knecht

2:55 499. Ultralong lifetime and efficient room temperature phosphorescent carbon dots through multiconfinement structure design. Y. Sun, S. Liu, A. Smith, W. Wang, Y. Liu, M. Zheng, **L. Sun**

3:15 Coffee Break.

3:40 500. Toward quantum confinement in graphitic carbon nitride-based polymeric monolayers. O. Olademehin, T.L. Ellington, **K.L. Shuford**

4:00 501. Mickey Mouse on nano caffeine. **B. Heyne**

Puerto Rico Convention Center 104 A

Puerto Rico NSF-PREM's Symposium I

U. M. Cordova-Figueroa, I. Ramos, *Organizers*
J. L. Colon, *Presiding*



1:25 Opening remarks.

1:35 502. Novel Materials and Operando Methods in Energy Conversion in Alkaline Media. **H.D. Abuña**

2:15 503. Effect of solvent composition on reaction rate and product distribution on C6 carbohydrates conversion using Sn-Beta as catalyst. **I. Hortal Sanchez**, N. Cardona-Martinez

2:35 504. Simulating Interfacial Spin Ordering in Transition Metal-Oxide Superlattices. **J.A. Santana**

2:55 505. Effect of oregano leaves biomass soft biotemplation on the properties of titanium dioxide. **L. Fuentes Claudio**, A. Colón, N. Santiago

3:15 Coffee Break.

3:40 158. Opportunities for PREM Research at CHESS. **J.D. Brock**, C.J. Pollock, L. Debeve, J. Ruff

4:20 507. Gallium derived nanoparticles for biomedical applications. **R. Oyola**

Puerto Rico Convention Center 201 A

Symposium on Forensic Chemistry I

J. Almirall, *Organizer, Presiding*

1:25 Introductory remarks.

1:35 508. Documentary standards and their role in the seized-drug laboratory. **S.E. Rodriguez-Cruz**

2:15 509. The use of the Fast -Blue BB and 4-Aminophenol color tests in combination with chemometrics for the indication of hemp-type and marijuana-type cannabis. **A. Acosta**, L. Li, M. Weaver, R. Capote, J. Perr, J. Almirall

2:35 510. Chemistry for the preparation of isotopically-barcoded Ni, Mo, and W oxide materials. **M.G. Bronikowski**, K. Samperton, S. Dowds, K. Reamer, S. Scott

2:55 Coffee Break.

3:20 511. Formation of spermine phosphate hexahydrate crystals in semen probed by Raman microspectroscopy. **S. Colón-Rodríguez**, I.K. Lednev

3:40 512. Enhanced Raman spectroscopy: Single-molecule detection, drug discovery, and forensics. **L.M. Almejadi**, I.K. Lednev

4:00 513. Optimization and Miniaturization of the 4-Aminophenol Colorimetric test for the Differentiation Between Hemp-type and Marijuana-

THURSDAY AFTERNOON

type Cannabis. **M. Kerpel dos Santos**, J. Ley, M. Quirke, A. Acosta, R. Capote, J. Almirall

Puerto Rico Convention Center 208 A

The Chemistry of Solar Fuels III

J. L. Colon, J. Velazquez, J. Y. Yang, *Organizers*
J. L. Dempsey, *Presiding*

1:25 Opening remarks.

1:35 514. Hybrid Photoelectrodes for Light-driven Carbon Dioxide Reduction: Catalyst Immobilization, Photoelectrode Characterization, and Product Analysis. **J.L. Dempsey**, B. Huffman, G. Pereira Feron, A. Bredar, A. Jordan

1:55 515. Using light for on-demand protonation in solar fuels chemistry. R. Bhide, S. Luo, C.N. Feltenberger, G.S. Phun, **S. Ardo**

2:15 516. Photochemical Applications of Highly Fluorescent Thiazolothiazole Materials. **M.G. Walter**, A. Brotherton, T.J. Adams, A. Shibu, P. Chakraborti, G. Martinez Ramirez, T. Perrell

2:35 517. Exploiting disordered photonics for light trapping in photoelectrochemical energy conversion applications. **R. Coridan**

2:55 518. Three terminal photoelectrodes for solar fuel production: enabling diurnal stability and cascade processes. **E. Warren**, N. Nesbitt, D. Collins, G. Rome, C. Kong, J. Ager, J. Zimmerman, A. Greenaway

3:15 Coffee Break.

3:40 519. Multi-Electron Transfer Photovoltages at p-Si Electrolyte Interfaces. N.D. Keller, G. Pereira Feron, R. Sampaio, J.L. Dempsey, **G.J. Meyer**

4:00 520. Nanoparticulate Silicon Photocatalysts for Solar-Driven Hydrogen Production. **M. Dasog**, I. Curtis, S. Putwa

4:20 521. III-V semiconductors for photo-electrochemical hydrogen production: Recent progress in efficiency, durability, and cost. **T.G. Deutsch**, K.W. Wyatt, M. Steiner, J. Young

Puerto Rico Convention Center 202 B

Undergraduate Oral Session I

B. J. Ramos-Santana, *Organizer*
A. M. Gonzalez, *Presiding*

1:25 Introductory remarks.

1:35 522. Development of cannabinoid testing method using blood plasma cards and LC-MS/MS. **L. Reynolds**, M.J. Vergne

1:55 523. Characterization of acetal formations in cherry and tangerine e-cigarette liquids as monitored via GC/MS. **H. Menees**, **H. Menees**, N. Hollabaugh, A. Thomas

2:15 524. Mechanisms of Fatty Acid Oxidation by Myeloperoxidase. **C. Powell**, K.M. Matera

2:35 525. Thermal contributions of AT-hook peptides and netropsin when competing for AT-Rich DNA. T. Townsend, **K.L. Buchmueller**

2:55 526. Developing the substrate scope of thiamine-dependent enzymes for abiological catalysis. **R.W. Peterson**, S. Bryant, K. Darrigrand, H. Debnam, E. Reynolds

3:15 Coffee Break.

3:40 527. Site-specific incorporation of p-benzoylphenylalanine in *Candida glabrata*. **C.S. Burdette**, R.E. Singer, M.E. Breen

4:00 528. Effects of Pdr1 phosphorylation on fluconazole resistance in *Candida glabrata*. **S.A. Stapleton**, E.W. Chandler, J.R. McCallum, M.E. Breen

4:20 529. *In silico* study of the interaction between the Autism Spectrum Disorder-associated gut microbiome metabolites p-cresol and 4-ethylphenyl sulfate bound to dopamine and serotonin receptors. **P.S. Diamandis**, J. Pajski

Puerto Rico Convention Center 209 C

Unusual Structure and Reactivity of Inorganic Molecules II

S. Westcott, *Organizer*
C. Martin, *Organizer, Presiding*

1:25 Opening remarks.

THURSDAY AFTERNOON

1:35 530. Undressing main-group elements. **G. Bertrand**

1:55 531. An isodesmic approach to metal-free C-H borylation reactions. V. Desrosiers, E. Rochette, Y. Soltani, **F.G. Fontaine**

2:15 532. Regio- and Stereoselective Hydro- and Phosphinoboration of Alkynes. **W.L. Santos**

2:35 533. Supercharging iodine(III) reagents. **J. Dutton**

2:55 534. Single or double? A radical approach to frustrated Lewis pairs. **R. Melen**

3:15 Coffee Break.

3:40 535. Pincer-based cobalt-diazoalkane complexes: investigations regarding bonding and reactivity. **S. Yruegas**, P.J. Chirik

4:00 536. La(III)-Catalyzed transesterifications for degradation of polyesters. **M. Hirano**

4:20 537. Tethered Alkylidenes at REMP Initiators Bearing an Unusually Stable Azoimido Ancillary Ligand. R. Yadav, A. Esper, I. Ghiviriga, K. Abboud, C. Ehm, **A.S. Veige**

Puerto Rico Convention Center 104 C

WCC Symposium: Crossing boundaries: The Resilience of Women Chemists Acá y Allá II

L. Tribe, *Organizer*
K. C. Caflin, *Presiding*

1:25 Introductory remarks.

1:35 538. Crossing boundaries: Organizing the Pan American Nanotechnology Conference 2: Growing Convergence in Nanotechnology Meeting. D.F. Rodrigues, V. Craver, **I.C. Escobar**

1:55 539. Negotiating an Academic Position in Chemistry. **J. Macdonald**

2:15 540. Female Student's Participation in STEM Majors at Puerto Rico's Higher Education Institutions. **E. Trujillo**

2:35 541. Different countries, different students but similar skills and difficulties. **M. Soriano**

2:55 542. Empowering the next generation of latin@s in STEAM: Histories of resilience. **L.M. Diaz**

3:15 Coffee Break.

3:40 543. Women, chemistry, and culture: intersectionality and belonging. **L. Tribe**

4:00 544. Broadening Participation: A Reconsideration of Undergraduate Research Topics. **P.M. Leggett Robinson**, **L.A. Royer**, T. Blue, N.L. Powell

Puerto Rico Convention Center 203

XRD in the Southeast - Advances in X-Ray Crystallography in Research II

W. E. Lynch, C. W. Padgett, D. M. Pinero Cruz, *Organizers, Presiding*

1:25 Welcome - Opening Remarks.

1:35 545. Synthesis, structural characterization, spectroscopic properties and Hirshfeld surface analysis of new dithiolene derivatives for multi-site coordination of 3d transition metals. **D.M. Pinero Cruz**, K.T. Cordero-Gimenez, G.I. Miranda Mendez, o. pichardo, C. González

1:55 546. Withdrawn

2:15 547. Crystallographic Characterization of Metallophthalocyanine and Magnetic Complexes Combined as Nanomaterials. **C. Metzler**, S. Flores, D.M. Pinero Cruz, D. Fonseca

2:35 548. Synthesis, structural characterization and chemical bonding of $\text{Sr}_7\text{Li}_6\text{Sn}_{12}$ and its quaternary derivatives with Eu and alkaline earth metal (Mg, Ca, Ba) substitutions. **S.S. Bobev**

2:55 Intermission - Coffee Break.

3:20 549. Crystal structures and physical properties in solid solutions of bismuth-containing mixed-metal oxides. **M. Lufaso**, D. Badger, A. Jessel

THURSDAY AFTERNOON

3:40 550. Flexibility of Porous Coordination Polymers upon Concomitant Hysteretic Carbon Dioxide Adsorption. **A.J. Hernandez**

4:00 551. Zinc oxides catalysts as candidates for dye sensitized solar cell applications. **M.B. Santiago-Berrios**, J. Del Pilar

Puerto Rico Convention Center 208 B

La Historia de Pioneros y Descubridores en Química I

M. Orna, D. Rabinovich, *Organizers, Presiding*

2:05 Introductory remarks.

2:15 552. Viva la tabla periódica: Hispanic contributions to the discovery of chemical elements. **D. Rabinovich**

2:35 553. Gil Chaverri Rodríguez's 1953 Periodic Table Re-Arrangement: A historical overview. **V. Castillo Salazar, M. Murillo-Soto, S. Sandi-Urena**

2:55 554. The lives, work and scientific contributions of famous Jamaican researchers. **R. Pryce**

3:15 Intermission.

3:40 555. Tungsten, friend or enemy? **D. Alequín-Torres**, I. Montes

4:00 556. Maya Blue: An intriguing and technologically savvy ancient pigment. **M. Orna**

4:20 Discussion.

Puerto Rico Convention Center Ball Room B

3:00 - 5:00 Undergraduate Poster Session I

N. M. Carballeira, *Organizer*

B. J. Ramos-Santana, *Presiding*

Physical Chemistry

557. Negative Ion Photoelectron Spectroscopy and Thermochemistry of Dinitrobenzenes. **K.T. Workman**, W.K. Gichuhi

558. Photochromic material using azobenzene and its derivatives: A theoretical study. **M. Gallman**, B.K. Dey

559. Investigation of the concentration dependence on the kinetics of aqueous nitrous acid decomposition. **A. Pehan**, D. Heintzelman, A. Rizzuto

560. Computational Analysis of Peptide Growth on Prebiotic Earth via Gas Phase Nano Water Droplets. **S. Warf**, S. Harold, G.C. Shields

561. Negative Ion Photoelectron Spectroscopy and Thermochemistry of Cyanoanthracene. **A. Usher**, W.K. Gichuhi

562. Proton Tunneling in the Complex of 3,5-difluorobenzoic Acid and Formic Acid. **M. Perez**, W. Lin

563. Elucidating steric effects on charge separation and trapping in sensitizer dyes with transient absorption spectroscopy. **C. Curiac, E.C. Lambert**, L.A. Hunt, N. Hammer, J.H. Delcamp

564. Propensities for halogen bonding for halides bonded to central atoms below period 2. **N. Robinson**, W. Rice, K. Donald

565. Utilizing nanostructure formation of cyclodextrins for drug-delivery in a biomimetic model. **S.E. Westervelt**, K.S. Aiken, S.M. Landge, D. Ghosh

566. Molecular junctions based on electrochemically exfoliated graphene. **Y.A. Falconí**, P.F. Ortíz, J.S. Narváez, K.S. Encalada, C.P. Santacruz, H.M. Osorio

567. Impacts of pH on decomposition of aqueous carbonic acid. **J. McNeil**, A.C. Sheinberg, A. Rizzuto

568. MoS₂-contacted rectifying single molecule junctions. **S.Y. Barragán**, H.E. Rodríguez, K.S. Encalada, C.P. Santacruz, H.M. Osorio

Biochemistry

569. Optogenetic investigation of the role of the actin ATP-binding site in actin-cofilin rod

THURSDAY AFTERNOON

formation: Insight into aberrant cytoskeletal phenotypes. **J.F. Sharp, R.M. Hughes**

570. Detecting novel RiPPs using structural approximation. **A.C. Ishee**, G. Rubin, Y. Ding

571. Accumulation and regulation of reactive oxygen species across cryptobioses in the tardigrade *Hypsibius exemplaris*. **T. Clark, S. Lutz, K. Tyler**, A. Smythers, L.M. Hicks, D. Kolling

572. Synthesis and Characterization of a Metalloenzyme Mimic. **J. Legaspi**, C. Akerson, J. Neidigk, A. Lajmi

573. Discovery of Small Molecules Stabilizing the Secondary Structure of CGG Repeat Expansion. **L. Wise**, W. Yang

574. Testing different BTK inhibition treatment therapies against Waldenström macroglobulinemia (WM) Lymphoma. **C. Clark**

575. Luteinizing-Hormone Releasing-Hormone (LHRH) ligated Cisplatin and 99m Technetium chelates as peptide drug conjugate agents in the fight against cancer. **A. Elliott**

576. Removal of Organic Solvents from Water using Novel Magnetic Microspheres. **O. Fisher**

577. Investigation of Synergistic Combinations of Chemotherapy Drugs for the Treatment of Oral Cancer. **M.M. Oby**, V.D. Moore

578. Determining if the M1 and M2 muscarinic acetylcholine receptors underlie the neuroprotective ERK 1/2 cascade in the telencephalon of zebrafish. **M. Thomas**

579. Characterization of Lipid Nanoparticle Assemblies for Cytochrome c Encapsulation. **G. Encarnación López**, J. Acosta Mercado, M.J. Bayro

580. Withdrawn

581. Design and Application of an Immobilized Protein Kinase. **A. Schulz**, R. Hughes, T. Cope, D. Deane

582. Evaluation of the dynamics of protein profiles obtained under different in vitro conditions during

the process of solid organ chimerization prior to transplantation in a porcine biomodel. **M. Frias**, S.M. Osorio Quinones

583. Production of Kombucha tea without a mother SCOBY. **C. Romo**

584. Products of peroxidase-catalyzed oxidation of estrogens. **S. Jackowski**, K.M. Matera

Organic Chemistry

585. Investigation into the biological function of the apolipoprotein AI propeptide. L.R. Frost, **P. Schray**

586. Synthesis of thermally responsive polymer for targeted drug-delivery applications. **A. Brueggemann**, O.T. Mefford

587. Mechanistic Study of Antibacterial Activity by Photoactivated Double-Stranded DNA Cleaver. **A. Tidwell**, T. Fraley, W. Yang

588. Withdrawn

589. A modular approach to solubilizing supramolecular cages via PEGylation of pyridyl imine components. **M.Y. Gessler**, J.D. Thoburn

590. Green Synthesis and Characterization of Manganese Oxide Nanostructures. **I.N. González**, M. Torres-Gonzalez, G. Galvis-Barreto, M. Taño-Gonzalez, D.I. Torres-Padilla

591. Synthesis of Fluorescent dyes for incorporation into Silica Nanoparticles. **K. Monheim**, T. Jia, S.S. Iyer

592. Synthesis of a tribenzo-18-crown-6 ether ligand for use in a face-capped M4L4 metal-organic cage. **K.T. Jones**, J.D. Thoburn

593. Withdrawn

594. The synthesis of 2,6-dicyanoazulene for use as a guest encapsulated by a porphyrin-based supramolecular cube. **W.T. Adair**, J.D. Thoburn

595. Adding a thermodynamic driving force to liquid membrane to separations mediated by metal-organic cages. **C.M. Halpin**, J.D. Thoburn

THURSDAY AFTERNOON

596. Bench-stable 2-halopyridinium ketene hemiaminals - new reagents for simple synthesis of bioactive 2-aminopyridines. I.C. Bote, Z.A. Krevlin, **M. Crespo**, **C.C. Lam**, A.M. Glanzer, H.L. Hutchinson, A.M. Blades, D. McConnell, C. Lin, K.V. Leiman, A. Thayaparan, **M.M. Majireck**

597. Withdrawn

598. Enantio- and chemoselective copper-catalyzed reduction of ketones using a disilane as the reductant. **D. Culley**, **C. Gernand**, R. Van Hoveln

599. Synthesis of tetrol aliphatic monomers and incorporation into easily degradable polymers. N. Johansen, **S. West**

600. Comparison of Synthesis Methods and Characterization of Cu Oxide Nanostructures. **L.D. Acevedo**, H.P. Diana, J.S. Rivera, M.T. Gonzales, D.T. Padilla

601. Withdrawn

602. Study of the chemical composition of the hexane extract from Simarouba. **N. Maldonado**, C. Ospina, P. Nieves

603. Progress towards the development of Aurora A degrading PROTACs. **S. Quigley**, V. Hasko, M.G. Prado, S. Nelson, L. Tierney, M. Beavers, B. Ody, J. Yin, M.L. Turlington

604. Isolation of simalikalactone D from Caribbean Simarouba species. **P.C. Nieves**, N. Maldonado, A. Garcia, C. Ospina, P. Vivas

605. Synthesis of Aromatic Compounds as Precursors to Porous Polymers. **J. Miles**, B. Aguila

Inorganic Chemistry

606. Withdrawn

607. Electrochemistry of Oxo-Bridged Heme/Copper Complexes. **M. Tapia**, F. Khan, R. Li, S. Hematian

608. Examination of 1,2-Bis(diphenylphosphine)benzene Nickel Complexes in C–N Cross-Coupling Reactions. **S. Goldberg**, M. Johnson

609. Generation of Novel N,N-chelating Trans-spanning Ligands. **L. Hair**, **N. Ribeiro**, C. McMillen, J.A. Pienkos

611. Well-defined Cp*Co(III) complexes involving bidentate chiral amine ligands for the activation of carbon-hydrogen bonds. **B. Newell**, C. McMillen, J.P. Lee

612. Withdrawn

613. Synthesis and Characterization of Copper (I) Proazaphosphatane Complexes. **W.E. Apostolou**, K. Kotera, J. Thomas, M. Johnson

614. CO₂ Reduction Using an Organocatalyst. **N. Asif**, M.R. Norris

615. Synthesis and functionalization of potassium bis(ethyleneglycol)organosilicates. **L. Hargrave**, C. Tierney, R. Van Hoveln

616. Excellent electrochemical performance of pristine Cobalt-based 2D metal organic frameworks supercapacitors. **J. Willier**, F.Z. Amir

617. Synthesis and NMR Characterization 5-Fluoroisatin and 7-Fluoroisatin Thiosemicarbazones and Semicarbazones. **E. Zachary**, B. Talent, E.C. Lisic

618. Synthesis and Characterization of Pd(II) and Cu(II) 5-Fluoroisatin and 7-Fluoroisatin Thiosemicarbazone Complexes for Biological Studies. **B.B. Talent**, E. Zachary, E.C. Lisic

619. Micelle Encapsulation for Electroactive Films of Homogeneous Catalysts. **A.E. McEntire**, M.R. Norris

620. Synthesis of CO₂ reduction electrocatalysts featuring Fe/Co porphyrin cores appended with Ru-H donors. **S. Kim**, R.J. Conk, M.R. Norris

621. Development of a C₂-Symmetric Chromium Catalyst for Asymmetric Aziridination. **C.W. Belcher**, K.M. Blatchford, D.M. Jenkins

Analytical Chemistry

THURSDAY AFTERNOON

622. Withdrawn

623. Iron chelation therapy drugs: Is curcumin as effective as current therapies? **W. O'Reilly**, M. Davis Mcgibony

624. Withdrawn

625. Bonding Interactions in Cerium (IV) and Uranium (II) Naphthylpyrasal and Salicylpyrasal Complexes. **T. Hoang**, A.E. Gorden, D. Gardner, D. Unruh

626. Structural analysis of fatty acids in Joro Spiders (*Trichonephila clavate*) using gas chromatography-mass spectrometry. **A. Sunshine**, L. Eubanks, **I. Agyekum**

627. Determining the bioconcentration and toxicity of phthalates in the swimming behavior of the land crab's larvae *Cardisoma guanhumi* in Puerto Rico. **C.P. Colon-Montalvo**, **M. Corujo Bonilla**, **B. Maldonado Aponte**, **D. Santiago Ferrer**, **A. Bermudez Adorno**, C. Rodriguez-Fourquet, N. Soares Quinete

628. Development and Improvement of Electrochemical Cell for X-ray Fluorescence and Absorption Spectroscopy. **H.J. Lopez-Astacio**, L. Cunci, C.J. Pollock

629. Development of a simple method for the assay of amino acid decarboxylases through ion exchange HPLC. **J. Helmy**, C. Clinger

630. Highly efficient photocatalytic degradation of organic dyes by ZnO nanostructures. **K.N. Torres-Torres**, V. Nash-Montes, J. Luciano-Velázquez, S. Bailón-Ruiz

631. Withdrawn

632. Inorganic Light Absorber for Transparent Solar Cells. **R. Zaher**, **D. Dugger**, F. Zuo

633. Quantitative measurements of ligand coated magnetic nanoparticle interactions during linear aggregation via magnetic particle spectroscopy. **A. Hunter**, O.T. Mefford

634. Functionalization of Iron Oxide Nanoparticles for use as an Interocular Magnetic Fluid. **A. Dixon**

635. Exploring the Photophysical Properties of Prodrug Delivery in Cationic Micelles. **A. Merhar**, D. Ghosh, S.M. Gopaul

636. Electrochemical Analysis of Neuropeptide Y Using NPY-specific Aptamers and Methylene Blue Redox Label. **L. Martinez**, L.F. Lopez, L. Cunci

637. ACS Inter Ponce: Innovated, adapted, and striving to reach new goals. **J.A. Figueroa Suarez**, **J.A. Vazquez**, S. Restrepo Maldonado, E.J. Ferrer Torres

638. From the ACS University of Puerto Rico-Arecibo chapter to the world: A creative chapter. **H.N. Vargas**, A. Delgado, Z. Cordero Molina, I. Ramos, M. Ramos

639. Binding Cyclodextrin to Cellulose via a Citric Acid Linker as a Step Toward Increasing Adsorption Capacity of Cotton Fiber. **D. Randolph**, C.L. Huffman

640. Withdrawn

641. Bioassay-guided-fractionation and isolation of SARS-CoV-2 ACE-2/spike inhibitors from the brown algae *Lobophora variegata*. **V.M. Casimir**, M.L. Matos Hernandez, G. Dyer, T. Messick, I. Tietjen, E.J. Caro-Diaz, C.L. Morales-Colón

642. Withdrawn

643. Identification of phosphosites in the *C. glabrata* Pdr1 transcription factor. **J.R. McCallum**, M.E. Breen

644. Withdrawn

645. Characterizing essential and toxic metal interactions with the regulatory domain of human cardiac troponin C: A differential scanning calorimetry study. **E.E. Lemus Rivera**, L. Oliveira, T. Vasquez, A.M. Spuches

646. Preparation of low dispersity, size-controlled PCDA liposomes with microfluidics. **A. Chadwick**, T.W. Hanks

647. FTIR identification of microplastics from the surface water at San Juan Estuary. **A. Rosado-Medina**, **A.M. Gonzalez**

THURSDAY AFTERNOON

648. Water quality monitoring in the Mayaguez Bay for the identification of total coliforms and *Escherichia coli*. **M.A. Flores-Rivera**, T. Rodriguez Lopez

649. Development of colorimetric biosensors through supported lipid bilayer by polydiacetylene vesicle fusion. T.W. Hanks, **S. Alapati**, C. Stueber, P. Dawson

650. Removal of cerium from aqueous solutions using NQSA-SC and TSC chelating resins. **S. Coulter**, A.J. Carroll

651. Cultivating root vegetables in Martian soil: An analysis of radishes by Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES) and Solid-Phase Microextraction (SPME) to Gas Chromatography Mass Spectrometry (GC-MS). **N. Kriegel**, K. Harper, K.W. Barnes

652. A functional SUMO-Interaction Motif (SIM) in the BRCA1 C-terminal (BRCT) domain implicated in its transcriptional regulation activity. **M. Wilchcombe**, B. Nicholson-Dews, A. Sekhar, J. Davis

653. Sodium channel Nav1.5: A potential drug target for metastatic pancreatic neuroendocrine tumors. P. Pukkanasut, **M. Sadanand**, J. Whitt, S.E. Velu, R. Jaskula-Sztul

654. Withdrawn

655. Using Artificial Intelligence to Formulate New Deep Eutectic Solvents. A. Varillas, L. Ayres, **C.D. Garcia**

656. Synthesis of chiral lanthanide complexes featuring SPINOL ligands for circularly polarized luminescence. **B. Willis**, D. Schnable, G. Ung

657. Substituent effects on a ruthenium-catalyzed oxidation of benzyl silyl ethers into benzyl silyl esters. **M. McKenna**, R.W. Peterson, J.T. Stokes, K.E. Poythress, B.C. Goess, S.K. Goforth

658. Total synthesis of hibiscone A. **F. Baerje**, B.C. Goess

659. Progress towards the Synthesis of a Novel Siderophore–Antibiotic Conjugate. **K. Carberry**, T. Whitaker, B.C. Goess

660. Pyrolysis product characterization of (2-chloroethyl)-benzene using matrix-isolation FTIR. **T. Courtney**, K. El-Shazly, L.R. McCunn

FRIDAY MORNING

FRIDAY MORNING

Puerto Rico Convention Center Ball Room A

Ligand and Biomolecular Contributions to Metal Bioactivity and Therapeutic Potential

A. D. Tinoco, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 661. Transport of chromium (III) by transferrin with aid from low-molecular-weight chromium-binding substance. **J.B. Vincent**

9:00 662. Measuring Biological Thiols: Examining Metal Effects on Glutathione Oxidation. N.L. Finch, L.A. Broughton, **J.L. Brumaghim**

9:20 663. Illuminating the Role of Magnesium (II) in Liver Disease. M. Brady, J. Gruskos, K.H. Chu, **D. Buccella**

9:40 664. Lessons learned from exploring the insulin enhancing properties of vanadium phosphatase inhibition. A.D. Tinoco, **D.C. Crans**, O.O. De Leon, J.A. Benjamin-Rivera, K. Gaur, S. Markham

10:00 Coffee Break.

10:25 665. Exciting anti-cancer results with cobalt (III) and copper (II) complexes: In vitro studies on a triple negative breast cancer cell line. **A. Holder**, D. Alajroush, C.B. Smith, B. Anderson, S.J. Beebe

10:45 666. Synthesis, structure, and applications of ferrocene-hormone conjugates in breast cancer. **E. Melendez**

11:05 667. Protic ruthenium anticancer compounds: Describing the role of ligand charge in both photodissociation and singlet oxygen production. **E.T. Papish**, O. Oladipupo, S. Das

11:25 668. Illuminating Heme Trafficking and Signaling in Health and Disease. **A.R. Reddi**

Puerto Rico Convention Center 104 B

Novel strategies for Localized Drug Delivery I

R. R. Kane, A. Unciti-Broceta, *Organizers*

8:30 Introductory Comments.

8:40 678. Click-chemistry to replenish drug delivery devices in live animals. **Y. Brudno**

9:00 679. Effects of chemical surface modifications on cell-based delivery vehicles. **M.E. Farkas**

9:20 680. Targeting nanomedicine in the vascular system. **V. Muzykantov**

9:40 681. Beta-eliminative linkers for Controlled-Release Drug Delivery. **E. Schneider**, G.W. Ashley, D.V. Santi

10:00 Coffee Break.

10:25 682. Cleavable radiotherapeutics. M. Vlastara, K. de Roode, I. kleijn, F. Hoeben, R. Versteegen, R. Rossin, **M. Robillard**

10:45 683. Priming tumor signaling and inflammation to enhance local prodrug action. **M. Miller**

11:05 684. Immunoengineering of orally ingestible Bile acid Nanocarriers for treatment of autoimmune disease. **T. Fahmy**

11:25 685. Designing enzyme-responsive polymeric nanocarriers with high molecular precision. **R.J. Amir**

Puerto Rico Convention Center 202 B

Organic Chemistry III Physical Organic Chemistry

D. J. Sanabria-Rios, *Organizer*

G. B. Dudley, *Presiding*

8:30 Opening Remarks.

8:40 686. Benzannulation reactions for synthesis of the illudalane sesquiterpenes. **G.B. Dudley**

9:00 687. Recent advances in catalysis of transesterification and benzoin condensation by carbenes and polycarbenes. **K. Marichev**

9:20 688. Cross conjugated broad spectrum benzothiophene based NIR dyes in dye sensitized solar cells. **R. Kaur**, D. Ndaleh, A. Hogue, J.H. Delcamp

FRIDAY MORNING

9:40 689. Vinyl diazonium ions as reactive intermediates for bond breaking and making. E. Howard, A. Peck, **M. Brewer**

10:00 Coffee Break.

10:25 690. Induction influences distal CH chemical shifts and CH coupling constants. **P. Wiget**, L. Middleton, H. Walker, N. Brandau

10:45 691. A cycloaddition-based approach to C-glycosylated heterocycles. **C.E. Marzabadi**, A. Abdullahi, K. Brogden

11:05 692. Trend of the photocatalytic degradation of the textile dyes using plant based green synthesized nickel oxide nanoparticles. **J. S**

11:25 693. Withdrawn

11:45 End of Session.

Puerto Rico Convention Center 104 A

Puerto Rico NSF-PREM's Symposium II

J. L. Colon, U. M. Cordova-Figueroa, *Organizers*
I. Ramos, *Presiding*

8:30 Opening remarks.

8:40 506. Sustainable chemistry and catalysis engineering: The need for interdisciplinary research. **I. Hermans**

9:20 703. Fabrication of cadmium selenide hierarchical metamaterials and their emerging properties. **J. Del Pilar**

9:40 704. Impurity charge compensation in ferroelectrically gated graphene and its effect on charge transport. **N.J. Pinto**, K. Figueroa, N. Zimbovskaya, C. Wen, A.T. Johnson

10:00 Coffee Break

10:25 705. Enhancement of Crystal Nucleation at a Liquid/Vapor Interface. **K. Borchardt**, X. Yao, H. Wu, L. Yu

11:05 706. Alternative Platforms for Colorimetric Assays. **V. Bansal**, D. Lee, G.A. Correa-Otero, G.B.

Gomez-Dopazo, R.J. Agosto Nieves, R.L.
Albarracin Rivera

11:25 707. Designer Capsules for Selective Binding of Polar Guests, Anions, and Xenon. Y. Lin, K. Du, **I.J. Dmochowski**

Puerto Rico Convention Center 204

Mass Spectrometry: Transcending Boundaries with Innovations in Methods & Technology I

C. D. Chouinard, *Organizer, Presiding*

8:30 Opening Remarks.

8:40 669. Leveraging Flow Injection and Ion Mobility-Mass Spectrometry for High-Throughput Multi-Omics. **K.M. Hines**

9:00 670. Noncovalent Complexation Strategies Combined with Ion Mobility-Mass Spectrometry and Theoretical Modeling to Reveal Structural Preferences of Isomers and Drugs. **E. Zlibut**, J.C. May, J.A. McLean

9:20 671. Profiling the Steroidome with Ion Mobility-Mass Spectrometry. D. Velosa, s.p. neal, R. Aderorho, **C.D. Chouinard**

9:40 672. Solar phototransformation of pharmaceuticals and persistent transformation products in the aquatic environment. **W. Cory**

10:00 Coffee Break.

10:25 673. Unraveling the spatial lipidome using gas-phase ion/ion reactions. **B.M. Prentice**

10:45 674. LC-FOX: A mass spectrometry-based approach for measuring the higher order structure of dynamic systems. **J.S. Sharp**, Z. Cheng, S. Choudhary, S.K. Misra, A. Shami, S. Mishra, R.J. Doerksen

11:05 675. Withdrawn

11:25 676. Contextualizing MALDI imaging: Technologies for improving molecular and biological specificity. **J.M. Spraggins**

11:45 677. A mass spectrometric guided approach to elucidate the transmetalation mechanism of an

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anticancer titanium (IV) complex that can target both intracellular iron and copper. **A.D. Tinoco**, K. Gaur, L.V. Fernandez-Vega, S. Loza, A.N. Maser, I. Rodriguez, S. Perez, J.A. Benjamin-Rivera, V. Ebenki, A. Vargas-Figueroa, M. Perez-Otero, A. Astachkine

Puerto Rico Convention Center 201 B

Photoinduced Processes in Macroscopic, Supramolecular and Nanoscale Inorganic Materials II

A. A. Marti-Arbona, *Organizer, Presiding*

8:30 Introductory remarks.

8:40 694. Shining New Light on Luminescent Low-Coordinate Organophosphorus Compounds. **J.D. Protasiewicz**

9:00 695. Towards complete characterization of the metastable state in photochromic ruthenium sulfoxides. **J. Rack**

9:20 696. Structures and activities of catalytic peptidic assemblies. **R. Prabhakar**

9:40 697. DFT study on the photo initiated intra and inter molecular C-H activation of disphenoidal metal (II) (Fe, Ni, and Co) nitridyl complexes. **D.C. Alamo**, D.A. Hrovat, T.R. Cundari

10:00 Coffee Break.

10:25 698. Withdrawn

10:50 699. Solution-Phase Synthesis of Quaternary Chalcohalide Semiconductors. **J. Vela**

11:15 700. Photochemical reduction of polyoxometalate frameworks. **A.M. Schimpf**, L. Chen, M.J. Turo

11:40 701. Origin and modulation of excitons in Thiazolothiazole based organic crystals. **A. Shibu**, D. Diaz, T.A. Schmedake, M. Walter

Puerto Rico Convention Center 201 A

Symposium on Forensic Chemistry II
J. Almirall, *Organizer, Presiding*

8:30 Introductory remarks.

8:40 708. Raman spectroscopy and machine learning for forensic purposes. **I.K. Lednev**

9:20 709. Analysis of Cannabis Labeled Vape liquids for Cannabinoid and Heavy Metal Content. **S. Moreno**, A. Trouten, C. Sullins, R. Quinones, L.L. Richards-Waugh

9:40 710. Fast Blue BB (FBBB) screening test applied to delta-9-tetrahydrocannabinol (THC) detection in oral fluid. **R. Gorziza**, N.B. Valdes, M. Tinoco, J. Almirall

10:00 Coffee Break.

10:25 711. Global Interlaboratory Study to Evaluate Background Databases of LA-ICP-MS Analysis of Trace Elements in Glass for the Calculation of Likelihood Ratios in the Interpretation of Glass Evidence. **K. Lambert**, J. Almirall

10:45 712. Influence of intra-personal variations in human hand odor on the determination of sample donor. **V.A. Gokool**, H. Holness, K.G. Furton

11:05 713. Highly selective differentiation of organic gunshot residues combining their elemental and molecular signatures. **S. Khandasammy**, L. Halámková, M. Baudelet, I.K. Lednev

11:25 714. Characterization of the 4-aminophenol (4-AP) colorimetric reaction with tetrahydrocannabinol (THC) and cannabidiol (CBD) to differentiate between marijuana and hemp plants; a collaboration between Miami-Dade College faculty and students with Center for Advanced Research in Forensic Science (CARFS) researchers at Florida International University (FIU). **J. Ley**, M. Kepel dos Santos, M. Quirke, A. Acosta, R. Capote, A. Berdalina, M. Mateo, M. Diaz de Villalvilla, J. Almirall

11:45 715. Withdrawn

Puerto Rico Convention Center 208 C

Symposium on Sustainable Green Chemistry II
H. Cheng, *Organizer*
J. C. Colberg, *Presiding*

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8:30 Opening Remarks.

8:40 716. Iron-based catalysts for Suzuki-Miyaura cross-coupling reactions. **J.A. Byers**, A. Wong, C. Tyrol, M. Crockett, B. Zhang, M. Neidig

9:20 717. Slimming the Synthetic Peptide Waste-line. **M.E. Kopach**

9:40 718. How Sustainable is your Chemistry? Effective and Useful Tools to Impact Decisions When Designing Chemical Processes. **I. Martinez**

10:00 Coffee Break.

10:25 719. Enabling Technologies Applied to Accelerating Oncology Projects in a Sustainable Manner. **P. Richardson**

10:45 720. Synthesis of Pharmaceutical Products and Intermediates with Engineered Enzymes. **E. David**

11:05 721. Driving Cycle Time Reduction, Agility and Greener Processes in API Supply Through Continuous Processing. **J.C. Colberg**

11:25 722. Aqueous Copper Free Method for Oxidative Dephosphorylation of Glyphosate. **J. Stewart**, D.W. Scott

11:45 723. Process Enablement of COVID-19 Oral inhibitor PF-07321332 at unprecedented speed: from mg to MT in 18 months. **J. Piper**

12:05 Closing remarks.

Puerto Rico Convention Center 208 A

The Chemistry of Solar Fuels IV

J. L. Colon, J. L. Dempsey, J. Y. Yang, *Organizers*
J. Velazquez, *Presiding*

8:30 Opening remarks.

8:40 724. Catalysts, interfaces, and devices for solar-driven H production and CO₂ reduction. **T.F. Jaramillo**

9:00 725. Extended surface electrocatalyst supports from self-assembled block copolymer templates. **C.G. Arges**, D. Bhattacharya

9:20 726. Establishing Structure-Function Relationships in Metal Sulfide Electrocatalysts to Drive CO₂ and CO Conversion to Alcohols. **J. Velazquez**

9:40 727. Molecularly based bifunctional electrocatalysts for water splitting. **D. Villagran**, Y. Ge, N. Ocuane

10:00 Coffee Break.

10:25 728. CO₂ Reduction to C₂⁺ Products on Copper Electrodes Modified with Organic Additives. **T. Agapie**, J. Peters, W. Nie, G. Heim, N. Watkins, Y. Wu

10:45 729. Design and characterization of integrated systems for solar fuel production. **F. Toma**

11:05 730. Evaluating Performance and Ion-Transport Dynamics in Impurity-Resilient Bipolar Membrane Water Electrolyzers. **J. Perryman**, D.H. Marin, M. Burke Stevens, A. Nielander, T.F. Jaramillo

11:25 731. Conversion of captured CO₂ directly into fuels. **C.P. Berlinguette**

11:45 732. Connecting chemistry from the nanoscale to the observable scale in artificial photosynthesis systems. **F.A. Houle**

Puerto Rico Convention Center 203

XRD in the Southeast - Advances in X-Ray Crystallography in Research III

C. W. Padgett, *Organizer*
W. E. Lynch, D. M. Pinero Cruz, *Organizers*,
Presiding

8:30 Welcome - Opening Remarks.

8:40 733. X-ray and computational study of halogen/halogen Interactions in haloaurate(III) complexes with heteroaromatic N-oxides. **W.E. Lynch**, C.W. Padgett, S. Lynch

9:00 734. Utilizing the N-oxide Functional Group to Tune the Properties of Transition Metal Compounds. **J.A. Pienkos**, C. McMillen, E. Stumbo, S. McDarmont, M. Shevlin

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9:20 735. Competitive nitrogen-iodine and oxygen-iodine halogen bonding studies using N-hetero diazine mono N-oxides: crystallographic and computational studies. S.N. Bailey, K. Hillis, A. Goetz, A. Cobb, A. Miller, R. Dean, W.E. Lynch, W.T. Pennington, C. McMillen, **C.W. Padgett**

9:40 736. Integration of a Benchtop Single-Crystal X-Ray Diffractometer into the Undergraduate Teaching Curriculum and Research Laboratory. **J.P. Lee**

10:00 Intermission - Coffee Break.

10:25 737. Group 12 complexes of a mixed aromatic amine-alkylthiolate ligand: Synthesis, structure and solution ¹H NMR studies. **D.C. Bebout**, M. Sturner, J. Owusu-Koramoah, S.M. Berry, R. Butcher

10:45 738. From Cocrystals to Deep Eutectic Solvents: The continuum of halogen bonding from

the solid to the liquid state. **W.T. Pennington**, A. Peloquin, M.M. Bandara, S.R. Watts, R. Dean, B. Sebastian-Olazabal, E. Haines, A. Cobb, A. Miller, C.D. McMillen, D. Rabinovich

11:05 739. Preparing of cationic, octahedral, ruthenium (II) complexes supported by bidentate ligands: Synthesis, characterization and reactivity. **B.P. Quillian**, K.D. Cartrette, G. Durrell, P.H. Ouedraogo, C.W. Padgett

11:25 740. Adventures in the Crystallography of Heterobimetallic Complexes Containing the Uranyl Ion. **J.D. Blakemore**, A. Kumar, R.R. Golwankar, J. Karnes, C. Dopp, J.A. Leseberg, E. Cosner

11:45 741. Synthesis and crystal structures of transition metal complexes based on 1-carboxylatepyrene ligand. **K. Gonzalez Nieves**, P.C. Ramis, A.C. Burgos, V. Nogué, D.M. Pinero Cruz

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Puerto Rico Convention Center 104 A

Puerto Rico NSF-PREM's Symposium III

J. L. Colon, I. Ramos, *Organizers*

U. M. Cordova-Figueroa, *Presiding*

2:30 Opening remarks.

2:40 702. Energy, work, entropy, and heat balance in Marcus-Hush molecular junctions. **A. Nitzan**, N. Zimbovskaya

3:20 End of Session

Puerto Rico Convention Center 208 C

La Historia de Pioneros y Descubridores en Química II

M. Orna, D. Rabinovich, *Organizers, Presiding*

2:30 Introductory remarks.

2:40 754. Latin American Nobel Laureates on postage stamps. **D. Rabinovich**

3:00 755. Mario Molina: from the Nobel Prize to the promotion of sustainable development in Mexico. **G. Lopez-Reyes**

3:20 756. Argentinian biochemist Rebeca Gerschman (1903-1986) was the first to connect free radicals and aging. **C.L. Ásquez Maldonado**

3:40 Intermission.

4:05 757. A forceful individual who changed the path of oncology: the connection between cancer and viruses. **J.C. Aquino**

4:25 758. Aztec Red: The real treasure on the Spanish galleons. **M. Orna**

4:45 Discussion.

Puerto Rico Convention Center 204

Mass Spectrometry: Transcending Boundaries with Innovations in Methods & Technology II

C. D. Chouinard, *Organizer, Presiding*

2:30 Opening Remarks.

2:40 759. Ionic liquid degradation: A mass spectrometric perspective. **A.L. Patrick**

3:00 760. Mass Spectrometry characterization of Menthol-based Deep Eutectic Solvents. **O.O. Olawuyi**, M. Halim

3:20 Coffee Break.

3:45 761. Preparation and testing of a paper-based volumetric absorptive microsampling (VAMS)-like device for use with the liquid microjunction – surface sampling probe (LMJ-SSP) coupled with mass spectrometry. **D. Reddy**, M. Hassan, L. Zhang, T. Covey, R. Oleschuk

4:05 762. Application of high-resolution mass spectrometry to environmental chemistry. **A.L. May**, F. Loeffler, S.R. Campagna

4:25 763. Solution-Cathode Glow Discharge (SCGD) Ionization Mass Spectrometry for the Detection and Quantification of Elements, Small Molecules, and Biopolymers. **J.T. Shelley**, C.L. Walton, G.M. MacLean, J. Wu, D.M. Wieland, M. Helling

Puerto Rico Convention Center 201 B

Photoinduced Processes in Macroscopic, Supramolecular and Nanoscale Inorganic Materials III

A. A. Marti-Arbona, *Organizer, Presiding*

2:30 Introductory remarks.

2:40 769. Luminescence studies of intercalated layered inorganic nanomaterials. **J.L. Colón**, R. Pervil

3:00 770. Photoinduced halide oxidation, release, and bond formation in supramolecular assemblies. A. Deetz, M.D. Turlington, M.J. Goodwin, J. Dickenson, N.D. Keller, **G.J. Meyer**

3:20 Coffee Break.

3:45 771. MOF photochemistry - Shining light on photocatalytic mechanisms. D.R. Cairnie, **A.J. Morris**

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4:05 772. Metal-organic frameworks (MOFs) for solar energy conversion: Antenna-like light-harvesting, energy transport, and catalyst sensitization. S. Goswami, B.V. Kramar, L.X. Chen, **J.T. Hupp**

Puerto Rico Convention Center 203

Project SEED Symposium I

D. Masterson, *Organizer*

A. Mallia, *Presiding*



2:30 Opening Remarks.

2:40 773. Reflections from the ACS Project SEED Puerto Rico. **I. Montes, A.D. Tinoco**

3:00 774. Increasing Chemistry Laboratory Experiences for High School Students at Boise State University. **D.L. Warner**

3:20 Coffee Break.

3:45 775. Mentoring ACS SEED students from a graduate student perspective. **T. Owens**, E. Choi, D. Masterson

4:05 776. Successfully Organizing ACS Project SEED Program. **A. Mallia**

4:25 777. Project SEED at Rhodes College: Lessons and Successes. **K. Mosley, L.W. Peterson**

Puerto Rico Convention Center Ball Room A

Symposium on Sustainable Green Chemistry III

J. C. Colberg, *Organizer*

H. Cheng, *Presiding*

2:30 Opening Remarks.

2:40 174. New materials and methods to address polymer sustainability. **J.N. Brantley**, A.D. Fried, N.G. Galan, B.J. Wilson

3:00 175. Dynamic Covalent Chemistry in Polymers for Improved 3D Printing. **R. Smaldone**

3:20 Intermission.

3:45 176. Simplifying the Synthesis of Conjugated Polymers with Electron-Rich Pyrrolopyrroles. **G.S. Collier**

4:05 177. Impact of side chain modification of donor polymer on optical and thermal properties of polymer non-fullerene blends. **B.R. Gautam**, S. Jones, Z. Kelly, S. Han, B. Kim

4:25 178. Sustainable Applications of Banana Skin. **L. Liu**, P. Van den Abbeele

Puerto Rico Convention Center 202 B

History of Chemistry - Puerto Rico's Impact on Chemistry

C. W. Padgett, *Organizer, Presiding*



2:30 Introductory remarks.

2:40 748. Puerto Rico's impact on chemistry. **C.W. Padgett**, T. Whiteside

3:00 749. Legacy of the Largest Telescope in the World. **R.C. Fortenberry**

3:20 Coffee Break.

3:45 750. Marine natural products in Puerto Rico: A historical perspective. **N.M. Carballeira**

4:05 751. Microbial Mats as platforms for Puerto Rican GEMS (Geochemical, Ecology and Microbiology Studies). **L. Casillas-Martinez**

4:25 752. Design of Hierarchical Porous Composite Materials for the Adsorption of Contaminants of Emerging Concern from Water. **A.J. Hernandez**

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4:45 753. A Puerto Rican classic, Coco Lopez. **C.E. MacGowan**

Puerto Rico Convention Center 202 A

Novel strategies for Localized Drug Delivery II
R. R. Kane, A. Unciti-Broceta, *Organizers*

2:30 Introductory Comments.

2:40 764. Carbon monoxide as a therapeutic agent: Targeted delivery through enrichment-triggered prodrug Activation. **B. Wang**

3:00 765. Next generation 3D-printed intravaginal ring for prevention of HIV and unplanned pregnancy. **S.R. Benhabbour**

3:20 Coffee Break.

3:45 766. Guns, Germs, and MOFs. **J.J. Gassensmith**

4:05 767. Insulin crystals grown in short peptide supramolecular hydrogels show enhanced thermal stability and slower release profile. **I. Alvarez de Cienfuegos**

4:25 768. Bioorthogonal nanozymes: Harnessing the power of transition metal catalysis for in situ therapeutic generation. **V.M. Rotello**

5:05 Closing Comments and Discussion.

Puerto Rico Convention Center 208 A

The Chemistry of Solar Fuels V
J. L. Colon, J. L. Dempsey, J. Velazquez, *Organizers*
J. Y. Yang, *Presiding*

2:30 Opening remarks.

2:40 742. Fundamental Studies on the Thermal Conversion of CO₂ to Alcohols on Metal-oxide and Metal-Carbide Interfaces. **J. Rodriguez**

3:00 743. Discovery of (photo)electrocatalysts with high throughput experiments and integration with theory. **J. Gregoire**

3:20 Coffee Break.

3:45 744. Application of in Situ X-Ray Absorption and Photoemission Spectroscopy for Studying CO₂ Reduction Reaction. **J. Yano**, X. Li, C. Kaminsky, A. Garcia Esparza, D. Sokaras, E. Crumlin

4:05 745. Tracking surface reconstruction of Cu catalysts under CO₂ reduction conditions. **W. Drisdell**, S. Lee, J. Lin, M. Farmand, A. Landers, J. Feaster, J.E. Avilés Acosta, J. Beeman, Y. Ye, J. Yano, A. Mehta, R. Davis, T.F. Jaramillo, C. Hahn

4:25 746. Operando elucidation of the working state of photocatalysts for the production of solar hydrogen. **A. Garcia-Esparza**, M. Qureshi, M. Reinhard, J. Lim, R. Alonso-Mori, D. Sokaras

4:45 747. Reversible and Selective CO₂ Reduction Catalysis. **J.Y. Yang**

Puerto Rico Convention Center Ball Room B

3:00 - 5:00 Sci-Mix Poster Session III
N. M. Carballeira, *Organizer*
J. L. Colon, B. J. Ramos-Santana, R. Rodriguez, *Presiding*

3:00 - 5:00

PR NSF-PREM

778. The NSF-PREM Center for interfacial electrochemistry for energy materials (CIEM): Confronting the energy and climate crises. J.L. Colon, **L. Fuentes Claudio**

779. Fabrication and Characterization of Perovskite based Hybrid supercapacitors for Energy Storage. R. Martinez, S. Zografos, **R. Palai**

780. Water splitting electrocatalysis within layered inorganic nanomaterials. J.L. Colon, **M. Ramos-Garcés**, K. La Luz-Rivera, A. Cortés-Ortiz, V.M. Figueroa-Lozada, Y. Serrano-Rosario, J. Sanchez, I. Barraza-Alvarez, Y. Wu, D. Villagran, T.F. Jaramillo

. Effects of pH and solvent on the binding affinity of salophen ligands to cerium (III) and cerium (IV) and its impact on structure. **D. Gardner**, T. Hoang, J.A. Williamson, D. Unruh, J.D. Gorden, A.E. Gorden

FRIDAY AFTERNOON

- 781.** Metal oxides catalysts as candidates for renewable energy applications. **M.B. Santiago-Berrios**, J. del Pilar-Albaladejo, C.R. Cabrera, H.D. Abruna
- 782.** Immobilization of hemicyptophane on cellulose for fluoride removal from drinking water. **F. Gonzalez**, A. Fodness, E. Fasoli, I.J. Dmochowski
- 783.** A Bimetallic Be/Cu Porous Pillared-Layered Coordination Polymer for the Removal of CO₂ via Adsorption. **A. Tous**, A.J. Hernandez
- 784.** BBFuels of Puerto Rico, LLC. A sustainable industrial model for bioethanol production in Puerto Rico. **J.L. Nina Espinosa**
- 785.** Gallium nitride nanoparticles as inhibitors for hIAPP amyloid formation. **N.V. Falcon**, K.M. Torres, A.S. Delgado, A. Melendez, I. Ramos, D. Du, R. Oyola
- 786.** Withdrawn
- 787.** Fluorogenic sensor for detection of the Pre-Exposure Prophylaxis (PrEP)-HIV drug emtricitabine (FTC). **R.L. Albarracin Rivera**, J.T. Sczepanski, C. Yu
- 788.** Integration of research into outreach program: Portable instrument for in situ preparation and electrical characterization of polymeric nanofibers. **D. Rivera Nazario**, A. Melendez, I. Ramos
- 789.** Synthesis of doped onion-like carbon nanoparticles as a support for non-precious metal electrocatalyst. **A. Del Valle-Perez**, L. Cunci
- 790.** Assessing surface and morphological effects in the adhesion of *L. casei* and *S. cerevisiae* onto Ag/polydimethylsiloxane nanocomposites. **R.F. Suárez-García**, M.A. De Jesus, C.H. Sotomayor Martinez, A. Ayala Ponce
- 791.** Titanium Dioxide: Oregano Fossil leaf biotemplation. **A.E. Colon Gueits**
- 792.** Manganese-doped zinc oxide as a photoanode candidate for dye sensitized solar cells. **E.G. Ramirez Aponte**, J. Rivera Rodriguez, J. Del Pilar, M.B. Santiago-Berrios
- 793.** Cellulose acetate microwell plates for enzymatic assays. **G.B. Gomez-Dopazo**, R.J. Agosto Nieves, D. Rivera Nazario, J. Rosenfeld, I. Ramos, D. Lee, V. Bansal
- 794.** Synthesis of Pillararene-and immobilization on cellulose matrix. **J. Crespo**, **G. Sanchez**, F. Gonzalez, E. Fasoli
- 795.** Spin structures in the perovskite heterostructures LaCoO₃/SrFeO₃ and LaMnO₃/SrFeO₃. **D. Gonzalez**, A. Rosario, J.A. Santana
- 796.** Emerging properties of CdSe hierarchical metamaterials. **R.A. Santos**, J. del Pilar-Albaladejo
- 797.** Paper based sensor for detection of Aromatic Fragrance: An Experimenta con PREM hands on workshop. **Y. Santa**, **B. Rios**, **G. Villafane**, E. Fasoli
- 798.** Silane Grafted Silica Nanoparticles based Liquid Marbles as Microreactors for Colorimetric Reactions. **R.J. Agosto Nieves**, G.B. Gomez-Dopazo, J. Rosenfeld, D. Lee, V. Bansal
- 799.** Earth-abundant transition metal-based catalytic systems on zirconium phosphate supports as electrocatalytic material for the Oxygen Evolution Reaction. **Y. Serrano Rosario**, **C. Marzant Ortiz**, K. La Luz-Rivera, A. Cortés-Ortiz, V.M. Figueroa-Lozada, B.L. Vargas Perez, M. Ramos-Garcés, C.J. Pollock, L.M. Debeffe, J.L. Colon
- 800.** Temperature dependent charge transport in poly(benzobisimidazophenanthroline) (BBL) thin films. **A. Cruz-Arzon**, W. Serrano, N.J. Pinto, A.T. Johnson
- 801.** Cyclodextrin-Modified gallium nanoparticles assessment for amoxicillin binding. **A.Y. Feliciano**, N.N. De Jesús
- 802.** UV photoresponse and electronic transport in Reduced Graphene Oxide/Silicon p-n heterojunction. **J. Perez Gordillo**, A. Melendez, N.J. Pinto, I. Ramos
- 803.** Operando Raman spectroscopic studies on the active species for promoted Ag-based propylene epoxidation with molecular oxygen. **J. Román Matías**, J.H. Jansen, I. Hermans

FRIDAY AFTERNOON

804. Viability of tamarind seeds as a source of activated carbon for supercapacitor applications. **S.P. Zografos**, R. Palai, D. Fontanez

805. Iron and Cobalt-based Catalyst on Doped Onion-like Carbon Nanoparticles. **L. Cunci**, B.L. Vargas Perez, A. Del Valle Perez, K. Vicente Ramos, H.J. Lopez-Astacio

806. TEM and SEM of Ag via magnetron sputtering physical vapor deposition for photonic sensing devices. **E. Díaz**, G. García

807. Optical studies of magnetron sputtering physical vapor deposition of Ag for ultra-sensitive, large-area plasmonic sensors. **C. Negron**

808. Tunability of Cobaloxime Scaffolds. **D.M. Diaz**, J. Lagana, O. Ahrens, K. Cartwright

Organic Chemistry

809. Design and Synthetic Progress Towards Two Small-Molecule Prodrugs for Use in Drug-Eluting Cellular Transplants. **C.A. Sells**, **P. Little**, R.R. Kane

810. Effect of Covalent Cell-Surface Modifications on a Hepatocyte-Mediated Clotting Cascade. **P. Little**, **C.A. Sells**, J. Mattke, R.R. Kane

811. Withdrawn

812. Palladium-catalyzed desymmetrization of meso-aziridines with pyrrole nucleophiles. **H. Nguyen**, J.B. Morgan

813. Chemical shift motifs in the spectroscopic characterization of liquid-state asthma drugs. **J. Thorn**, A.F. Callender, O.A. Cojocar

814. Accessing Tosyl Amines Through Continuous Flow Intermolecular Aziridination of Terminal Olefins Featuring In-Situ Nitrene Formation. **J. Tomlin**, E. Chandler, E. Stryker, M. Jaskowski, A. Chin

815. Investigation of adamantyl-based phenyl sulfonyl acetamide and analogs as antileishmanial agents. **I.V. Ogungbe**, B. Kolawole, O. Adeyinka, O. Crown

816. Novel Route to Fluoroquinolone Antibiotics through Friedel-Crafts Acylation. **J. Noble**, T.Y. Yue, F. Gupton

817. Withdrawn

818. Implications of reaction and cargo types on cell surface modifications. **K.J. Winters**, J.D. Cullen, B.P. Joshi, J.A. Mas-Rosario, M.E. Farkas

819. Tertiary Amines as Switchable Polarity Solvents for Carbon Dioxide Removal. **J. Cruz-Lebron**, P.E. Cruz Tato, E. Nicolau

820. Synthesis of α -aryl- α -sulfonyl aldehydes via HFIP-induced rearrangement of 2-aryl epoxysulfones. **T.C. Coombs**, A. Anderson Uritis, H. Phillips

821. Withdraw

822. Expanding the scope of carbon-carbon bond formation using visible light activated electron donor-acceptor complexes. **M. Allen**, T.C. Coombs

823. Relating bromonium ion structure to alkene addition regioselectivity. N. Johansen, **B. Tutkowski**

Undergraduate

824. Biophysical characterization of a putative amino acid binding protein from *Thematoga maritima*. **S. Wenger**, J.D. Dattelbaum

825. Nanomaterial-Doped Xerogel Biosensors for Enhanced Measurement of Xanthine and Hypoxanthine in Clinical and Industrial Applications. **Q. Dang**, **A.H. Wemple**, M.C. Leopold

826. Dual-ionic liquid functionalized cellulosic materials: Thermal, mechanical and conductive properties. **E.A. McGrew**, G. Eicher, K.M. Miller

827. Swelling capacity of hydrogels with incorporated Sn and Cu nanostructures. **K. Lassala Almazan**, **K. Lassala Almazan**, **I. Gonzalez Vega**, **J. Ortiz Santana**, D.I. Torres-Padilla, M.P. Alvarez

FRIDAY AFTERNOON

- 828.** Mesoporous silica for the delivery of liquid state phenothiazine drugs. **B.C. Copeland**, L.G. Pipkin, O.A. Cojocar
- 829.** Diffusion of choline-based ionic liquid coated nanoparticles in nasal mucus. **M. VanLandingham**, R. Heintz, E.E. Tanner
- 830.** Isothermal Titration Calorimetry of the Pyridine Exchange of CdSe Semiconductor Nanocrystals. **E.A. Hall**, J.D. Keene
- 831.** Nanoparticles for latent fingerprints development: Comparison study of traditional and nanoparticles-based development methods. **B. Rodriguez Cardona**, P. Garcia, J. Pagan Soto, E.J. Ferrer Torres
- 832.** Evaluation of Moringa Oleifera extraction methods and their application for the synthesis of metallic and metal oxide nanoparticles with plant extract. **S. Restrepo Maldonado**, **M.D. Rodriguez Natali**, E.J. Ferrer Torres
- 833.** Detection of Neonicotinoids Using Functionalized Gold Nanoparticles and Halogen Bonding. **S. Reiff**, **M. Sherard**, **Q. Dang**, M.C. Leopold
- 834.** Exploring the potential toxicity of gold nanoparticles (AuNPs) on Zooxanthellae, Symbiodinium microadriaticum. **L. Llovet**, L. Diaz, M. Torres
- 835.** Confirmation of cannabielsoin (CBE) structure and utility of 1,2-CBD epoxide. **A. Monroe**, J.B. Morgan, W. Gordon, R. Williamson, J. Wood, G. Martin
- 836.** From Benzonitrile to Dicyanobenzenes: The Effect of an Additional CN group on Thermochemistry and Vibrational Spectra of Deprotonated Radical Isomers. **R.A. Firth**, W.K. Gichuhi
- 837.** Physicochemical properties of urethane-containing imidazolium ionic liquids from a non-isocyanate synthetic approach. **G.M. Timmermann**, P. Perdue, K.M. Miller
- 838.** Preparation and physical properties of dyes based on 2H,10H-anthra[1,9,8-c,d,e,f]-2,7-naphthyridine-1,6,11-trione. **H.S. Mitchel**, Y. Lysandrou, D. Sangani, **J.T. Markiewicz**
- 839.** Evaluation and characterization studies on the stability of acetals within a deuterated physiological buffer by ¹H NMR Spectroscopy. **C. Scott**, **H. Menees**, N. Hollabaugh, A. Thomas
- 840.** Synthesis and photophysical properties of SiRosindolizine derivatives for in vivo SWIR fluorescence imaging. **T. Lewis**, W.E. Meador, A.K. Shaik, N. Hammer, J.H. Delcamp
- 841.** Withdrawn
- 842.** Withdrawn
- 843.** Withdrawn
- 844.** Self-diffusion coefficients of aliphatic phenothiazine double salt ionic liquids. **D. Popa**, E.E. Etheridge, O.A. Cojocar
- 845.** Withdrawn
- 846.** Synthesis of 2,3-dihydroisoxazoles from N-benzylhydroxylamine and chalcones promoted by trimethylsilyl trifluoromethanesulfonate. **G. Hughes**, **O. Lambertson**, R. Goodner, C.W. Downey
- 847.** Trimethylsilyl trifluoromethanesulfonate-promoted alkylation of amides with allyl and propargyl propionates. **T. Chong**, **M. Hussein**, A. Helbling, C.W. Downey
- 848.** Investigation of guanidinium molecules as antisolvent additive to increase halide perovskites performance. **Z. Yang**, Y. Shi, D. Ginger
- 849.** Withdrawn
- 850.** Optimization of Paper Spray Mass Spectrometry via Chemically Patterned Paper Substrates. **A. Arias**, W.M. Gilliland
- 851.** Investigation of the impact of structural rigidity on the photophysics and photochemistry of titanocene arylamine compounds. **T. Whittemore**, H. London, E. Harris, M. Barker, P.S. Wagenknecht

FRIDAY AFTERNOON

- 852.** Application of 1,8-ANS fluorescent probe to identify hydrophobic patches on the surface of native Ca (II) binding EF-hand proteins upon heavy metal binding. **O.R. Warfel**, A.M. Spuches
- 853.** Qualitative Detection of Illicit Drug Use in Hair Samples Via GC/MS Analysis. **P.C. Griffeth**, **P. Mosayebi**, C.H. Lisse
- 854.** Mechanisms of multielectron reactions at the plasma/water interface: Interfacial catalysis, RONS, nitrogen fixation, and plasma activated water. **G. Taengwa**, A.G. Volkov
- 855.** Modification of the surface of titanium to support soft tissue growth. **M. Roberts**, T.W. Hanks
- 856.** Selectivity of controlled release from surface-modified polypyrrole films. **G. Richter**, A. Knepper, T.W. Hanks
- 857.** Interactions of silver cations and DNA using isothermal titration calorimetry. **A. Sorescu**, J.T. Petty
- 858.** 3D-Printed prototype socket for BIDEA's Biosensing Strip (BBS) as an innovative point-of-care cancer screening test. **Y.A. Avellanet Crespo**, J.L. Colón Quiles, C.R. Cabrera, R. Diaz-Ayala
- 859.** Development of a super hydrophilic zwitterionic membrane for forward osmosis water reclamation. **L. Lizardi**, E. Nicolau
- 860.** Polyunsaturated fatty acid incorporation into membrane phospholipids of *Aeromonas salmonicida*. **B.C. House**, A. Lin, D.K. Giles, S.J. Symes
- 861.** Investigating the degradation of atrazine and associated activity of manganese peroxidase in white-rot fungi. **J.S. Wirth**, J.F. Wheeler, S.K. Wheeler
- 862.** Investigating the Novel Histidine Kinase Regulator NtrZ. **M. Lutey**, B. Stein
- 863.** Interaction between the FixL kinase and its feedback inhibitor. **E. Travers**, B. Stein
- 864.** The degradation of atrazine by white-rot fungi using a mixed inoculum. **M.L. Schroder**, C.S. Webber, J.S. Wirth, J.F. Wheeler, S.K. Wheeler
- 865.** Photodynamic therapy agents: The power of Mjöllnir to eradicate cancer. **S. Hopper**, M. Davis McGibony
- 866.** Conformational analysis and docking study of Retinol-binding protein 4 (RBP4) antagonists. **C. Brown**, G.C. Shields
- 867.** Withdrawn
- 868.** Investigating transthyretin aggregates link to oxidative damage of HDL cholesterol carriers. **A. Lahetta**, K.M. Matera
- 869.** Characterization of modified catheter surface with antimicrobial polymer-peptide conjugate used to combat infection disease. **A. Gomez Cardona**, V. Ortiz Gomez, R. Maldonado Hernandez, E. Nicolau Lopez
- 870.** Computational Investigation of Triglycine Peptide Formation: A Study of Prebiotic Earth. **E. Shaikh**, S. Warf, S. Harold, G.C. Shields
- 871.** Isolating an E. Coli adhesin protein (fimH) for future thermodynamic characterization. **A.T. Mikael**, A.C. Sarcona, S.A. Hinson, M.T. Regaa, T.B. Cavitt
- 872.** Isolating an E. Coli adhesin protein (papGII) for future thermodynamic characterization. **M.T. Regaa**, S.A. Hinson, A.T. Mikael, A.C. Sarcona, T.B. Cavitt
- 873.** Synthesis, Characterization, and In-Vitro Analysis of Antiviral Peptides Targeting the Spike Protein and Angiotensin-Converting Enzyme-2. **R. Faddis**, M. Halim
- 874.** Scientific and pedagogical analysis of Gil Chaverri Rodriguez's 1953 Periodic Table Arrangement. **M. Murillo-Soto**, **V. Castillo Salazar**, S. Sandi-Urena
- 875.** Oxidative self-dimerization of indoles for the synthesis of bisindoles. **M. Mancin**, C. Rountree, **M.A. Lnu**

FRIDAY AFTERNOON

876. Sulfinamides and benzylamines as chiral auxiliary for the enantioselective amination of α -diazo esters. m. vescio, **M.A. Lnu**

877. Spiropyran-based mechanochromism in polyurethane foam. **K. Hooper**, M.H. Barbee

878. Design and synthesis of a new aminotropinimate supported zinc complex for hydroamination. **C. Dral**, R.J. Harris

879. Structure and properties of the binary mixtures of hydrogen bond acceptors and simple alcohols. **C. Mitchell**, S.W. Huffman

880. Bottom-up synthesis of graphene nanoribbons via iterative Suzuki-Miyaura cross-coupling. **A. Conde-Del Moral**, D. Pyle, G. Dong

881. Optimization of reaction conditions for the ruthenium-catalyzed oxidation benzyl silyl ethers to benzyl silyl esters. **R.W. Peterson**, A.G. Riccardi, M. McKenna, K.E. Poythress, B.C. Goess, S.K. Goforth

882. Electrophilicity as a means of describing free-radical scavenging mechanism of antioxidants: A Computational Study. **D. Young**, B.K. Dey

883. Synthesis of Annulated Pyridones via [2+2] Photocycloaddition–Cyclobutane Fragmentation. **C. Slough**, A. Davis, M.E. Daub

884. Synthesis and characterization of covalently modified poloxamers. **D. Taylor**, R.J. Harris

SATURDAY MORNING

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Puerto Rico Convention Center 201 A

Analytical Chemistry IV - Mass Spectrometry

L. Cunci, *Organizer*

L. V. Fernandez-Vega, *Presiding*

9:55 Introductory remarks.

10:05 885. Withdrawn

10:25 151. Withdrawn

10:45 886. Pattern recognition approach to headspace analysis of crude oils. **V.A. Gokool**, S. Vaughn, L. DeGreeff

11:05 887. Evaluation of a non-targeted analysis approach for identifying chemicals of environmental concern in soil and dust and children's exposure. **J. Cox**, D. Cui, E. Mejias, D. Bagner, P.R. Gardinali, N. Soares Quinete

11:25 888. Intestinal Permeability Analysis by UHPLC-MS/MS method. **M.J. Vergne**, L. Reynolds, J. Townsend

11:45 889. Polycyclic Aromatic Hydrocarbons in the Alternative Tobacco Product Midwakh: A major concern. **F. Samara**, Y. Elsayed

12:05 890. Identification of cannabinoids and terpenes profile in some vegetative and commercial samples using GC/MS and HPLC. **J.S. Torres-Rodriguez**, M. Rivera-Isaac, A. Báez-Rodríguez, E. Resto-Rodriguez, I. Montes Gonzalez

Puerto Rico Convention Center 201 B

Inorganic Chemistry III -CO₂ catalysis

M. B. Santiago-Berrios, *Organizer, Presiding*

9:55 Introductory Remarks.

10:05 891. Withdrawn

10:25 892. Visible-Light Driven Photocatalytic CO₂ Reduction by a Series of Self-Sensitized Ruthenium Complexes. A. Devdass, K. McCardle, A. Dorris, D.K. Buettner, N. Hammer, J. Panetier, **J.W. Jurss**

10:45 893. Low Valent Cobalt Pincer Complexes as catalysts for CO₂ Hydrogenation. **W. Yao**, C.M. Boudreaux, E.T. Papish

11:05 894. Combined CO₂ capture and reduction using electrochemically generated metal hydrides. **M.R. Norris**, S. Moise

11:25 895. Development of ROMP polymers to support and enhance electrocatalytic CO₂ reduction by Cobalt Phthalocyanine. **W.W. Kramer**, F. Valoy, N. Keyes

11:45 896. Dialing-In Molecular Electrocatalytic CO₂ Reduction Onset Potentials with Meridional Quinoline-Derived Ligands. J. Stober, J. Dickenson, T. Tarring, D. Turner, C. Brown, K. Cartwright, **D.P. Harrison**

Puerto Rico Convention Center 202 C

Organic Chemistry IV Chemical Biology

D. J. Sanabria-Rios, *Organizer, Presiding*

9:55 Opening Remarks.

10:05 897. High-throughput discovery and development of antifungal peptoids. **K. Bicker**, R.M. Green

10:25 898. Structure-activity relationship study of disubstituted benzoxazoles as inhibitors of sphingosine-1-phosphate transporter Spns2. **A. Burgio**, C. Shrader, Y. Kharel, T. Huang, K. Lynch, W.L. Santos

10:45 899. Synthesis and characterization of improved β -eliminative linkers for the bioconjugation and sustained release of the TLR4 inhibitor TAK-242 (Resatorvid) for applications in transplantation. **J.H. Kostyo**, A.T. Lallande, R.R. Kane

11:05 900. Withdrawn

11:25 901. Synthesis and evaluation of small molecules that modulate antibiotic resistance, biofilm formation, and virulence in methicillin-resistant *Staphylococcus aureus* (MRSA). **M.S. Blackledge**

SATURDAY MORNING

11:45 Moved

12:05 906. Structure Activity Relationship (SAR) of heterocyclic ferrocenyl chalcones towards lung cancer cell line. **A.M. Sanchez**, E. Ormé, I. Rodriguez, S. Delgado, A.D. Tinoco, I. Montes

Puerto Rico Convention Center 204

Physical Chemistry I

M. J. Bayro, *Organizer, Presiding*

9:55 903. Kinetics and mechanistic study of polymer functionalized fluorographite - a radical assisted defluorination and exfoliation process. **J.C. Poler**, A. Sahu, S. Schmal

10:15 904. On the PhotoPhysical Characterization of Novel Organic Small Molecule Dyes in the NIR. **C. Smith**, D. Ndaleh, M. Loku Yaddehige, A.K. Shaik, D.L. Watkins, N. Hammer, J.H. Delcamp

10:35 905. Probing local changes to model nanoparticle-bound α -helical structures with 2D IR spectroscopy and isotope labeling. K.R. Webb, K.A. Hess, **A. Schmidt**, K.D. Segner, L.E. Buchanan

10:55 906. Predicting the protonation state of side chains in proteins with electric fields. **V. Vaissier Welborn**

11:15 907. Understanding and Tuning the Spectroscopic and Photophysical Properties of Flavin Binding Fluorescent Proteins. **M. Kabir**, Y. Orozco-Gonzalez, D. Ouedraogo, G. Gadda, S. Gozem

11:35 908. Membrane composition drives sidechain ionization and assembly of transmembrane protein domains. **T. Smirnova**, M.A. Voinov, G. Cook, A.I. Smirnov

11:55 909. Establishing the role of structure and dynamics in radiation brightening from virus-like particles. R.L. Ranawaka, P.E. Jones, B. Dragnea, **J.A. Hadden-Perilla**

Puerto Rico Convention Center 208 C

Symposium on Sustainable Green Chemistry IV

J. C. Colberg, *Organizer*

H. Cheng, *Presiding*

9:55 Opening Remarks.

10:05 910. Withdrawn

10:25 911. Strategies toward diverse functionalized nanocelluloses and products. **Y. Hsieh**

10:45 912. Cellulose nanomaterials from cotton gin byproducts: processing and applications. **J.H. Jordan**, M. Easson

11:05 913. Withdrawn

11:25 914. Engineering reversible carbon dioxide-based processes for biorefining of lignocellulosic biomass. **J. Sheehan**, K.A. Agwu, S.R. Belmont

11:45 915. Microwave Pretreatment for Enhanced Cellulase Enzymatic Activity. **D.W. Scott**

Puerto Rico Convention Center 202 B

Undergraduate Oral Session II

B. J. Ramos-Santana, *Organizer, Presiding*

9:55 Introductory remarks.

10:05 916. Withdrawn

10:25 917. How do undergraduate students studying general chemistry approach designing multiple-choice questions in learner sourcing communities? **K. Medina**, C. Randles

10:45 918. Tuning diamine appended metal-organic frameworks for post-combustion CO₂ capture. **O.A. Conde**, B.E. Snyder, J.R. Long

11:05 919. A rare earth metal modulates *Pseudomonas putida* chemistry and physiology: Examining bacterial biofilm formation and the conversion of toxic intermediates. **D. Thompson**, S. Sathish, D.E. Williams

11:25 920. Microbiological assessment in “El Yunque” Tropical Rainforest: Bacterial identification in the Freshwater River Mameyes. **L.V. Vivas Garcia**, **A. Suarez**, **K. Perez**, G.S. Vega

SATURDAY MORNING

11:45 921. Mass transfer in the adsorption of siloxanes derivatives compounds in water. **S. Espina**, A. Aviles, P.J. Tarafa

12:05 922. Withdrawn

Puerto Rico Convention Center Ball Room B

10:00 - 12:00 Sci-Mix Poster Session IV

N. M. Carballeira, *Organizer*

M. J. Bayro, B. J. Ramos-Santana, S. Sandi-Urena,

W. Torres, *Presiding*

10:00 - 12:00 i-RIPS Abstracts

923. Withdrawn

924. Development and validation of analytical method for quantification of ethanol on a 70% alcohol base. H.J. Solis Xicara, **J.A. Garcia Bolanos**

925. Optimization of a method for extraction and analysis of polybrominated diphenyl ethers in passive resin adsorption samplers. **R. Ayala Guzman, I. Gavilán García, E. Beristain**

926. First Central American woman in Chemistry. **Y.J. Tzian**

927. Determination of the adsorption rate of atrazine in a passive-type atmospheric aerosol sampler in a wind tunnel. **Z. Ayala**, E. Beristain

928. Design of a low cost and low volume active sampler. **F. Maqueda**, E. Beristain

929. Periodycart: An interdisciplinary activity proposal for the teaching of Periodicity through Art. **J.O. Júnior**, F.L. Silva, C.V. Nobre, G.R. Lopes, Y.L. Silva, E.S. Santos, H.H. Fiuza, M.d. Oliveira

930. Development of Time and Resource Diagrams for the Costing of the Productive Process of Local Agroindustrial Companies. **P.F. Martinez Guendulain**

931. Single-step production of green butadiene over bimetallic silica-supported catalysts. **S. Silva**, L. Cardoso Cintra, M. Murta Valle

932. Prediction of the resistome of family of spore-forming bacteria of the gut microbiome. **B.M. Espino Jurado**, A. Romero Rodríguez

934. Portable sustainable practicals in college experimental chemical education. **K. Villalobos Morera, S. Sandi-Urena**

935. Design, synthesis and biological evaluation of quinazoline derivatives as potential inhibitors of Lactate Dehydrogenase A. **L. Chávez Vargas**

936. Electronic compatibility of unnatural nucleotides in the DNA double helix. **C.A. Hernández**, J. Barroso-Flores

937. BODIPYS molecular rotors as viscosity sensors. **I. Martinez Sulvaran**

938. Nanoprecipitation and characterization of PMMA and PVC nanoparticles for biological and chemical testing. **B.A. Ulate Caballero**, B. Honnorat, K. Wende

939. Sustainable Source Of Electrical Energy From Chemical Reactions In Organic Matter. **P. Peña Reséndiz**

940. Field work, my experience in the Environmental Chemistry course in the Chemistry school at UNAM. **Z. López Vega**, I. Gavilán García

941. Water, analysis of the use of the water system in Mexico: a review. **A.E. Salinas Pérez**

942. Bioremediation of soil polluted with oil by *Pleorutus ostreatus*. **G.M. Marquez Portillo**

943. Reactivity and detection methods of Gamma-hydroxybutyrate. **F.Y. May Moreno**, F.J. Rivera Mendoza

944. In vitro study of the effect of *Parietaria officinalis* extracts obtained by different methodologies on calcium oxalate and its antibacterial activity against *E. coli* and *S. aureus*. **S. Velasquez**

945. Polypyrrole-based materials as electrochemical capacitors. **C.C. Moreno**, M.T. Cortes

SATURDAY MORNING

946. Evangelina Villegas: Woman who developed QPM. **K. Vazquez-Cervantes**

947. Optimization of an extraction method for the quantification of metribuzin, atrazine and 2,4-dichlorophenol in agricultural soils and their leachates from an agricultural area of CDMX (Mexico City). **K. Valtierra**, E. Beristain

948. Withdrawn

950. Female undergraduate students' leaders experience and achievements in the ACS Student Chapter, UNA. **M. Porras**, M.F. Camacho Murillo, J. Mora Martinez, L. Vega Fernández, P. Zúñiga Muñoz, J.Á. Rodríguez Corrales

951. Cheap and easy colorimetric biosensor made from curcumin: A home lab experience. **E.O. Pérez**, B.J. Lopez Mayorga, J.A. Solis-Portillo

952. Introducing green chemistry to undergraduate students: a mentoring project on green polyamide routes. **S. Silva**, G.A. Rodrigues, P.R. Seidl, E. Freire

Project SEED

953. Extraction and characterization of fatty acids from green Caribbean macroalgae *Ulva fasciata*. **A. Ojeda**

954. Qualitative Determination of Heavy Metals through the use of Tetra Hydroxyphenyl Porphyrin-Doped Silica Sol-Gels. **M. Collins**, C. Miller, C. Smith, C.H. Lisse

955. Synthesis of a Reusable Colorimetric pH Sensor using Doped Silica Sol-Gels. **W. Ratajczak**, C. Miller, C. Smith, C.H. Lisse

956. Synthesis and Characterization of Silica-Porphyrin Heterogenous Sol-Gel Catalysts. **C. Buck**, C. Miller, C. Smith, C.H. Lisse

957. Synthesis and Characterization of Silica Sol-Gel Monoliths as Glucose Biosensors. **N. Walsh**, C. Miller, C. Smith, C.H. Lisse

958. Synthesis of a Reusable Colorimetric Silica Sol-Gel Sensor for Detection of Methamphetamine. **T. Johnson**, C. Miller, C. Smith, C.H. Lisse

959. Towards the development of multimodal ferroptosis inducing compounds for hard-to-treat lung cancer. **J. Vega Díaz**, A.M. Orta-Rivera, A.D. Tinoco

960. Non-Coding mutations alter the binding affinity of the cardiac transcription factor NKX2-5. **B.M. Rosario**, E.G. Rodríguez -Martínez, A. Rivera-Madera, L. Sanabria, J.A. López Gonzales

961. Assessing the virion stabilization effect of HIV maturation inhibitors. **V. Santiago-Excia**, M.J. Bayro, K. Reyes Colon, D. Rodriguez, G. Michel

962. Enhanced cycling performance of the SnO₂ anode by using LiFSI-based electrolyte. **F. Camacho**

963. Synthesis and analysis of oil dispersants derived from the wax of *A. mellifera*. **S. Albury**, B. Corbett

964. Isolation and utility of *C. atlantica*, *C. verum*, *L. angustifolia*, *C. aurantifolia*, *O. vulgare*, and *M. piperita* as natural antibiotics: Structural supports toward enhanced utility. **S. Joshi**, B. Corbett

965. Protein hydrolysis toward mineral chelation: Improving iron and calcium absorption. **R. Tikkala**, B. Corbett

Organic Chemistry

966. Gas phase mechanistic studies on the formation of 2-thiohistidine under biomimetic conditions. **T. Owens**, R. Nuckels, F. Hawkins, S. Gusa, D. Masterson

967. Hotplate temperature studies: Variability and reproducibility of thermal sources for organic synthesis. **K. Williamson**, D. Herr, H.P. Rathnayake

968. Wacker-type oxidation of aryl-substituted alkenes over various Pd (II) organometallic heterogeneous catalysts under microwave. **H. Yin**, J. Barton

SATURDAY MORNING

969. Development of cryptochrome-targeting PROTACs to investigate effects of protein degradation on circadian rhythms. **C.W. Yan**, K. Chhe, E.F. Rivera Iglesias, M.E. Farkas

970. Withdrawn

971. Withdrawn

972. Diphenylpyrrolone Analogues Behave as Cannabinoid 1 Receptor Agonists. **J.J. Harp**, K. Eldeeb, T. Reeves

973. Synthesis and Characterization of Chemical Probes to Elucidate the Mechanism of HIV-1 Maturation Inhibitors. **C. Diaz**, K. Reyes Colon, C.P. Vlaar, M.J. Bayro

974. Live-cell RNA imaging with metabolically incorporated fluorescent nucleosides. D. Wang, **A. Shalamberidze**, E. Arguello, B.W. Purse, R. Kleiner

975. Compound activity mapping for SARS-CoV-2 antiviral marine cyanobacterial extracts. **M.L. Matos Hernandez**, G. Dyer, C.L. Morales-Colón, J. Cassel, T. Messick, I. Tietjen, E.J. Caro-Diaz

976. Development of a greener, continuous preparation of the tuberculosis drug rifapentine. **E. Stryker**, A. Matthews, T.Y. Yue, F. Gupton

977. Chemoinformatic synthesis and analysis of cyanobacterial pseudonatural products. **W.O. Mendoza Morales**

978. Development of novel palladacycles by C–H activation of azetidines. **T.A. Rossman**, J.B. Morgan

979. Biological Properties of Nitrogen Containing Ferrocenyl Chalcones Derivatives. **S.M. Delgado-Rivera**, S.A. Henriquez-Lopez, G.E. Perez-Ortiz, I. Montes Gonzalez, A. Baerga-Ortiz, D.M. Pinero Cruz

980. Use of Dimethyldioxirane as a reliable oxidizing agent. **D. McTush-Camp**

981. Examining the chemical reactivity of boron-based carbon monoxide donor, CORM-A1. **N. Bauer**, X. Yang, Z. Yuan, F. Vazquez, B. Wang

982. Metal-organic Frameworks(MOFs) for Sustainable Energy Using Computational Simulations. **R. Kyung**, J. Lee

983. Optimization of warfarin synthesis using biocatalysts and adjuvants for enantioselectivity: A CURE approach. **A.I. Wurz**, R. Hughes, J. Walker

Physical Chemistry

984. Rad26 powers RNA polymerase II forward translocation by an allosteric mechanism. **C. Yan**, T. Dodd, I.N. Ivanov, D. Wang

985. Evaluating the Physical Properties of 12-n-12 Gemini Surfactants. **D. Aguilar**, R.D. Sheardy

986. Withdrawn

987. Residue Interaction Networks and the Cheminformatics of Atomic-Level Enzyme Models. **N.J. Deyonker**

988. Spectroscopic and Computational Studies of Nitrogen and Sulfur-Containing Dipole-Bound Anions as Components in Light-Harvesting Materials. **N. Kruse**, R.C. Fortenberry, N. Hammer

989. Thermal Decomposition Pathways of Dihydrofuranones. **L.R. McCunn**, H.N. Legg, T.D. Martin, G.J. Brown, K. Narkin, K. El-Shazly, T. Courtney

990. Computational analysis of water catalysis on prebiotic peptide bond formation. **S. Harold**, S. Warf, G.C. Shields

991. Comparative DFT study of the Isomerization barrier and Global Descriptive Indices of 2-butenedioic acid and its Methyl substituted derivatives. **J.K. Agbo**, C.A. Mebi

992. Withdrawn

993. Penta-Hexagonal Graphane: A New Promising 2D Anode Material for Li-ion Batteries. **L. Lu**

Undergraduate

994. Reaching non-STEM students of Erskine College through campus wide events. **O. Jans**, T.R. Hayden

SATURDAY MORNING

- 995.** Withdrawn
- 996.** Investigating student resource use. **K. Oliver**, J.N. Orvis, L. Padgett, S.E. Conti, L. Williams
- 997.** Application of machine learning approaches towards spectral deconvolution and secondary structure quantification in infrared hyperspectral imaging. **L. Verace**, B.M. Holcombe, A. Ghosh
- 998.** Chemometrics of honey: Design and development of spectroscopic and spectrophotometric experiments for a first-year undergraduate research experience. **D. Rodriguez**, **L. Harrison**, **B. Dominguez**, A. Edlin, A.J. Rodriguez
- 999.** Chemometrics of honey: Design and development of stoichiometry experiments for a first-year undergraduate research experience. **M. Bonilla**, **S. Serrano**, **M. Carrion**, **A. Perez**, A.J. Rodriguez
- 1000.** Chemometrics of honey: Design and development of fundamental and exploratory experiments for a first-year undergraduate research experience. **L. Caballero**, **L. Harrison**, **A. Edlin**, **Q. Rodriguez-Manzanares**, A.J. Rodriguez
- 1001.** Driving Effects of Common Atmospheric Molecules for Formation of Prenucleation Clusters. **C.J. Bready**, V. Fowler, L. Juechter, L. Kurfman, G. Mazaleski, G.C. Shields
- 1002.** Effect of thermal diffusivity on wood torrefaction process at various temperature and duration (part 1). **T.N. Nguyen**, L. Richa, A. Petrisans, R.L. Quirino, D. Florez, R. Remond, B. Colin, V. Fierro, M. Petrisans
- 1003.** Monitoring water quality in Abbeville County, South Carolina- A citizen science project. **H. Holcomb**, T.R. Hayden
- 1004.** Titania photocatalysis for fish aquaculture. A. Giammarinaro, **J.E. Boyd**
- 1005.** Sucralose (C₁₂H₁₉Cl₃O₈) impact on microbial activity in estuarine and freshwater marsh soils. **A. Westmoreland**, T. Schafer, K. Breland, T. Osborne
- 1006.** Benchmark study of water clusters (H₂O)₂₋₃₀. **V. Fowler**, T. Odbadrakh, G.C. Shields
- 1007.** Remediation of cerium from water utilizing ISA- PTSC and PSC chelating resins. **C. Morris**, A.J. Carroll
- 1008.** Development of an automated process to measure the regeneration, reuse and sustainability of nanoresin water purification materials. **J. Costelloe**, C. Reid, A. Sahu, S. Schmal, T. Sharma, J.C. Poler
- 1009.** Contamination of Coliform bacteria on bioluminescence Mosquito Bay in Vieques. **C.A. Rios Rosa**, V.V. Duarte, **K.H. Rodriguez**, S.N. Santana, F.N. Alvarado
- 1010.** Computational investigation of the secondary aerosol system H₂SO₄-HNO₃-HCl-NH₃-(CH₃)₂NH-(H₂O)_n. **A. Byerly**, G.C. Shields
- 1011.** Bacillariophyta Diatom. **V.V. Valerio Duarte**, C.A. Rios Rosa, K.H. Rodriguez, S. Mercado Santana, F.N. Alvarado
- 1012.** Microplastics in cave environments. **B. Larmon**
- 1013.** Bioaccumulation of heavy metals by aquatic plants from a natural wetland in the Northern Part of Puerto Rico. **P.Y. Rodriguez Lopez**, M. Ramos
- 1014.** Obtaining eco-friendly biofilms and microwave extraction of chitosan from *Aspergillus niger* mycelium. **C. Rodriguez**, J. Vargas
- 1015.** Microorganism assesment in the bodies of water surrounding the Guayanés river in Yabucoa. **J.D. Pinto Burgos**, A. Rodríguez Lebrón, D. Alequin Torres
- 1016.** Sustainable Medicine: Investigating Green Solvents in Conversion of Sugars. **C. McGrath**
- 1017.** Solar photodegradation of metoprolol in simulated natural water samples. **H. Sabatini**, W. Cory
- 1018.** Permeation of choline-based ionic liquid nanoparticles through porcine nasal mucosa. **R. Heintz**, M. VanLandingham, E.E. Tanner

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- 1019.** Single chain polymer nanoparticles with silyl ether crosslinks. **G. Ford**, M.H. Barbee
- 1020.** Biomimetic Design of Single Chain Nanoparticle Polymers Networks. **S. Robinson**, M.H. Barbee
- 1021.** Photocatalytic degradation of 6PPD-quinone. D. Ashley, **J.E. Boyd**
- 1022.** Intramolecular [2+2] Photocycloadditions of 2-Pyridones. **A. Davis**, C. Slough, M.E. Daub
- 1023.** MoS₂/WO₃@N-rGO@polyaniline nanocomposites for high-performance supercapacitors. **M. Thompson**, A. Rodriguez, M.H. Kabir
- 1024.** Antibacterial synergistic properties of silver nanoparticles and Manuka honey solutions for treatment of antibiotic resistant Escherichia coli and Staphylococcus aureus infections. **J.Y. Taylor**, W.F. Mays, K. LaiHing
- 1025.** Understanding nanomaterial toxicity and the potential for resistance evolution in bacteria. E.E. Carlson, A. Gavin, **Y.L. Peña Señeriz**
- 1026.** Comparison of photochemical decomposition and efficiency of different sunscreens. **A. Blake**, D. Craig, A. Labossiere, K. LaiHing, S. LaiHing
- 1027.** Fabrication of 30-100 nanometer Fluorescent Dye Encapsulated Silica Nanoparticles. **N. Singleton**, T. jia, S.S. Iyer
- 1028.** Withdrawn
- 1029.** Measuring the effect of interparticle spacing on the magnetic interactions of iron oxide nanoparticles with variable silica shell thicknesses. **A. Nozka**, O.T. Mefford
- 1030.** Spectral tuning of a green fluorescent silver cluster. **C. Setzler**, J.T. Petty, D. Lewis
- 1031.** Blue Ridge Blues: A Computational Study of Deep-Blue Emitters for use in Organic Light Emitting Diodes. **E.M. Smith**, A.L. Tomlinson
- 1032.** Synthesis of hybrid ferrocenyl-urea-chalcones : Exploring their potential as antitumorogenic agents. **L. Birriel Rodriguez**, J.A. Mendez, I. Montes
- 1033.** Synthesis and characterization of isomeric monodentate pyrrolyl phosphine ligands. **N. Sykes**, S. Pa, V. Osenga, M. Bambha, M. Johnson
- 1034.** Synthesis and characterization of ferrocenyl-indole chalcones as potential anticancer compounds. **J.L. Llera**, I. Montes
- 1035.** Continuous flow synthesis of chloroenals. **E. Ramirez**, F. Minami, K. Dwomoh, R.N. Dominey, E.W. Goldman
- 1036.** Continuous flow synthesis of polyfunctionalized pyrroles. **F. Minami**, **K. Dwomoh**, C. Perez Mandry, A. Kim, R.N. Dominey, E.W. Goldman
- 1037.** Quantifying electronic effects through Halogen bonding: A Computational assessment. **N.H. Pham**, K. Donald
- 1038.** Colorimetric and fluorescent probe for hydrogen sulfide and thiols. **A. Smith**, R. Osbourn, E. Adogla
- 1039.** Structure and Activity Relationships in Acridine Derivatives. **G. Blount**, K.S. Aiken, J. Kocerha
- 1040.** Synthesis of α -Ketoalkynes via alkylation. **J.J. Jaramillo Gonzalez**, B.D. Feske
- 1042.** Color of dyes and indicators: Natural resonance theory of excited states. **D.M. Hiatt**, E. Glendening
- 1043.** Detection of Nitroaromatic compounds using Porphyrin-Doped Silica Sol-Gels. **A. Ortiz**, **N. Snyder**, D.N. Collins, C.H. Lisse
- 1044.** Using Multi-Step Synthesis for the Production of Hydrogels with Adhesive Properties. **C. Smith**, T. Newar, C.H. Lisse
- 1045.** Optimization of product isolation for ruthenium-catalyzed oxidations of benzyl silyl ethers to silyl esters. **A.G. Riccardi**, R.W. Peterson, M. McKenna, J.T. Stokes, B.C. Goess, S.K. Goforth

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1046. Enabling targeted carbon monoxide delivery through click chemistry-based prodrug design and synthesis. **F. Vazquez**, S. Bansal, N. Bauer, B. Wang

1047. Withdrawn

1048. Investigation of S-nitrosylation in neuroblastoma cells exposed to silver nanoparticles. L.R. Frost, **H. Mays**

1049. The role of H121 in FtrB and its interaction with FtrA. **A. Kerkan**, E. Arias, D.W. Martin, S. Banerjee

1050. Chemical Analysis and Biological Properties of the Native Plant *Schinus terebinthifolius*. **S. Elias Rodriguez**

1051. Progress on the synthesis and analysis of the chemical and physical properties of 1-bromo-1-chloro-2,2,3,3-tetramethylcyclopropane. **D. Saakov**, R.L. King, J.R. Boone, C. Clinger

1052. Progress in the synthesis of tetrahalotricyclooctanes. **J. Osipchuk**, J.R. Boone, C. Clinger

1053. Synthesis, characterization, and reactivity of nickel and platinum complexes stabilized by multidentate ligands. **W. Ryder**, S. Schreiner

1054. Exploring transmetalation as an anticancer therapeutic strategy via localization and mechanistic studies for drug optimization. **Y. Del Valle**, A.D. Tinoco, J.A. Benjamin-Rivera, J. Acosta Mercado

1055. Computational investigations of the Morita-Baylis-Hillman reaction for E/Z-isomerization of α,β -unsaturated carbonyls by phosphines and arsines. **G. Scuderi**, D.A. Clabo

1056. Computational investigation of the fluorescence of substituted naphthylimides. **R. Osbourn**, E. Adogla, D.A. Clabo

610. Metal complexes of 2-pyridyl-naphthyridine ligands. **B. Solomon**, M. Ortiz, R.N. Dominey, E.W. Goldman

1057. Withdrawn

1058. Withdrawn

1059. S Withdrawn

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Puerto Rico Convention Center 202 A

Biochemistry IV Enzyme Activity / Kinetics

E. I. Pares-Matos, *Organizer*

J. A. Rodríguez-Martínez, *Presiding*

1:25 Introductory Remarks.

1:35 1068. Impact of Multivalency and Encapsulation of Affinity Reagents and Catalysts. **B. Manuel**, S. Das, A. Sanford, J.M. Heemstra, M. Finn

1:55 1069. Exploring how rare earth elements modulate bacterial growth and physiology in *Pseudomonas putida*. **D.E. Williams**

2:15 1070. Kinetics of *Escheria coli* upon treatment with antimicrobial ionic liquids. **C. Chism**, S. Plash, D. Zuckerman, G. Dasanayake, M. Bennett, S.K. Tripathi, S. Pedigo, E.E. Tanner

2:35 1071. Tanshinone derivatives inhibits of SARS-CoV-2 specific 3-chymotrypsin like protease (3CLpro) and papain like protease (PLpro) enzymatic activity in vitro. **D. Lewis**, A. Kawall, A. Sharma, K. Chavada, S. Rayalam, V.V. Mody, S. Taval

2:55 Coffee Break.

3:20 1072. Development of a DNase Activity Kinetic Assay. **J.J. Colón-Morales**, O. Soto-Berrios, A. Baerga-Ortiz

3:40 1073. Identification of phytochemicals that inhibit the enzymatic activity of SARS-CoV2 3-chymotrypsin like protease (3CLpro) in vitro. **A. Sharma**, A. Kawall, D. Lewis, K. Chavada, S. Taval, V.V. Mody, S. Rayalam

4:00 1074. Functional Roles of Coupled Motions in Enzymes: A case Study on Deubiquitinase A. **Y. Li**, S.D. Fether, A. Kabra

4:20 1075. Soft electrophile-based growth inhibitors of trypanosomes with oral in vivo efficacy. **I.V. Ogungbe**, D. Metibemu, O. Ajayi, O. Crown, O. Adeyinka

Puerto Rico Convention Center 201 B

Inorganic Chemistry IV -Catalysis

M. B. Santiago-Berrios, *Organizer, Presiding*

1:25 Welcoming remarks.

1:35 1076. Electrochemical and Light-driven Carbon Dioxide Reduction by Molecular Manganese Catalysts: Exploring the Positional Effect of Second-Sphere Hydrogen-Bond Donors. S. Sinha Roy, K. Talukdar, **J.W. Jurss**

1:55 1077. Light-Assisted Halide Perovskite Film Deposition and Photocatalytic Properties. **C. Lai**, J. Gonzalez-Moya

2:15 1078. Didodecylditelluride: a versatile reagent in the synthesis of metal telluride nanocrystal. D.N. Penk, E.H. Robinson, A.Y. Nuriye, **J. Macdonald**

2:35 1079. Association Constants of Various Rh(II) Paddlewheel Complexes with Tethered Thioether Ligands: Towards Establishing Structure-Activity Correlations. **D. Moore**, A. Darko

2:55 Coffee Break.

3:20 1080. Aluminum-Containing Late Metal Heterobimetallic Complexes: Synthesis and Reactivity. **T. Brewster**, N. Taylor, R.M. Charles, N.J. Deyonker, K. Young

3:40 1081. Understanding the challenges of biomimetic nitrogen fixation from computational analysis. Z. Benedek, **T. Szilvasi**

4:00 1082. Activity evaluation of two substituted-Nickel-Bis-dithiolene systems in MDA-MB-231 cancer cell line as a photothermal agent candidate. **K.T. Cordero-Gimenez**, D.M. Pinero Cruz

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4:20 1083. Fluorescence studies of Cucurbit[n]ril-Coumarin host-guest complexes. **R. Spencer**, K. Christensen, A. Watson, **F.A. Khan**, J.E. Hansen

Puerto Rico Convention Center 202 C

Organic Chemistry V Catalysis

D. J. Sanabria-Rios, *Organizer*
N. M. Carballeira, *Presiding*

1:25 Opening Remarks.

1:35 1084. Efficient Solvent-Free hydrosilylation of aldehydes and ketones catalyzed by palladium nanodispersed in organically modified silicate (Pd@MTES). **J. Fotie**, H.S. Drago, T. Tolar, J.E. Wroblewski

1:55 1085. Palladium/Silver Catalyzed Alkenylation of Partially Fluorinated Benzenes. **T. Brewster**, A.A. Mercado, D. Griffin, A.E. Lobos, T.J. Ricks

2:15 1086. S Withdrawn

2:35 1087. Copper Hydride-Catalyzed Reductive Coupling of Azatrienes and Ketones for the Synthesis of (Z)-Allylic anti-1,2-Amino Alcohols. **J. Zhu**

2:55 Coffee Break.

3:20 1088. Synthesis of heteroleptic Rh(II) paddlewheel complexes with axial coordination for selective carbene transfer reactions. **A. Darko**

3:40 1089. Non-directed palladium-catalyzed C-H activation of fluorinated arenes. **A. Mercado**, D. Griffin, A.E. Lobos, T.J. Ricks, T. Brewster

4:00 1090. Investigating engineering strategies to enable biocatalytic scalable syntheses of tropolone natural products. **J.R. Hernandez**, J. Perkins, A. Narayan

4:20 1091. Biocatalytic oxidation of indoles. **S. Champagne**, C. Chiang, A. Narayan

4:40 End of Session.

Puerto Rico Convention Center 203

Physical Chemistry II

M. J. Bayro, *Organizer, Presiding*

1:25 Introductory Remarks.

1:35 1092. Computational Quest of High-Performance Sorbents for Water Treatment: From Mechanism Understanding to Big-Data-Driven Prediction. **Z. Chen**, A.J. Hernandez

1:55 1093. A Search for Benzonitrile Relatives in the Interstellar Garden: The Negative Ion spectra of Deprotonated Dicyanobenzenes. **W.K. Gichuhi**

2:15 1094. Withdrawn

2:35 1095. Withdrawn

2:55 Coffee Break.

3:20 1096. Molecular Spin Qubits Based on High-Symmetry Lanthanide Complexes. M. Gakiya-Teruya, R. Stewart, S. Hill, **M. Shatruk**

3:40 1097. The unrestricted natural orbital active space decomposition approach for strongly correlated electronic structure. **L.M. Thompson**

4:00 1098. M-H Bond Activation Mediated by Sigma Hole Interactions. **K. Donald**

4:20 1099. Exploring C-H Activation with Quantum Chemistry and Machine Learning. **K.D. Vogiatzis**

Puerto Rico Convention Center 204

Project SEED Symposium II

D. Masterson, *Organizer*
A. Mallia, *Presiding*

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1:25 Opening Remarks.

1:35 1100. Project SEED: Positively impacting the interest and engagement in chemistry for rural high school students. **C.H. Lisse**

1:55 1101. Computational studies of carbon cycle reactions: A virtual summer experience. **L. Tribe**

2:15 1102. Learning Computational Drug Design: High School Student Investigations. **D. McTush-Camp**

2:35 1103. Project SEED at the University of Vermont – a mentor’s perspective. **M. Brewer**

2:55 Coffee Break.

3:20 1104. Integration of ACS Project SEED Students an Ongoing Undergraduate Research Program. **K. Dungey**, J.A. Pienkos, W. Yang

3:40 1105. Seed research experience in computational chemistry. **R. Prabhakar**

4:00 1106. Polymer-Protein Biomaterials Research with Project SEED. **M. Gaines**, G. Brim, D. Ingabire, A. Mancina, M. Smith, K.M. Jackson

Puerto Rico Convention Center Ball Room A

Symposium on Sustainable Green Chemistry V
J. C. Colberg, *Organizer*
H. Cheng, *Presiding*

1:25 Introductory Remarks.

1:35 1107. Development and application of self-assembled active agents to create sustainable green materials. **W. Hart-Cooper**, J. McManus, K. Johnson, L. Torres, **W.J. Orts**

1:55 1108. Reversible actives: Disinfectant applications, hazard analysis and use in agriculture to prevent mastitis and heal wounds.

W. Hart-Cooper, J. Wilson-Welder, J. McManus, L. Torres, X. He, W.J. Orts

2:15 1109. Fabrication of water treatment membranes using eco-friendly solvents and recycled polyethylene terephthalate. **D.J. Lu**, **I.C. Escobar**

2:35 1110. Biodegradable mulch films produced from soy-filled polymer resins. **K. Candlen**, M. Haque, S. Martey, J. Ratto, **W. Chen**

2:55 Intermission.

3:20 1111. Recycling polypropylene: A balance between stiffness and impact and story of compatibilizers. **H.B. Nulwala**, C. Diaz-Acosta

3:40 1112. Sophorolipids and their component hydroxy fatty acid amide derivatives as antimicrobial compounds. **R. Ashby**, J. Msanne, H. Yosief, M. Olanya, X. Fan

4:00 1113. Polymer Blends as a Platform for Sustainable Green Chemistry. **H. Cheng**, Z. He, K. Klasson, A. Biswas

Puerto Rico Convention Center 202 B

Undergraduate Oral Session III
B. J. Ramos-Santana, *Organizer, Presiding*

1:25 Introductory remarks.

1:35 1114. Molecular orbital study of a new class of large cage fullertube. **E.C. Lee**, **K.E. Smith**, **F. Steinour**, T.J. Fuhrer

1:55 1115. Viability of HEP-G2 and CHO-K1 cells after exposure to tin nanoparticles. **L. Alamo-Nole**, M. De Jesús Torres

2:15 1116. Synthesis of SnS nanoparticles using microwave irradiation. **J. Colon Dedos**, L. Alamo-Nole

2:35 1117. Friedel–Crafts alkylation of indoles with diarylmethyl acetates promoted by

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trimethylsilyl trifluoromethanesulfonate. **H. Xia**,
B. Bicalho, C.W. Downey

2:55 Coffee Break.

3:20 1118. Adamantane Ferrocenyl Derivatives
as a pharmacological approach towards SARS-
CoV-2. **D. Caraballo**, I. Montes Gonzalez

3:40 1119. Characterization of 4-Pyrone
Pyrolysis Products via Computational Modeling
and Matrix-Isolation FT-IR. **K. El-Shazly**, H.N.
Legg, K. Narkin, E.R. Sparks, T. Courtney, L.R.
McCunn

4:00 1120. Synthesis and Characterization of
Novel Meridional Quinoline-Derived Ligands
and their Homoleptic Complexes. **J. Stober**, J.
Dickenson, D.P. Harrison

4:20 1121. Synthesizing unnatural nanocrystal
phases: Understanding the role of alkyl selenol
reactivity with common solvents and ligands. **A.**
Peng, E.A. Ho, J. Macdonald

Puerto Rico Convention Center 201 A

Analytical Chemistry V - Spectroscopy

L. Cunci, *Organizer, Presiding*

1:25 Introductory remarks.

1:35 1060. Mosquito Species Classification
from Infrared Spectroscopy and Chemometrics
of Eggs. **S.W. Huffman**, C. Larmore, B.
Guilliams, H. Edmonds, C. Mitchell, T.
Gregory, B. Byrd

1:55 1061. Electrochemical flow reactor design
for operando surface enhanced infrared
absorption spectroscopy with tunable mass
transport. **J.E. Avilés Acosta**, J. Lin, T.F.
Jaramillo, C. Hahn

2:15 1062. Density functional theory to guide
the interpretation of platinum x-ray emission
spectroscopy. **L.M. Debeve**, C.J. Pollock

2:55 Coffee Break.

3:20 1063. Determination of polycyclic aromatic
hydrocarbons in surface water of an urban
wetland by gas chromatography-mass
spectrometry (GC-MS). **P.J. Berrios-Rolon**, F.
Marquez, M. Cotto-Maldonado

3:40 1064. Ultrasensitive Detection of SARS-
CoV2 Nucleocapsid Proteins Using Multi-
Photon Nonlinear Laser Wave-Mixing
Spectroscopy. **N. Shatirishvili**

4:00 1065. Metabolomics investigation of
intestinal contents reveal exercise induces
changes in the presence of western style diets.
K.A. Jones, A.J. Richard, A.J. Bruce-Keller,
J.M. Stephens, S.R. Campagna

4:20 1066. Streamline developability assessment
of therapeutic proteins without any sample
preparation requirements. **B. Pastrana-Rios**, D.
Dimitrov

4:40 1067. Metabolomics suggests potential sex
differences in renal mitochondrial epigenetic
signaling. **C. Christopher**, R. Schibalski, S.R.
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Destinee L Manning	811	Emmanuel Fernando Rivera Iglesias	380
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Devin Shane Lewis	1071	Eric Schneider	681
Devon Taylor	884	Erin Stryker	976
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Diana Sanchez	15	Ethan Chase Lambert	563
Dillon McBee	466	Evan Michael Smith	1031
Dino Villagran	727	Evelyn Ramirez	1035
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Dirk Guldi	495	Fabiola Vazquez	1046
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Lyza Martinez	636	Matthias Brewer	1103
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Shannon W Boettcher	168	Theodor Agapie	728
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Sharon Kennedy	305	Thomas F Jaramillo	724
Shawn Paul Zografos	804	Thomas Owens	966
Shawna Coulter	650	Thomas Owens	775
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Sierra Madison Neudorfer	588	Timothy Brewster	1080
Silmara Silva	931	Timothy Lewis	840
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Victoria Marie Casimir	641	Xu Simon	294
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Vincent Zollo	498	Yeriel Andrés Avellanet Crespo	858
Vladimir Muzykantov	680	Yessenia Alexandra Falconí	566
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