Siemens Competition
Math : Science : Technology
Regional Finalist

Name: Edric Chen
High School: The Kew Forest School
Mentor: Dan Ismailescu, Hofstra University
Project Title: *Triangle-Free 4-Chromatic Unit Distance Graphs And Related Problems*

A *unit distance graph* is a graph that can be drawn in the plane so that every pair of adjacent vertices corresponds to points that are unit distance apart. A graph that does not have this property is said to be a *forbidden graph*.

The *chromatic number of a graph* is the minimum number of colors needed color the vertices, so that no two adjacent vertices are assigned the same color.

The main unsolved problem is to determine how large the chromatic number of a unit distance graph can be. It is known that certain unit distance graphs require 4 colors, while 7 colors are sufficient for any unit distance graph.

Erdos inquired about the existence of *triangle-free* unit distance graphs with chromatic number 4. The problem was solved in the affirmative in the mid 1990's; the current record graph has 23 vertices.

In this paper we construct triangle-free 4-chromatic unit distance graphs with 21, 19, and 17 vertices, respectively. We also show that 17 cannot be replaced by any smaller number.

A forbidden graph is said to be *edge minimal* if all of its subgraphs are unit distance graphs. It is known that there are exactly six edge minimal forbidden graphs of order up to 7. In this paper, we find all edge minimal forbidden graphs of order 8; there are thirteen of them.

A graph is said to be *edge critical* if the removal of any edge results in a graph with strictly smaller chromatic number. We determine all edge critical 4-chromatic unit distance graphs of order

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Names: Jun Yan He & Bongseok Jung
High Schools: Manhasset Senior High School & Herricks High School
Mentor: Dr. Patrick Cadet
Project Title: *Salicin as a Multipurpose Therapeutic Approach for Colorectal Cancer: Striking a Balance in the Regulation of COX to Maximize Benefits While Minimizing Side Effects*

Tumor viability, inflammation, carcinogenesis, pain, and metastasis represent essential targets required for effective colorectal cancer (CRC) treatment. Growing evidence points to Cyclooxygenase-2 (COX2) inhibition as a multi-therapeutic option in CRC. Through cellular and molecular analysis, our study investigated the potential of the natural COX inhibitor salicin as a multipurpose drug void of complications found with the use of conventional COX2 inhibitors. Salicin's therapeutic potential was modeled at three time points in CRC development: before carcinogenic changes, during carcinogenic changes, and after cells turned cancerous. Cellular results demonstrated salicin's ability to selectively kill and hamper the growth of human CRC cells while protecting healthy cells from carcinogenesis. Molecular results suggest that salicin normalizes oncogenic gene expressions. Specifically, salicin promoted apoptosis and cell cycle arrest in CRC cells while interfering with metastatic, pain, and inflammatory pathways. Most importantly, salicin's significant inhibition of COX2 was accompanied by a minimal inhibition of COX1. This balance of COX inhibition suggest that salicin may be accompanied with minimal to no intestinal toxicity and atherosclerotic complications. Overall, our study proposes salicin as a safe, effective, multipurpose therapeutic drug that may potentially improve current CRC treatment options and CRC patient outcomes.

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Name: Sarah Lee
High School: Syosset High School
Mentor: Dr. Iwao Ojima, Stony Brook University
Project Title: *Next Generation Fatty Acid Binding Protein Inhibitors: Computer-Aided Drug Design and Synthesis of Novel Truxillic Acid Diesters for Chronic Pain Inhibition*

Pain is a pervasive aspect of daily life—one associated with potential tissue damage and diseases. As such, it is necessary to develop small drug molecules that can target the two fatty acid binding proteins, FABP5 and FABP7, responsible for anti-nociception. Previous studies have demonstrated SB-FI-26 to be a potent inhibitor of FABP5, but a poor binder to FABP7, which has prompted the development of next-generation FABP inhibitors for greater pain relief. This study aims to optimize SB-FI-26 and identify all key components that can contribute to the selective inhibition of both FABP5 and FABP7 in order to amplify endocannabinoid-mediated agonistic effects. To do so, a four-part methodology was employed: (a) library optimization, (b) computational modeling, (c) chemical syntheses of analogs, and (d) biological tests. Of the forty-nine compounds assessed, two were predicted to inhibit both FABPs better than SB-FI-26. This ultimately revealed that the diesters with the octahydro-1H-inden2-yl moiety increased the number of intermolecular interactions with the FABP5 active site. In addition, the charged carboxylic moiety present in SB-FI-26 may not be completely necessary for potent FABP binding, which points to the prospect of using these drug candidates as a novel approach to pain relief and management.

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Names: Alia Rizvon & Vishal Nyayapathi
High School: Half Hollow Hills High School East
Mentor: Dr. Ken-ichi Takemaru
Project Title: *A Vesicular Interaction Between Basal Body Protein Chibby and CCDC11: Implications for Ciliogenesis and Related Ciliopathies*

Cilia are hair-like organelles responsible for essential biological functions. They are classified as either motile cilia or primary cilia; motile cilia are necessary for processes such as mucociliary transport, while primary cilia are responsible for mechanosensation, photoreception, and the establishment of left-right asymmetry. Defective primary cilia have been linked to laterality defects, including situs inversus and heterotaxia. Chibby (Cby) and CCDC11 are two ciliary proteins; Cby functions in ciliary vesicle formation and basal body docking, while specific CCDC11 functions are largely unknown. Recently a large-scale, in silico functional proteomics study postulated an interaction between Cby and CCDC11. We performed Co-IP assays in HEK293 cells transfected with Cby and FLAG-CCDC11, confirming a Cby/CCDC11 interaction. Furthermore, immunofluorescence and structured illumination microscopy (SIM) demonstrated that Cby and CCDC11 colocalize at vesicular structures. Consequently, we hypothesize that these proteins interact to regulate vesicle trafficking within the transition zone during ciliogenesis. Validation of a Cby/CCDC11 interaction provides further insight into the mechanisms of cilia formation and growth. This interaction may serve as an interesting model for primary ciliary dyskinesia (PCD) patients, as phenotypes of Cby-knockout (Cby-/-) mice are similar to those of PCD patients. Additionally, approximately 50% of PCD patients also present laterality defects, like situs inversus, a phenotype commonly associated with mutations in CCDC11.

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Name: Dominick Rowan
High School: Byram Hills High School
Mentor: Dr. Stefano Meschiari, The University of Texas at Austin
Project Title: *Determining The Frequency Of Jupiter Analogs And The Announcement Of A Jupiter Analog Orbiting HD32963.*

Using 109 radial velocity measurements from Keck Observatory for the Sun-like star HD32963, we identified a Jupiter analog with a 6.5-year period and a minimum mass of 0.70 Jupiter masses. Since Jupiter was a catalyst for the developing Solar System, calculating the frequency of Jupiter analogs is a precursor to determining the occurrence of Solar System analogs. Due to the long period of Jupiter analogs, an extensive baseline of observation is needed. Stars in the Keck radial velocity survey have accumulated baselines up to 18 years, providing ample data for analysis. We first fit planets using local minimization and the Markov-Chain Monte Carlo algorithm in the Systemic application. Planets with periods between 5 – 15 years and mass between 0.3 – 3 MJup, with an eccentricity < 0.3, are considered Jupiter analogs. The raw frequency was calculated to be .71%, since there are 8 Jupiter analogs within the Keck radial velocity survey. We then calculated the detection limit to assess the ability to recover Jupiter analogs within the parameter space for each star in the sample. Using this information to correct the raw frequency for detectability, we found the frequency of Jupiter analogs to be 3%.

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Names: Kevin Sadhu & Arvind Sridhar
High Schools: Manhasset Senior High School & Bellarmine College Prep School
Mentor: Dr. Miriam Rafailovich, Stony Brook University
Project Title: *Synthesis and Application of Novel, Cost-Effective, Biomimetic Hydrogels Doped with Nanoscale Graphene Oxide as Scaffolds for Tissue Engineering and Drug Delivery Abstract*

As the fields of tissue engineering and drug delivery move closer to clinical applications, challenges of engineering inexpensive scaffolds with biomimetic properties persist. To address these issues, previous studies have synthesized water-swollen, cross-linked hydrogels; however, the gels' weak mechanical properties limited their viability. The discovery of versatile nanoscale graphene oxide (nGO) has opened up avenues for hydrogels to overcome these limitations and demonstrate enhanced structural stability, biocompatibility, and physiological viability. Therefore, this study engineered cross-linked, nGO-doped gelatin hydrogels and characterized them through Rheology, FTIR, Contact Angle, and Thermogravimetric Analysis. The nGO-doped hydrogels exhibited a stiffer structure (~17.9 kPa elastic modulus) with increased biocompatibility and water retention capacity. Furthermore, the gels showed potential as anti-cancer drug delivery vehicles when they suppressed cancerous keratinocyte growth. Additionally, they exhibited significant dermal fibroblast cytotoxicity, indicating their potential as scaffolds for anti-fibrotic tissue engineering. Finally, the nGO-doped hydrogels were optimized for the loading and sustained release of curcumin, a common cancer therapeutic, to expand their applicability as drug delivery vehicles. Overall, this study proposed nGO-doped gelatin hydrogels as novel and cost-effective scaffolds to tackle the issues facing tissue engineering and drug delivery.

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Names: Kameron Sedigh
High School: Kings Park High School
Mentor: Dr. Peter J. Tonge, Stony Brook University
Project Title: *Domain Modeling and Kinetics Studies of MenE, an acyl-CoA Synthetase of the Bacterial Menaquinone Biosynthesis Pathway, and Other Adenylate-Forming Enzymes*

The increasing drug resistance among Gram-positive bacteria such as methicillin-resistant Staphylococcus aureus (MRSA) has become a growing threat and thus the necessity for novel antibacterial targets is as imperative as ever. Bacterial menaquinone biosynthesis and the enzymes within its pathway are promising targets for novel drug discovery and development against drug-resistant bacteria because menaquinone functions as the lipid-soluble electron carrier in the electron transport chain of bacteria and humans lack this biosynthetic pathway. This study focused on MenE, the o-succinylbenzoate-CoA Synthetase of the biosynthesis pathway. In order to gain insight on the structure and function of the domains and specific residues of the enzyme, S. aureus MenE was compared to other ANL superfamily enzymes, and steady-state kinetics and isothermal titration calorimetry was run on saMenE mutants. 3D alignment and analysis of saMenE and ANL enzymes identified a potential function of the C-terminal domain of ANL enzymes to be that of a binding domain and ITC results of a removed C-terminus saMenE confirmed that the C-terminal domain is necessary for binding to ligands. Steady-state kinetics of site-directed saMenE mutants discovered important catalytic residues in the active site of MenE, elucidating the molecular details of each half reaction. Therefore, the C-terminal domain and key conserved catalytic residues can serve as novel targets for antibacterial drug development against MenE and the entire ANL superfamily of enzymes.

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Names: Kunal Shah, Brian Rhee & Roshan Patel
High Schools: Syosset High School, Half Hollow Hills High School East & Ward Melville Senior High School
Mentor: Mr. Hongfei Li
Project Title: *Enhanced Power Output and Tolerance to Fuel Impurities Demonstrated in a Polymer Electrolyte Membrane Fuel Cell Utilizing a Graphene Oxide Nanoparticle Coated Nafion® Membrane*

Polymer electrolyte membrane fuel cells (PEMFC's) are promising frontrunners of the future's green energy production; however, they are not widely used today because of their low efficiency under impure fuel sources containing carbon monoxide, a poison that destroys platinum catalysts in the fuel cell. When used as an internal component of the Nafion® membrane, graphene oxide (GO) nanoparticles (NPs) demonstrated potential in increasing the self-humidification and proton conductivity of the PEMFC. Specifically, the role of GO NPs in possibly mitigating CO poisoning or in assisting in hydrogen dissociation at the anode was studied. GO NPs were prepared as 1 mg/mL solutions in either water/methanol (GO-WM) or dimethylformamide (GO-DMF) solvents. Subsequently, a Langmuir-Blodgett (LB) trough was used to obtain isothermal curves to determine optimal GO-monolayer coating pressures. GO-DMF membranes coated at 8 mN/m produced the highest maximum power output of 267 mW, representing a 102% increase over the uncoated membrane. Furthermore, CO poisoning tests demonstrated that the 8 mN/m GO-DMF coated membrane underwent a 150% increase in maximum power output as compared to uncoated membranes in the CO poisoning environment. The increased efficiency under pure and impure fuel sources may allow PEMFCs to be more cost-efficient and viable in new applications.

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Names: Kimberly Te & Christine Yoo
High School: Manhasset Senior High School
Mentor: Peter Guastella
Project Title: *Natural, Cost-Effective Anodes for Optimized Sediment Microbial Fuel Cells: Engineering a Novel Approach to Harvesting Energy and Cleaning Up Oil-Polluted Regions*

To address clean energy and pollution issue, microbial fuel cells (MFCs) were hypothesized to simultaneously generate electricity and remediate oil spill pollution. The purpose of this study was to engineer efficient, cost-effective MFC anodes that optimize electrical output and oil remediation using structural and surface coating configurations. For structure, carbonized Luffa aegyptiaca, loofah sponges (LS), were tested as cheaper 3-dimensional (3D) alternatives to commercial materials (carbon fiber and RVC). For surface coating, hybrids were synthesized to increase electrical properties. Coatings were uncoated, TiO2, graphene, and graphene/TiO2 composite. Nine anode designs were made from these structure/coating combinations. MFCs were implemented in different conditions to assess oil remediation. A multimeter measured electrical outputs; UV-VIS spectroscopy measured oil degradation. Results showed anodes improved oil degradation. LS-structure groups had significantly higher power densities than standard 2D and 3D anodes. LS-graphene/TiO2 had the highest power density (2087.1 mW/m2) and oil remediated (93%). This suggests structure and surface coating synergistically improve surface area, biocompatibility, and electrical conductivity for optimized MFC performance. LS are over 90% cheaper than RVC and come from accessible, sustainable sources. This MFC design shows potential towards remediating oil spills and providing clean energy for industries, remote sensors, and developing nations.

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Name: Julian Ubriaco
High School: Kings Park High School
Mentor: Tobiloba Oni
Project Title: *Identification and Characterization of Novel Diagnostic and Therapeutic Targets in Pancreatic Ductal Adenocarcinoma Using an Antibody-based Approach*

Pancreatic Ductal Adenocarcinoma (PDAC) is the fourth-leading cause of cancer related death in the U.S. with a median survival period of less than six months. Better means of detection and more effective therapeutics are needed to improve PDAC survival. In other types of cancer, antibody-based diagnostics and therapeutics such as Herceptin have experienced success in the clinic (Baselga, 2001). This project employed an antibody-based approach to the recently developed 3D pancreatic organoid culture system to identify and characterize novel PDAC biomarkers to be used in the detection and treatment of malignancy. Tumor-specific monoclonal antibodies (mAbs) and Antigen-binding Fragments (Fabs) were developed using the hybridoma and phage display technologies, respectively. Antibodies were then validated for tumor organoid binding and cell surface localization using cell-based ELISA, immunofluorescence, immunoprecipitation-western blot, and flow cytometry. Hybridoma mAb 31 was identified, validated as tumor-specific and shown to bind a tumor-associated cell surface antigen via IP western blot. Fabs A3 and B2 were identified and validated as tumor-specific Fabs that localize to the cell surface as determined by flow cytometry. In conclusion, this study identified three novel antibody-based molecules targeting PDAC-associated antigens and validated the potential of a pancreatic organoid-based antibody approach in antigen discovery.