Welcome to our Annual Winter Research Review.

Today’s program of research presentations by our fourth-year graduate students provides a wonderful opportunity to learn about the scientific discoveries and training pathways of our senior graduate students and their faculty advisors. Throughout the day, you can also visit research posters presented by our third-year students.

Our graduate program is one of the central foundations of the department’s mission towards scholarship and education. We hope that you will enjoy this opportunity to learn more about our department and its activities, as well as to meet the students and faculty. We are pleased that you can join us!

Millicent Sullivan
Alvin B. and Julie O. Stiles Professor and Department Chair
Department of Chemical and Biomolecular Engineering

Cailin D’Ambrosio and Emma Sudduth
Co-Presidents of Colburn Club
The Graduate Student Organization

Colburn Club is the graduate student organization in the Chemical and Biomolecular Engineering Department, which is comprised of representatives from each year as well as a number of members filling specialized roles. The primary functions of the club are to organize research reviews and social events for the department, in addition to serving as one line of contact between the students and the faculty. We hope you enjoy this event and can join us again in the future.

The Colburn Club
https://sites.udel.edu/colburnclub/
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<td>ALI KAMALI “Two-Dimensional (2D) Catalyst Materials for Plastic Recycling”</td>
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<td>10:00 – 10:20 AM</td>
<td>AKASH AJIT WARTY “Electrochemical Synthesis of Zeolite Films on Metal Substrates”</td>
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<td>NEFELI KAMARINOPOULOU “Direct HCN Synthesis Via Plasma-Assisted Conversion of Methane and Nitrogen”</td>
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<td>1:30 PM – 1:50 PM</td>
<td>DARIAN K. NGUYEN “Plasma-Assisted Upcycling of Plastic Waste Derivatives”</td>
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ROOM 101B

1:50 – 2:10 PM  ERHA ANDINI
“Chemical Recycling of Mixed Textile Waste”
Advisor: Dionisios Vlachos
Committee Members: Raul Lobo and Dongxia Liu

2:10 – 2:30 PM  TEJAS B. GOCULDAS
“Biomass to Biobased Chemicals”
Advisor: Dionisios Vlachos
Committee Members: Raul Lobo and Dongxia Liu

2:30 – 2:50 PM  BREAK

2:50 – 3:10 pm  ALFRED WORRAD
“Ab Initio Molecular Dynamics Spectra for Characterization of Hydrated Supported Metal Oxide Catalysts”
Advisor: Dionisios Vlachos
Committee Members: Raul Lobo and Antony Beris

3:10 – 3:30 pm  JASON CONRADT
“Multiscale Analysis of the Dissipative Self-assembly of Polarizable Colloids”
Advisor: Eric Furst
Committee Members: Arthi Jayaraman and Norman Wagner

3:30 – 3:50 pm  MICHELLE GEE
“Closed-Loop Modeling of Central and Intrinsic Cardiac Nervous System Circuits Underlying Cardiovascular Control”
Advisor: Abraham Lenhoff and Rajanikanth Vadigepalli
Committee Members: Aditya Kunjapur

4:00 PM  END

4:00 – 5:00 PM  FREEFORM INDUSTRY SESSION (101A)
ROOM 125

8:00 – 9:00 AM  BREAKFAST (Lobby)
9:00 – 9:05 AM  WELCOME/Opening Remarks: Colburn Club (Room 101B)
9:05 – 9:15 AM  REMARKS: Dr. Raul Lobo, Associate Department Chair (Room 101B)

SESSION I  9:20 AM – 1:00 PM  ROOM 125

9:20 – 9:40 AM  PHILIP GITMAN
“Engineering Y. Lipolytica for Stable & Carbon-Efficient Production of Commodity Chemicals”
Advisor: Mark Blenner
Committee Members: Aditya Kunjapur and Terry Papoutsakis

9:40 – 10:00 AM  THOMAS LEIBIGER
“Proteomic Analysis of Residual Host Cell Protein Retention Across Adeno-Associated Virus Affinity Chromatography Processes”
Advisor: Kelvin Lee
Committee Members: Abraham Lenhoff and Wilfred Chen

10:00 – 10:20 AM  KATHERINE RAUDENBUSH
“Modeling the Effect of Gradients on Cell Culture Performance in Large Scale Bioreactors”
Advisor: Marianthi Ierapetritou and Terry Papoutsakis
Committee Members: Richard Grenville, Christopher Roberts, and Christopher Kloxin

10:20 – 10:40 AM  CHRISTOPHER MAYHUGH
“Genetic Code Expansion for The Development of Novel Bacterial Vaccines”
Advisor: Aditya Kunjapur
Committee Members: Wilfred Chen and Catherine Fromen

10:40 – 11:40 AM  POSTER SESSION

11:40 AM – 1:00 PM  ROOM 101A: LUNCH AND FEATURED SPEAKER, YUSHAN YAN

SESSION II  1:10 PM – 4:00 PM  ROOM 125

1:10 – 1:30 PM  AMANDA FORTI
“Design of Orthogonal and Obligate Commensalism for Organism-Based Biological Containment”
Advisor: Aditya Kunjapur
Committee Members: Mark Blenner and Terry Papoutsakis
ROOM 125

1:30 PM – 1:50 PM  
JOHN HILL  
“Applications of Species-Specific rRNA-FISH Probes in Synthetic Clostridial Consortia”  
Advisor: Terry Papoutsakis  
Committee Members: Aditya Kunjapur and Kevin Solomon

1:50 – 2:10 PM  
TESSA POSEY  
“Coiled-Coil Peptides as Nanoscale Building Blocks”  
Advisor: Christopher Kloxin  
Committee Members: Millicent Sullivan, April Kloxin, and Darrin Pochan

2:10 – 2:30 PM  
KENNETH CRANE-MOSCOWITZ  
“Ionic Strength Determines Self-Assembly, Solution Stability, and Interactions between Coiled-Coil Nanoparticles”  
Advisor: Eric Furst, Christopher Kloxin, and Darrin Pochan  
Committee Members: Arthi Jayaraman

2:30 – 2:50 PM  
BREAK

2:50 – 3:10 PM  
ROMAN DICKEY  
“Genome Engineering Allows Selective Conversions of Terephthalaldehyde to Multiple Valorized Products in Bacterial Cells”  
Advisor: Aditya Kunjapur  
Committee Members: Catherine Fromen and Wilfred Chen

3:10 – 3:30 pm  
SHELBY ANDERSON  
“The Elimination of Nitroreductases in E. Coli Enables the Retention of Many Nitro Compounds for Biosynthesis and Biosensing Applications”  
Advisor: Aditya Kunjapur  
Committee Member: April Kloxin and Wilfred Chen

3:30 – 3:50 pm  
MADAN R. GOPAL  
“Reductive Enzyme Cascades for Valorization of Polyethylene Terephthalate Deconstruction Products to Aldehydes and Amines”  
Advisor: Wilfred Chen and Aditya Kunjapur  
Committee Members: Mark Blenner, Arthi Jayaraman, and Joshua Michener

4:00 PM  
END

4:00 – 5:00 PM  
FREEFORM INDUSTRY SESSION (101A)
The elimination of nitroreductases in *E. coli* enables the retention of many nitro compounds for biosynthesis and biosensing applications

Shelby Anderson
Advisor: Dr. A. Kunjapur
Committee Members: Dr. A. Kloxin, Dr. W. Chen

Nitro groups are important components of small molecule pharmaceuticals, energetic materials, commodity chemicals, and natural products such as antibiotics. One challenge associated with the detection or production of nitro compounds using microbial hosts is their context-dependent instability in and around cells. In this study, we measured the stability of diverse nitroaromatic compounds in the presence of *E. coli* and found that we could improve stability substantially by engineering combinatorial gene inactivations. The identity and position of the other ring substituents strongly affects stability, which reflects the preferences of natively expressed enzymes that have nitroreductase activity in *E. coli*. Through combinatorial gene deletions of candidate nitroreductase targets, we engineered a collection of Nitro Aromatic Reductase Knockout Strains (NARKOS). With five deletions in the MG1655 progenitor strain (MG1655-NARKOS.d5), we observed retention of 1 mM of *meta*-nitrobenzoic acid and *para*-nitrobenzoic acid 20 h after addition to live cells compared to complete instability when added to cultures of the progenitor MG1655 strain. However, some compounds such as the di-nitro compound 3,4-dinitrobenzoic acid remained rapidly degraded in cultures of this engineered strain. Therefore, we performed additional inactivations of candidate nitroreductase genes, targeting as many as 12. With this MG1655-NARKOS.d12 strain, we enabled the retention of as much as 50% of the di-nitro compound supplemented at 1 mM after 20 h. We also demonstrate that we can use genome engineering to stabilize another set of compounds that are otherwise fully degraded: nitroaldehydes. We achieve more than 50% retention of multiple nitroaldehydes 4 h after supplementation at 1 mM concentration to cell cultures by performing the NARKOS gene deletions in the *E. coli* RARE strain background. This includes the versatile *ortho*-nitrobenzaldehyde synthon for photochemistry applications. Using these strains, we show that the biosynthesis of certain nitroaromatic compounds in live cells can be improved by up to 10-fold. Finally, we show that the use of the NARKOS strains can improve the dynamic range of nitro compound detection by genetically encoded biosensors. Our study represents a major advance in the understanding of nitro compound metabolism and the ability of engineered biological systems to access this important chemistry.
Chemical Recycling of Mixed Textile Waste

Erha Andini
Advisor: Dionisios G. Vlachos
Committee Members: Raul F. Lobo and Dongxia Liu

Less than 0.5% of post-consumer textile waste generated globally is recycled, while the rest is incinerated, accumulated in landfills, or leaks into the environment. Today, many post-consumer textiles produced consist of mixed fibers. Recycling mixed fibers is challenging due to the blend of materials and contaminants such as additives, dyes, and finishes. Mechanical recycling has been the predominant recycling means. However, mechanically recycled textiles exhibit reduced fiber strength, with applications limited to low-value products such as carpeting and upholstery. The inadequacy of mechanical recycling has led to a surge in chemical recycling technologies such as hydrolysis, methanolysis, and glycolysis. The high energy demands associated with these processes can lead to significant CO₂ production. The textile industry, with its ever-growing environmental footprint, needs sustainable recycling technologies for mixed textiles.

In this work, we demonstrate that the coupling of microwave assisted heating for glycolysis and solvent dissolution can efficiently separate the four major textiles (polyester, cotton, nylon, and spandex) from post-consumer mixed textile waste, allowing to overcome the energy-related challenge of conventional heating. We show rapid depolymerization of polyester into bis(2-hydroxyethyl) terephthalate (BHET) and spandex into its monomers in the presence of an earth-abundant heterogeneous catalyst. Cotton remained intact, and nylon turned into powders which were separated easily through solvent dissolution. Quality of each component was confirmed by NMR, FTIR, TGA, XRD, and DSC techniques. This development provides a solution to address the problem of recycling post-consumer mixed textile waste containing all major textiles while retaining their properties.
Non-oxidative Ethane Dehydrogenation over Cobalt in Dealuminated BEA Zeolite at Lattice Tetrahedral Sites

Antara Bhowmick
Advisor: Dr. Dongxia Liu

Committee Members: Dr. Raul Lobo, Dr. Yushan Yan, Dr. Dionisios G. Vlachos

The catalysts for on-purpose non-oxidative dehydrogenation of ethane (NDE) have been challenged by coke deposition from side reactions and thermal sintering of active species. Herein, we report a catalyst mechanism that overcomes both challenges to enable highly stable, active and selective NDE. The catalyst is made of sub nanometric cobalt (Co) species (i.e., single atoms and clusters) habituated in the silanol nests of dealuminated BEA zeolite (DeAl-BEA) support. The dealuminated BEA zeolite provides high silanol groups and weak acid sites. The former property incorporated Co species into the silanol nest of zeolite framework that creates strong metal-support interaction leading to well-dispersed Co species against thermal sintering. The later characteristic prohibits acid catalyzed side-reactions to avoid coking. Sub-nanometer clusters and nanoparticles are formed in the DeAl-BEA support with increasing Co loadings. The nanoparticles lead to lower EDH catalytic performance and X-ray absorption spectroscopy (XAS) reveals that during reaction, parts of Cobalt exist as metallic cobalt which leads to carbon formation. Therefore, these carbons stay as carbon nanotubes which don’t block the active site, providing stable catalytic performance. Consequently, the DeAl-BEA supported Co catalyst exhibited high stability, durability and regeneration capability in the NDE.
Multiscale Analysis of the Dissipative Self-assembly of Polarizable Colloids

Jason Conradt
Advisor: Eric M. Furst
Committee Members: Arthi Jayaraman and Norman J. Wagner

Colloids of paramagnetic spheres phase separate in the presence of sufficiently powerful magnetic fields. By toggling the field, suspensions can be directed to self-assemble into highly anisotropic, dynamic phases. Suspensions of spherical particles (0.26, 0.48, and 1.02 μm diameters) were subjected to toggled magnetic fields with field strengths ranging from 627 A/m to 2276 A/m over a frequency range of 0.25 Hz to 20 Hz and a duty ratio range of 0.10 to 0.50 in microgravity. At long experiment times, the mesoscopic shapes of self-assembled structures exhibited strong dependence on toggle frequency and duty ratio, displaying morphologies ranging static columnar aggregates to dynamic, ribbon-like structures.

Startling variation is observed in aggregate structures as a function of field conditions. We analyze the assembled structures in terms of the overall suspension energy across multiple length scales. Bulk and surface energies for crystalline structures are calculated using an induced multipolar Ewald sum method to clarify the energy landscape at the particle-scale. We confirm literature calculations that the body-centered tetragonal crystal structures represent the low-energy particle configuration of polarizable spheres and calculate lattice surface energies to clarify surface stabilities for assembled aggregates.

A continuum, mean-field model is developed to explain qualitative behaviors of aggregates too large for direct simulation. The model suggests that the energy costs associated with shape anisotropy are relatively low and gives predictive estimations for the equilibrium shapes of self-assembled bodies at long times. This concept is carried forward into a Monte Carlo technique which assesses the low-energy distributions of many large aggregates throughout a sample volume. The correlation between simulation results and experimental imaging in microgravity provide insight into the mechanisms governing the self-assembly process and can enable tuning of structures beyond the particle scale.
Electrochemical CO₂ Reduction Towards Multi-Carbon Chemicals and Food

Bradie S. Crandall
Advisor: Prof. Yushan Yan
Committee Members: Prof. Feng Jiao, Prof. Dionisios Vlachos

The urgent need for affordable carbon capture technology in the fight against climate change has prompted the exploration of innovative approaches for carbon utilization. The valorization of captured carbon emissions via the electrochemical conversion of CO₂ into multi-carbon commodity chemicals and food has emerged as a promising carbon utilization strategy. This frontier in carbon utilization has previously been restricted to the Watt-scale, limiting industrial insights. Here, a kW-scale tandem CO₂ electrolyzer stack designed for producing multi-carbon products is introduced. A 1,000-cm² CO electrolyzer was successfully operated at 0.71 kW alongside a 500-cm² CO₂ electrolyzer at 0.40 kW. The CO electrolyzer stack demonstrated stable performance at 300 A for over 125 h. This pre-pilot system yielded 98 L of 1.2 M acetate at 96% purity. Notably, the CO electrolyzer stack also maintained high performance in the presence of common industrial contaminants. Techno-economic analysis revealed the competitiveness of electrochemical acetate production against conventional fossil-based production methods. Beyond the role of acetate as a valuable commodity chemical, the integration of acetate into biological systems for food production in arid environments is explored. Efforts towards a fully integrated electrocatalytic-biocatalytic system to support an astronaut crew in deep space travel to Mars will be showcased. Furthermore, analysis suggests that this same system can be deployed on earth to improve food market stability and substantially reduce agricultural land usage. These advancements underscore the industrial feasibility of CO₂ electrolysis and electro-agriculture technology, presenting a transformative opportunity for global carbon emission reduction efforts.
Ionic Strength Determines Self-Assembly, Solution Stability, and Interactions between Coiled-Coil Nanoparticles

Kenneth Crane-Moscowitz
Advisor: Eric M. Furst, Christopher J. Kloxin, Darrin J. Pochan
Committee Members: Arthi Jayaraman

Anisotropic nanoparticles are a broad range of materials of interest to the colloid science community. The assembly of anisotropic nanoparticles leads to unique self-assembled structures and properties not found in their isotropic counterparts. One interesting anisotropic dimension that has not been extensively studied is surface charge anisotropy, or how the positioning of locally dense regions of like-charges influences the resulting nano- and micro-structure in colloidal dispersions. Peptide-based coiled-coil nanoparticles, termed “bundlemers”, are well-suited to this type of study given their inherent shape anisotropy, facile synthetic scheme, and their exact display of surface chemistry. While a large library of bundlemers now exist in the literature, their solution dynamics and interactions are largely uninvestigated.

In this work, light scattering techniques are used to develop insight into the static and dynamic properties of bundlemers in solution. We are interested in examining the role of surface charge on the formation of hierarchical structures within and between bundlemers. Based on the results of static light scattering, highly charged peptide sequences require electrostatic screening to properly assemble into discrete coiled-coil domains. Once this assembly occurs, the bundlemers remain well-dispersed in solution until high ionic strengths, at which point aggregation dominates. Additionally, bundlemers with more surface charge (Lys, Arg, Glu, and Asp), and more charge homogeneity (i.e. less ampholytic) exhibit aggregation behavior at higher ionic strengths than ampholytic and charge neutral bundlemers. By studying the role of electrostatic screening in bundler/self-assembly and solution stability, we can better understand how charge “patchiness” plays a role in the modeling of other nanoparticle systems, including proteins.
Genome engineering allows selective conversions of terephthalaldehyde to multiple valorized products in bacterial cells

Roman Dickey
Advisor: Dr. Aditya Kunjapur
Committee Members: Dr. Catherine Fromen, Dr. Wilfred Chen

Deconstruction of polyethylene terephthalate (PET) plastic waste generates opportunities for valorization to alternative products. We recently designed an enzymatic cascade that could produce terephthalaldehyde (TPAL) from terephthalic acid (TPA). In this work, we showed that the wild-type MG1655 E. coli strain rapidly reduces TPAL in metabolically active cells to diol 1,4-benzenedimethanol (BDM), a valuable building block that can be utilized for the production of pesticides, perfumes, or dyes. We showed that the addition of TPAL to growing cultures of an engineered strain for reduced aromatic aldehyde reduction (RARE) strain resulted in partial reduction to 4-(hydroxymethyl) benzaldehyde, a polymer precursor. We then investigated if we could mitigate this reduction using multiplex automatable genome engineering (MAGE) guided by RNA-seq to create an E. coli strain with up to 10 additional knockouts in RARE. Encouragingly, we found this newly engineered strain enabled a 2.5-fold higher retention of TPAL over RARE after 24 h. We applied this new strain for the production of para-xylylenediamine (pXYL), a useful building block for polymeric materials, and observed a 6.8-fold increase in pXYL titer when compared with the RARE strain. Additionally, we showed a 2.5-fold increase in our newly engineered strains for TPAL production from TPA when compared to the RARE strain. Overall, our study exploits genome engineering and heterologous expression to demonstrate selective microbial biosynthesis routes of TPAL to diverse chemicals that are derived from waste PET.
Design of orthogonal and obligate commensalism for organism-based biological containment

Amanda Forti
Advisor: Aditya Kunjapur
Committee Members: Mark Blenner & Eleftherios Papoutsakis

Biological containment is a critical safeguard for genetically engineered microbes prior to their environmental release to prevent proliferation in unintended regions. However, few biocontainment strategies can support the longer-term microbial survival that may be desired in a target environment without repeated human intervention. In addition, few strategies have been evaluated for their ability to function in the presence of other microbes. Here, we introduce the concept of an orthogonal and obligate commensalism for the autonomous creation of environments that are permissive for survival of a biocontained microbe. We show that this obligate commensalism is highly effective, with the survival of our commensal organism during co-culture dependent on the presence of our producer strain. We also show that this commensalism is orthogonal to a microbial consortium derived from maize root, with survival of the biocontained strain conditional upon the addition of the producer strain to the consortium. Overall, our study demonstrates a transition from a chemical to a biological dependence for biocontained organisms that could lay the groundwork for biocontained synthetic ecologies.
Closed-loop modeling of central and intrinsic cardiac nervous system circuits underlying cardiovascular control

Michelle Gee

Advisors: Abraham Lenhoff, Rajanikanth Vadigepalli
Committee Members: Aditya Kunjapur

The baroreflex is a multi-input, multi-output physiological control system that regulates short-term blood pressure by modulating motor and sensory vagus nerve activity between the brainstem and the heart. The primary objective of the baroreflex is to maintain near-constant blood pressure while balancing multiple demands for blood flow to different organs, including coping with disturbances such as those caused by respiration or exercise. Existing computational models of the baroreflex do not explicitly incorporate the heart’s “little brain”, the intrinsic cardiac nervous system (ICN), which mediates central control of heart function. We have developed a computational model of closed-loop cardiovascular control by integrating a network representation of the ICN within brainstem control reflex circuits. We used the model to examine brainstem and ICN contributions to the control of heart rate, ventricular functions, and the synchronization of heart rate and respiration known as respiratory sinus arrhythmia (RSA). Our simulations match the experimentally observed relationship between RSA and lung tidal volume. Furthermore, we used the model to simulate multiple scenarios of vagus nerve stimulation (VNS), an emerging bioelectronic treatment for heart failure. Our model was able to capture the hemodynamic changes in response to VNS. We found that a lower relative activation of vagal motor fibers compared to vagal sensory fibers was necessary to produce heart rate changes consistent with the experimental results. Thus, our results support the notion that VNS activates vagal sensory and motor fibers differentially, likely in varying proportions depending on the parameters of stimulation.

We have also extended our previously published computational model of closed-loop cardiovascular control to represent the disease state following myocardial infarction (heart attack). A hallmark of these changes is decreased vagus nerve activity. Loss of cardiac function following myocardial infarction is accompanied by neural adaptation in baroreflex systems that are compensatory in the short term but then become associated with long-term disease progression. The closed-loop feedback structure of the baroreflexes confounds the source of neural adaptation following myocardial infarction. Neuronal adaptations leading to decreased vagal activity could occur in neuronal groups located centrally in the brainstem or peripherally at the heart and vasculature, so we developed alternative models to reflect these hypotheses. Of the alternative models, only the model representing adaptation in the baroreceptors that sense blood pressure changes predicted both physiological baroreflex function and a decrease in vagus nerve activity. These findings suggest that decreased vagal activity after myocardial ischemia may be due, at least in part, to a decrease in baroreceptor sensitivity. We also link these model predictions with experimental evidence from the literature.
Engineering *Y. lipolytica* for stable & carbon-efficient production of commodity chemicals

Philip Gitman  
Advisor: Dr. Mark Blenner  
Committee Members: Dr. Aditya Kunjapur & Dr. Terry Papoutsakis

There is a need to develop efficient and scalable biomanufacturing platforms for industrially relevant chemical production to reduce humanity’s reliance on fossil fuels. The optimization of titer as well as titer stability during long fermentations is a critical feature of industrial production of commodity chemicals from microorganisms such as the model oleaginous yeast species, *Y. lipolytica*. However, microbial fermentations often exhibit a tendency to yield high titers for short durations or low titers for long durations. These challenges will be addressed through (1) the development of methodologies to screen and mitigate titer instability in a *Y. lipolytica* strain engineered for β-carotene production and (2) the engineering of *Y. lipolytica* to efficiently assimilate methanol to achieve high product titers.

The titer instability problem is exemplified by an engineered β-carotene producing *Y. lipolytica* strain that was developed by enhancing flux from acetyl-CoA to terpene precursors and overexpressing carB and carRP enzymes. This engineered strain produced ~4 g/L β-carotene titer using benchtop bioreactors. However, when moving this strain to a larger bioreactor, cell performance significantly dropped during 60 generations of growth. We hypothesized that loss of productivity is due to accumulation of mutations in genes for β-carotene production during prolonged generations of culture growth. To test this hypothesis, we collected samples from shake flask, ambr250 and 2L bioreactor cultures grown under high and low stress continuous fermentation conditions and performed whole genome sequencing as well as global and targeted proteomics, metabolomics and lipidomics. The mutation rate and locations of the β-carotene producing strain were determined at various time points in culture growth. Additionally, targeted and global metabolomics and proteomics of the time course samples was then used identify correlations between growth conditions, mutation rates and pathway regulation. The goal of this work is to investigate the nature of titer instability in this β-carotene strain as a model to understand more broadly factors that lead to instability during cell-line development and scaleup.

Low product titers in microbial fermentations may be the direct result of pyruvate oxidation which results in a maximum cellular carbon efficiency of 62% due to the release of CO₂. To address this problem, we integrated a synthetic methanol assimilating pathway into the host species, *Y. lipolytica*. Using methanol as the primary substrate, this methanol assimilating pathway can achieve a 21% higher theoretical pathway yield than traditional glucose-oxidizing pathways. A higher theoretical pathway yield means that more of the substrate can be converted commodity chemical titers, making the pathway more carbon efficient. We have developed high-throughput screening methods to both evolve and test enzyme candidates to improve the whole pathway activity *in vivo*. Additionally, isoprenol production will be used as a proof-of-principle compound to demonstrate how low value substrates can be used to efficiently produce value-added products at high titers. Then, strategies learned from the β-carotene work will be used to improve the isoprenol titer stability in this *Y. lipolytica* strain. Overall, both strategies will aid in the development of microbial workhorses capable of producing high chemical titers for long culture durations at industrial scales.
Biomass to Biobased Chemicals

Tejas. B. Goculdas
Advisor: Dr. Dionisios G. Vlachos
Committee Members: Dr. Raul Lobo and Dr. Dongxia Liu

Most commodity chemicals originate from non-renewable fossil fuels, with industrial synthesis methods posing significant hazards and yielding environmentally harmful products. To address this, we emphasize the necessity for improvements in production methods and the resulting products. Biomass, an underutilized renewable resource, holds significant potential for fine and commodity chemical production. To unlock this potential, we illustrate various strategies for valorizing biomass, from organic synthesis to process intensification.

We start by creating a novel route to biobased carbamate insecticides. We circumvent hazardous chemicals such as isocyanates, traditionally used in carbamate synthesis, by creating a novel two-step synthesis using reductive amination and carbonylation to create the carbamate functional group on a renewably derived furan core. The proposed synthetic strategy is validated by the competitive toxicity of our compound to target pests; the furan moiety used in the starting material has unique electronic properties, resulting in extremely favorable ecological impacts of our compound compared to existing industrial carbamates.

We then develop catalysts to improve ketonization, an existing biobased route to precursors of oleo-furan surfactants and lubricants. This is an attractive route to upgrade furan and fatty acids. We explored various alkaline earth metals and mixed metal oxides for the ketonization reactions and found that MgO is extremely effective, improving product yield from cross-ketonization of furoic and lauric acid by order of magnitude. We elucidate that a distinct ketonization mechanism is instrumental in the high selectivity of our catalyst. Building on this breakthrough, we apply our insights to streamline and enhance the self-ketonization of lauric acid to 12-tricosanone. Overcoming separation challenges, we designed an efficient packed bed reactor that is capable of kilogram scale solventless synthesis of 12-tricosanone, enhancing productivity by a factor of 20. TEA simulations reveal a 50% decrease in the minimum selling price of the lubricant, showcasing favorable economic and environmental impacts. These improvements position our process at an industrially relevant scale.

In conclusion, our research advances biobased solutions across multiple fronts. Utilizing principles of organic chemistry, catalyst synthesis, and characterization, reactor design and construction, we have elucidated strides in producing biobased chemicals.
Reductive Enzyme Cascades for Valorization of Polyethylene Terephthalate Deconstruction Products to Aldehydes and Amines

Madan R. Gopal
Advisor: Wilfred Chen and Aditya M. Kunjapur
Committee Members: Mark A. Blenner, Arthi Jayaraman, and Joshua K. Michener

To better incentivize the collection of plastic wastes, chemical transformations must be developed that add value to plastic deconstruction products. Polyethylene terephthalate (PET) is a common plastic whose deconstruction through chemical or biological means has received much attention. However, a limited number of alternative products have been formed from PET deconstruction, and only a small share could serve as building blocks for alternative materials or therapeutics. Here, we demonstrate the production of useful monoamine and diamine building blocks from known PET deconstruction products. We achieve this by designing one-pot biocatalytic transformations that are informed by the substrate specificity of an ω-transaminase and diverse carboxylic acid reductases (CAR) toward PET deconstruction products.

We first establish that an ω-transaminase from Chromobacterium violaceum (cvTA) can efficiently catalyze amine transfer to potential PET-derived aldehydes to form the monoamine para-(aminomethyl)benzoic acid (pAMBA) or diamine para-xylylenediamine (pXYL). We then identified CAR orthologs that could perform the bifunctional reduction of terephthalic acid (TPA) to terephthalaldehyde or the reduction of mono-(2-hydroxyethyl) terephthalic acid (MHET) to its corresponding aldehyde. After characterizing 17 CARs in vitro, we show that the CAR from Segniliparus rotundus (srCAR) had the highest observed activity on TPA. Given these elucidated substrate specificity results, we designed modular enzyme cascades based on coupling srCAR and cvTA in one pot with enzymatic cofactor regeneration. When we supply TPA, we achieve a 69 ± 1% yield of pXYL, which is useful as a building block for polymeric materials. When we instead supply MHET and subsequently perform base-catalyzed ester hydrolysis, we achieve 70 ± 8% yield of pAMBA, which is useful for therapeutic applications and as a pharmaceutical building block. This work expands the breadth of products derived from PET deconstruction and lays the groundwork for eventual valorization of waste PET to higher-value chemicals and materials.
Escaping our dependence on fossil fuels will ultimately depend on many emergent technologies, working synergistically, to provide for the material and energy demands of industrial society. The generation of energy dense fuels and materials from plant derived biomass seems to be the most promising approach to re-establishing a circular carbon economy. Thermochemical, enzymatic, and hydrolytic process are capable of converting inedible, waste biomass feedstocks into a diverse landscape of substrates (e.g. xylose, CO, and H₂) for microbial metabolic conversion to biofuels, solvents, and other chemical precursors. For decades, researchers have largely employed strategies which leverage either a single, genetically engineered organism or a complex, naturally occurring microbial consortia. Though in its infancy, the concept of synthetic microbial consortia, that is a consortium consisting of two or more organisms that are not naturally co-inhabitants, seems to be a promising approach. Synthetic consortia offer some benefits over pure-cultures such as division of labor, modularity, and the compartmentalization of incompatible metabolic reactions. Furthermore, they can be engineered unlike naturally occurring consortia. Collectively, researchers agree that the primary issues facing synthetic consortia is stability, specifically the effect of environmental factors and interspecies interactions on subpopulation viability and growth. Theoretical approaches hoping to characterize subpopulation dynamics mathematically are too simple and too abstracted to be applied to real systems, so experimental methods leading to effective heuristics are essential at this state. Additionally, the nature of interspecies interactions (especially in an industrial production context) is crucially understudied, limiting our ability to understand experimental observations in the first place. Generally speaking, *Clostridia spp.* are heavily employed in synthetic consortia owing to their wide substrate utilization and fast growth rates. As a result, I have chosen to address the aforementioned problems with synthetic consortia based on this species. In this work I describe the development of two novel ribosomal RNA-fluorescence in situ hybridization probes, ClosAcet and ClosLjun, and a streamlined hybridization technique which enables high-throughput subpopulation tracking. I also demonstrate the first application of this technique to a synthetic consortium containing three unique species: *C. acetobutylicum*, *C. ljungdahlii*, and *C. kluyveri*. I then use this technique to characterize patterns of ribosomal localization in the above clostridial species. Finally, I explore interspecies ribosomal and protein material exchange between members of the synthetic consortia and discuss the implications of this phenomenon.
Two-Dimensional (2D) Catalyst Materials for Plastic Recycling

Ali Kamali
Advisor: Prof. Dongxia Liu
Committee Members: Prof. Raul F. Lobo, Prof. Dionisios G. Vlachos, Prof. Yushan Yan

The amount of plastic product consumption globally in 2019 reached 460 million tons and this is projected to continue grow exponentially. Although recycling appears to be a promising solution to plastic waste management, the rate of recycling in the United States is only 5-6%. Plastic waste polyolefins such as high- and low-density polyethylene (HDPE and LDPE) are of specific concern as their strong C-C backbone makes them challenging to depolymerize and recycle. Therefore, diffusion is expected to limit the performance of traditional cracking catalysts when applied to the depolymerization of polymers. Emerging research has shown great potential in plastic waste upcycling via hydrogenolysis. This process produces fuel-range hydrocarbons facilitated by a catalyst at lower operating temperatures (200-300°C). Utilizing ruthenium (Ru) as a catalyst has been demonstrated to be more active in C-C bond hydrogenolysis of LDPE. In this work, we study the effects of two-dimensional materials (2DM) on plastic waste depolymerization. Recently, these materials showed catalytic activities, however, their catalytic activities in different applications such as plastic depolymerization have not been explored. Based on our results, 2DM precedes the reaction selectivity towards more value-added products in LDPE hydrogenolysis. This data shows a promising way to use 2DM for selective plastic depolymerization. Different catalyst characterizations pave the way for discovering other 2DM structure–property relations in plastics depolymerization.
Direct HCN synthesis via plasma-assisted conversion of methane and nitrogen

Nefeli Kamarinopoulou
Advisor: Dionisios G. Vlachos
Committee Members: Raul Lobo, Dongxia Liu

Hydrogen cyanide (HCN) is synthesized from ammonia (NH$_3$) and methane (CH$_4$) at $\sim$1200 °C over a Pt catalyst. Ammonia synthesis via the Haber-Bosch entails several complex and highly emitting processing steps. Plasma-assisted hydrogen cyanide (HCN) synthesis directly from CH$_4$ and nitrogen (N$_2$) could be pivotal for on-demand HCN production. Here, we evaluate the potential of dielectric barrier discharge (DBD) N$_2$/CH$_4$ plasma for decentralized catalyst-free selective HCN production. We demonstrate a single-step conversion of methane and nitrogen to HCN with a 54% yield at $<$300 °C. HCN is favored at low CH$_4$ concentrations with ethane (C$_2$H$_6$) as the secondary product. We propose a first-principles microkinetic model considering essential electron impact reactions. The model accurately predicts primary product yields and elucidates that methyl radical (∙CH$_3$) is a common intermediate in HCN and C$_2$H$_6$ synthesis. Compared to current industrial processes, N$_2$/CH$_4$ DBD plasma can achieve minimal CO$_2$ emissions.
Proteomic Analysis of Residual Host Cell Protein Retention Across Adeno-Associated Virus Affinity Chromatography Processes

Thomas Leibiger
Advisor: Kelvin H. Lee
Committee Members: Abraham Lenhoff, Wilfred Chen

To meet growing clinical and commercial demand for recombinant adeno-associated virus (rAAV) vector therapies, higher titer production systems and increased manufacturing scales are needed. Improvements in rAAV upstream processes will require accompanying changes in purification strategies, which must be scalable and robust to accommodate increased volumes and vector titers while meeting critical quality attribute (CQA) specifications. One important CQA that must be defined and monitored in the downstream processes is residual host cell protein (HCP) impurity levels. Residual HCPs can pose immunogenicity risks to patients due to high rAAV dosing requirements and have been shown to impact in vivo rAAV transduction efficiency. Proteomic analysis techniques including liquid chromatography tandem mass spectrometry (LC-MS/MS) have been applied to better understand HCP expression levels and retention across production and purification for different biotherapeutic modalities including monoclonal antibodies (mAbs). The use of these techniques has improved the design of both upstream and downstream mAb bioprocesses by informing targeted protein knockouts, modification of cell culture conditions, and chromatography wash development as strategies to reduce levels of problematic and difficult-to-remove HCPs. For rAAV downstream processing, the use of affinity chromatography resins with cross-linked single domain antibody fragments has emerged as a leading technique for scalable primary purification. However, the ability of these resins to clear process-related impurities is not well understood. To better understand HCP retention in rAAV downstream processes we applied data-dependent acquisition (DDA) LC-MS/MS and sequential window acquisition of all theoretical mass spectra (SWATH-MS) to identify and quantify HCPs carried through primary purification across different rAAV serotypes and affinity chromatography resins. Using our LC-MS/MS workflows, we studied the impacts of rAAV serotype, genome packaging, and resin selection on residual HCP profiles after affinity purification. Identification of difficult-to-remove HCPs in rAAV purification can inform next-generation downstream process designs and contribute to the manufacture of safer, more potent gene therapies.
Genetic Code Expansion for The Development of Novel Bacterial Vaccines

Christopher C. Mayhugh
Advisor: Dr. Aditya Kunjapur
Committee Members: Drs. Wilfred Chen, Catherine Fromen

Vaccines are one of the most important innovations in modern medicine and are largely responsible for the development of society today. However, some bacterial pathogens remain elusive to vaccinate against. This is generally due to antigenic variation between serotypes, as well as the inability to direct immune responses towards desired sequences of antigens that will result in a robust, protective immune response. As more bacterial pathogens grow resistant to current antibiotic treatments, there is a need for novel treatments and prophylactic measures.

With advancements in synthetic biology, we can genetically encode structurally distinct amino acids that possess functional groups that differ from the 20 standard amino acids. In this work, we show preliminary evidence that the aromatic nonstandard amino acid (nsAA) para-nitro-L-phenylalanine (pNPhe) can be used to enhance bacterial antigen immunogenicity in a site-specific manner and represents a potential strategy to overcome current limitations in vaccine design. Immunogenicity was assessed via in vivo studies using a mouse model, and mucosal immunization with nitrated antigen induced high-titer, cross-reactive systemic IgG and mucosal IgA antibody responses relative to wild-type antigen in the absence of an adjuvant. Future studies will assess protective immunity resulting from nitrated antigen immunization and characterize T cell response. Overall, this strategy may provide a general method for enhancing bacterial antigen immunogenicity for vaccine design and a potential strategy to combat antimicrobial resistance.
Plasma-Assisted Upcycling of Plastic Waste Derivatives

Darien K. Nguyen  
Advisor: Dr. Dionisios G. Vlachos  
Committee Members: Dr. Raul Lobo and Dr. Yushan Yan

The pervasive and ubiquitous plastic pollution necessitates an eco-friendly solution to mitigate this issue. In this context, the oxidative functionalization of plastic waste derivatives, particularly long aliphatic alkanes, using non-thermal, atmospheric plasma processing, is presented as a green, catalyst-free step for plastic waste upcycling. The direct upgrading of the saturated hydrocarbons to value-added oxygenates can compete with petrochemicals-based manufacturing in many applications, such as the production of surfactants and lubricants. Two distinct plasma reactor designs, namely a batch pin-to-plate reactor and a modular biphasic microreactor, were employed to functionalize liquid n-alkanes using Ar/O₂ gas mixtures. Secondary alcohols and ketones emerged as the main products resulting from oxygen radical hydrogen abstraction and sequential radical recombination and disproportionation reactions. Higher conversions led to the formation of difunctional oxygenates, oligomerized oxygenates, and lighter hydrocarbon products stemming from carbon cleavage. Plasma parameters such as applied power, treatment time, and O₂ molar fraction were optimized to achieve optimal molar and energy yields. Utilizing the geometry of the microreactor, the plasma-liquid interface was enhanced by modifying gas and liquid flow rates, resulting in the highest energy yields reported among plasma systems. Alkane conversion using the microreactor can be further improved by increasing the length of the plasma region while maintaining excellent energy efficiencies. This system is also amenable to treating mixtures of liquid n-alkanes, confirming the process's applicability for utilizing plastic waste derivatives from processes such as catalytic hydrogenolysis. The results hold promise for upcycling plastic waste degradation products under ambient conditions using green, catalyst-free plasma discharges.
Coiled-Coil Peptides as Nanoscale Building Blocks

Tessa Posey
Advisor: Christopher Kloxin
Committee Members: Millicent Sullivan, April Kloxin, Darrin Pochan

A coiled-coil peptide assembly can act as a nanoscale building block to build higher-order structures. Through selective modification, click chemical functional groups can be incorporated at the ends of these coiled-coil peptide bundle units, or bundlemers, enabling bundlemer polymerization to form polybundlemers rods. Additionally, amino acids that reside at the periphery of the bundlemer can be modified to impart additional functionality. Here, we will explore two types of modifications: 1) reactions between amino acid side groups, or peptide stapling, to impart greater stability to the bundlemer, and 2) polymerization from the amino acid side group of the bundlemer, creating a bundlemer-polymer conjugate. Internal stapling was achieved through computational design, which predicted the close placement of cysteine and vinyl sulfonamide from two different peptides that are adjacently spaced. Upon the introduction of a base, a rapid thiol-Michael addition results in the stapling of the bundlemer assembly. The linkage was confirmed through LC-MS and the impact these linkages have on bundlemer stability was observed using circular dichroism. To create a bundlemer-polymer conjugate, a bromide handle was selectively installed on the bundlemer exterior to enable subsequent atom transfer radical polymerization (ATRP). ATRP of 2-(dimethylamino) ethyl methacrylate (DMAEMA) was performed, producing a thermally responsive star polymer with a bundlemer core. In a second experiment, a polybundlemer rod was formed through the Diels–Alder cycloaddition, followed by ATRP of DMAEMA to produce a bottlebrush-like architecture. Conjugate structure was confirmed using NMR, GPC, CD, turbidity measurements, and TEM. This work highlights the potential use of the coiled-coil peptide assembly to build complex architectures via click chemistry and living polymerization, advancing a unique platform for the design of responsive bio-inspired materials.
Modeling the effect of gradients on cell culture performance in large scale bioreactors

Katherine Raudenbush
Advisor: Professor Marianthi Ierapetritou and Professor Eleftherios (Terry) Papoutsaklis
Committee Members: Dr. Richard Grenville, Dr. Christopher Roberts, and Dr. Christopher Kloxin

Monoclonal antibodies (mAbs) have emerged as pivotal therapeutic agents in treating various diseases such as cancer, autoimmune diseases, and Covid-19. Most are produced by Chinese hamster ovary (CHO) cells grown in bioreactors. Bioreactor scale-up is necessary for the industrialization of mAb production, however scale-up often leads to the formation of spatial gradients in critical process parameters (CPPs) of cell culture, such as dissolved oxygen, dissolved carbon dioxide, and pH. Cell culture is sensitive to these CPPs, and optimal values are determined in small scale experiments. Because cells are exposed to fluctuating environmental conditions in large scale bioreactors, scale up could have detrimental effects on mAb production and product quality.

Modeling the interplay between fluid dynamics and bio-phase kinetics in large scale mixing tanks can provide insights into expected effects of the oscillating and suboptimal conditions observed in large scale bioreactors, minimizing expensive scale-up experiments. This objective is achieved through 1) small scale experiments of CHO cell growth and mAb production under constant and oscillating conditions, 2) kinetic modeling of CHO metabolism under fluctuating conditions based on experimental data, and 3) computational fluid dynamics (CFD) integrating hydrodynamics, multiphase mixing, mass transport and the developed kinetic reactions to predict mAb production and quality under heterogeneous conditions in large scale bioreactors. The framework for integrating the three components is described.

Small scale experiments were performed to characterize the effect of dissolved oxygen (DO) and the compounding effect of DO oscillations on CHO cell culture performance. VRC01 producing CHO cells were grown at 5%, 10%, 20%, and 40% DO levels in a 1L Eppendorf BioFlo320 system. There is an apparent shift in cell culture performance at 5% compared to 10% and above. An oscillating condition was also performed with 20 minute oscillations between 5% and 75% DO to determine the effect of large oscillations on cell culture, and the cell line tested was shown to be robust to these oscillations. Future work is planned to study the effect of oscillating pH levels on culture performance, as pH level has been shown to have significant impact on this cell line. Duplicate experiments are also planned for bioreactors held at different stationary DO levels to better characterize the switch from oxygen sufficient to oxygen limited conditions and model the unique metabolic behavior at these conditions.

Industrial collaborators performed a full experimental design of scale down simulator experiments in AmBR miniaturized bioreactors. These experiments varied dissolved oxygen and pH levels for two of their cornerstone mAb producing CHO cells at different oscillation frequencies and amplitudes. Results are discussed. To make predictions based on expected large scale bioreactor oscillations, a CFD model of the production bioreactor has been developed. Validation of the CFD model against experimental measurements of impeller power, mixing, and gas transfer is discussed.
Electrochemical Synthesis of Zeolite Films on Metal Substrates

Akash Ajit Warty
Advisor: Dr. Dongxia Liu
Committee Members: Dr. Raul Lobo, Dr. Yushan Yan

Zeolites and zeolite coatings are studied as catalysts, adsorbents, and molecular sieves for membrane separation, membrane reactor, and chemical sensor applications. Zeolite coatings have also been studied as anti-corrosive films for metals and alloys, antimicrobial and hydrophilic films for HVAC (i.e., heating, ventilation, and air conditioning), and dielectrics for semiconductor applications. Different synthesis techniques have been developed for depositing zeolite coatings on substrates to impart functionalities to the component on which it is deposited. In situ crystallization being the most widely researched technique in the past two decades because it allows the direct growth of zeolite crystals on the support, which offers high adhesion and cohesion between the zeolite coating and the underneath support. The in-situ synthesis of zeolite coatings can be done by hydrothermal, ionothermal and dry-gel conversion approaches, which require high process temperature and long synthesis times (i.e., from several hours to days).

This work demonstrates a novel electrochemical synthesis of zeolite coatings that is formed within sub-hourly duration thus reducing time and energy costs. The new zeolite film synthesis method was successful in developing hydroxy sodalite (SOD) and NaA (LTA) coatings on a titanium substrate. The coating morphology and crystallinity depend on temperature, time, zeolite precursor composition, and applied current. The growth mechanism is dominated by the in-situ water electrolysis that promotes the local pH and high growth rate on the cathode. Electrochemical synthesis is a novel, simple, fast, and environmentally friendly approach to preparing zeolite coatings with a potential to be generalized for developing zeolite coatings with diverse framework structures, morphologies, and orientation for substrates with complicated geometries.
Ab Initio Molecular Dynamics Spectra for Characterization of Hydrated Supported Metal Oxide Catalysts

Alfred Worrad
Advisor: Dionisios G. Vlachos
Committee Members: Raul Lobo, Antony Beris

Vibrational spectroscopy is an essential tool to determine the structure and active site of supported catalytic materials. However, due to these materials' vastly complex configurational space, it is virtually impossible to accurately gain clear insights into these systems based solely on well-established single-crystal experiments. To circumvent this challenge, we turn to computational spectra to provide a direct mapping between structure and spectra.

We compute Raman and power spectra for molybdenum oxide on γ-alumina via ab initio molecular dynamics (AIMD) and compare them to conventional 0 K density functional theory spectra. AIMD spectra can capture anharmonicities and features present at finite temperatures, making them more amendable for comparison with experimental data. We find that the hydration conditions, often neglected for modeling simplicity, significantly affect spectral signatures. Interestingly, the trends of hydration on these vibrational frequencies and modes are not uniform across examined systems. Additional analysis of the isolated hydroxyl group frequencies from power spectra suggests that the changes seen experimentally in infrared spectra can be related to surface reconstruction upon anchoring MoOx species on alumina. We also highlight system conditions that lead to different predicted frequencies between AIMD and traditional methods, which should be taken into consideration when directly comparing experimental and computational spectra.
Poster Presentations
Advisor: Yushan Yan

Avaniek Cabales  “Engineering Bacillus Subtilis for Control Over Persistence and Production”  
Advisor: Aditya Kunjapur

Rafael Castro  “Design and synthesis of bioactive collagen mimetic peptides”  
Advisor: April Kloxin

Marco Colin Martinez  “Investigating the Ion Transport in a Hydroxide Exchange Membrane Carbon Capture (HEMCC) Device”  
Advisor: Yushan Yan

Caitlin DAmbrosio  “Biosynthesis of Bundlemer Proteins with Orthogonally Reactive Handles”  
Advisor: April Kloxin

Ted Egnaczyk  “Relating the Early-Age Reaction Kinetics and Material Property Development of a Model Metakaolin Geopolymer Binder”  
Advisor: Norman Wagner

Sean Farrington  “Thixotropy of Blood and the Impact of Rouleaux”  
Advisors: Norman Wagner and Antony Beris

Chas Fields  “Intensification of Renewable 4,4’-Dimethylbiphenyl Synthesis”  
Advisors Raul Lobo and Dionisios Vlachos

Quent Harttt  “Multi-Fidelity Meta-Modeling of Complex Fluids Using Rheology-Informed Neural Networks”  
Advisor: Norman Wagner

Jinzen Hu  “Histone Tails Peptide Based Non-Viral Gene Delivery System for Treatment of Monogenic Lung Disease”  
Advisor: Millicent Sullivan

Bree Huntington  “Assessing Cellular Response in Viscoelastic Supramolecular Hydrogels for Bioinspired Three-Dimensional Cell Culture”  
Advisors: Eric Furst and April Kloxin

Dat Huynh  “Optimal Biorefinery Design Considering Carbon Pricing and Uncertainty”  
Advisors: Marianthi Ierapetritou and Dionisios Vlachos
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