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Type them into the questions box!

"Why am I muted?"

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https://chemidp.acs.org

Career Consultant Directory

- ACS Member-exclusive program that allows you to arrange a one-on-one appointment with a certified ACS Career Consultant.
- Consultants provide personalized career advice to ACS Members.
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www.acs.org/careerconsulting
Atlantic Basin Conference on Chemistry
Linking the World through Chemistry
13-16 December 2022 | Marrakech, Morocco

HOTEL: MöVENPICK HOTEL MANSOUR EDDAHBI MARRAKECH CONVENTION CENTER: PALAIS DES CONGRÈS MARRAKECH
ABCChem.org  #ABCChem2022

ACS Career Resources

Register for a 2022 Virtual Office Hour

<table>
<thead>
<tr>
<th>Date</th>
<th>Event</th>
<th>Description</th>
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<tr>
<td>1 Sep</td>
<td>Leadership and Soft Skills Development—What You Need to Advance in Your Career</td>
<td>September 1, 2022</td>
</tr>
<tr>
<td>4 Oct</td>
<td>Developing Innovative Ideas and Intellectual Property</td>
<td>October 4, 2022</td>
</tr>
<tr>
<td>3 Nov</td>
<td>Finding and Succeeding in Internships</td>
<td>November 3, 2022</td>
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<tr>
<td>1 Dec</td>
<td>Careers in Academia</td>
<td>December 1, 2022</td>
</tr>
</tbody>
</table>

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Volunteer to meet with ACS members at all stages of their careers to discuss advice and career guidance.

https://www.acs.org/content/acs/en/careers/personal-career-consulting.html

https://www.acs.org/content/acs/en/careers/developing-growing-in-your-career.html
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ACS Scholar Adunoluwa Obisesan
BS, Massachusetts Institute of Technology, June 2021
(Chemical-biological Engineering, Computer Science & Molecular Biology)

“The ACS Scholars Program provided me with monetary support as well as a valuable network of peers and mentors who have transformed my life and will help me in my future endeavors. The program enabled me to achieve more than I could have ever dreamed. Thank you so much!”

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ACS OFFICE OF DEIR
Advancing ACS' Core Value of Diversity, Equity, Inclusion and Respect

Resources

- Inclusivity Style Guide
  Designed to help staff and members use language and images that respect diversity in all its forms.

- ACS Webinars on Diversity
  Covering diversity and inclusion in the workplace.

- ACS Publications DEIR Hub
  See what ACS Publications is doing for fostering diversity in scholarly publishing.

- ACS Volunteer and ACS Meetings Code of Conduct
  Promoting a positive and welcoming environment for attendees, volunteers, and staff.

- C&EN Trailblazers
  C&EN highlights scientists from different backgrounds who are making an impact in chemistry.

- NEW Download DEIR Educational Resources
  Download this educational guide for additional recommendations on essays, articles, books, portraits, and more on diversity, inclusion, and related topics.

- Quick Guide: Inclusion Moments
  Learn more about what inclusion moments are and one idea to host them during your meetings.

- Quick Guide: How to host inclusive in-person events
  Recommendations and best practices to ensure that your events can accommodate everyone.

Diversity, Equity, Inclusion, and Respect

**Diversity**
- The representation of varied identities and differences (race, ethnicity, gender, disability, sexual orientation, gender identity, national origin, religion, age, social-economic status, thinking and communication styles, etc.) collectively and as individuals. ACS seeks to proactively engage, understand, and draw on a variety of perspectives.

**Equity**
- Seeks to ensure fair treatment, equality of opportunity, and fairness in access to information and resources for all. We believe there's only equality in an environment built on respect and dignity. Equity requires the identification and elimination of barriers that have prevented full participation of some groups.

**Inclusion**
- Describes a culture of belonging by actively inviting the contribution and participation of all people. Every person's value adds value, and ACS strives to create balance in the face of power differences. In addition, no one person can or should be relied upon to represent an entire community.

**Respect**
- Ensures that each person is treated with professionalism, integrity, and ethics undergirding all interpersonal interactions.

https://www.acs.org/content/acs/en/about/diversity.html
Circular Nutrient Economy
Recovering nutrients from waste streams for reuse as fertilizers

Wednesday, December 14, 2022  @ 2-3PM ET

Featuring Panelists: Expert Environmental Engineers from UMBC

Dr. Hui Chen (Team Lead) postdoctoral research associate, UMBC, Dr. Blaney’s lab. (Completed her PhD in Chemistry at Stonybrook University)

Dr. Ushar Shashratt postdoctoral research associate, UC Berkeley (Completed her PhD in Chemistry at Stonybrook University – Dr. Blaney’s lab)

Mr. Michael Fleming Ph.D. candidate, UMBC, Dr. Blaney’s lab (environmental engineering program)

Ms. Ouriel Ndalamba BS student, UMBC (chemical engineering major)

Ms. Kaylyn Stewart BS student, UMBC (chemistry major)

Key Learning Objectives:
• Importance of circular nutrient economy
• Basics of Donnan dialysis
• Current progress in Donnan dialysis technologies for nutrient recovery

Who Should Attend:
• Analysts, technicians, engineers and chemists who are either currently involved in environmental issues
• Wastewater professions and farmers who are interested in employing new strategies to solve nutrient pollution
• Students and researchers working on environmental issues

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THIS ACS WEBINAR® WILL BEGIN SHORTLY...

👋 Say hello in the questions window!

Chemistry Tools to Help Achieve Zero World Hunger

MIKE MORELLO, MS
Member, ACS Committee on Science ACS Division of Agricultural & Food Chemistry

MICHAEL APPELL, PhD
Research Chemist, Agricultural Research Service, U.S. Department of Agriculture

OMOWUNMI "WUNMI" SADIK, PhD
Distinguished Professor and Chair, Department of Chemistry and Environmental Sciences, New Jersey Institute of Technology

H.N. CHENG, PhD
Past President, American Chemical Society

This ACS Webinar® is co-produced with the ACS Committee on Science and the ACS Division of Agricultural and Food Chemistry as part of the 2022 Frontier Fridays Series.
Initiated by 2021 ACS President H.N. Cheng & ACS Committee on Science

**Skin-Inspired Organic Electronics**

*Zhenan Bao* K.K. Lee Professor of Chemical Engineering & Chair, Dept of Chemical Engineering, Stanford University

https://www.acs.org/content/acs/en/acs-webinar/library/organic-electronics.html

**Artificial Molecular Machines**

*Sir Fraser Stoddart* 2016 Nobel Laureate in Chemistry, Board of Trustees Professor of Chemistry, Northwestern University


**Lithium-ion Batteries**

*Amy Lucía Prieto* Professor, Department of Chemistry, Colorado State University & Founder, Prieto Battery, Inc.

https://www.acs.org/content/acs/en/acs-webinar/library/lithium-ion-sustainability.html

**Putting Sustainable Chemistry to Work in Manufacturing**

*Mark Mascal* Professor of Chemistry, University of California Davis

*Ryan Lively* Assistant Professor, Georgia Institute of Technology

https://www.acs.org/content/acs/en/acs-webinar/library/sustainable-chemistry-work.html

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**ACS Committee on Science (COMSCI)**

ComSci is a joint Board-Council Committee. It aims to identify new frontiers of chemistry, examine the scientific basis of and formulate public policies related to the chemical sciences, and recognize outstanding chemical scientists. It is structured to provide a forum for collaboration, coordination, and communication of the scientific activities of diverse units of the SOCIETY and to provide an interface between and among such units.

https://www.acs.org/content/acs/en/about/governance/committees/science.html
Chemistry & the SDGs

https://www.acs.org/content/acs/en/sustainability/chemistry-sustainable-development-goals.html

ACS Technical Division
Agricultural & Food Chemistry (AGFD)

Vision:
Enhance quality of Life by advocating safe, nutritious, and sustainable food and agricultural supplies that meet global challenges.

Mission:
Lead and foster a diverse community to promote and advance agricultural and food chemistry research, education, outreach, and communication.

https://www.agfoodchem.org
The U.N. Sustainable Development Goal of “Zero Hunger” aims to end hunger and achieve food security by 2030.

There is an intense need for more and better food: over 690 million people are without enough to eat, and world population is growing.

Chemists and engineers have a vital role to play in the fight against world hunger.

https://www.acs.org/content/acs/en/sustainability/zero-hunger-summit.html
Chemistry Tools to Help Achieve Zero World Hunger

Michael Appell
USDA, Agricultural Research Service
National Center for Agricultural Utilization Research
Peoria, IL USA

Agricultural and Food Chemistry

• Vision: Enhance quality of life by advocating safe, nutritious and sustainable food and agricultural supplies that meet global challenges.
• Mission: Lead and foster a diverse community to promote and advance agricultural and food chemistry research, education, outreach and communication
• Membership is insurance for your career
• National Meetings are like family reunions
• Active community in Sustainability, Greentech, and the FEW Nexus
• agfoodchem.org

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Zero Hunger
= End World Hunger

- Chemistry plays an important role in agriculture and food
- AGFD was founded in 1908 as one of the four original technical divisions of ACS (AGRO and BIOT)
- Agricultural problems need solutions:
  - Shifts in weeds, pests, diseases due to extreme changes in weather
  - Improving long-term crop production
  - Reducing food packaging and food waste
  - Reducing greenhouse gases in agriculture
  - Food, Energy, Water (FEW) Nexus

Sustainable Food Security and Production

- The world needs to produce at least 56% more food by 2050 to feed and meet the needs of a projected 10 billion people
- 11% of the world (925 million people) lack access to a safe and nutritious food supply
- 13% of the world is obese and 39% is overweight
- Approximately 2/3 of adult Americans are overweight or obese (dramatic increase since the mid 1970s)
- Sustainable practices support meeting these needs

https://ourworldindata.org/obesity#what-share-of-adults-are-obese
Waste Food and Sustainable Agricultural Commodity Recycling

• "In the United States, 31 percent— or 133 billion pounds—of the 430 billion pounds of the available food supply at the retail and consumer levels in 2010 went uneaten. The estimated value of this food loss was $161.6 billion using retail prices. For the first time, ERS estimated the calories associated with food loss: 141 trillion in 2010, or 1,249 calories per capita per day."

• "1/3 of the food in the USA is wasted (every third aisle in a grocery store)"

Significant increase in corn yields through technology

- 2021 National Corn Growers highest yield:
  - 602 bu/acre
- 1870 to 1940s corn yields about 25 bu/acre
- Recent average yields are around 160+ bu/acre

The NCAUR is at the center of high yield corn and soybean production
Sustainability and Food Safety are Complementary

- Almost 48 million cases of foodborne illness in the USA each year resulting in 128,000 hospitalizations and 3000 deaths
- Foodborne illnesses are a public burden, difficult to detect, and harm humans and other animals
- Food hazards, including microorganisms and chemical contaminants, can enter the food supply at any point from farm to table
- Most of these hazards cannot be visually detected in food when it is purchased or consumed
- Food contamination can be detected by frequent monitoring using analytical instrumentation


https://www.fda.gov/food/consumers/what-you-need-know-about-foodborne-illnesses
Mycotoxins and Food Safety

- Environmental stresses cause commodities to become susceptible to contamination to harmful microbes
- Some microorganisms produce toxins; certain fungi produce mycotoxins
- Mycotoxin contamination reduces food quality and impacts food security
- Some mycotoxins are very toxic, others have no noticeable effects at low levels
- Some recent analytical methods can detect very low toxin levels that are significantly below the advisory and regulated levels

The Dose Makes the Poison

Analyzing Risks of Mycotoxins

- 85% of commodity samples tested from around the world had detectable levels of mycotoxins
- Joint FAO/WHO Expert Committee on Food Additives reported that Asia and Africa were highly affected
- High variability of mycotoxin concentrations
- Many samples have multiple mycotoxins

https://www.pigprogress.net/specials/whats-the-truth-behind-the-faos-25/

Mycotoxins

- Chemically diverse compounds
  - Hundreds of known mycotoxins
- Mycotoxins are structurally diverse and number over 800+
- Defined by toxic and fungal origin (not structure)
- FGIS Mycotoxin Handbook provides approved examples of testing
- Why are mycotoxins produced?

https://www.ams.usda.gov/publications/content/fgis-pdf-handbooks

Mycotoxin Exposure

100,000 turkeys died from aflatoxin exposure in 1962
- Due to Aspergillus flavus contaminated peanuts
- Spurred interest in mycotoxin research

155 of 452 elementary school children in U.S. became ill within 15 minutes of eating school lunch in 1997
- 15 other outbreaks in the U.S. from October 1997 to October 1998
- 1700 students affected overall
- 2 million pounds of burritos recalled
- Vomitoxin contamination (deoxynivalenol) at 0.3 ppm

In 2021, over 70 dogs died from exposure to aflatoxins in pet food, resulting in FDA recall.

https://www.ams.usda.gov/publications/content/fgis-pdf-handbooks
Computational Approaches to End Mammal Testing

U.S. EPA to eliminate all mammal testing by 2035

All-Party Parliamentary Group is urging the UK government to bypass animal tests, due to their high failure rate, in place of human-relevant research

European Parliament votes for EU-wide plan to phase out animal testing

https://www.science.org/content/article/us-epa-eliminate-all-mammal-testing-2035

What fraction of people in the U.S. become sick due to foodborne illness each year?

• 1 out of 2 people
• 1 out of 6 people
• 1 out of 10 people
• 1 out of 20 people
• 1 out of 50 people

* If your answer differs greatly from the choices above tell us in the questions window!
Sustainable Approaches for Food Safety and Security

Computational Chemistry and Toxicology

- Reduces costs and needs for mammal sacrifice
- High-throughput *in silico* screening
- Solves problems that cannot be addressed experimentally
  - Machine Learning/AI models for toxicity and detection
  - Antifungal development

Materials

- Unique properties and large surface areas
- Enable new approaches to address agricultural problems
- Overcome the limitations of existing methods
  - Biochar
  - Nanospponge materials
  - Biomimetic technology

Design, Create, and Applications

Quantum chemistry and cheminformatics

Quantum Chemical – energetic preferences, toxicological potential, spectroscopic properties

Unusual Properties of Natural Products

Computational Toxicology using DFT

TD-DFT Properties

QSAR – predictive models for toxicity, ADMET, detection, and antifungal activity

<table>
<thead>
<tr>
<th>Activity</th>
<th>Eq.</th>
<th>Equation</th>
<th>$R^2$</th>
<th>$Q^2$</th>
<th>$R^2_{Adj}$</th>
<th>$q^2$</th>
<th>PRESS</th>
<th>n</th>
<th>s</th>
<th>F</th>
<th>p</th>
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<tbody>
<tr>
<td>cytotoxicity NIH3T3</td>
<td>X1</td>
<td>$pIC_{50} = 0.6764(E_{LOMO}) + 0.24(2)(\log P) + 8.1073$</td>
<td>0.517</td>
<td>0.273</td>
<td>0.443</td>
<td>0.815</td>
<td>16</td>
<td>1.001</td>
<td>6.95</td>
<td>0.0088</td>
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<td></td>
<td>X2</td>
<td>$pIC_{50} = 0.7752(\Delta t) + 0.164(\log P) + 2.5737$</td>
<td>0.540</td>
<td>0.304</td>
<td>0.470</td>
<td>0.979</td>
<td>16</td>
<td>0.795</td>
<td>7.64</td>
<td>0.0064</td>
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<td>X3</td>
<td>$pIC_{50} = 1.4771(MTOC_{10}) - 1.9890(\log P) + 0.1896 X(\log P) + 6.9024$</td>
<td>0.789</td>
<td>0.616</td>
<td>0.729</td>
<td>0.757</td>
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<td>14.39</td>
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<tr>
<td></td>
<td>X4</td>
<td>$pIC_{50} = 1.5089(MTOC_{10}) - 1.7746(\log P) + 7.3778$</td>
<td>0.773</td>
<td>0.663</td>
<td>0.738</td>
<td>0.681</td>
<td>16</td>
<td>0.559</td>
<td>22.12</td>
<td>0.0001</td>
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</tbody>
</table>
Antifungals

- Some potent mycotoxins are regulated, and these toxins are generally associated with *Fusarium*, *Aspergillus*, and *Penicillium* species.

- Essential oil components and alkaloids are of interest as antifungal compounds due to their reported antifungal activity and favorable properties (including anti-oxidant).

- **Goal:** Identify GRAS mixtures of safer phenolic compounds that can be used as better antimicrobials.

*Approach:* Identify the contributions of electronic structures and topological properties of popular phenolic compounds to antifungal activities to aid the development of improved antifungal compounds against mycotoxin producing fungi.

USDA - Paige Pierson, Kervin Evans, Dave Compton, Eric Johnson, Mark Doehring

Bradley University – Wayne Bosma

National Taiwan University – Yufeng Jane Tseng, Yi-Shu Tu
Phenolic compounds as antifungals

MIC<sub>50</sub> of six fungi
- *Fusarium verticillioides* - fumonisin, deoxynivalenol
- *Fusarium oxysporum*, fruit rot
- *Aspergillus flavus* – aflatoxins
- *Aspergillus fumigatus* - gliotoxin
- *Penicillium expansum* – patulin
- *Penicillium brevicaespactum* - mycophenolic acid

Principal Component Analysis:
- 1<sup>st</sup> component explained 93.5% of the variance
- 2<sup>nd</sup> component explained 2.95%
- Phenolic compounds exhibit similar antifungal activities across species; however, the compounds exhibit some species-specific antifungal profiles

**QSAR** (Quantitative Structure–Activity Relationship)
- Chemical Structures

- Predictive mathematical models are developed on the assumption that molecules with similar structures have similar properties
- Properties of molecules are related to their electronic structure
- Popular descriptors
  - Quantum chemical
  - Electrostatic
  - Electronic
  - Lipophilic
  - Topological
  - Constitutional
  - Geometric
  - Steric
The biological activity data used in the structure activity studies were obtained from previously published reports. Structures were built using Spartan'16 and the B3LYP density functional and 6-311+G** basis set. QSAR models were built using BuildQSAR and QSARINS v2.2.4 software.

785 Descriptors were considered, including 18 quantum-based descriptors and 777 descriptors using Mold2 bioinformatics programs developed by the FDA for toxicity prediction.

Descriptor selection was based on systematic search and multiple genetic algorithm experiments with 1-2 descriptor models, 10000 generations, and 10 models per generation on mean centered and scaled descriptor values.

---

### Quantum Chemistry: Electrophilicity Index

- Theorem of Koopman

- Electrophilicity index, $\omega$, is an indicator of the reactivity and stability

- Compounds with a conjugated double bond have higher electrophilicity index values

- Phenolic compounds with greater antifungal activity possessed a lower electrophilicity index values
• Thymol, 1, and carvacrol, 2, are antioxidant components of essential oils from several popular plants, including the widely used herb thyme.

• Thymol and carvacrol have historically been used as food preservatives against spoilage and as insecticides.

• It has been proposed that the antifungal properties of thymol are associated with inhibitory effects on hyphae formation of fungi, and the lack of viability of the resulting fungal aggregates.

- Biological Methods
  - Biotransformations
  - micro-organisms – enzymes
  - Probiotics
  - Non-mycotoxin producing fungi

- Chemical/Physical processing
  - Food/product processing

- Sorbents – binders
  - Agro-based biomaterials

- New uses of materials
  - Feed to organisms not affected by the toxins
  - Fertilizers
  - Value-added biobased materials

Value proposition?
Zearalenone and Biochar

- Burning or decomposing biomass releases 99% of the carbon as CO₂
- Biochar is a charcoal made from biomass through pyrolysis that captures 50% of the carbon
- The feedstock influences the properties
- Functionalization is possible
- Switchgrass vs. corn stover for binding estrogenic compounds in water

<table>
<thead>
<tr>
<th>Biochar sample</th>
<th>C (%)</th>
<th>H (%)</th>
<th>N (%)</th>
<th>O (%)</th>
<th>Ash (%)</th>
<th>Total surface area (m²/g)</th>
<th>Micropore surface area (m²/g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CSB</td>
<td>45.14</td>
<td>1.86</td>
<td>0.44</td>
<td>12.96</td>
<td>39.60</td>
<td>74</td>
<td>14</td>
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<tr>
<td>SB</td>
<td>43.65</td>
<td>3.71</td>
<td>0.78</td>
<td>24.99</td>
<td>26.87</td>
<td>46</td>
<td>23</td>
</tr>
</tbody>
</table>

USDA-ARS: Mike Jackson, Steve Peterson, Steve Vaughn

Biochar: Unique Physical Properties

SEM Switchgrass vs. Corn Stover

FTIR Switchgrass vs. Corn Stover
Biochar Summary

- Corn stover and switchgrass are two very affordable, renewable feedstocks from which to make biochar
- These results suggest that micropore surface area is a key factor in predicting sorptive quality of a given biochar
- The surface area of corn stover biochar was greater than switchgrass biochar; however, switchgrass biochar had greater micropore surface area
- Switchgrass biochar could bind more estrogenic compounds

Nanosponge Materials for Patulin & Ochratoxin A

- Cyclodextrin polyurethane polymers have been developed to detect patulin in apple juice and shown suitable to remove ochratoxin A from wine
- Three dimensional scaffolds synthesized around the cyclic cyclodextrin carbohydrate
- Previous applications include toxin sorbents from water, controlled release materials for pharmaceutical/bioactive delivery
- Transition from using TDI to MDI for safer polyurethanes
- Polymers were designed, synthesized, characterized, and applied to detect mycotoxins
- Researchers at Shinshu University in Japan used these materials to develop a rapid and very sensitive method to detect the mycotoxin patulin in apple juice

**USDA-ARS:** Mike Jackson, Atanu Biswas, H.N. Cheng, Julie Wang, Dave Compton, Kervin Evans  
**Shinshu University:** T. Goto, T. Shirasawa, M. Ueda
• Nanoscopic scale (1-100 nm) is where quantum mechanics retains influence on properties - larger sizes are dominated by classical (Newtonian) mechanics

Applications in Food Safety:
• Detection
• Delivery
• Sequestration

Sustainability

Patulin
• Associated with apple juice and apple rot
• Children are especially susceptible to this toxin – apple juice is used in beverages targeted toward children
• Exposure to the toxin is associated with
  • gastrointestinal diseases
  • potential for carcinogenicity
  • genotoxicity
  • immunotoxicity
  • Neurotoxicity
• Regulated in the US and other countries at 50 μg/L for certain apple-based products
• A validated 10 μg/L method exists that is very labor intensive
Health Benefits of Apples

- Apple juice has health-promoting properties apart from the basic nutritional characteristics and is considered a functional food

- Apples are packed with vitamins, calcium, potassium and magnesium

- The pectin and fiber of apple juice helps boost energy

- Apple is a rich source of phenolic compounds, that can aid in the fight against common infections

- Benefits include: enhances skin, weight control, heart health, liver health, cures constipation, diabetes, hydrates the body, prevents anemia, vision

Researchers at Shinshu University in Japan used these materials to develop a rapid and very sensitive method to detect the mycotoxin patulin in apple juice

<table>
<thead>
<tr>
<th>Patulin concentration (ng mL⁻¹)</th>
<th>Patulin recovery (%)</th>
<th>RSD (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>Cannot be calculated (Tr., Tr., 170)</td>
<td>60*</td>
</tr>
<tr>
<td>10</td>
<td>78</td>
<td>16</td>
</tr>
<tr>
<td>20</td>
<td>71</td>
<td>9.4</td>
</tr>
<tr>
<td>50</td>
<td>78</td>
<td>14</td>
</tr>
<tr>
<td>80</td>
<td>71</td>
<td>5.0</td>
</tr>
<tr>
<td>100</td>
<td>67</td>
<td>2.0</td>
</tr>
</tbody>
</table>

Method developed using polyurethane nanosponge materials prepared by MDI to detect patulin at 10-100 μg/kg in apple juice

The nanosponge-based method has quantitative range that covers the 50 μg/kg patulin regulated limits
Ochratoxin A in Wine and Grape Juice

- The recoveries were between 77.0-89.4% for wine and 69.1-86.5% for grape juice.
- The method reported is suitable to detect ochratoxin A in wine and grape juice at levels between 20 ng mL\(^{-1}\) to 0.5 ng mL\(^{-1}\).
- The limit of detection (LOD) was 0.2 ng mL\(^{-1}\).

- One of the most common mycotoxins
- Occurs in grains, meats, fruits, including grapes and wines
- Associated with carcinogenicity and neurotoxicity

Health benefits of grapes and wines
Packed full of vitamin C and polyphenols, grape products reduce inflammation, supports heart health, immune function, and digestion.

Key Points

- Chemists can address important problems to ensure safe and nutritious food supplies and support the goals of Zero Hunger.
- Computational models can reduce costs, the need for animal sacrifice, and can solve problems that cannot be addressed experimentally.
- Materials science and nanotechnology offer a means to produce economical biomaterials to address food safety problems.
• **Vision:** Enhance quality of life by advocating safe, nutritious and sustainable food and agricultural supplies that meet global challenges.

• Join -> agfoodchem.org

Thank you!
Chemistry Tools to Help Achieve Zero World Hunger

Omowunmi “Wunmi” Sadik
Distinguished Professor and Chair
Department of Chemistry and Environmental Science

Sustainable Agriculture

• **Goal 2.** End hunger, achieve food security and improved nutrition, and promote sustainable agriculture

• By 2030, the goal is to end hunger and ensure that everyone (particularly those most vulnerable) has access to safe, nutritious, and sufficient food year-round
What do we mean by zero hunger and undernutrition? (Select all that apply)

- Access to safe, nutritious, and sufficient food
- Access to physical and economic food resources that meets dietary needs and food preferences for an active and healthy life
- Access to an adequate amount of food at all times
- Ending malnutrition of all forms

* If your answer differs greatly from the choices above tell us in the questions window!

Pillars of Sustainability

People 1
- Measurements of education, equity, and access to social resources

Planet 2
- Measurements of natural resources and influences to its viability

Profits 3
- Measurements of income, expenditures, taxes, and employment

Roland M. Miller, Francis J. Osonga, & Omowummi A. Sadik, Synthesis and Biological Applications of Greener Nanoparticles, In CRC on “Interfaces between microbes and nanomaterials, Gupta Editor, April 2021, 10.1201/9780429321269-11
Sustainable Nanotechnology

Green chemistry and "safe-by-design" approaches

Responsible development at corporate and societal level

Development of advanced methodology tools

Nano-ES: nanoscience and engineering for sustainability

Diverse and effective means of waste and waste-free approaches

To develop low-cost, low power sensing technologies using sustainable and biodegradable materials and processes that leave no environmental footprints
Sustainable Nanosynthesis


Greener One-Pot Nanosynthesis using Glycoconjugates

ACS Agric. Sci. Technol. 2021, 1, 4, 379–389, Publication Date: July 20, 2021
https://doi.org/10.1021/agscitech.1c00093
Flavonoids Acetamides


Scheme 1: Steps in the synthesis of 2,2'-((4-(3,7-bis(2-amino-2-oxoethoxy)-4-oxo-4H-chromen-2-y1)-1,2-phenylene)bis(oxy))diacetamide (3S3), 2,2',2''-((2-(4-(2-amino-2-oxoethoxy)phenyl)-4-oxo-4H-chromene-3,5,7-triyl)tris(oxyl)triacetamide (4S3) and 2,2'-((4-(5,7-bis(2-amino-2-oxoethoxy)-4-oxo-4H-chromen-2-y1)-1,2-phenylene)bis(oxyl)diacetamide (5S3) derivatives.

TEM and XRD Characterization

Figure R: Formation of L-α-Aconitine (10 μg/mL) and CEGA (10 μg/mL) using L-α-Aconitine and CEGA (10 μg/mL).

Figure S: Formation of L-α-Aconitine (10 μg/mL) and CEGA (10 μg/mL) using L-α-Aconitine and CEGA (10 μg/mL).
**Fusarium**

The genus of *Fusarium* is a wide group of fungi that have a broad impact on the food and drug industry, medicine, and agriculture. This disease is lethal to a variety of plants.

- *F. oxysporum* is also pathogenic to humans and animals causing fungal keratitis, onychomycosis, and hyalohyphomycosis.
- *F. solani* can cause Fusarium crown, foot rot, and dry rot in squash, pumpkin, bananas, and also other plants. Both of these fungi can survive in the soil for long periods of time which negates the effect of crop rotation.

**Penicillium italicum Infection**

**Citrus infection**

- *P. italicum* is a plant pathogen commonly found in citrus fruits.
- Early symptoms include a soft water-soaked area on the peel, followed by development of a circular colony of white mold.

Antifungal Activities of Greener Nanostructured Copper against *Penicillium italicum*

Influence of Particle Size and Shapes on the Antifungal Activities of Greener Nanostructured Copper against *Penicillium italicum*

Francis J. Osonog, Gadji Eshun, Sanjay Kalra, Idiris Yazeen, Laura Sakharee, Renata Ohtman, Shaojie Jiang, and Omowammi A. Sadik

**ABSTRACT:** Pathogenic microorganisms cause diseases that play a limiting role in food production. The growth of blue mold set on citrus fruits caused by *Penicillium italicum* poses substantial economic loss due to food decay. The control of *P. italicum* using toxic synthetic fungicides raises serious concerns about food safety and quality. There is a need to develop safe fungicide-management techniques to prevent economic loss in the agro-industry. Copper nanoparticles (CuNPs) are typically prepared at elevated temperatures (200 °C) using toxic surfactants such as octylphenolpolyethoxylate bromide (CTAB) and harsh organic solvents. We hereby report, for the first time, a novel greener and eco-friendly one-pot aqueous method for synthesizing copper nanoparticles (CuNPs) and well-defined copper nanosheets (CuNNS) with controlled shape and size using copper(II) sulfate (CuSO₄) precursor and water-soluble quaternary phosphine (QFQ) in a bio-enhancing and capping agent at room temperature. The CuNPs were characterized by transmission electron microscopy (TEM), energy-dispersive X-ray (EDX) spectroscopy, and X-ray diffraction (XRD). CuNPs with average edge lengths of 150-250 and 60-180 nm were designed using QFQ and CuSO₄, in the ratios of 5:1, respectively. The metrics of sustainability obtained include atomic economy (73.34%), molar efficiency (68.0%), and environmental factor (3.49%). The antifungal activity of CuNPs and CuNNS was tested against *P. italicum* using the Kirby-Bauer method. The study demonstrated the comparative effectiveness of CuNCS and CuNNS on the growth of *P. italicum* spores in a dose-dependent manner. The results indicated that CuNCS and CuNNS showed antifungal activity against the growth of *P. italicum*, with the minimum inhibitory concentration (MIC) of 100 and 200 μg/mL, respectively. At a constant particle size, it was evident that CuNCS showed significant inhibitory activity of *P. italicum* at a low-dose treatment (100 μg/mL) in comparison to CuNNS. The particle size and shape effect of CuNCS played a vital role in its antifungal activity. QFQ-modulated synthesis of CuNCS and CuNNS could serve as a potent biocide for the natural remediation of citrus-based fungal diseases.

**KEYWORDS:** sustainability, antifungal, naturally derived, macroalgae, nanosheets, fungicides, antifungal, *Penicillium italicum*

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**How can chemical science help to achieve zero hunger?** (Select all that apply)

- Extend the shelf life of food through advances in packaging and maintain food quality and safety
- Develop new products to protect crops from pests and diseases
- Develop food additives to prolong the shelf life of foods
- Develop sustainable insecticides and pesticides, plant growth regulators, fertilizers and animal growth supplements

* If your answer differs greatly from the choices above **tell us in the questions window!**
The Role of Chemistry and Healthy Foods

Chemistry plays a role in improving the access to healthy foods through improved post-harvest storage loss. Chemistry is core to food utilization and combinations — by improved biofortification, food processing and essential medicines. Chemistry has contributed much to the food security agenda.

The Food and Agriculture Organization urges countries to...

- Meet the immediate food needs of their vulnerable populations
- Boost social protection programs
- Keep global food trade going
- Keep the domestic supply chain gears moving, and
- Support smallholder farmers’ ability to increase food production

The Food and Agriculture Organization estimates that we entered 2022 with 828 million hungry people.
A paper-based diagnostic tool for smallholder farmers

A smart phone based biosensor / nanoremediation system that helps smallholder farmers address the devastating effects on the production of vegetative crops (sweet yams, oranges, bananas) due to the epidemics of *Colletotrichum gloesporioides*.

---

BREAD: Basic Research to Enhance Agricultural Development

The goal of BREAD is to support innovative, basic scientific research designed to address key constraints to smallholder agriculture in the developing world.
Paper-based Biosensor Concept

Sensing Platform  Microbial Battery

Smart Biosensors

With Professor S. Choi, Binghamton University

Smartphone-based biosensors to detect anthracnose disease caused by fungus, *Collectotrichum gloeosporioides*
Biobattery Testing

The electric bacteria were revolutionarily freeze-dried for long-term storage and were readily rehydrated for power generation by using a finger-activated, self-contained media pouch.

This work ensured for the first time the practical efficacy of the explored paper-based battery pack, generating on-demand energy even in resource-limited environments to power a light-emitting diode and an electric calculator.

With Professor S. Choi, Binghamton University

Problem with Anthracnose

• Sweet Yams are plagued with anthracnose
• Small-holder farms typically grow this yam species
  • Need for cheap, rapid, and reliable sensor and greener fertilizers
• Farmers currently use a fungicide called Topsin and Glider
  ➢ Methyl thiophanate (active ingredient)
  ➢ \( C_{12}H_{14}N_4O_4S \)
• Also, use various fertilizers (Miracle Grow) and some herbicides.
Sweet Yams *(Dioscorea species)*

- **Sweet Yams** *(Dioscorea species)* are among the primary agricultural commodities and major staple crop
  - Africa, India, Southeast Asia, South America, and the Caribbean
- Production problems due to anthracnose disease
  - *Colletotrichum gloeosporioides*

### Impact of Yam Anthracnose in Jamaica

**Production estimates for Sweet Yam in Jamaica (MICAF) from 2005 to 2014**

<table>
<thead>
<tr>
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<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>PRODUCTION (TONNES)</td>
<td>6313</td>
<td>6275</td>
<td>5185</td>
<td>3765</td>
<td>4411</td>
<td>3907</td>
<td>3291</td>
<td>2609</td>
<td>1805</td>
<td>1768</td>
</tr>
</tbody>
</table>

The Rural Agricultural Development Authority (RADA) recommends the use of **Topsin** as treatment to counteract the effect of this disease *(JIS, 2004)*.

Sadik, O., Asemota H. Grant T., Miller R., Osonga F., Eshun G., unpublished results
# Field Testing and Biometrics

## Sampling Location: Mr. Young Farm, Bilby

<table>
<thead>
<tr>
<th></th>
<th>Sample 1</th>
<th>Sample 2</th>
<th>Average</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weight of tubers</td>
<td>13.0g</td>
<td>33.0g</td>
<td>23.0g</td>
</tr>
</tbody>
</table>

## Sampling Location: Mr. Kirkland Farm, Grove place

<table>
<thead>
<tr>
<th></th>
<th>Sample 1</th>
<th>Sample 2</th>
<th>Average</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weight of tubers</td>
<td>322.0g</td>
<td>192.6</td>
<td>257.3g</td>
</tr>
</tbody>
</table>

Sadik, O., Asemota H. Grant T., Miller R., Osonga F., Eshun G., unpublished results

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# Yam plants post Nanoparticle Treatment

Sadik, O., Asemota H. Grant T., Miller R., Osonga F., Eshun G., unpublished results
Collaboration

- National Science Foundation Project and Bill and Melinda Gates Foundation
- International collaboration SUNY-Binghamton, University of the West Indies Mona Campus (UWI), and the Northern Caribbean University (NCU)
- Southern Trelawny Environmental Agency (STEA)
- Efforts to help sweet yam small holder farmers in Manchester and Trelawny areas of Jamaica

Nano US-Africa Supplement (CBET)
* CREATES is an African Center of Excellence (ACE), which was established at the NM-AIST through the World Bank’s African Centers of Excellence (ACE II) initiative.

The NM-AIST is part of a network of African Institutions of Science and Technology (AISTs), established as a brainchild of the late Nelson Mandela and the World Bank.

TROPICAL PESTICIDES RESEARCH INSTITUTE (TPRI)

Central Goal

To isolate the causative agent of the disease plaguing Sweet yam in Jamaica and conduct field trials for fungal disease suppression and crop yield augmentation using nanotechnology.

1. Determine if a mode of application of selected nanoparticles has the potential to control the yam anthracnose causing organism

2. Determine if a mode of application of selected nanoparticles when mixed with Topsin has greater effectiveness in controlling the yam anthracnose pathogen over an 'unmixed' Topsin treatment

3. Examine the response of tissue culture Sweet yam foliage to inactive fungal inoculum in vitro

Sadik, O., Asemota H. Grant T., Miller R., Osonga F., Eshun G., unpublished results
Isolation of fungi from yam samples showing symptoms of infection

Biotechnology Centre, UWI
- Cut bits of leaf and tuber adjacent to diseased regions
- Surface sterilized the bits with 0.5% sodium hypochlorite solution and 70% ethanol then rinse with sterile distilled water
- Sub-cultured in an attempt to produce pure cultures

Plant Pathology Laboratory in the Research and Development Division of MICAF
Procedure similar to that above

Identification of Isolates: Genetic and Morphological Identifications (MICAF)
Sadik, O., Asemota H. Grant T., Miller R., Osonga F., Eshun G., unpublished results

Study Overview

- **Synthesis of three different nanoparticles:**
  - L nano (Lactose PDA nanoparticles)
  - G nano (Galactose PDA nanoparticles)
  - LQ nano (Lactose PDA Quercetin Diphosphate nanoparticles)

- Conduct trial of various nanoparticle treatments along with negative and positive controls

- Collect and analyze field data and biometrics

Sadik, O., Asemota H. Grant T., Miller R., Osonga F., Eshun G., unpublished results
**Pathogen Identification**

The following fungi were identified genetically:

- *Fusarium oxysporum*
- *Fusarium solani*
- *Fusarium verticillioides*
- *Fusarium spp.*
- *Colletotrichum alatae*
- *Xenoacreomoium falcatus*
- *Aspergillus flavus*
- *Colletotrichum gloeosporioides*

Sadik, O., Asemota H. Grant T., Miller R., Osonga F., Eshun G., unpublished results

**Morphological Identification**

The following isolates were identified morphologically:

- *Curvularia* sp.
- *Aspergillus* sp.
- *Cephalosporium* sp.
- *Penicillium* sp.
- *Verticillium* sp.
- *Colletotrichum* sp.
- *Cladosporium* sp.
- *Colletotrichum gloeosporioides*

Sadik, O., Asemota H. Grant T., Miller R., Osonga F., Eshun G., unpublished results
Yield as a Measure of Disease Severity

- At harvest, all the Sweet Yam plants had symptoms of the yam anthracnose disease

- **Yield** used as a measure of the disease severity since weight of tubers is expected to be inversely proportionate to the level of infection.

Mean Tuber Weights for Controls and Batches of Plants Treated with Unmixed Nanoparticles

<table>
<thead>
<tr>
<th>Treatments</th>
<th>Weight of Tubers/lbs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Negative Control</td>
<td>4.00</td>
</tr>
<tr>
<td>Topsin</td>
<td>6.00</td>
</tr>
<tr>
<td>G nano 10</td>
<td>8.00</td>
</tr>
<tr>
<td>G nano 20</td>
<td>10.00</td>
</tr>
<tr>
<td>G nano 30</td>
<td>10.00</td>
</tr>
<tr>
<td>G nano 30</td>
<td>10.00</td>
</tr>
<tr>
<td>LQ nano 10</td>
<td>8.00</td>
</tr>
<tr>
<td>LQ nano 20</td>
<td>6.00</td>
</tr>
<tr>
<td>LQ nano 30</td>
<td>4.00</td>
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<tr>
<td>L nano 10</td>
<td>2.00</td>
</tr>
<tr>
<td>L nano 20</td>
<td>2.00</td>
</tr>
<tr>
<td>L nano 30</td>
<td>2.00</td>
</tr>
</tbody>
</table>

Sadik, O., Asemota H. Grant T., Miller R., Osonga F., Eshun G., unpublished results
Mean Tuber Weights for Controls and Batches of Plants Treated with Topsin mixed with Nanoparticles

Sadik, O., Asemota H. Grant T., Miller R., Osonga F., Eshun G., unpublished results

The Fertilizer Effect of Nanoparticles

**Nanoparticles without compound Q:** Plant growth is inversely proportional to concentration. Possibly the nanoparticles caused growth to be concentrated in tubers since yield was directly proportionately-attributed to a fertilizer effect.

**L-nano Topsin with compound Q:** caused great foliage growth but relatively low storage of tubers possibly because the nanoparticles where nullified and did not have a fertilizer effect.

**Control:** Plants are considerably long, possibly due to hypersensitivity response.

Sadik, O., Asemota H. Grant T., Miller R., Osonga F., Eshun G., unpublished results
Nanotechnology vs. Topsin Fungicides

• Since all the plants had a significant amount of necrosis at harvest it is presumed that the Sweet yam plants have a mutualistic relationship with *Colletotrichum gloeosporioides* and the fungus is widespread.

Topsin only treated plants produced a relatively good yield because Topsin kills viruses affecting the plants and when this happens the plants are able to flourish because the viruses are the main hindrance to the plant’s development.

Sadik, O., Asemota H. Grant T., Miller R., Osonga F., Eshun G., unpublished results

Nanotechnology - A Fertilizer Effect

• The nanoparticles only treated plants may have grown prolifically because the nanoparticles have a fertilizer effect. When the plants are well nourished they are possibly able to suppress the effect of the virus.

For the plants treated with nanoparticles and Topsin the nanoparticles, the effect of both substances are nullified so the plant suffers from the full impact of the virus. Therefore, the nanoparticles used may be having a primary fertilizer effect based on this field analysis.

Sadik, O., Asemota H. Grant T., Miller R., Osonga F., Eshun G., unpublished results
Overall Finding

- Field studies demonstrate the prospects of sustainable nanotechnology as a tool to address the devastating effect of the Yam Anthracnose Disease on the Sweet Yam crop.

Sadik, O., Asemota H. Grant T., Miller R., Osonga F., Eshun G., unpublished results

Summary and Conclusions

- Chemistry is helping to achieve zero hunger through sustainable precision nanosensors and nanofertilizers
- Chemistry tools are helping to achieve food security and improved nutrition, and promote sustainable agriculture
- Greener nanosynthesis is enabling the development of sustainable insecticides and pesticides, plant growth regulators, fertilizers and animal growth supplements
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• Asemota (UWI)
• Biotech Center
• RADA
• Tamara Grant (UWI)
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