Siemens Competition
Math : Science : Technology
Regional Finalist

Names: Sriharshita Musunuri
High School: Henry M. Jackson High School
Mentor: Dr. Chris Lausted, Institute for Systems Biology
Project Title: Computational and Experimental Design of MIP Nanoparticles: A Novel Theranostic Solution to Detect and Neutralize Endotoxins

Lipopolysaccharides (LPS) are harmful biomolecules found on the surface of gram-negative bacteria and are responsible for over 50% of sepsis cases, the leading cause of death in US hospitals. Past efforts to detect and extract LPS effectively have been hampered by high synthesis costs, or incompatibility with body fluids. In this research, the lock-and-key mechanism of molecularly imprinted polymers was utilized to design selective fluorophore-conjugated nanoparticles capable of simultaneous LPS detection and neutralization. A novel polymer matrix was modeled by utilizing GROMACS to optimize LPS affinity and simulate several template-monomer interactions. Analysis of reaction spontaneity and non-bonding interactions indicated that itaconic acid copolymerizes with EGDMA to form the most effective LPS-imprints. These computational results were translated to experimental synthesis of MIP nanoparticles by precipitation polymerization. FT-IR results showed the formation of LPS-specific bonds between the template and polymeric nanoparticles, while SPR confirmed sensitivity on the order of 2.2 pM under blood plasma-like conditions, and fluorescence spectroscopy indicated a correlation between LPS concentration and fluorophore intensity ($p<0.05$). Based on comparisons to the standard LAL assay, these polymers bind endotoxins for a fraction of the cost and could be applied both in vivo and in pharmaceuticals to decrease the effects of gram-negative sepsis and LPS contamination.

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Names: Arnob Das
High School: Jesuit High School
Mentor: Dr. Shankar Rananavare
Project Title: Room Temperature Tunable Ferromagnetism in Solution Grown Mesoscopic Doped Conjugated Polymer Rings

Conventionally, ferromagnetic materials are restricted to metals such as iron and nickel. Although syntheses in the literature have been attempted to induce ferromagnetism in organic polymers, most require sufficiently low temperature, have low magnetic strength, and no tunability, inhibiting practical applications. This research demonstrated a method for synthesizing tunable ferromagnetic conjugated polymers at room temperature without aid of metals. Room temperature existence of the Peierls instability in mesoscopic ring structures of doped conjugated polymers was hypothesized as rationale for ferromagnetism. Modified one-pot solution based templating method was employed to form doped polyaniline rings/cylinders, evidenced in Atomic Force Microscopy (AFM) and Scanning Electron Microscopy (SEM) images. Vibrating Sample Magnetometry (VSM) data for low radii (mean ~39 nm) polyaniline ring demonstrated hysteresis loop, indicating ferromagnetic signature. With increasing ring size (~300 nm) hysteresis loop shrunk and magnetic strength reduced, completely diminishing for larger rings (~25 μm). Chemical shift from liquid Nuclear Magnetic Resonance (NMR) corroborated VSM data, demonstrating tunability of magnetic strength with size variation by controlling templating. Saturated DC magnetization of the low radii doped polyaniline rings was 0.421 emu/g from Physical Property Measurement System (PPMS), the highest ever magnetic strength achieved for fully organic polymer magnets at room temperature.

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Names: Sohini Kar
High School: Saratoga High School
Mentor: Dr. Simon Rubinstein-Salzedo
Project Title: *Factorization of Recurrence Relations*

This paper presents a new integer sequence $a_n = u_{\lfloor \frac{n}{k} \rfloor + 1}^{k-z} u_{\lceil \frac{n}{k} \rceil + 1}^{z}$ where the equation $u_n = pu_{n-1} + qu_{n-2}$ is a generalized second-order or Horadam recurrence relation with $n, k, p, q, z \in \mathbb{Z}$, $u_0 = 0$, $u_1 = 1$, and $z = n - k\lfloor \frac{n}{k} \rfloor$. The pictorial representation for this sequence is illustrated by the number of ways we can tile a $1 \times n$ board broken into k almost-equal pieces with 1×1 square with p colorings and 1×2 rectangles with q colorings. A recurrence relation and the generating function is derived for this new sequence. The results are used to show the recurrence relation between Horadam sequence and this new sequence. The illustration of this result shows how the new sequence can be constructed by breaking the Horadam sequence.

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Names: Pushkar Shinde
High School: Oregon Episcopal School
Mentor: Dr. Monika Davare
Project Title: Aptamer Based Disruption of the CD47:SIRPα interface for Anticancer Applications

Cancer – the uncontrolled proliferation of abnormal body cells – is a leading cause of morbidity, mortality, and healthcare expenditures worldwide. Cancerous cells often upregulate evasive pathways in order to elude innate and adaptive immune responses. One such pathway involves the ubiquitously expressed receptor CD47, which interacts with macrophage expressed SIRPα to inhibit the phagocytic response. Agents that disrupt this interaction have been shown to revive the innate anticancer immune response *in vitro* and *in vivo*, and a humanized monoclonal antibody against CD47 is currently entering clinical trials. However, antibodies have significant functional limitations that complicate therapeutic use, and major questions remain regarding the mechanism of action and the reproducibility of the tumoricidal effects of this antibody. Thus the development of a tool to disrupt the CD47:SIRPα interaction without the limitations associated with antibodies is critical. This project seeks to develop and characterize nucleic acid aptamers – small sequences of nucleic acids or derivatives that can be selected to bind to a variety of targets with extraordinary affinity and specificity – that target the CD47:SIRPα interaction. Several candidate aptamer sequences were obtained, and five were screened. Three aptamers, PS04, PS35 and PS65, demonstrated affinity ranging from 2-10 μM for SIRPα and can bind to surface expressed SIRPα in U937 cells. Further screening, characterization and optimization are underway.

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Names: Muhammad Shahir Rahman
High School: Westview High School
Mentor: Mourad Souag
Project Title: A Smart-Burn/Spill Proof "SAFE" Microwave That Spares the Salad: Novel Application of Levenberg-Marquardt Algorithms and Machine Learning for Real-time Thermodynamic Modeling

The microwave oven is a commonplace appliance used by millions worldwide. Even after half a century from its commercialization, no fundamental improvement has occurred. Although economical, the platform remains relatively unsafe. All common cooking apparatus are primarily user-selected time driven, with no understanding of the food status causing over/undercooking. Even the smartest of the breeds require food-type, weight, volume, as inputs. Detecting food properties without input parameters, although an essential objective, has not been possible until this interdisciplinary innovation.

This project pioneers a novel application of mathematical optimization and machine learning analysis for real-time thermodynamic modeling of heat propagation, and radiation focus management. Employing a multi-iterative systems engineering approach, many heat-absorption scenarios have been analyzed resulting in complete auto-detection of a broad spectrum of food-types. Using a low-cost, touchless thermopile-array-sensor, virtual real-time optimization leads to customized user-differentiated, cooking/reheating experience for lip-ready food. With only single parameter measurement, bounded interdependent food characteristics have been solved.

A plethora of smart features are included such as selective heating, infrared-map-telemetry and temperature personalization. This patent-pending original work introduces sophisticated IoT architecture, allowing a truly burn/spill-proof and zero-user-input experience. A fully-functional prototype was created by retrofitting an ordinary oven with a microcontroller.

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Regional Finalist

Names: Guanpeng Xu, Wendy Wu
High School: Phillips Academy Andover
Mentor: Guangyi Yue
Project Title: Higher Gonalities of Erdös-Rényi Random Graphs

In this report, we consider the asymptotic behavior of the second and higher gonalities of an Erdös-Rényi random graph and provide upper bounds for both via the probabilistic method. Our results suggest that for sufficiently large n, the second gonality of an Erdös-Rényi random Graph G(n,p) is strictly less than and asymptotically equal to the number of vertices under a suitable restriction of the probability p. We also prove an asymptotic upper bound for all higher gonalities of large Erdös-Rényi random graphs that adapts and generalizes a similar result on complete graphs. We suggest another approach towards finding both upper and lower bounds for the second and higher gonalities for small $p=c/n$ using the Riemann-Roch theorem, and fully determine the asymptotic behavior of arbitrary gonalities when $c \leq 1$.

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Names: Arjun Subramonian and Kelly Ho
High School: Monta Vista High School and Cupertino High School
Mentor: Dr. Graeme Smith
Project Title: A Novel Method for Age Estimation in Solar-Type Stars Through *GALEX* FUV Magnitudes

Utilizing an inverse association known to exist between Galaxy Evolution Explorer (*GALEX*) far ultraviolet (FUV) magnitudes and the chromospheric activity of F, G, and K dwarfs, we explored a method of age estimation in solar-type stars through *GALEX* FUV magnitudes. Sample solar-type star data were collected from refereed publications and filtered by B-V and absolute visual magnitude to ensure similarities in temperature and luminosity to the Sun. We determined FUV-B and calculated a residual index *Q* for all the stars, using the temperature-induced upper bound on FUV-B as the fiducial. Plotting current age estimates for the stars against *Q*, we discovered a strong and significant association between the variables. By applying a log-linear transformation to the data to produce a strong correlation between *Q* and log_e *Age*, we confirmed the association between *Q* and age to be exponential. Thus, least-squares regression was used to generate an exponential model relating *Q* to age in solar-type stars, which can be used by astronomers. The Q-method of stellar age estimation is simple and more efficient than existing spectroscopic methods and has applications to galactic archaeology and stellar chemical composition analysis.

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Regional Finalist

Names: Charles Huang, Ethan Hsiao
High School: Lynbrook High School and Cupertino High School
Mentor: Dr. Mervin Zhao
Project Title: Characterization of 2D Molybdenum Disulfide CVD Crystal Growth for Nano Scale Photonics and Transistors

The electronic and optical properties of molybdenum disulfide make it a potential material for the scaling down of transistors and the engineering of 2D optoelectronic devices. Chemical Vapor Deposition (CVD) is a developing method of MoS_2 synthesis, with the potential of synthesizing consistent monolayer crystal. Currently, there is no systematic study focused on the relationship between the number of MoS_2 crystal layers and solid state MoO_3 : Sulfur precursor ratios. This information would aid in the implementation of MoS_2 in industrial settings. By analyzing a proposed reaction mechanism and the effect of sulfur pressure, we hypothesized that higher molar ratios of MoO_3 : S are correlated with greater yields of monolayer crystal. The effect of precursor molar ratio on crystal layering was analyzed through the preparation of 6 molar ratio variants and subsequent microscopy, photoluminescence, and Raman spectroscopy. From the scanning optical microscopy, a sample was observed with a new undocumented wire structure with unique optical properties. The Raman and photoluminescence spectra were analyzed to characterize the degree of layering and their viability as nano-photonic materials, respectively. From the analysis of three data forms, a higher ratio of MoO_3:S was shown to be correlated with greater yields of monolayer crystal.

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Names: Rachana Madhukara, Kevin Ren, and Anlin Zhang
High School: Canyon Crest Academy, Torrey Pines High School
Mentor: Professor Laura Schaposnik
Project Title: Epidemic Dynamics on Symmetric Networks

Since social interactions have been shown to lead to symmetric clusters, we propose here that symmetries play a key role in epidemic modeling. Mathematical models on d-ary tree graphs were recently shown to be particularly effective for simple networks by Seibold-Callender. To account for symmetric relations, we generalize this to a new type of network modeled on d-cliqued tree graphs, which are obtained by adding edges to regular d-trees to form d-cliques. This setting gives a more realistic model for social networks which consist, for instance, of families or a group of cities. Specifically, we quantify how an infection starting in a clique (e.g. family) can reach other cliques through the body of the graph (e.g. public places). Moreover, we propose and study the notion of a *safe zone*, a subset that has a negligible probability of infection. Finally, since many of society's interactions are described by random networks satisfying non-random constraints (e.g. spacial proximity), we make this problem mathematically precise by introducing M-Rado graphs, which are random graphs dependent on a function M, and give bounds on their connectivity and clique density. Thus, our new results provide a mathematical foundation for implementing symmetric constraints in epidemic modeling.

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Names: Thomas Chen[1], Alexander Wang[2], Kevin Gao[3]
High School: Mission San Jose High School[1], Dougherty Valley High School[2], Amador Valley High School[3]
Mentor: Miriam Rafailovich
Project Title: P12 Peptide's Suppressive Effects on Fibrinogen Fiber Formation and Novel Application of Machine Learning in Fiber Counting

Abstract: P12 is a recently discovered fibronectin-derived peptide that has been shown to reduce erythrocyte aggregation in burn wounds, which suggests its usefulness in countering thrombosis [1, 11]. This paper further shows that both types of P12 -- linear P12 and circular P12 --inhibit fibrinogen fiber formation by inhibiting fibrin's αC domains. The substrates on which fibers were grown were spun-cast with monodispersed polystyrene (200k molecular weight). Two types of purified fibrinogen-fibrin solutions—50P (fibrin-rich) and 50S (fibrin-poor)—were added with or without P12 onto the wafers for either 10 minutes, 1 hour, or 8 hours. ImageJ and Machine Learning were utilized to count the area covered by fibers in the optical and atomic-force microscope images. For the 8-hour samples, the mean fiber densities of the P12 substrates showed a ten-fold decrease from those of the control substrates, demonstrating that P12 inhibited the formation of fibrinogen fibers in the 50P solution. Furthermore, the results for the fibrin-poor 50S show that fibrin monomers are necessary in clot formation, suggesting that P12 inhibits fiber formation by interacting with the αC domains on the fibrin monomers. Finally, studies have shown that the endothelial cells are critical in preventing vascular thrombosis since they block platelet binding, in turn preventing the release of thrombin to induce clotting [13]. In this paper, incubation with endothelial cells show no significant difference regardless of presence of P12, indicating that P12 inhibits clot formation while preserving endothelial cells. Thus, the results provide evidence that P12 can be effectively used to counter thrombosis.