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Questions
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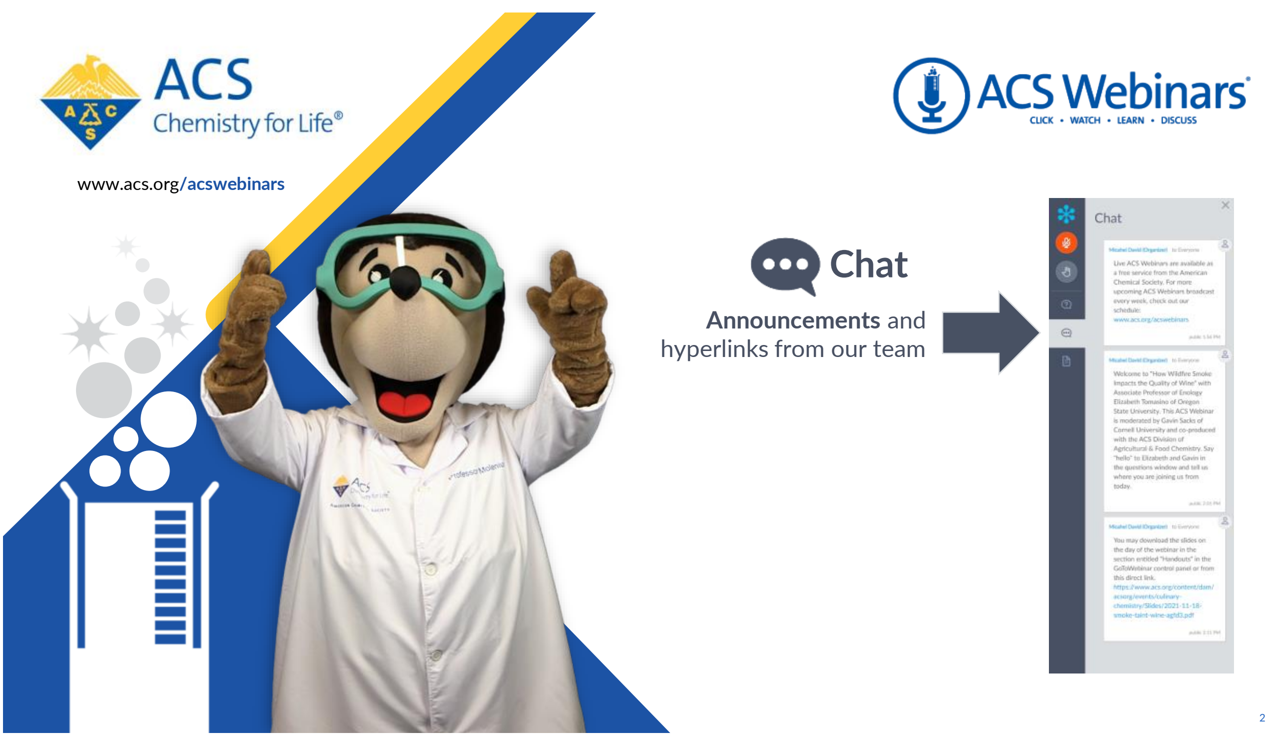
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Where is the Webinar Recording?

24h

www.acs.org/acswebinars

All Registrants

Watch the unedited recording linked in the **Thank You Email for 24 hours.**

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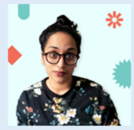
Looking for a new science podcast to listen to?

Check out Tiny Matters, from the American Chemical Society.

Sam Jones, PhD
Science Writer & Exec Producer



Deboki Chakravarti, PhD
Science Writer & Co-Host

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ACS Industry Member Programs

- **ACS Industry Matters**

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Preview Content: **acs.org/indnl**

- **ACS Innovation Hub LinkedIn Group**

Connect, collaborate and stay informed about the trends leading chemical innovation.

Join: **bit.ly/ACSinnovationhub**

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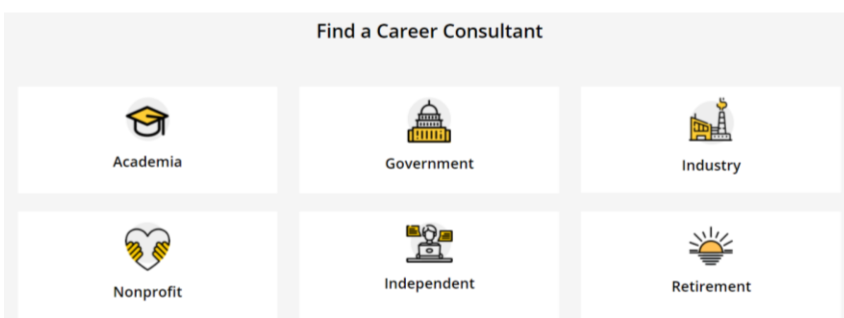
A Career Planning Tool For Chemical Scientists

ChemIDP is an Individual Development Plan designed specifically for graduate students and postdoctoral scholars in the chemical sciences. Through immersive, self-paced activities, users explore potential careers, determine specific skills needed for success, and develop plans to achieve professional goals. **ChemIDP** tracks user progress and input, providing tips and strategies to complete goals and guide career exploration.

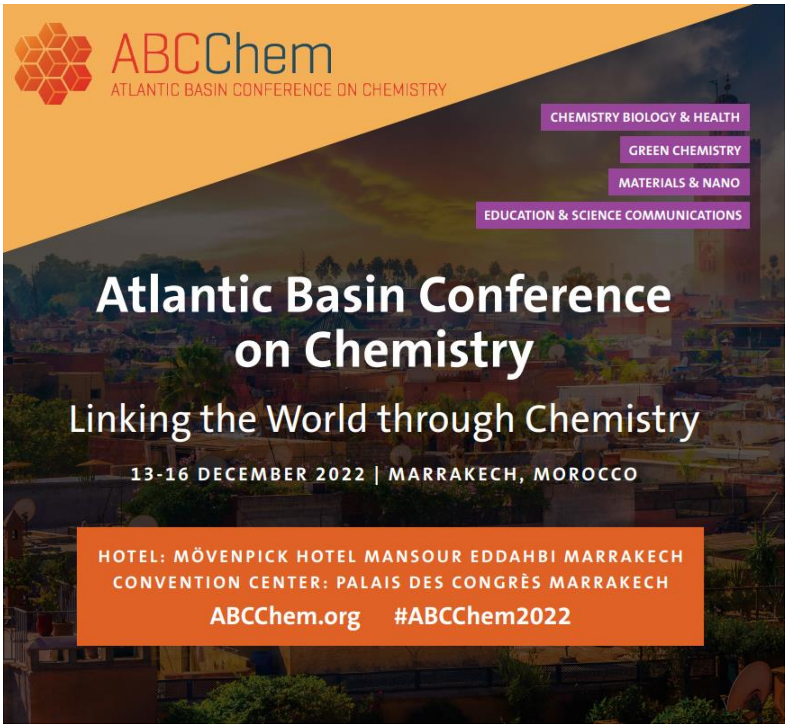
https://chemidp.acs.org

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.
- Browse our Career Consultant roster and request your one-on-one appointment today!

www.acs.org/careerconsulting



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ACS Career Resources

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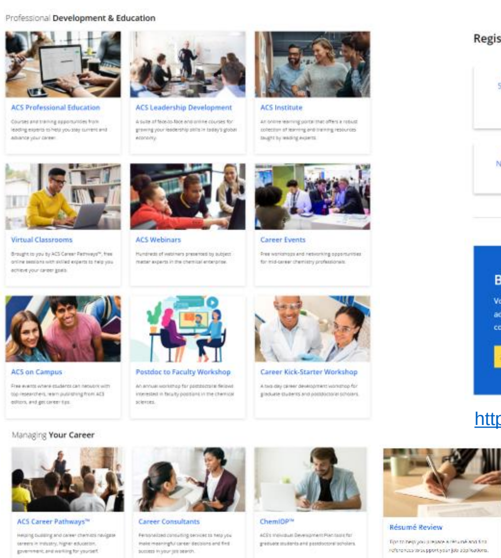
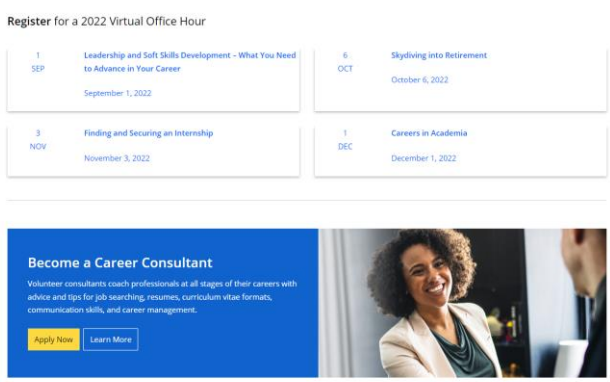


https://www.acs.org/content/acs/en/careers/developing-growing-in-your-career.html



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

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If you are a student from a group underrepresented in the chemical sciences, we want to empower you to get your graduate degree!

The ACS Bridge Program offers:

- A FREE common application that will highlight your achievements to participating Bridge Departments
- Resources to help write competitive grad school applications and connect you with mentors, students, and industry partners!

Learn more and apply at www.acs.org/bridge

Email us at bridge@acs.org

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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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TWENTY-SEVENTH ANNUAL

GREEN CHEMISTRY & ENGINEERING CONFERENCE

June 13-15, 2023 | Long Beach, CA

Closing the Loop: Chemistry For a Sustainable Future

Call for Abstracts

Will Open January 2023

gcande.org

ACS Green Chemistry Institute
Chemistry for Life

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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 at the workplace

ACS Publications DEIR Hub
See what ACS Publications is doing for fostering inclusivity in scholarly publishing

ACS Volunteer and ACS Meetings Code of Conduct
Fostering 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 videos, articles, books, podcasts, and more on diversity, inclusion, and related topics.

Quick Guide: Inclusion Moments
Learn more about what Inclusion Moments are and see ideas 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

**Adapted from definitions from the Ford Foundation Center for Social Justice:

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

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

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

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

https://www.acs.org/content/acs/en/about/diversity.html

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ACS Local Section Maryland

CHEMICAL BIOCHEMICAL AND ENVIRONMENTAL ENGINEERING
UMBC

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 Ph.D. in Chemistry at Stonybrook University)

Dr. Utsav Shashvatt **postdoctoral research associate, UC Berkeley** (Completed his Ph.D. in environmental engineering at UMBC – 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

Register Now! https://morganstate.zoom.us/webinar/register/WN_qjp23X-HSey30c99cTPe9w

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Mon., Nov. 21, 2022 | 2:00pm–3:00pm ET

Shear Thickening Fluids
(Rebroadcast)

Co-produced with ACS Industry Member Programs and ACS Division of Polymer Chemistry

Wed., Nov. 23, 2022 | 2:00pm–3:00pm ET

Espresso Chemistry
(Rebroadcast)

Co-produced with the ACS Division of Agricultural Food and Chemistry

Thurs., Dec. 1, 2022 | 2:00pm–3:00pm ET

The Search for the Worst Science Stock Photo!

Co-produced with ACS Productions

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WILL BEGIN SHORTLY…
Say hello in the
questions window!
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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 Institutes 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.
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FRONTIER FRIDAYS Initiated by ***2021 ACS President H.N. Cheng & ACS Committee on Science***

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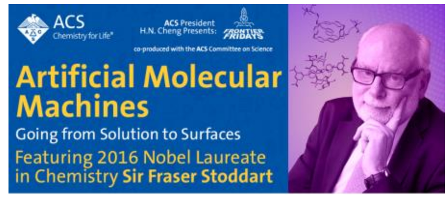
Zhenan Bao K.K. Lee Professor of Chemical Engineering & Chair, Dept of Chemical Engineering, Stanford University
https://www.acs.org/content/acs/en/acs-webinars/library/organic-electronics.html



Sir Fraser Stoddart 2016 Nobel Laureate in Chemistry, Board of Trustees Professor of Chemistry, Northwestern University
https://www.acs.org/content/acs/en/acs-webinars/library/molecular-machine.html

Amy Lucía Prieto Professor, Department of Chemistry, Colorado State University & Founder, Prieto Battery, Inc.
https://www.acs.org/content/acs/en/acs-webinars/library/lithium-ion-sustainability.html

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-webinars/library/sustainable-chemistry-work.html

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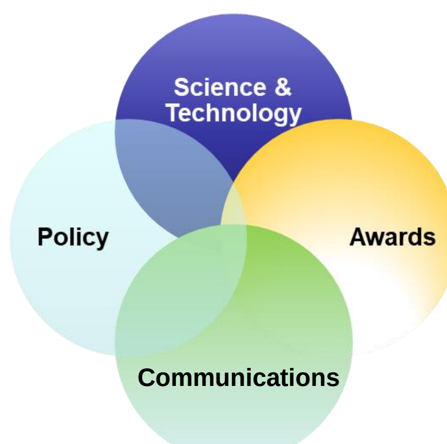
ACS Committee on Science (COMSCI)

ACS Chemistry for Life®

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

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Chemistry & the SDGs

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

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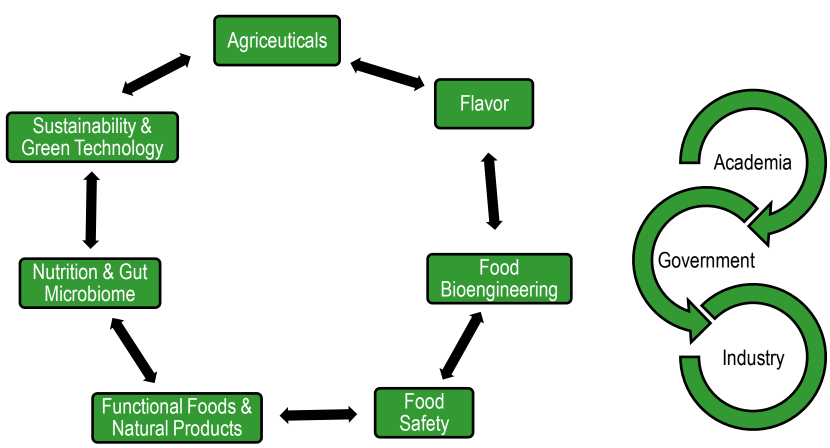
ACS Technical Division
Agricultural & Food Chemistry (AGFD)

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

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Free Virtual Event See acs.org/ZeroHungerSummit

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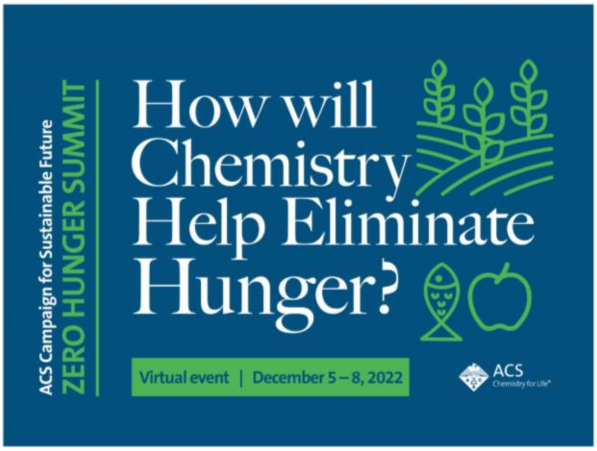

- The U.N. Sustainable Development Goal of “Zero Hunger” aims to end hunger and achieve food security by 2030
- There is an intense need for more and better food: over 690 million people are without enough to eat, and world population is growing
- Chemists and engineers have a vital role to play in the fight against world hunger

https://www.acs.org/content/acs/en/sustainability/zero-hunger-summit.html

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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 Institutes of Technology

H.N. CHENG, PhD

Past President, American Chemical Society

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Chemistry Tools to Help Achieve Zero World Hunger

Michael Appell

USDA, Agricultural Research Service

National Center for Agricultural Utilization Research

Peoria, IL USA

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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 ass 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**

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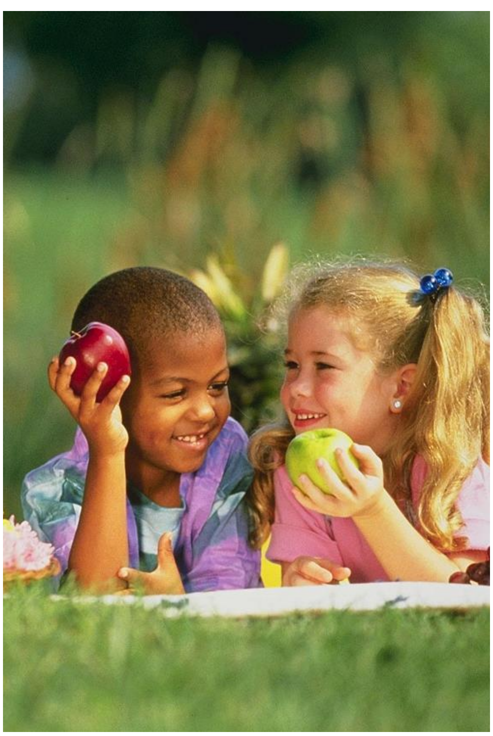

Sustainable Food Security and Production

- **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**

http://www.worldbank.org/en/topic/foodsecurity
https://www.un.org/en/chronicle/article/feeding-world-sustainably
https://ourworldindata.org/obesity#what-share-of-adults-are-obese
https://www.ers.usda.gov/topics/food-choices-health/obesity/

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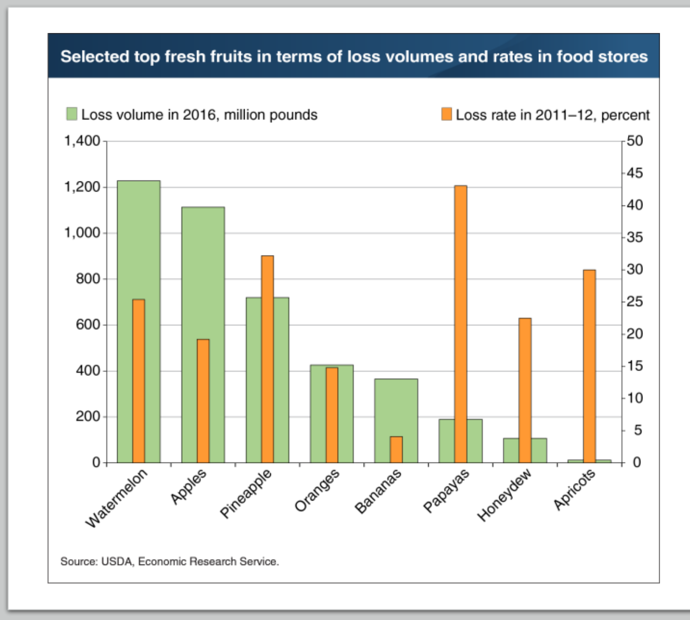
Waste Food and Sustainable Agricultural Commodity Recycling

- **"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)



http://www.ers.usda.gov/publications/eib-economic-information-bulletin/eib121.aspx

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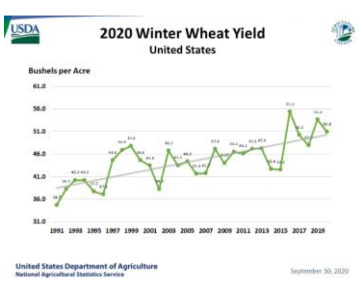

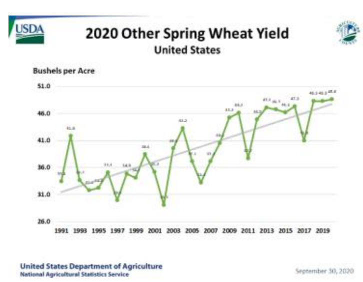

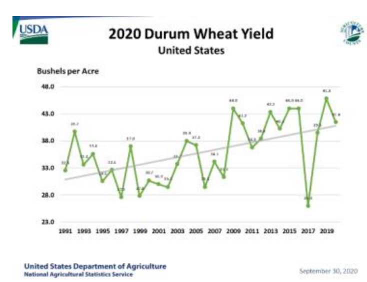

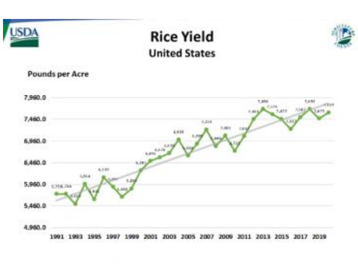

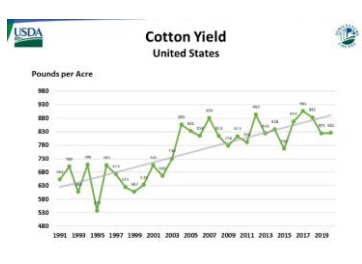

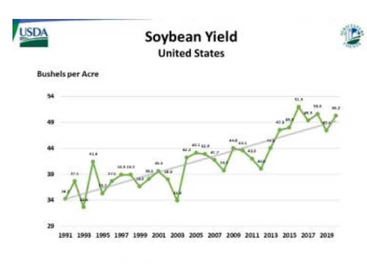

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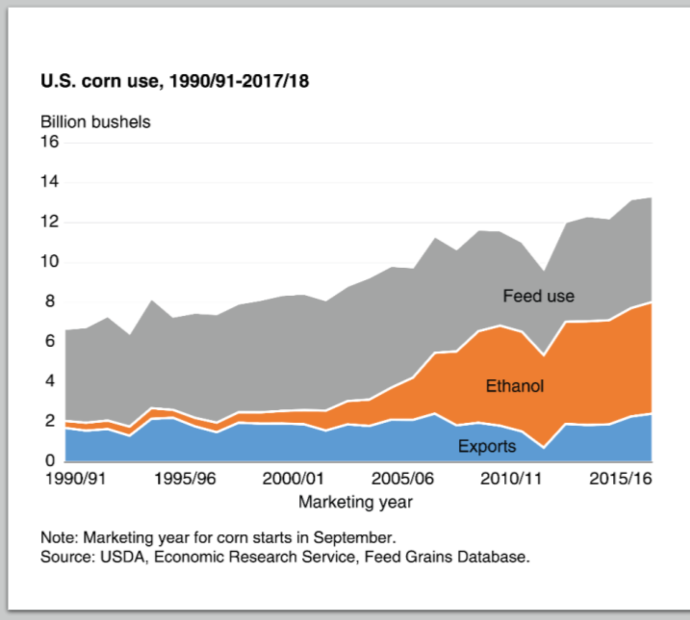
Significant increase in corn yields through technology

- **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**



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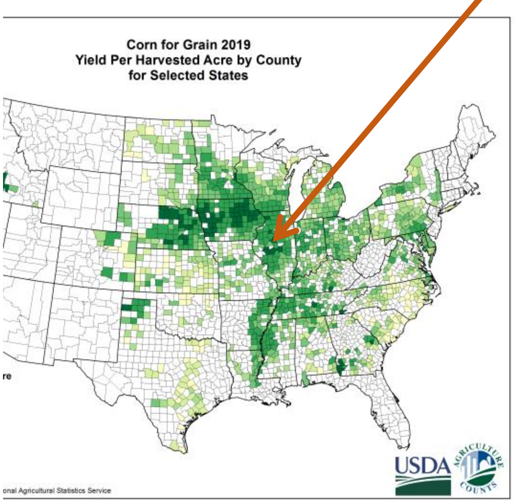
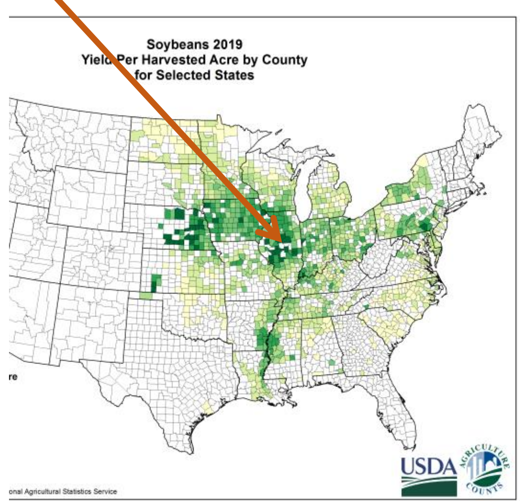
USDA

The NCAUR is at the center of high yield corn and soybean production





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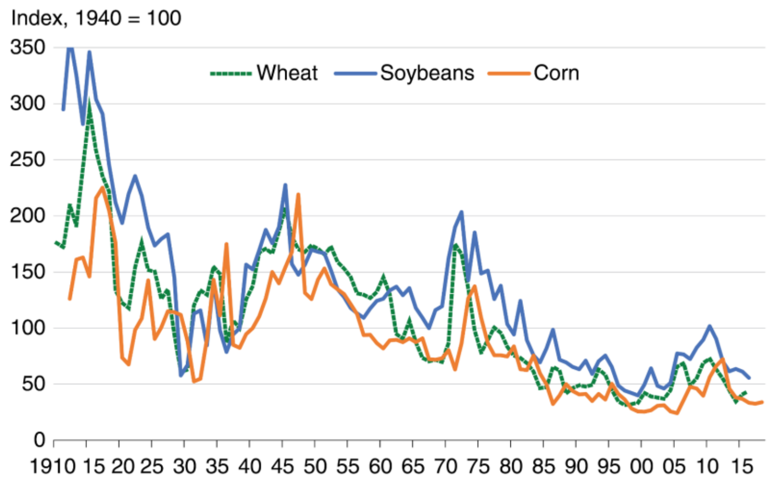
Inflation-adjusted corn, wheat, and soybean prices, 1912-2018



Source: USDA, Economic Research Service calculations using data from USDA, National Agricultural Statistics Service and U.S. Department of Labor, Bureau of Labor Statistics.

USDA

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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

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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

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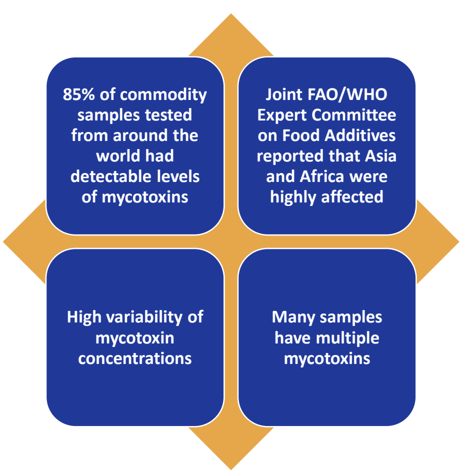
Analyzing Risks of Mycotoxins



https://www.pigprogress.net/specials/whats-the-truth-behind-the-faos-25/
Eskola M, Kos G, Elliott CT, Hajšlová J, Mayar S, Krska R. Worldwide contamination of food-crops with mycotoxins: Validity of the widely cited 'FAO estimate' of 25. Crit Rev Food Sci Nutr. 2020;60(16):2773-2789.

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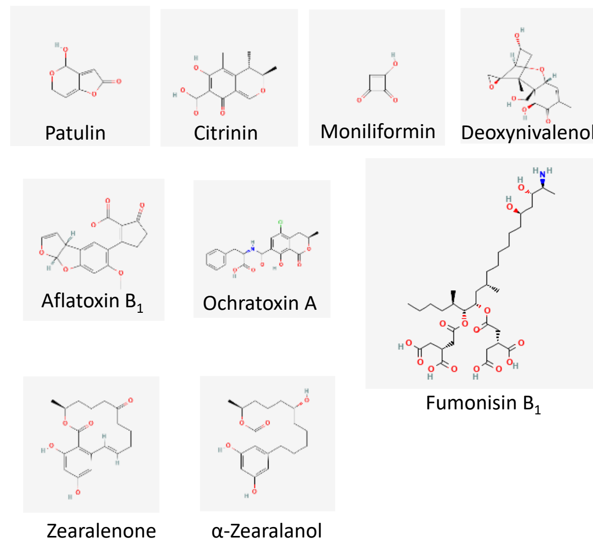
Mycotoxins

- **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



https://pubchem.ncbi.nlm.nih.gov/

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Mycotoxin Exposure

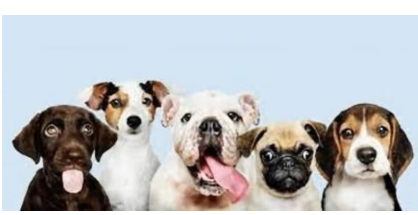
100,000 turkeys died from aflatoxin exposure in 1962

- 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.



Centers for Disease Control and Prevention. Outbreaks of gastrointestinal illness of unknown etiology associated with eating burritos. In: Morbidity and Mortality Weekly Report. U.S. Centers for Disease Control and Prevention, 1999, 48(10):210-3.

https://www.akc.org/expert-advice/news/fda-recalls-dog-food-fatal-aflatoxin-levels-70-dogs-die/

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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

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Audience Survey Question

ANSWER THE QUESTION ON THE INTERACTIVE SCREEN IN ONE MOMENT

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!**

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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
  - Nanosponge materials
  - Biomimetic technology

Design, Create, and Applications

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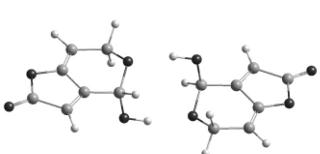
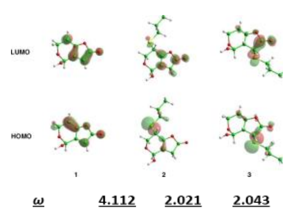
Quantum chemistry and cheminformatics

Quantum Chemical – energetic preferences, toxicological potential, spectroscopic properties

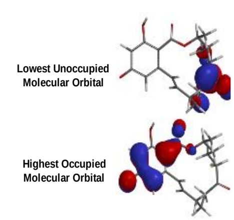
Unusual Properties of Natural Products



Computational Toxicology using DFT



TD-DFT Properties



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

Activity	Eq.	Equation	R^2	Q^2	R^2_{adj}	sPRESS	n	s	F	p
cytotoxicity NIH3T3	X1	$pIC_{50} = 0.6764 (E_{LUMO}) + 0.2482(logP) + 8.1073$	0.517	0.273	0.443	0.815	16	1.001	6.95	0.0088
	X2	$pIC_{50} = 0.7792 (\Delta\varepsilon) + 0.1640(logP) + 2.5737$	0.540	0.304	0.470	0.979	16	0.795	7.64	0.0064
	X3	$pIC_{50} = 1.4711(MTOci3) – 1.5989(\chi) + 0.1886 X(logP) + 6.9024$	0.783	0.616	0.728	0.757	16	0.569	14.39	0.0003
	X4	$pIC_{50} = 1.5080(MTOci3) – 1.7740(\chi) + 7.3779$	0.773	0.663	0.738	0.681	16	0.559	22.12	0.0001

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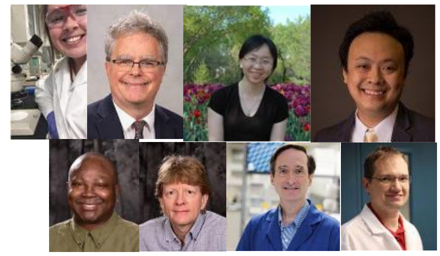
Antifungals

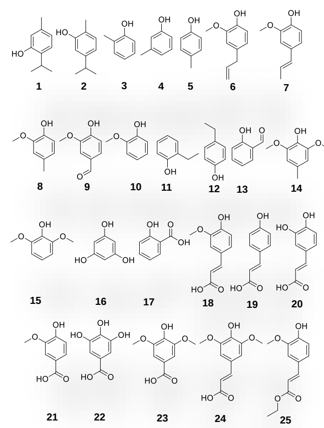


- Some potent mycotoxins are regulated, and these toxins are generally associated with *Fusarium, Aspergillus*, and *Penicillium* species

- 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

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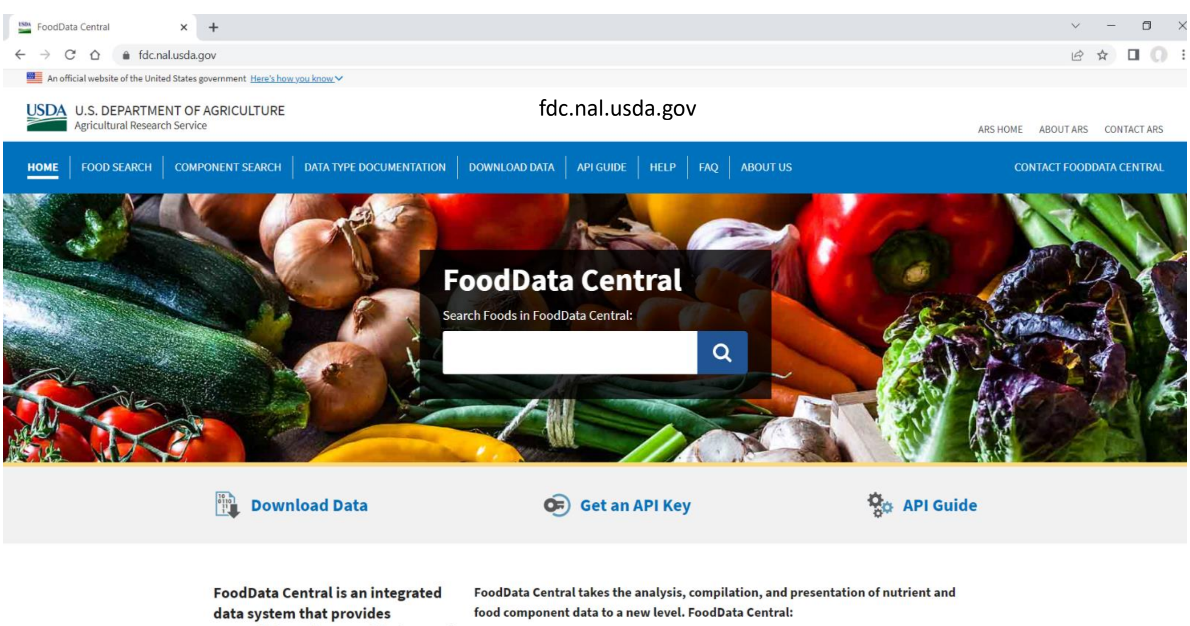

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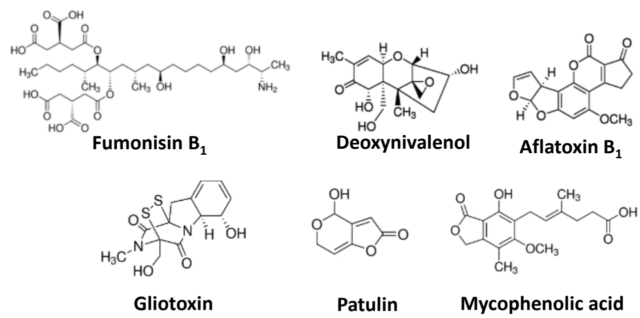
Phenolic compounds as antifungals

MIC_{50} of six fungi
- *Fusarium verticillioides* - fumonisin, deoxynivalenol
- *Fusarium oxysporum,* fruit rot
- *Aspergillus flavus* – aflatoxins
- *Aspergillus fumigatus* - gliotoxin
- *Penicillium expansum* – patulin
- *Penicillium brevicompactum* - mycophenolic acid

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



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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

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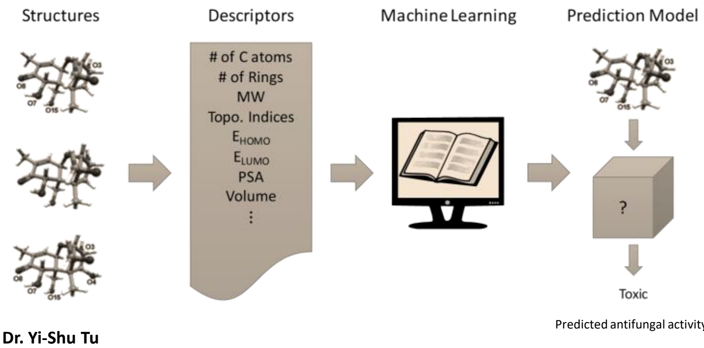

Dr. Yi-Shu Tu

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

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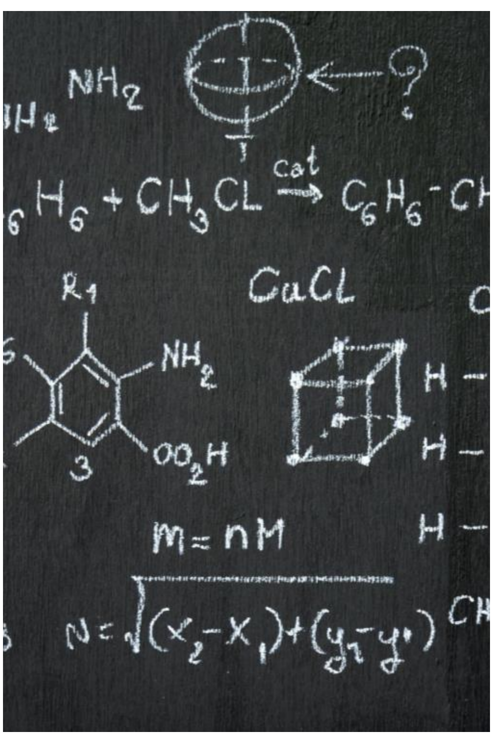

Quantum Chemistry: Electrophilicity Index

- Theorem of Koopman
- Electrophilicity index, ω, 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

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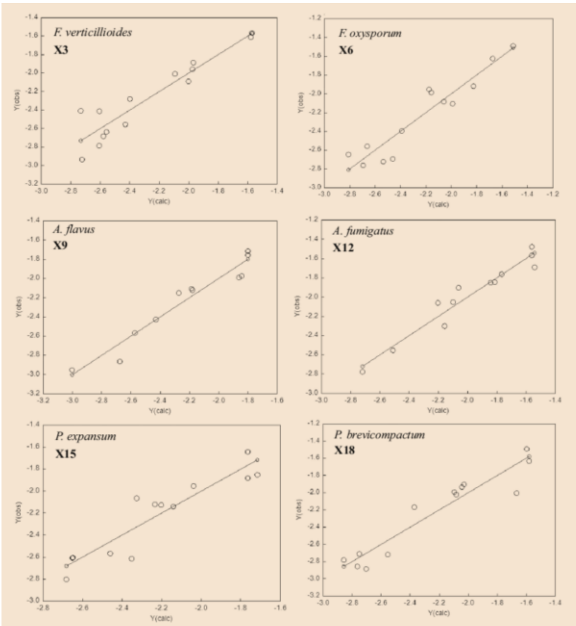
Plots of predicted vs observed antifungal activities of phenolic compounds



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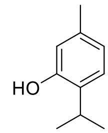

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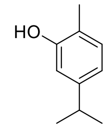

- Thymol, **1**, and carvacrol, **2**, are antioxidant components of essential oils from several popular plants, including the widely used herb thyme.
- Thymol and carvacrol have historically been used as food preservatives against spoilage and as insecticides.
- It has been proposed that the antifungal properties of thymol are associated with inhibitory effects on hyphae formation of fungi, and the lack of viability of the resulting fungal aggregates.

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- **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?

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Zearalenone and Biochar

- Burning or decomposing biomass releases 99% of the carbon as CO_2
- 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

Biochar sample	C (%)	H (%)	N (%)	O (%)	Ash (%)	Total surface area (m^2/g)	Micropore surface area (m^2/g)
CSB	45.14	1.86	0.44	12.96	39.60	74	14
SB	43.65	3.71	0.78	24.99	26.87	46	23

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

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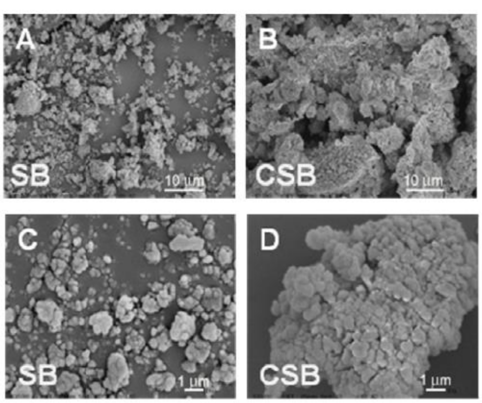
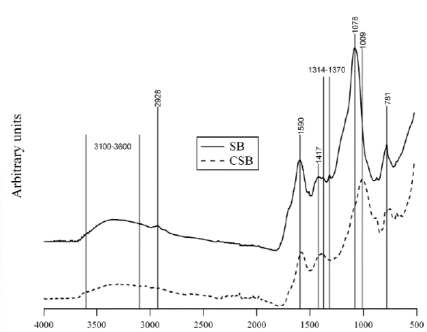
Biochar: Unique Physical Properties



SEM Switchgrass vs. Corn Stover



FTIR Switchgrass vs. Corn Stover

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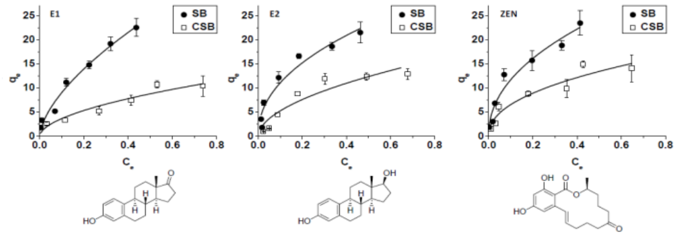
Biochar Summary



Estrone Estradiol Zearalenone

- 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

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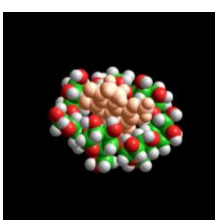
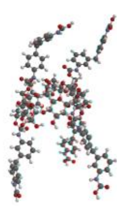
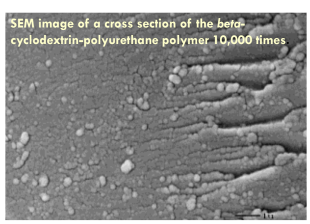
Nanosponge Materials for Patulin & Ochratoxin A







- **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

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- **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

Nanotechnology

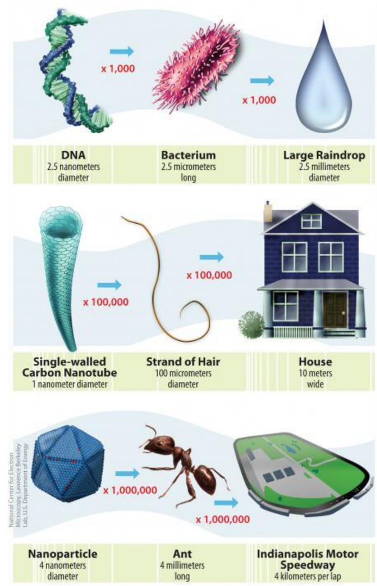
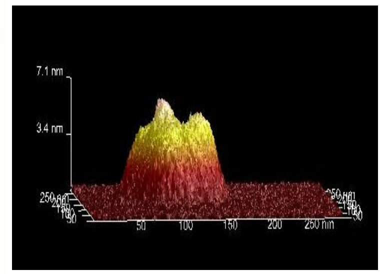


Illustration from nano.gov

Atomic Force Microscopy



Experiments by Dr. Kervin Evans (USDA-ARS)

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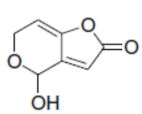
Patulin



- **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 $\mu g/L$ for certain apple-based products**

- **A validated 10 $\mu g/L$ method exists that is very labor intensive**

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

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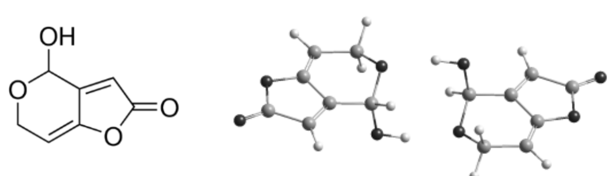
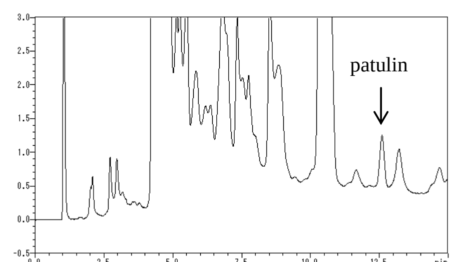
Researchers at Shinshu University in Japan used these materials to develop a rapid and very sensitive method to detect the mycotoxin patulin in apple juice





Patulin concentration (ng mL^{-1})	Patulin recovery (%)	RSD (%)
5	Cannot be calculated (Tr., Tr., 170)	69*
10	78	16
20	71	9.4
50	78	14
80	71	5.0
100	67	2.0

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

The nanospongebased method has quantitative range that covers the 50 μg/kg patulin regulated limits

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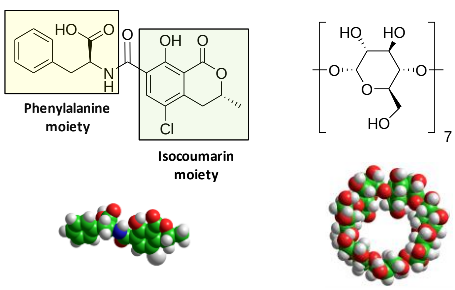
Ochratoxin A in Wine and Grape Juice

- **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

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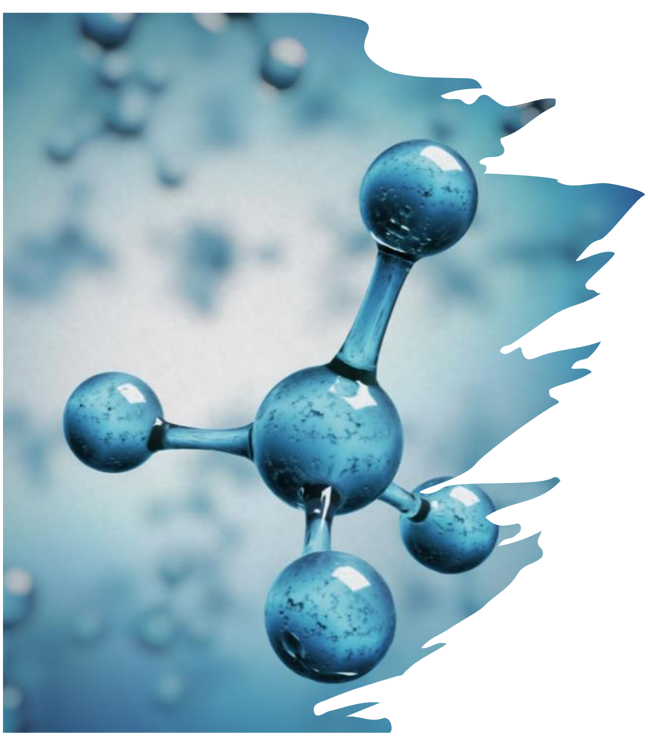

Key Points

- 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

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- **Vision:** Enhance quality of life by advocating safe, nutritious and sustainable food and agricultural supplies that meet global challenges.
  - **Join -> agfoodchem.org**

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Chemistry Tools to Help Achieve Zero World Hunger

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

BIOSMART
New Jersey Institute of Technology

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

Audience Survey Question

ANSWER THE QUESTION ON THE INTERACTIVE SCREEN IN ONE MOMENT

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!**

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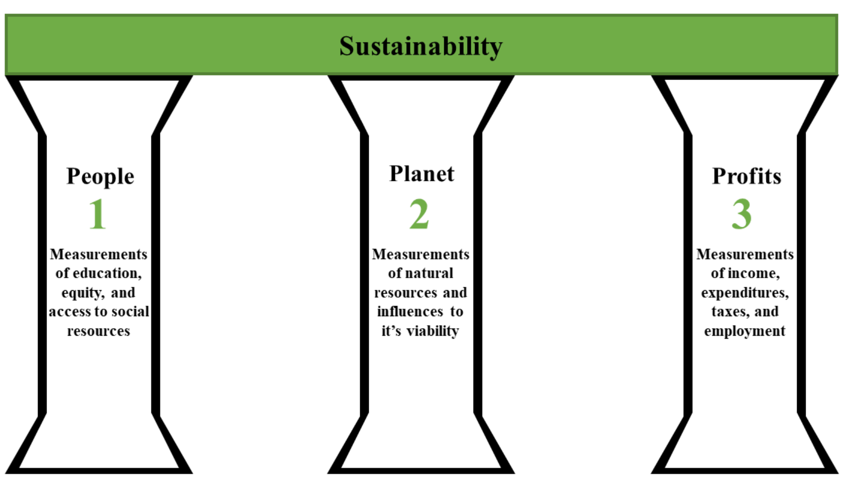
Pillars of Sustainability



Roland M. Miller, Francis J. Osonga, & Omowunmi 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

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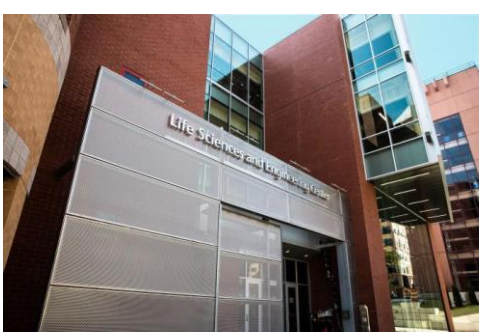
Sustainable Nanotechnology

Sadik, Demokritou, Karn, Nature Nano

SNO
Sustainable Nanotechnology Organization
Research | Education | Responsibility
www.susnano.org

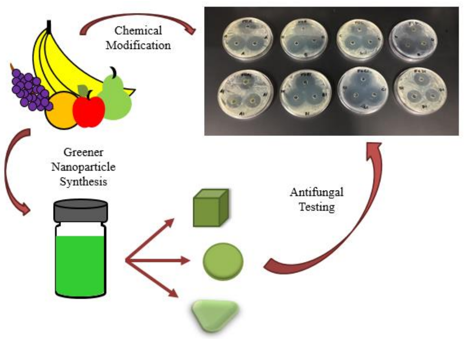
The BioSMART Center at NJIT

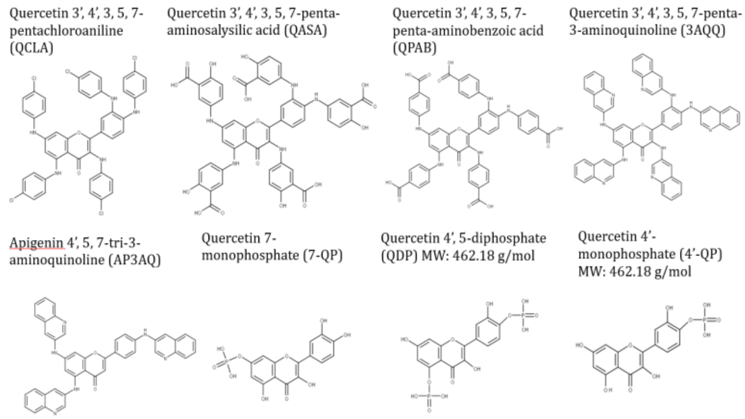


Biosensor Materials for Advanced Research & Technology

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

Sustainable Nanosynthesis





Francis J. Osonga, *Sanjay Kalra, Roland M. Miller, Daniel Isika and Omowunmi A. Sadik, Synthesis, characterization and antifungal activities of eco-friendly palladium nanoparticles, ***RSC Adv.***, 2020, **10**, 5894-5904.

Sadik et. al., Tetrahedron Letters 58 (**2017**) 1474–1479).

Greener One-Pot Nanosynthesis using Glycoconjugates

Figure 2. Digital images of some of the synthesized AuNP-GCs using different sugar ligand concentrations. From left to right: (1) L3AP, (2) G3AP (30 mg/mL), (3) LPSA/M5AS mixture, (4) G3AP (6 mg/mL), (5) L5AS (1 mg/mL), (6) L5AS (0.2 mg/mL), (7) LSA (3 mg/mL), (8) LPSA/M5AS mixture (0.3 mg/mL), (9) M5AS (1 mg/mL), (10) M5AS (2 mg/mL), (11) LPDA, (12) LpAB (0.3 mg/mL), (13) M5AS (0.5 mg/mL), (14) L5AS (1 mg/mL), (15) GAEA (0.1 mg/mL), (16) G3AP (3 mg/mL), and (17) LAEA. If not specified otherwise, the Au^{3+} concentration was 0.1 mg/mL while the sugar ligand concentrations were 10 mg/mL.

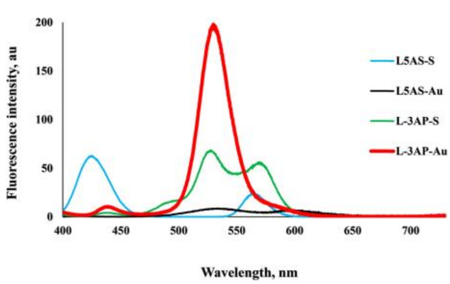


Figure 10. Synchronous fluorescence of selected sugar ligands and corresponding AuNP-GCs. S refers to sugar ligands alone, while Au refers to the gold nanoparticle. $\Delta\lambda_{Ex-Em}$ was 10 nm.

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

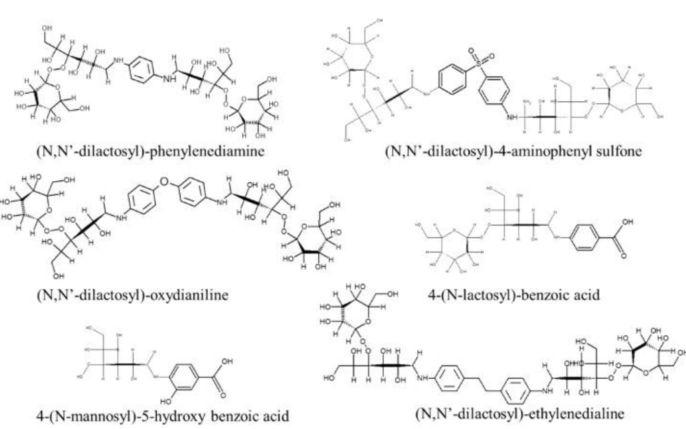
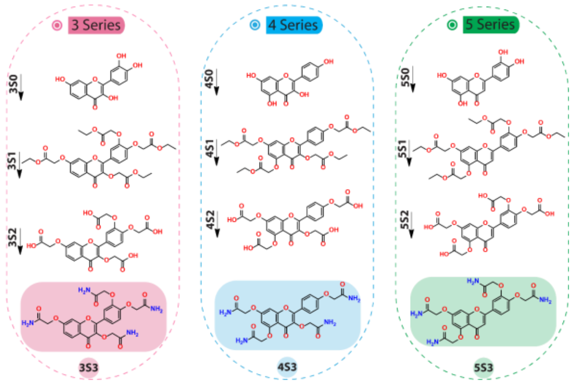


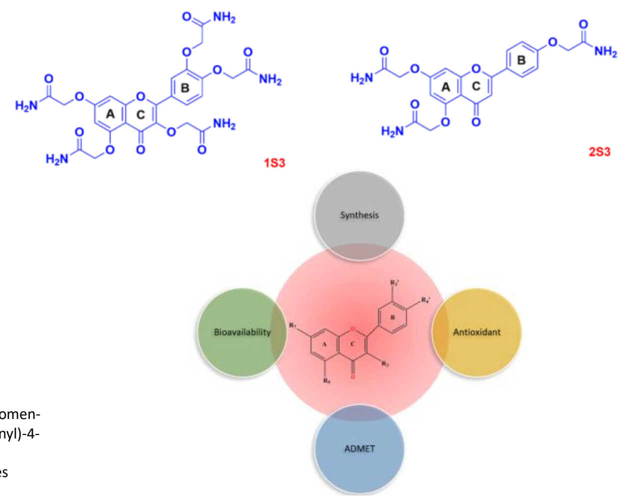
Figure 6. Sugar ligands that resulted in the formation of stable AuNP-GCs.

Flavonoids Acetamides

Daniel K. Isika, Fatma Nur Ozk¨omeç, Mustafa Çesme and Omowunmi A. Sadik, derivatives, **RSC Advance,2022, DOI: 10.1039/d2ra01375d.**



Scheme 1: Steps in the synthesis of 2,2'-((4-(3,7-bis(2-amino-2-oxoethoxy)-4-oxo-4H-chromen-2-yl)-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(oxy))triacetamide (4S3) and 2,2'-((4-(5,7-bis(2-amino-2-oxoethoxy)-4-oxo-4H-chromen-2-yl)-1,2-phenylene)bis(oxy))diacetamide (5S3) derivatives



TEM and XRD Characterization

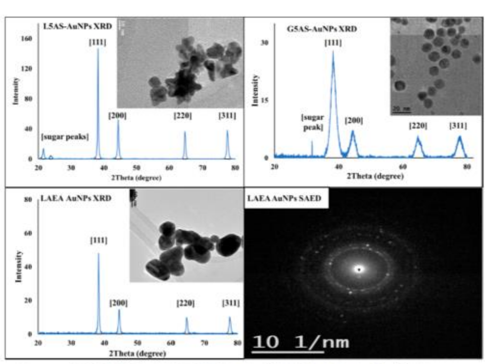
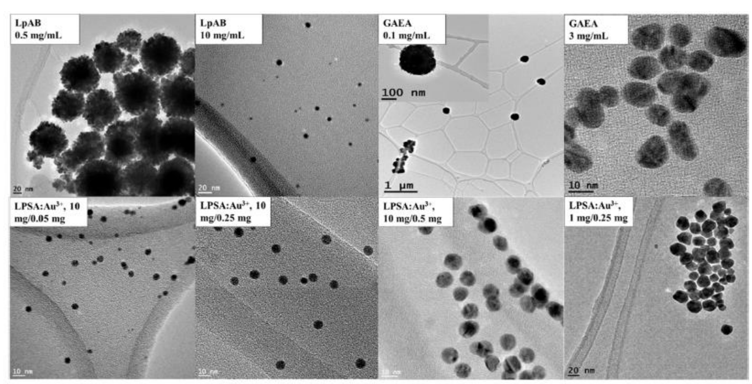
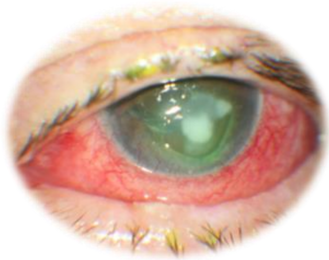


Figure 5. Formation of LSAS-AuNPs (~20 nm), GSAS-AuNPs (~5 nm), and LAEA-AuNPs (~50 nm) confirmed by XRD.



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.



https://eyewiki.aao.org/Fungal_Keratitis

iStock/vidka: Brown rot damages the tomato plants and makes the fruit inedible.

- *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

Brown and Eckert (1988).
Brown (1994).

- *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*

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

Francis J. Osonga, Gaddi Eshun, Sanjay Kalra, Idris Yazgan, Laura Sakhaee, Renata Ontman, Shaojie Jiang, and Omowunmi A. Sadik*

Cite This: *ACS Agric. Sci. Technol.* 2022, 2, 42–56 Read Online

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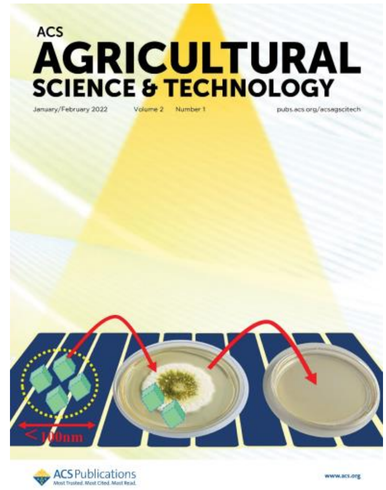
ABSTRACT: Pathogenic microorganisms cause diseases that play a limiting role in food production. The growth of blue mold rot on citrus fruits caused by *Penicillium italicum* poses postharvest economic loss due to food decay. The control of *P. italicum* using toxic synthetic fungicide raises serious concerns about food safety and quality. There is a need to develop safe fungi 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 cetyltrimethylammonium 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 nanospheres (CuNS) and well-defined copper nanocubes (CuNCs) with controlled shape and size using copper(II) sulfate ($CuSO_4$) precursor and water-soluble quercetin diphosphate (QDP) as a bio-reducing 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). CuNCs with average edge lengths of 150–250 and 80–180 nm were designed using QDP and $CuSO_4$ in the ratio of 3:1, respectively. The metrics of sustainability obtained include atom economy (73.56%), molar efficiency (0.9019), and environmental factor (3.429). The antifungal activity of CuNCs and CuNSs was tested against *P. italicum* using the Kirby–Bauer method. This study demonstrated the comparative effect of CuNCs and CuNSs on the growth of *P. italicum* spores in a dose-dependent manner. The results indicated that CuNCs and CuNSs 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 CuNS. The particle size and shape effect of CuNCs played a vital role in its antifungal activity. QDP-mediated synthesis of CuNC and CuNS could serve as a potent biocide for the natural remediation of citrus-based fungal diseases.

KEYWORDS: *sustainability, anisotropy, naturally derived, macromolecules, nanocubes, fungi, antifungal, Penicillium italicum*



ACS Agricultural Science & Technology, 2022, 2, 1, 42-56, https://doi.org/10.1021/acsagscitech.1c00102 , (Featured in Cover Art).

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Audience Survey Question

ANSWER THE QUESTION ON THE INTERACTIVE SCREEN IN ONE MOMENT

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*.

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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.

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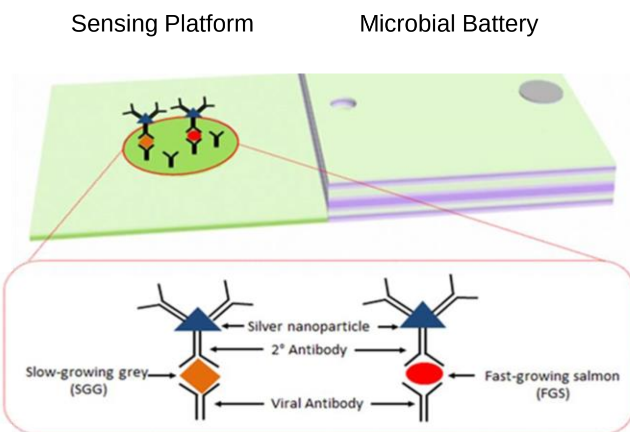
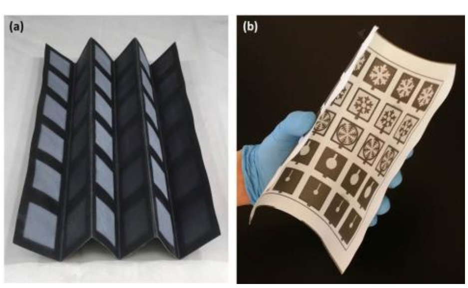
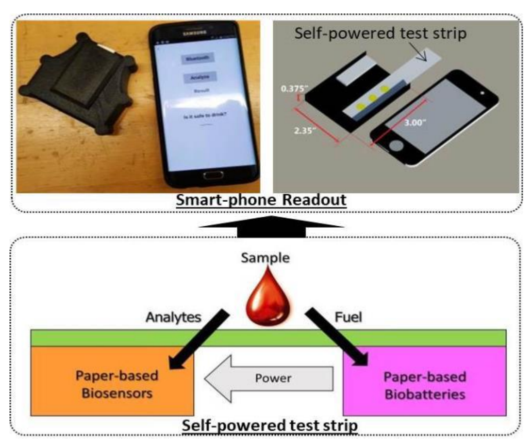
Paper-based Biosensor Concept



Smart Biosensors

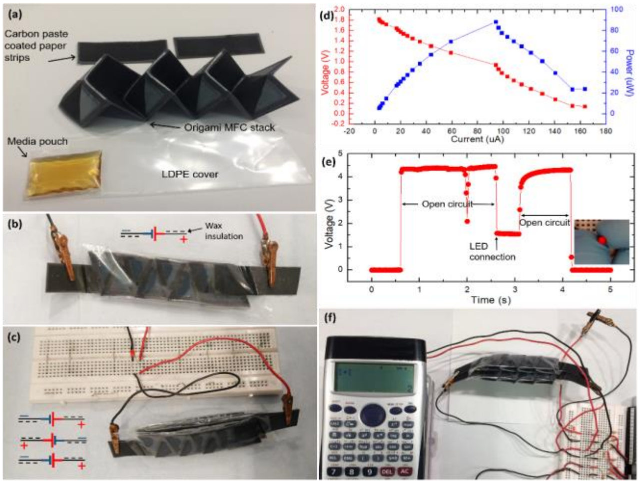


With Professor S. Choi, Binghamton University



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

Biobattery Testing



Mohammadifar, K. Zhang, and S. Choi (2017). A saliva-powered paper biobattery for disposable biodevices. IEEE MEMS 2017 Proceedings. pp.121-124.M. Mohammadifar, J. Zhang, I. Yazgan, V. Kariuki, Omowunmi Sadik, and S. Choi (2016). High performance paper-based microbial fuel cells using nanostructured polymers. IEEE Sensors 2016 Proceedings. pp.1727-1729

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**
  - *Collectotrichum gloeosporioides*

Impact of Yam Anthracnose in Jamaica

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

YEAR	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014
PRODUCTION (TONNES)	6313	6275	5185	3765	4411	3907	3291	2609	1805	1768

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

	Sample 1	Sample 2	Average
Weight of tubers	13.0g	33.0g	23.0g

Sampling Location: Mr. Kirkland Farm, Grove place

	Sample 1	Sample 2	Average
Weight of tubers	322.0g	192.6	257.3g

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

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*

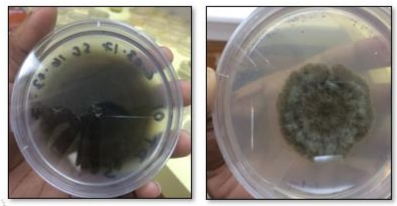
-*Fusarium spp.*

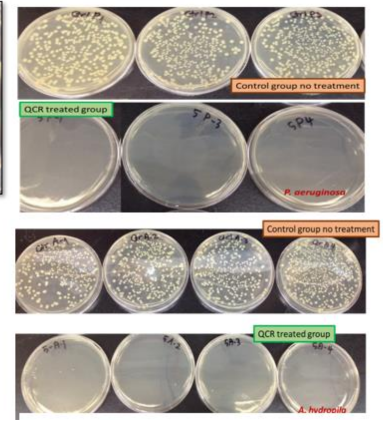
-*Colletotrichum alatae*

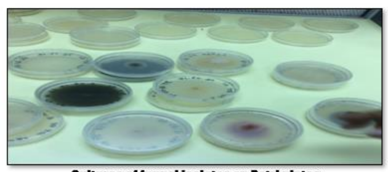
-*Xenoacremoium falcatus*

-*Aspergillus flavus*

-***Colletotrichum gloeosporioides***







Cultures of fungal isolates on Petri plates containing potato dextrose agar (Asemota

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***

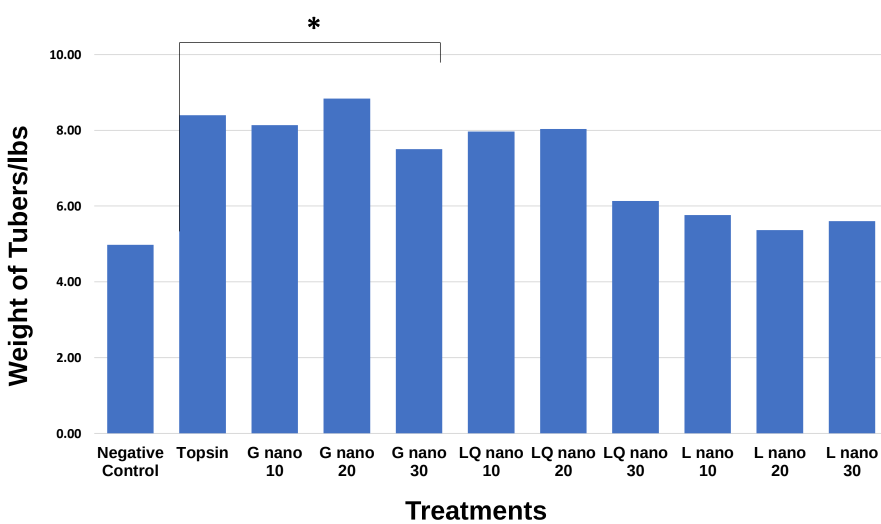
Sadik, O., Asemota H. Grant T., Miller R., Osonga F., Eshun G., unpublished results

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.

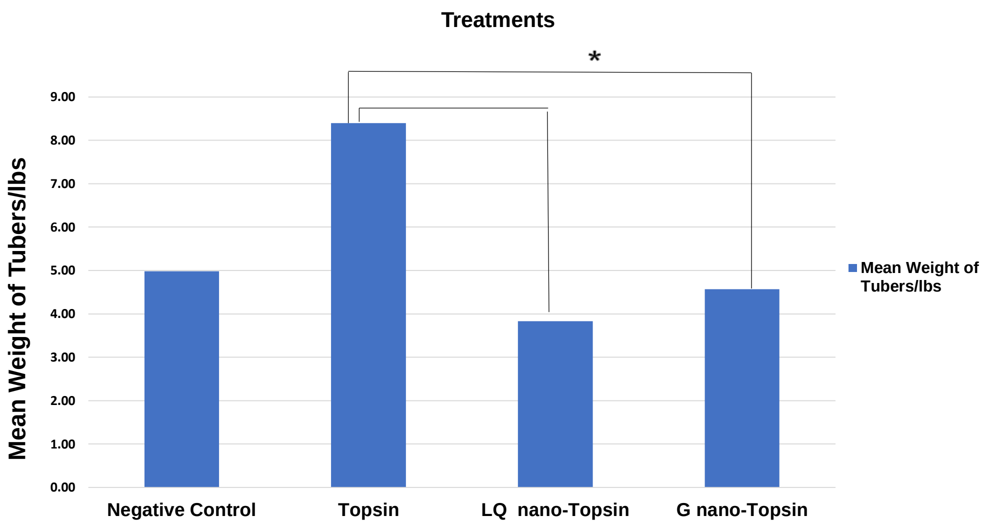
Sadik, O., Asemota H. Grant T., Miller R., Osonga F., Eshun G., unpublished results

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



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 gloeosporiodes* 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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- Biotech Center
- RADA
- Tamara Grant (UWI)

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NJIT New Jersey Institute of Technology

BIOSMART New Jersey Institute of Technology

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