

ANALYTICAL RESOURCES CORE

COLORADO STATE UNIVERSITY

ARC MONTHLY BULLETIN JANUARY 2024 SHAPPY NEW YEAR! S

Welcome to the ARC Bulletin, a monthly newsletter to keep you informed about the latest happenings in the ARC. Here you will find information about our team, job opportunities, equipment and facilities, upcoming seminars, and other exciting news!

RESEARCH SPOTLIGHT

For this month's research spotlight, we interviewed Dr. Shiva Kumar Angala and Dr. Zuzana Palcekova about their recent publication in Nature Communications on mycobacteria glycerolipid synthesis pathways (https://www.nature.com/articles/s41467-023-42478-x). Both are Research Scientists and members of the Jackson Research Group within the Department of Microbiology, Immunology, and Pathology at CSU. The Jackson group studies cell wall biosynthesis of the human pathogen Mycobacterium tuberculosis, which causes the disease tuberculosis.



UPLC-QTOF mass spectrometry measurements in the ARC confirmed that PIsM is the sole acyltransferase capable of transferring C16:0 onto position sn-2 of G3P in Mycobacterium smegmatis, as the enzymatic products of glycerolipid were found to be separated between sn-1 and sn-2"



What is the best point-to-point resolution that can be obtained on our JEOL JEM-2100F Transmission Electron Microscope?

ARC TRIVIA

HTTPS://WWW.RESEARCH.COLOSTATE.EDU/ARC/

We look forward to featuring more of our users' research. Want to have your research in the spotlight? Be sure to cite our RRID (SCR_021758) so that we can find you!

For this particular publication, Shiva, Zuzana, and colleagues were able to identify the enzymes responsible for the unique glycerolipid synthesis pathways in mycobacterial cell walls, which may have consequences for the physiology of mycobacteria, including the fluidity, permeability, and various other functions of their cell envelope.

"Glycerophospholipids are a class of lipids containing *sn*-glycerol-3-phosphate (G3P) backbone to which one or two long-chain hydrocarbons (fatty acids) are attached to the hydroxyl groups via carboxylic acid ester linkages. Phospholipids are the primary building blocks of cell membranes and define the lipid bilayer permeability barrier of membranes. Phospholipids of mycobacteria have a unique structure," explained Zuzana. "On the contrary, with phospholipids from other bacterial species, in mycobacteria, unsaturated or branched fatty acids esterify position 1 of the glycerol, while C16:0 (palmitoyl acid) principally occupies position 2 of the glycerol. How this unusual positional distribution of acyl chains influences the physiology of mycobacteria remains unclear. However, we believe that it is crucial for bacterial survival."



Shiva (right, first author) and Zuzana (left, coauthor) next to the ARC Agilent 6545 UPLC-QTOF mass spectrometer (funded by OVPR, CNS, CVMBS, and ARC).

"In our publication, we have proposed two novel biosynthetic pathways of mycobacterial phospholipids and identified two enzymes, PIsM and PIsB2, catalyzing the acylation of G3P. We showed that PIsM is the first example of bacterial *sn*-2 G3P acyltransferase outside the plant kingdom, while PIsB2 is the first example of a 2-acyl-G3P acyltransferase."

The ARC was able to aid the researchers through the use of mass spectrometry analyses, data collection, and data analysis. "The most valuable part of working in the ARC is the independence provided to us," explained Shiva. "In depth training to become proficient in instrument operation allowed us to plan extremely time-sensitive experiments and schedule instrument time accordingly. Having that flexibility as well as the access to high end instrumentation here at CSU was a game changer for our experiments, so that we didn't have to send the samples elsewhere, allowing us to maintain critical sample conditions all the way up to the time of analysis, and achieve consistent results."

Shiva also expressed his thanks to ARC mass spectrometry staff scientist Claudia Boot, specifically, for her guidance during advanced LC-MS method development and for her expertise that allowed the researchers to see how the enzymes were behaving as well as their positions, helping to prove their hypothesis correct. "The new Agilent 6454 UPLC-QTOF mass spectrometer the ARC recently acquired allowed us to measure the change in abundance and structure of the cell wall lipids upon gene silencing of the essential enzymes."

"Our group is one of the few in the world diligently studying the structure and biosynthesis of cell wall macromolecules of mycobacteria," said Zuzana. "Our projects rely heavily on mass spectrometry and other structural analyses. We are proud that we can do the majority of analytical studies here at CSU. Without the ARC, none of the structural studies would be possible. The progress in analytical techniques in recent years is also very exciting, in particular the recent additions of the new Agilent UPLC-QTOF and the new Bruker MALDI-TOF/TOF has opened new possibilities for our projects as well, and we hope to keep close collaboration with ARC also in the future."

The ARC is excited to continue to support research in the field of microbiology and infectious disease here at CSU through the use of mass spectrometry and other analytical studies, in addition to providing expert training and guidance!

Thank you, Shiva and Zuzana, for speaking with us! We are thrilled to hear how our facilities have aided in advancing your high-impact research.

MEET THE INSTRUMENT AND EXPERT!

Explore our self-use Gas Chromatography Mass Spectrometry (GC-MS) instruments in Chemistry C5:

Thermo TSQ8000-EVO Triple Quadrupole Mass

Spectrometer is designed for the quantitative analysis of small molecules. Employing a triple quadrupole design, it selectively filters and measures ions for precise detection and quantification of specific molecules in fields such as chemistry, microbiology, biochemistry, and environmental science.

Thermo ISQ Single-Quadrupole Mass Spectrometer with Markes Unity/ULTRA-xr Thermal Desorption is designed to analyze volatile and semi-volatile compounds in samples. The thermal desorption system facilitates the release of compounds from a sample matrix by heating. This configuration is particularly useful for identifying and quantifying trace levels of volatile substances in atmospheric, environmental, food, and industrial samples.



Paul Mathews is your go-to person for GC-MS self-use operations in the ARC. With 1.5 years of experience at the ARC and a master's in food science and human nutrition from CSU, Paul is dedicated to assisting you with user training, maintenance, repairs, method development, and troubleshooting. Feel free to connect with Paul for any assistance – from science and food to hockey!

INSTRUMENT UPDATES

Become trained on our new SEM!

The loaner IT700HR SEM arrived and has been installed! ARC SEM manager Dr. Rebecca Miller, has started user training. Training can be requested through iLab and by contacting Rebecca.Miller@colostate.edu. It's been a joy observing happy trainees' amazement by the incredible imaging improvements and software automation compared to our older SEM. Thank you again, OVPR, for making this possible!



Rebecca Miller (ARC SEM Manager) and trainee Emma Rettner (Miyake research group)



Biochar sample. Imaged by Kerry Miller (Borch research group)

Here are a few updates on instruments that are currently down for repair, and the ARC is working hard on getting back online as soon as possible:

- Bruker ASC400 NMR (walkup NMR in CHEMR): The probe is currently being serviced at Bruker for cleaning and repair. We expect the NMR to be back online by mid February. In the meantime, users are advised to use the Bruker US400 and Agilent 400MR. Contact <u>Michele.Mailhot@colostate.edu</u> for more information.
- 500 NMR has been down for several months due to a failure with the room AC unit. A new AC unit will likely not be installed until April. For high-temperature experiments, contact <u>Michele.Mailhot@colostate.edu</u>.
- Single Crystal XRD: The broken generator is being serviced at Bruker. We expect the system to be back online in 2-3 weeks. Contact <u>Indrani.Bhowmick@colostate.edu</u> for more information and local alternatives for analyses.
- **SAXS:** still down for the foreseeable future. Users are encouraged to go to CU Boulder, which has a new Xenocs SAXS/WAXS system, and they are happy to train our users on it while our system is pending repair. Contact <u>Alyssa.Winter@colostate.edu</u> for more information.
- Orbitrap Eclipse: has been down for repair, and is expected to come online later this week.

ON THE CALENDAR



FEB

2

FEB

First Friday ARC Tour 12-1:30pm.

A chance to see the different ARC facilities and learn about ARC services. Meet in Chemistry C3 (basement). Registration required: <u>https://www.research.colostate.edu/arc/tour-demo-</u> class-support-request/

ARC Monthly Seminar. 2-3 pm.

"Metaproteomics - who is doing what in microbial communities." By Dr. Gustavo Diaz, ARC Proteomics Research Scientist.

The Microbiome, a community of microorganisms in a specific environment or area (e.g., soil, gut), is extensively studied using metagenomic approaches like 16S RNA or whole shotgun sequencing. While these approaches identify microbial members and their gene potential, they lack insights into biological functions. Metaproteomics, a large-scale characterization of proteins in a microbiome, reveals molecular processes and the major contributors. At the ARC, we are developing workflows to enable the CSU community and beyond to conduct metaproteomic studies. Join our seminar for an overview of metaproteomics, its applications, and examples of our current developments.

Register here: https://www.research.colostate.edu/arc/arc-seminar-series/



ARC FALL & SPRING SEMINAR SERIES

Hosted by the Analytical Resources Core Office of the Vice President of Research



ANALYTICAL RESOURCES CORE COLODADO STATE UNIVERSITY

Learn about the ARC's latest developments and newly added technologies available to CSU researchers and regional companies. This year the ARC experts themselves will present the technologies, analytical services, and educational resources each of their labs have to offer. Join us as we delve into a diverse array of scientific instruments and methodologies, enabling you to harness the full potential of our facilities.

Date	Presenter	Торіс
September 6	Karolien Denef	Overview of the Analytical Resources Core
October 4	Corey Broeckling	Mass spectrometry-based metabolomics
November 1	Jackie Chaparro	Inductively coupled plasma mass spectrometry and ionomics applications
December 6	Roy Geiss	Electron microscopy
January 10	Linxing Yao	Targeted quantitative analysis
February 7	Gustavo Diaz	Metaproteomics - who is doing what in microbial communities
March 6	Claudia Boot	Self service mass spec offerings in the ARC
April 3	Indrani Bhowmick	Materials analysis techniques
May 1	Alyssa Winter May	MALDI mass spectrometry and macromolecular analysis
June 5	Rebecca Miller	Surface analysis techniques
July 3	Michele Mailhot	Nuclear Magnetic Resonance (NMR)
August 7	TBD	X-ray diffraction and scattering techniques

First Wednesday of the month | 2-3 pm

www.research.colostate.edu/arc/arc-seminar-series/ Join our mailing list to stay receive further updates

TEAM UPDATES

Welcome to the Team, Ethan Crace!

Greetings! I am Dr. Ethan Crace, and I am joining ARC this year as the X-ray Crystallographer and X-ray Diffraction Scientist. I earned my PhD in Chemistry at Stanford University, working for Prof. Hemamala Karunadasa. During my thesis, I developed techniques for preparing hybrid organic-inorganic perovskite materials exhibiting broadband light emission at room temperature. My training focused on organic and inorganic materials synthesis and analysis, X-ray crystallography and diffraction techniques, and optical characterization of materials. I then worked as a postdoctoral associate in Prof. David Mitzi's lab at Duke University.



I continued working on hybrid perovskite materials but shifted my focus to developing structure-property relationships between structural deformation in perovskites and thermal, magnetic, and spin-splitting properties. My favorite aspect of my work has been X-ray crystallography and related diffraction techniques. For me, being able to determine the structure and composition of unknown or novel compounds is an extremely powerful tool for understanding the world around us and allowing us to fine-tune materials to improve everyone's lives. I also love how beautiful and colorful crystals can be. I look forward to working at ARC to further my expertise in these techniques and help solve interesting problems. When I am not in the lab, I am usually in a pottery studio covered in clay, reading fantasy/horror novels, playing board games with my fiancé Sarah, or walking/playing with our dog Fenrir.

Ethan will arrive at CSU on March 4 to start his position in the ARC. Please join us in giving him a warm welcome!

We are incredibly grateful to those in ARC and Chemistry who played a crucial role in maintaining the operations and services in the X-ray facility. Indrani Bhowmick, Alyssa May, Thinh Tran, Amanda Kale, and Autumn Peters: your dedicated efforts have been truly invaluable. Thank you for your tremendous assistance!

WE NEED YOUR INPUT!





REMINDERS AND UPDATES

PLEASE WEAR YOUR EYE PROTECTION!

Please remember to wear eye protection at all times when working in or visiting our laboratory spaces. Safety glasses are available in the ARC. We kindly ask you to return these when leaving the laboratory.

ILAB RESERVATIONS

Trained users: an iLab calendar reservation is always required before using the instrument (NMR being the exception). Repeated failure to do so will result in revoked access to the lab and instrument.

INSTRUMENT RE-TRAINING

For a number of instruments, re-training will be required if users do not use the instrument within six months following initial training. This will be clearly communicated in the training guidelines for each instrument.

ARC FIRST FRIDAY TOURS

The ARC will start hosting monthly tours of the facilities for all interested students, researchers and faculty starting in 2024.

- When: Every first Friday of the month 12-1:30pm.
- Register: <u>https://www.research.colostate.edu/arc/tour-demo-class-support-request/</u>
- Contact: <u>Karolien.Denef@colostate.edu</u>.

Scan me to register!







Check out recent publications using the ARC:

Tipton M, Baxter BA, Pfluger BA, Sayre-Chavez B, Muñoz-Amatriaín M, Broeckling CD, Shani I, Steiner-Asiedu M, Manary M, Ryan EP. Urine and Dried Blood Spots From Children and Pregnant Women Reveal Phytochemicals, Amino Acids, and Carnitine Metabolites as Cowpea Consumption Biomarkers. Molecular Nutrition & Food Research. 2024 Jan 17:2300222. <u>https://onlinelibrary.wiley.com/doi/full/10.1002/mnfr.202300222?</u> casa token=jIdPPQXoyOwAAAAA%3A8k2KSyPw_clCUwk9JVi9uvJo6Nu8gEVE_hCgmIaWqfI7hIUi7PKzBiSuJIzKbqJkEic51D7VtMEECk

Randall CR, Zou L, Wang H, Hui J, Rodríguez-López J, Chen-Glasser M, Dura JA, DeCaluwe SC. (School of Mines) Morphology of Thin-Film Nafion on Carbon as an Analogue of Fuel Cell Catalyst Layers. ACS Applied Materials & Interfaces. 2024 Jan 11. <u>https://pubs.acs.org/doi/full/10.1021/acsami.3c14912</u>

Gia Thinh Tran, Allison Wustrow, Daniel O'Nolan, SongSheng Tao, Christopher J. Bartel, Tanjin He, Matthew J. McDermott, Brennan C. McBride, Karena W. Chapman, Simon J. L. Billinge, Kristin A. Persson, Gerbrand Ceder, and James R. Neilson. Selective Synthesis of Defect-Rich LaMnO3 by Low-Temperature Anion Cometathesis. Inorganic Chemistry. 2023 Dec 27. <u>https://pubs.acs.org/doi/full/10.1021/acs.inorgchem.3c03305?</u> casa token=yU4Qh7IXJ4AAAAAA%3A3dlkPOI-2HmSIS2P7aocEiW7gxbwwI36e4neb7OpyJZ75ejc 9asmkKrar x2cfuv gr05CyA17dQY

Neisius NA, MacHale LT, Snyder ER, Finke RG, Prieto AL. Copper Selenophosphate, Cu3PSe4, Nanoparticle Synthesis: Octadecane Is the Key to a Simplified, Atom-Economical Reaction. Nano Letters. 2023 Dec 12. https://pubs.acs.org/doi/full/10.1021/acs.nanolett.3c02620? casa token=Tzzu aGrl4YAAAAA%3AZ261jA-8NAEII c3r90ECsKdvF3K7L1jo4Ty7RH9YZkvU12D1qc-aXSIFUIutethdZckDBSJ0IBsRpo

Broeckling CD, Beger RD, Cheng LL, Cumeras R, Cuthbertson DJ, Dasari S, Davis WC, Dunn WB, Evans AM, Fernández-Ochoa A, Gika H. Current practices in lc-ms untargeted metabolomics: a scoping review on the use of pooled quality control samples. Analytical Chemistry. 2023 Dec 6.<u>https://pubs.acs.org/doi/full/10.1021/acs.analchem.3c02924</u>

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in publications that include any data generated in or by our facility