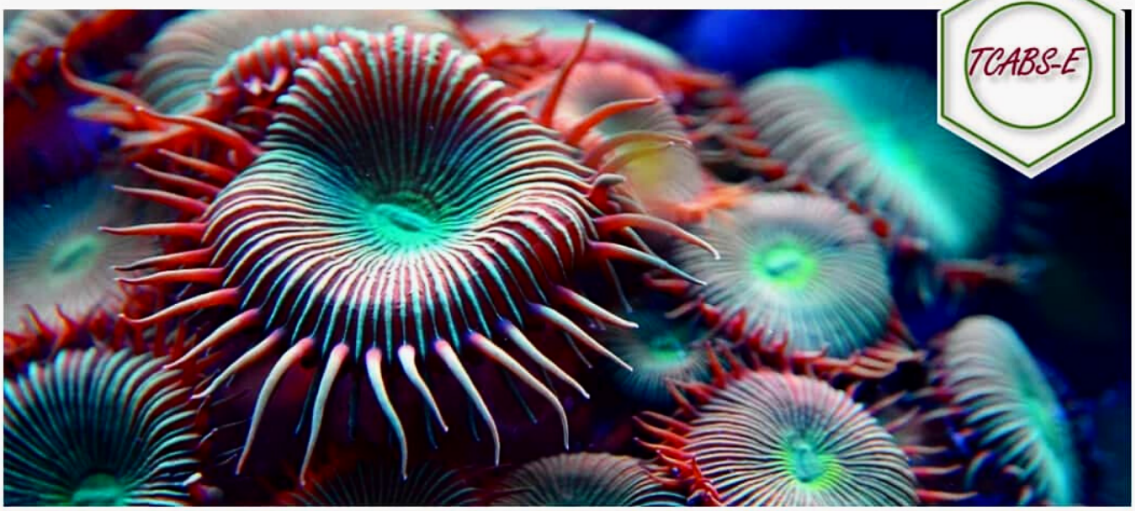
VISAKHA LIFE SCIENCES & ENTREPRENEURSHIP (VLSE) SYMPOSIUM 2022



DATE: 24TH & 25TH Nov, 2022

Venue: Andhra University

No registration fee for students with valid ID cards but registration is mandatory

Exciting prizes for best oral and poster presentations e-certificates will be provided

LAST DAY FOR ABSTRACT SUBMISSION: 10TH NOV 2022

https://tcabse.org/vlse-2022

tcabse.india@gmail.com

+91-8660301662

SCAN & REGISTER

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INTRODUCTION

The Visakha Life Sciences & Entrepreneurship (VLSE) Symposium is a unique opportunity for Undergraduates, Postgraduates, Research scholars, Faculty members, Scientists and Entrepreneurs created by The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E) in collaboration with the prestigious Andhra University in Visakhapatnam, Andhra Pradesh, India. This year the VLSE Symposium-2022 is focused on all the local educational institutions within the vicinity of Visakhapatnam. The goal of VLSE Symposium-2022 is to primarily give an opportunity to the students to show off their original research work! However, we understand that not everyone has their own original research work so we encouraged literature review presentations as well as any topic of public importance that has relevance to either Life Sciences or Entrepreneurship or both.

ORGANIZERS

The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E) is proudly organizing the Visakha Life Sciences & Entrepreneurship (VLSE) Symposium in collaboration with the prestigious Andhra University in Visakhapatnam, Andhra Pradesh, India.

MoU signing and exchange ceremony between TCABS-E and Andhra University. Delegates present in this ceremony: (from left to right) Mr. Ravi Eswarap (CEO, AU Incubation centre); Prof. U. Shameem (Emeritus faculty, Department of Zoology, AU); Prof. V. Krishna Mohan (Registrar, AU); Prof. P.V.G.D. Prasad Reddy (Hon'ble Vice Chancellor of AU); Dr. Ravikiran Yedidi (Founder of TCABS-E); Prof. K. Samatha (Rector, AU) and Prof. K. Srinivasa Rao (Principal, College of Science & Technology, AU).

PROGRAM OVERVIEW

Day-1, Nov 24th (9:30 am - 5:00 pm), Venue: Department of Zoology, Andhra University.

09:30 am-11:00 am: Registrations at the door! Valid student/faculty ID cards issued by their respective institutions are required for registration fee waivers.

11:00 am-11:30 am: Inauguration & Introduction.

- Inauguration by the Hon'ble V.C. of Andhra University, Prof. P. V. G. D. Prasad Reddy and the Registrar of Andhra University, Prof. V. Krishna Mohan.
- Introduction to TCABS-E and VLSE Symposium-2022 by Dr. Ravikiran S. Yedidi, Founder, TCABS-E.

11:00 am-11:15 am: Snacks & Beverages!

11:00 am-01:00 pm: Poster session - 1 (P1 to P20).

11:30 am-12:30 pm: Guest Lecture by **Dr. Ramesh Babu, Boga.**
President & Managing Director, BogaR Laboratories LLC, USA & India.

01:00 pm-02:00 pm: Lunch Break!

02:00 pm-04:00 pm: Poster session - 2 (P21-P40).

02:00 pm-04:00 pm: Oral presentations session - 1 (T1-T8).

04:00 pm-05:00 pm: TCABS-E Internship certificate issue ceremony.

Day-2, Nov 25th (9:00 am - 5:00 pm), Venue: Department of Zoology, Andhra University.
(*e-Posters will be on display throughout the day*).

09:30 am-11:00 am: Workshop on Bioinformatics.

11:00 am-01:00 pm: Poster session - 3 (P41-P60).

11:00 am-01:00 pm: Oral presentations session - 2 (T9-T16).

01:00 pm-02:00 pm: Lunch Break!

02:00 pm-04:00 pm: Poster session - 4 (P61-P80).

02:00 pm-04:00 pm: Oral presentations session - 3 (T17-T24).

04:00 pm-05:00 pm: VLSE Symposium-2021 concluding remarks and prizes for winners!

Guest Lecture: Newer Trends of Drug Discovery and Development

Dr. RameshBabu Boga
President and Managing Director.
BogaR Laboratories LLC, Suwanee (GA), USA.
BogaR Laboratories, Peddapuram (A.P.), INDIA.

Dr. RameshBabu Boga is the President and Managing Director of BogaR Laboratories in USA and India, and he is Visiting Professor/Corporate Advisory Member in Reva University, Bangalore (Karnataka), and an Adjunct Professor in VIT University, Vellore (Tamil Nadu) and Shri Vishnu College of Pharmacy, Bhimavaram (Andhra Pradesh) and Jamia Hamdard (Deemed University), New Delhi (Delhi). In that past, he was an adjunct faculty in the Department of Pharmacology at Emory University School of Medicine, Atlanta (USA). Dr. Boga received his Ph.D., (1990) from Indian Institute of Technology (IIT-Madras), Chennai (India) and had his pre-doctoral and postdoctoral experience at Kyoto University (Japan) and University of Michigan Medical School (Ann Arbor, USA). He was appointed as Research Assistant Professor in Department of Biochemistry at Medical college of Wisconsin (Milwaukee, USA), and later he took several industry positions in pharma and diagnostic companies before starting his own company, BogaR Laboratories in 2007.

Dr. Boga is a diversified scientist and entrepreneur, and his contributions are significant in organic chemistry, biochemistry, medicinal chemistry, clinical chemistry, and food chemistry. He has published 24 research articles, and obtained over 30+ patents (23 US patents, 2 European, and 6 Indian patents). His research contributions are significant in developing Nitric Oxide Synthase (NOS) inhibitors, selective neuronal NOS inhibitor of Vinyl-L-NIO, and also other inhibitors for kinases, food mycotoxins, and TB. In the area of sensors and diagnostics, he has contributed several patented technologies for hormonal and bone-resorption biomarkers, bacterial vaginosis, H. Pylori infection, and ovulation. He is the member of American Chemical Society (ACS) and American Society for Biochemistry and Molecular Biology (ASBMB). His current focuses are promotion of science and its importance to the younger generation in India by visiting various universities/institutions and also involving more of the industry-academic collaborations.

Selected publications and patents:

1. Agarwal, B., Karthikeyan, R., Gayathri, P., Babu, B.R., Ahmed, G., Jagannadham, M.V.: "Studies on the mechanism of multidrug resistance Acinetobacter baumannii by proteomic analysis of the outer membrane vesicles of the bacterium", J. Proteins Proteomics, 10, 1-15 (2019).
2. Dhanamjayulu, P., RameshBabu, B., Alka, M.: "Inhibition of Aflatoxin B1 biosynthesis and down regulation of aflR and aflB genes in presence of benzimidazole derivatives without impairing the growth of Aspergillus flavus", Toxicon, 170, 60-67 (2019)
3. RameshBabu, B.: "Antibody pair screening methods" U.S. Patent, No. 6,998,241 dated February 14, 2006.
4. RameshBabu, B., Frey, C., Griffith, O.W.: "L-Arginine binding to nitric oxide synthase: The role of H-bonds to the non-reactive guanidinium nitrogens" J. Biol. Chem., 274, 25218-25226 (1999).
5. RameshBabu, B., Griffith, O.W.: "N5-(1-Imino-3-butenyl)-L-ornithine: A neuronal isoform selective mechanism-based inactivator of nitric oxide synthase. J. Biol. Chem., 273, 8882-8889 (1998).
6. RameshBabu, B., Vaz, A.D.N.: "1,2,3-Thiadiazole: A novel heterocyclic heme ligand for the design of Cytochrome P450 inhibitors" Biochemistry, 36, 7209-7216 (1997).

Details of Oral presentations:

Session-1 (T1-T8): Nov 24th, 2:00pm-4pm.

T1. 2:00pm-2:15pm: Design, Synthesis & Evaluation of "The HelicoTAC©" a PROTAC-based small molecule targeting the *Helicobacter pylori* virulence factor, Cag-A protein as a potential therapeutics for gastric ulcers, gastritis and gastric cancers.

Presented by: ***Madhumita Aggunna**, Juniorette Assistant Professor, **TCABS-E**.*

T2. 2:15pm-2:30pm: Success of Current COVID-19 Vaccine Strategies vs. the Epitope Topology of SARS-CoV-2 Spike Protein-Receptor Binding Domain (RBD): A Computational Study of RBD Topology to Guide Future Vaccine Design.

Presented by: ***Santhinissi Addala**, Juniorette Assistant Professor, **TCABS-E**.*

T3. 2:30pm-2:45pm: Basics of Biofloc technology and its importance in aquaculture.

Presented by: ***Khadem Hussain Saeedi**, Research Scholar, Department of Zoology, **Andhra University**.*

T4. 2:45pm-3:00pm: Screening of human-friendly bacteria and redesigning them using Synthetic Biology, to develop a potential synthetic bacterium with built-in genetic circuits for PETase based plastic bio-degradation.

Presented by: ***Madhuri Vissapragada**, Juniorette Assistant Professor, **TCABS-E**.*

T5. 3:00pm-3:15pm: Photocatalytic Degradation of Indigo Carmine Dye using $CuBi_2O_4$ Nanocatalyst and Effect of Various Operational Parameters.

Presented by: ***Dr. Sailaja, B. B. V.**, Associate Professor, Department of Chemistry, **Andhra University.***

T6. 3:15pm-3:30pm: Sequence homology-based identification of paracetamol metabolizing enzymes in chicken liver homogenates for *in vitro* drug metabolism studies.

Presented by: ***Niharikha Mukala**, Juniorette Assistant Professor, **TCABS-E**.*

T7. 3:30pm-3:45pm: Converting Trash to usable biofuels for homes and automobiles in the campaign to save the climate by reducing climate change and Greenhouse emissions.

Presented by: ***Kiryowa Idrisa**, Student, **GITAM deemed to be University.***

T8. 3:45pm-4:00pm: Biophysical Approach For Treating Esophageal Squamous Cell Carcinoma With The Help Of Protein Liquid Liquid Phase Condensates.

Presented by: ***Manikanta Sodasani**, Program Manager, **TCABS-E**.*

Session-2 (T9-T16): Nov 25th, 11:00am-1pm.

T9. 11:00am-11:15am: A spotlight on host-microbiome interactions and their therapeutics.

Presented by: ***Dr. Sudhakar Pola****, Assistant Professor, Dept. of Biotechnology,* ***Andhra University****.*

T10. 11:15am-11:30am: A Radical Solution for Human health.

Presented by: ***Jahnavi Chintalapati****, Program Manager,* ***TCABS-E****.*

T11. 11:30am-11:45am: Structural analysis of TP53 in association with different ligands in the context of Cancer.

Presented by: ***Srividya Inemella****, Student, Dept. of Pharmaceutical Biotechnology,* ***Andhra University****.*

T12. 11:45am-12:00pm: Inhibiting Matrix Metalloproteinases by the Tissue Inhibitors of Metallo-proteinases in intimal thickening and atherosclerotic plaque rupture.

Presented by: ***Hemsai Palla****, Scientist Trainee,* ***TCABS-E*** *& student, Dept. of Biotechnology,* ***Andhra University****.*

T13. 12:00pm-12:15pm: Review on phytochemical secondary metabolites of five wild mushroom extracts and their Antimicrobial activity.

Presented by: ***Jayalakshmi Rompilli****, Student, Dept. of Microbiology,* ***St. Ann's College for Women****.*

T14. 12:15pm-12:30pm: Industrial wastewater treatment with a bioelectrochemical process: assessment of depuration efficiency and energy production.

Presented by: ***Sumaiyah Soghra****, Student,* ***M. V. R. Degree and P. G. College****.*

T15. 12:30pm-12:45pm: Narcotics And Its Constituents.

Presented by: ***Anandsai Sahini*** *&* ***Anilkumar Budi****, Students,* ***Aditya Degree College-Gopalapatnam****.*

T16. 12:45pm-1:00pm: Comparative Evaluation of Wheat Protein Extract from Natural and Commercial Wheat Flour.

Presented by: ***Nandhini Perla****, Student, Dept. of Microbiology,* ***St. Ann's College for Women****.*

Session-3 (T17-T24): Nov 25th, 2:00pm-4pm.

T17. 2:00pm-2:15pm: Structural analysis of Rev protein in association with different ligands in context of HIV.

Presented by: ***Raviteja Kolluru****, Student, Dept. of Pharmaceutical Biotechnology,* ***Andhra University****.*

T18. 2:15pm-2:30pm: Synergistic effects of Aq. Theobroma Extract and Doxorubicin on Therapeutic Resistant Cervical Cancer Cells.

Presented by: ***Prasanthi Chittineedi****, Student, Dept. of Biochemistry,* ***GITAM deemed to be University****.*

T19. 2:30pm-2:45pm: An Analysis Of BRCA1 Gene Taking Breast Cancer Into Account.

Presented by: ***Hanisha Penta****, Student, Dept. of Microbiology,* ***Andhra University****.*

T20. 2:45pm-3:00pm: Lumpy skin disease in cattle.

Presented by: ***Chandrika Kona****, Student,* ***Andhra University****.*

T21. 3:00pm-3:15pm: A preliminary screening on biodegradability of face masks and their impact on plant growth of *Hibiscus sabdariffa*.

Presented by: ***Atheena Paul****, Student, Dept. of Microbiology,* ***St. Ann's College for Women***.

T22. 3:15pm-3:30pm: Design, Synthesis & Evaluation of "Rheumatoid Arthritis" novel topology of antibody-antigen interaction: human IgM rheumatoid factor Fab bound to its autoantigen IgG Fc.

Presented by: ***Sapana Kumari****, Student,* ***St. Joseph's College for Women***.

T23. 3:30pm-3:45pm: Edible Oil And Its Constituents.

Presented by: ***Dineshchandra Ponaganti*** & ***Shyamprasad Karri****, Students,* ***Aditya Degree College-Gopalapatnam***.

T24. 3:45pm-4:00pm: Preparation and comparison of herbal sanitizer with different extracts- anti microbial activity and phytochemical activity.

Presented by: ***Vasanthalakshmi Surisetty****, Student, Dept. of Chemistry,* ***St. Ann's College for Women***.

T25. 4:00pm-4:15pm: Increase in the predicted mRNA stability of certain SARS CoV-2 mutant spike proteins compared to wild type may pose potential risk to vaccines.

Presented by: ***Abinav Grandhi****, Scientist Trainee,* ***TCABS-E***.

Details of Poster presentations:

Day 1 - Nov 24th, 2022.

Poster session - 1 (P1 to P15): 11:00am-1pm.

- P01 - Ahila, B.
- P02 - Charles, K.
- P03 - Esther, G.
- P04 - Gangadhar, K.
- P05 - Joel, Ch.
- P06 - Mythili, A.
- P07 - Nirmala, K.
- P08 - Nombuso Lolo, F.
- P09 - Phaneendra, G.
- P10 - Pranavi, A.
- P11 - Ruby, P.
- P12 - Sai Mounika, P.
- P13 - Sravan Kumar, V.
- P14 - Subhakanth, S.
- P15 - Vineetha, L.

Poster session - 2 (P16 to P30): 2:00pm-4pm.

P16 - Alekhya, A.
P17 - Anjani, Ch.
P18 - Anupama, D.
P19 - Jayasurya, N.
P20 - Lakshmi Meghana, M.
P21 - Muskan, B.
P22 - Rachana, G.
P23 - Ramya Saisri, J.
P24 - Reshma, K.
P25 - Sai Rupa, R.
P26 - Siri Hanuma, V.
P27 - Swapna, T.
P28 - Swaroop Rao, J.
P29 - Varahallika, M.
P30 - Venkat Sushma, B.

Day 2 - Nov 25th, 2022.

Poster session - 3 (P31 to P45): 11:00am-1pm.

- P31 - Afeez, U.
- P32 - Chamanthi, P.
- P33 - Gayathri, P.
- P34 - Geetika Priya, S.
- P35 - Haradeep, K.
- P36 - Hemasri, M.
- P37 - Kamalakumari, G.
- P38 - Mahalakshmi, V.
- P39 - Naga Prathyusha, G.
- P40 - Neelima Devi, A.
- P41 - Pravallika, S.
- P42 - Ramya, T.
- P43 - Roopini, G.
- P44 - Sathvika, G.
- P45 - Yathiraj, Ch.

Poster session - 4 (P46 to P60): 2:00pm-4pm.

P46 - Bindusha, S.
P47 - Gayathri, E.
P48 - Jayasree, G.
P49 - Nandini, T.
P50 - Pravallika, L.
P51 - Ratna Priya, G.
P52 - Sai Tejasri, M.
P53 - Sasi Prathyusha, P.
P54 - Sonia Kumari.
P55 - Sowjanya, V.
P56 - Sowmya, S.
P57 - Tanuja, I.

Design, Synthesis & Evaluation of "The HelicoTAC©" a PROTAC-based small molecule targeting the *Helicobacter pylori* virulence factor, Cag-A protein as a potential therapeutics for gastric ulcers, gastritis and gastric cancers.

Madhumita Aggunna* and Ravikiran S. Yedidi*

The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Rajahmundry, AP, India. (*Correspondence to MA: aggunnamadhumita@gmail.com & RSY: tcabse.india@gmail.com)

Abstract (Oral presentation):

Stressful lifestyle and unusual food habits often lead to acidity problems causing acid reflux issues. However, gastric ulcers, gastritis and gastric cancers can be caused by other reasons such as bacterial infections by Helicobacter pylori. During the infection, H. pylori protects itself by neutralizing the local acidic environment through urease and hacks the host cell by injecting its virulence factor, cytotoxin associated gene A (Cag-A), through its type-4 secretion system (T4SS). Cag-A controls cellular proliferation and apoptotic pathways in a variety of different ways ultimately resulting in severe pathologies. In this strategic communication, we designed a proteolysis targeting chimera (PROTAC)-based small molecule, HelicoTAC©, that specifically targets the H. pylori Cag-A to the host cell ubiquitin-proteasome-mediated degradation. By permanently removing the Cag-A one can hypothesize that the bacterium will automatically be removed by the host immune system thus reducing further potential pathological effects that might be caused by the bacterium.

Keywords: *Helicobacter pylori*, cytotoxin associated gene A (Cag-A), proteolysis targeting chimera (PROTAC), type-4 secretion system (T4SS), HelicoTAC©, gastric ulcers, gastritis and gastric cancers.

Success of Current COVID-19 Vaccine Strategies vs. the Epitope Topology of SARS-CoV-2 Spike Protein-Receptor Binding Domain (RBD): A Computational Study of RBD Topology to Guide Future Vaccine Design.

Santhinissi Addala* and Ravikiran S. Yedidi*

The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Rajahmundry, AP, India (*Correspondence to SA: santhinissiaddala@gmail.com & RSY: tcabse.india@gmail.com).

Abstract (Oral presentation):

Coronavirus disease-2019 (COVID-19) is a pandemic with a high morbidity rate occurring over recent years. COVID-19 is caused by the severe acute respiratory syndrome causing coronavirus type-2 (SARS-CoV-2). COVID-19 not only challenged mankind but also gave scope to the evolution of various vaccine design technologies. Although these vaccines protected and saved many lives, with the emerging viral strains, some of the strains may pose a threat to the currently existing vaccine design that is primarily based on the wild type spike protein of SARS-CoV-2. To evaluate the risk involved from such mutant viral strains, we performed a systematic *in silico* amino acid substitution of critical residues in the receptor binding domain (RBD) of the spike protein. Our molecular modeling analysis revealed significant topological changes in the RBD of spike protein suggesting that they could potentially contribute to the loss of antigen specificity for the currently existing therapeutic antibodies/vaccines, thus posing a challenge to the current vaccine strategies that are based on wild type viral spike protein epitopes. The structural deviations discussed in this article should be considered carefully in the future vaccine design.

Keywords: Coronavirus, SARS-CoV-2, Wild type, vaccine design, receptor binding domain (RBD), spike protein and Epitope topology

Converting Trash to usable biofuels for homes and automobiles in the campaign to save the climate by reducing climate change and Greenhouse emissions.

Kiryowa Idrisa*

GITAM University, Visakhapatnam, AP, India. (*Correspondence to KI: kidrisa@gitam.in)

Abstract (Oral presentation):

The increasing global cost of fossil fuels and their negative impact on the ecosystem poses many questions. It is a cause for concern for many researchers, which increases our desire to seek alternative sources of fuel. Paper waste has become more abundant since the start of the pulp and paper industries, a source of rich biomass as it contains cellulose in higher concentrations for biofuel production. Homes and automobile users are the key targets for these fuels. This paper will enlighten the critical dangers of fossil fuels, including greenhouse emissions, and show the usefulness of biofuels, i.e., renewable and sustainable, and survey a given population to find out how much they know about biofuels and the dangers of fossil fuels. Recent studies have shown that increased demand for fossil fuels has led to the earth's temperature rising by one degree yearly. This leads to global warming; hence using plant-based biofuels, we are improving the ecosystem by reducing emissions of greenhouse gases from fossil fuel combustion. In the target study, where we gave out a questionnaire to a few hundred people, we found out that more than 70% of people in the survey have loads of paper trash they throw every day, and above 90% were willing to give it in for biofuel production, support the campaign for biofuels, and encourage the environment and reduce the usage of fossil fuels. The study concludes that more than half of the study population was knowledgeable about the dangers of fossil fuels and had heard of plant-based alternative sources of fuels. However, there is more need for how biofuel production can be enhanced in production as biomass produces relatively fewer fuels than identical amounts of coal and petroleum.

Keywords: Biofuel, fossil fuels, renewable, global warming, plant-based fuels, coal and petroleum.

A preliminary screening on biodegradability of face masks and their impact on plant growth of *Hibiscus sabdariffa*.

Atheena Paul (3rd year BSc student)

Department of Microbiology, St. Ann's College for Women, Malkapuram, Visakhapatnam, AP, India. (*Correspondence to AP, atheenapaul2001@gmail.com)

Abstract (Oral presentation):

Outbreak of the COVID-19 pandemic led to tremendous increase in the production of facemasks across the world. Face masks are for monitoring origins to avoid transmission from infected persons. The purpose of facemask is like air filters which protect airborne infectious pathogens. Filtering face masks are either pharmacologically or non-pharmacologically used. There are many types of facemasks that are in use now-a-days. They include surgical masks, N95 and cloth masks where they have three layered structures. The primary raw materials for the manufacturing of the surgical and N95 face masks are non-biodegradable synthetic polymers made of polypropylene fibers. Disposal of these synthetic facemasks increases solid waste-load in the environment causing damage to natural flora and fauna. The present study was aimed to analyze the biodegradability of two different kinds of face masks by using three different soil types to know the natural degradation of facemasks and also by artificial pure microbial plate method. The degradation of 2 different face masks was not observed in both the mentioned methods during the study period from the Month of March 2022 to the end of August 2022. But there was a good sign in our identification that there was a quick biodegradability when it was converted into ash form. The time of biodegradability was about 1-2 days/ 3 gms of ash in both the natural and artificial methods. The use of reusable cloth masks is recommended to avoid soil pollution. The present study concluded that cloth masks have more potential degradation capability when compared with surgical masks within a short period of time. Further research should focus on assessing soil profile status, efficacy of cloth mask and surgical masks when dumped in the soil directly. The present literature review aims to evaluate these determinants and provide a framework for future interventions directed at increasing facemask usage as an effective public health measure to curb airborne infectious disease outbreaks.

Keywords: Covid-19, Face masks, Biodegradability, polymers and Ash.

Structural Studies Of Bovine Prion Protein Bound To The Fab Fragment Of Monoclonal Antibody POM1.

Esther, Gottapu* and RaviKiran S. Yedidi *

The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, A.P, India. (*Correspondence to EG: esthergottapu2001@gmail.com and RSY: tcabse.india@gmail.com)

Abstract (Poster presentation):

BSE (Bovine spongiform encephalopathy, commonly known as “mad cow disease”) is a progressive neurological disorder of cattle that results from infection by an unusual transmissible agent called prion. Prion is a misfolded, transmissible protein. Prion diseases are caused when the normal cellular prion protein PrP (present on brain cells surface) is converted to a pathogenic conformer PrP sc . The latter propagates by recruiting the non-pathogenic PrP, imposing its conformation upon it and ultimately aggregating into insoluble deposits known as amyloid fibrils, which are identified in the diseased tissue. This can be controlled by designing monoclonal antibodies that bind to the prion protein. Structurally, the monomeric form of PrP consists of an unstructured N-terminal segment or flexible tail and a globular folded domain. The monoclonal antibody POM1 binds to the globular domain of PrP and does not allow the replication of the cellular prion protein PrP which in turn reduces the propagation of BSE.

Keywords: Bovine spongiform encephalopathy (BSE), mad cow disease, prion protein (PrP), Pathogenic and amyloid fibrils.

Review on phytochemical secondary metabolites of five wild mushroom extracts and their Antimicrobial activity.

Jayalakshmi, Rompilli* (3rd year Bsc student)

Department of Microbiology, St.Ann's college for women, Malkapuram, Visakhapatnam, AP, India. (*Correspondence to RJ: jannujayalakshmi74@gmail.com)

Abstract (Oral presentation):

Wild mushrooms are a vital rich source of natural nutrients and they are occasionally consumed for their supposed medicinal value. There are numerous reports on wild edible mushrooms, which doubt and confusion persist regarding which species are safe and suitable to consume. They are known as highly valued non-wood products today, thus wild mushrooms have played an important role in providing new sources of medicine in the whole World. Our review highlights the need for further information on wild species. They can be used in the treatment of disease through their antimicrobial properties. Five different wild mushrooms were identified and collected from the campus of St. Ann’s college for women, Malkapuram, Visakhapatnam. The result revealed that all mushroom extracts were having antimicrobial activity with high potential effectiveness in suppressing bacterial cell growth when compared with fungal cell growth. The maximum zone of inhibition was 1mm against E.coli by Brown wild mushroom and minimum zone of inhibition was 0.1mm on Staphylococcus aureus. In the present study the presence of phytochemicals like flavonoids, alkaloids and terpenoids were also analyzed by using standard methods. The need for greater clarity on wild species of mushrooms is further underlined to know their nutritional values and phytochemical analysis with their molecular interactions.

Keywords: Wild Mushrooms, phytochemicals, Antimicrobial activity and medicinal values.

Role of Simian virus 40 in inactivating tumor suppressor protein.

[a, b] Subhakanta Sethi* and [b]Ravikiran S. Yedidi*

[a]Centre for Biotechnology, Department of chemical engineering, Andhra university college of engineering (A), Visakhapatnam, AP, India. [b]The center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India.
(*Correspondence to SS: skofficial.9134@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Cancer is characterized by proliferation of cells that have managed to evade central endogenous control mechanisms. Tobacco use is the cause of about 22% of cancer deaths. Another 10% are due to obesity, poor diet, lack of physical activity or excessive drinking of alcohol, 15% of cancers are due to infections such as Helicobacter pylori, hepatitis B, hepatitis C, human papillomavirus infection, Epstein–Barr virus and human immunodeficiency virus (HIV). These factors act, at least partly, by changing the genes of a cell. Proto-oncogenes and tumor suppressor genes are such genes which contribute to cancer when their genetic makeup is altered. Retinoblastoma is a tumor suppressor protein which prevents the entry of cells from G1 phase to S phase. Inactivation of the retinoblastoma (Rb) tumor suppressor by Simian virus 40 (SV40) large T antigen is one of the central features of tumorigenesis induced by SV40. The two central helices and a connecting loop in large T antigen have structural similarities with the J domains of the molecular chaperones DnaJ and HDJ-1, suggesting that large T antigen may use a chaperone mechanism for its biological function. However, there are significant differences between large T antigen and the molecular chaperones in other regions and these differences are likely to provide the specificity needed for large T antigen to inactivate Rb.

Keywords: Cancer, Tobacco, Proto-oncogenes, tumor suppressor proteins, G1 Phase, chaperone and T antigen.

Structural analysis of BCL-2 in association with BH3 domain of Bax.

[a, b] Joel Cherian Jacob* and [b]Ravikiran S. Yedidi*

[a]Centre for Biotechnology, Department of chemical engineering, Andhra university college of engineering (A), Visakhapatnam, AP, India. [b]The center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India.
(*Correspondence to SS: joelcherianjacob777@rediffmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Apoptosis is a process of programmed cell death where the cell brings up its own demise through a series of molecular events. It is a very effective mechanism of the body to eliminate cells that have the tendency to become cancerous. The BCL-2 family of proteins are found to be the chief regulators of mitochondria mediated apoptotic cell death. They are characterized by containing up to four conserved stretches of amino acids, known as BCL-2 homology (BH) domains. The protein family consists of various pro-apoptotic and anti-apoptotic proteins. The interaction between various conserved domains of these proteins is what regulates apoptosis. One such interaction occurs between BCL-2 and the BH3 domain of Bax which inhibits the pro-apoptotic activity of Bax. Stress induced over-expression of anti-apoptotic proteins like BCL-2 may have the tendency to cause cancer due to its inhibition of pro-apoptotic proteins.

Keywords: Apoptosis, BCL-2 homology (BH) domains, pro-apoptotic proteins, Cancer and Over-expression.

Design, Synthesis & Evaluation of Novel inhibitors targeting DBD of Androgen receptor (AR) to inhibit Androgen synthesis which is a Steroidal hormone, whose hyperproduction is responsible for Polycystic Ovary Syndrome (PCOS).

[a, b] S. N V D Sowmya* and [b] Ravikiran S. Yedidi*

[a]Department of Biotechnology, Andhra university, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to SS: sowmya.snvd@gmail.com & RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Stress, unhealthy food and unhealthy lifestyle often leads to hormonal imbalance especially in women. However, hormonal imbalance can also be caused by some other reasons such as suppression of genes or over expression of genes. Among the steroidal hormones Androgen is highly responsible for polycystic ovary syndrome (PCOS). Higher levels of androgen is also responsible for insulin resistance (IR), type 2 diabetes, obesity, and cardiovascular disease and kidney diseases, so it is important to suppress androgen receptor to control androgen synthesis, To address this challenge, we have developed a novel class of inhibitors targeting the DNA-binding domain (DBD) of the receptor, which is distanced from the androgen binding site (ABS) targeted by all conventional anti-AR drugs and prone to resistant mutations. While many members of the developed 4-(4-phenyl thiazol-2-yl)morpholine series of AR-DBD inhibitors demonstrated the effective suppression of wild-type AR, a few represented by 4-(4-(3-fluoro-2-methoxyphenyl)thiazol-2-yl)morpholine (VPC14368) exhibited a partial agonistic effect toward the mutated T878A form of the receptor, implying their cross-interaction with the AR ABS.

Keywords: Androgen Receptor, polycystic ovary syndrome (PCOS), DNA-binding domain (DBD), Androgen binding site and cross-interaction.

Mechanism of dimerization and structural features of human LI-cadherin.

[a, b]Muskan Nargis Baig* and [b]Ravikiran S. Yedidi*

[a]Centre for Biotechnology, Department of chemical engineering, Andhra university college of engineering (A), Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Rajahmundry, AP, India. (*Correspondence to MNB: nargismuskan786@gmail.com and RSY: tcabse.india@gmail.com)

Abstract (Poster presentation):

Gastric cancer (GC) is the third leading cause of cancer-associated death worldwide . More importantly, it is predicted that deaths from gastric cancer will rise from the 15th to the 10th cause of mortality from all causes globally by 2030. LI-cadherin leads to cell aggregation .Soon after the identification of LI-cadherin it was found that LI-cadherin is a functional cell-adhesion molecule. Liver intestine (LI)-cadherin is a member of the cadherin superfamily, which encompasses a group of Ca 2+-dependent cell-adhesion proteins. The expression of LI-cadherin is observed on various types of cells in the human body, such as normal small intestine and colon cells, and gastric cancer cells. Because its expression is not observed on normal gastric cells, LI-cadherin is a promising target for gastric cancer imaging. I downloaded the 3-D structure of LI-Cadherin EC1-2 using PyMOL to perform structural analysis. Therefore ,I successfully performed the secondary structural analysis of LI-Cadherin EC1-2.

Keywords: Gastric cancer, LI-cadherin, PyMOL, Ca^{2+}-dependent cell adhesion proteins, and Structural Analysis.

Prevalence of various gynecologic cancers.

Nirmala, Kalidindi and Manjulatha C.

Department of Zoology, Andhra University, Visakhapatnam, AP, India. (*Correspondence to NK: nirmala.zoo34@gmail.com)

Abstract (Poster presentation):

Cancer that begins in a woman's reproductive organs is known as gynecologic cancer. Cervical, ovarian, endometrial, vaginal, and vulvar cancers are all examples of gynecologic cancer. The sixth kind of gynecological cancer is fallopian tube cancer, an incredibly rare subtype. Measures of the burden of the disease are frequently based on cancer incidence, death, and prevalence. In order to create cancer control plans and organize healthcare services, the burden of cancer must be calculated. On 5524 patients with gynecological malignancies, a data analysis was done. Cervical cancer accounted for 3118 (56.44%) of the cases, ovarian cancer for 1433 (24.9%), uterine cancer for 636 (11.5%), vaginal cancer for 276 (4.83%), and vulvar cancer for 70 (1.27%) of the patients. It was found that cervical cancer and vaginal cancer were more prevalent in the low-income category, occurring in 76% and 70% of cases, respectively, by looking at the socioeconomic status of all these cases. Endometrial cancer occurred in 75% of cases in the middle-class and upper-middle-class groups, which was more common. The prevalence of ovarian and vulvar cancer is the same across all socioeconomic levels. 90% of all gynecological malignancies were found to occur most frequently in women between the ages of 41 and 70, peaking at 32% between 41 and 50. The age range between 41 and 60 is when 61% of cases of cervical cancer develop. 69% of endometrial cancer cases and 63% of vulvar cancer cases were observed in people between the ages of 51 and 70. Ages between 41 and 70 were observed in 78% of cases of ovarian cancer and 76% of cases of vaginal cancer.

Keywords: Gynecologic cancers, prevalence, socioeconomic status and age.

Design, Synthesis And Evaluation Of "HIV-1 Protease"in complex with amprenavir.

[a, b]Venkat sushma Bokka* and [b]Ravikiran S. Yedidi*

[a]Centre for Biotechnology, Department of chemical engineering, Andhra university college of engineering (A), Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Rajahmundry, AP, India.
(*Correspondence to VSB: venkatsushma24@gmail.com and RSY: tcabse.india@gmail.com)

Abstract (Poster presentation):

PDB ID: 4RVJ is a Crystal structure of multidrug-resistant clinical isolate A02 HIV-1 protease in complex with amprenavir. HIV (human immunodeficiency virus) is a virus that damages the cells in your immune system and weakens your ability to fight everyday infections and disease.AIDS (acquired immune deficiency syndrome) is the name used to describe a number of potentially life-threatening infections and illnesses that happen when your immune system has been severely damaged by the HIV virus. Globally, 38.4 million [33.9–43.8 million] people were living with HIV at the end of 2021. The retroviral protease of human immunodeficiency virus (HIV) is an excellent target for antiviral inhibitors for treating HIV/AIDS. Despite the efficacy of therapy, current efforts to control the disease are undermined by the growing threat posed by drug resistance.The virally encoded protease is an important drug target for AIDS therapy. Despite the potency of the current drugs, infections with resistant viral strains limit the long-term effectiveness of therapy. Highly resistant variants of HIV protease from clinical isolates have different combinations of about 20 mutations and several orders of magnitude worse binding affinity for clinical inhibitors.So I downloaded the 3D structure of HIV-I protease protease and used PyMOL for structural analysis.

Keywords: Human Immunodeficiency Virus (HIV), Immune system, retroviral protease, mutations, PyMOL and binding affinity.

Interaction of colipase on pancreatic lipase for digestion of fats – its structure analysis and its inhibition by C11 Alkaline phosphonate.

[a, b]Sravan Kumar Viyyapu* and [b]Ravikiran S. Yedidi*

[a]Centre for Biotechnology, Department of chemical engineering, Andhra university college of engineering (A), Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences and Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to VSK: sravan9288@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Human pancreatic lipase in duodenal secretions was studied under conditions of maximal activation by porcine colipase and maximal inhibition by sodium taurodeoxycholate. In almost all samples, total lipase activity in 4 mM sodium taurodeoxycholate was activated by the addition of porcine colipase. Activation was linear until saturation by cofactor was reached, and maximum activity was greater than that obtained in the absence of bile salts. At pH 8.0 in 4 mM sodium taurodeoxycholate, lipase activity was due to pancreatic lipase in samples from normal and steatorrhea individuals and was proportional to the concentration of endogenous colipase in samples that could be activated by exogenous colipase. In these samples, therefore, colipase activity could be conveniently assayed as the lipase activity at pH 0.8 in 4 mM sodium taurodeoxycholate. Colipase to total pancreatic lipase ratios varied widely from individual to individual and on average were significantly lower in steatorrhea patients. In individual samples, colipase secretion was stimulated by pancreozymin and secretin roughly in parallel with total pancreatic lipase, but some variation in the ratio of the two was often seen in successive collection periods. Because pancreatic lipase is usually unsaturated with respect to cofactor, lipolytic activity in duodenal secretions may be finely controlled by modulation of colipase secretion.

Keywords: Human pancreatic lipase, porcine colipase, pancreozymin, secretin and cofactor.

Screening of human-friendly bacteria and redesigning them using Synthetic Biology, to develop a potential synthetic bacterium with built-in genetic circuits for PETase based plastic bio-degradation.

Madhuri Vissapragada* and Ravikiran S. Yedidi*

The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Rajahmundry, AP, India. (*Correspondence to MV: vissapragadamadhuri5@gmail.com & RSY: tcabse.india@gmail.com).

Abstract (Oral presentation):

Plastic waste accumulation, especially of PET (Polyethylene terephthalate) plastics has been an issue of global concern since decades. Since PET plastics have a wide range of applications in several fields, the production and usage of PET plastics is inevitable. Till date, in the year 2022, 26.3 million metric tons of plastic waste was produced alone in India, with India being in second place in global plastic waste producers ranking. Discovery of a novel bacterium called *Ideonella sakaiensis* that produces PETase capable of degrading PET has created new opportunities to develop potential solutions targeting PET plastic waste accumulation. We believe that synthetic biology, which involves redesigning the organisms for useful purposes to be a powerful tool to solve the problem of PET accumulation. In order to build a synthetic bacterium, choosing the right host bacterial cell is an important step as both efficacy of the bacterium in fulfilling the purpose and also safety to humans and environment has to be ensured. Since probiotics are human-friendly bacteria, our first goal is to screen the available probiotic bacterial species to get a suitable strain for PETase cloning. Thus, selected bacterial species are tested for the expression and efficiency of PETase by cloning.

Keywords: Synthetic biology, *Ideonella sakaiensis*, PETase, plastic degradation and human-friendly bacteria.

The HECT-type ubiquitin ligase E6AP (UBE3A) is critically involved in several neuro-developmental disorders and human papilloma virus-induced cervical tumorigenesis.

[a, b]Alekhya Adhikari* and [b]Ravikiran S. Yedidi*

[a]Department of Biotechnology, Andhra University, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to AA: alekhyaadhikari3441@gmail.com & RSY: tcabse.india@gmail.com)

Abstract (Poster presentation):

Cervical cancer begins in the cells of the cervix. Cervical cancer is a type of cancer that occurs in the cells of the cervix — the lower part of the uterus that connects to the vagina. Various strains of the human papillomavirus (HPV), a sexually transmitted infection, play a role in causing most cervical cancer. Epidemiologic evidence showed that HPV16 and HPV18 are correlated with cervical cancer. Only a minority of HPV infections lead to integration into the host genome, resulting in abnormal gene structures and functions and malignant transformation of cervical cells. Two viral oncoproteins E6 and E7 could play a key role in the HPV-infected cervical cancers. When the viral genome integrates into the host DNA genome, E6 and E7 will be upregulated and subsequently deregulate critical proteins in cellular signaling pathways, such as inhibition of two important tumor suppressor proteins, p53 and pRb.

Keywords: Cervical cancers, Human papillomavirus (HPV), onco-proteins, Viral genome integration and cellular signaling pathways.

Design, Synthesis & Evaluation of "Rheumatoid Arthritis" novel topology of antibody-antigen interaction: human IgM rheumatoid factor Fab bound to its autoantigen IgG Fc.

[a, b]Sapana Kumari* and [b]Ravikiran S. Yedidi*

[a]St. Joseph's College for Women, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Rajahmundry, AP, India. (*Correspondence to SK: sapanakumari2111@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Oral presentation):

Rheumatoid factors are the characteristic autoantibodies of rheumatoid arthritis, which bind to the Fc regions of IgG molecules. Here we report the crystal structure of the Fab fragment of a patient-derived IgM rheumatoid factor (RF-AN) complexed with human IgG4 Fc, at 3.2 A resolution. This is the first structure of an autoantibody-autoantigen complex. The epitope recognized in IgG Fc includes the C gamma 2/C gamma 3 cleft region and overlaps the binding sites of bacterial Fc-binding proteins. The antibody residues involved in auto recognition are all located at the edge of the conventional combining site surface, leaving much of the latter available, potentially, for recognition of a different antigen. Since an important contact residue is somatic mutation, the structure implicates antigen-driven selection, following somatic mutation of germline genes, in the production of pathogenic rheumatoid factors. In rheumatoid arthritis, the body's immune system attacks its own tissue, including joints. In severe cases, it attacks internal organs. Rheumatoid arthritis affects joint linings, causing painful swelling. Over long periods of time, the inflammation associated with rheumatoid arthritis can cause bone erosion and joint deformity. While there's no cure for rheumatoid arthritis, physiotherapy and medication can help slow the disease's progression. Most cases can be managed with a class of medications called anti-rheumatic drugs (DMARDS). This is the first crystal structure analysis of a complex between an autoantibody and its autoantigen, and it reveals a mode of interaction never before seen in an antibody-antigen complex.

Keywords: Rheumatoid Arthritis, autoantibody-autoantigen complex, IgG Fc and IgM rheumatoid factor.

Casein kinase 2 (CK2) is a ubiquitous pleiotropic enzyme that is highly conserved across eukaryotic kingdoms.

[a, b]Jyothi Swaroop Rao Mylapilli* and [b]Ravikiran S. Yedidi*

[a]Centre for Biotechnology, Department of chemical engineering, Andhra university college of engineering (A), Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to JSRM: jyothiswaroopraom@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Casein kinase 2 (CK2) is a ubiquitous pleiotropic enzyme that is highly conserved across eukaryotic kingdoms. CK2 is singular amongst kinases as it is highly rigid and constitutively active. Arabidopsis thaliana is widely used as a model system in molecular plant research; the biological functions of A. thaliana CK2 are well studied in vivo and many of its substrates have been identified. Here, crystal structures of the α subunit of A. thaliana CK2 in three crystal forms and of its complex with the non hydrolyzable ATP analog AMppNHp are presented. While the C-lobe of the enzyme is highly rigid, structural plasticity is observed for the N-lobe. Small but significant displacements within the active cleft are necessary in order to avoid steric clashes with the AMppNHp molecule. Binding of AMppNHp is influenced by a rigid-body motion of the N-lobe that was not previously recognized in maize CK2.

Keywords: Casein kinase 2, ubiquitous pleiotropic enzyme, crystal structure, α subunit and ATP.

Crystal Structure of *Bacillus Halodurans* Ribonuclease H1 in Complex with an RNA/DNA Hybrid.

[a, b]Anupama Kavya Priya Dwarapureddy* and [b]Ravikiran S. Yedidi*

[a]Centre for Biotechnology, Department of chemical engineering, Andhra university college of engineering (A), Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to AKPD: anupama.kavya.priya@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Through the analysis of DNA synthesis in crystallo by time-resolved X-ray crystallography, our group has shown that binding of two canonical Mg 2+ ions by DNA pol η is insufficient to initiate the reaction, and a third Mg 2+ ion transiently bound to the incoming dNTP is required for catalysis. Catalysis by members of the RNase H superfamily of enzymes is generally believed to require only two Mg2+ ions that are coordinated by active-site carboxylates. By examining the catalytic process of *Bacillus halodurans* RNase H1 in crystallo, however, we found that the two canonical Mg2+ ions and an additional K+ failed to align the nucleophilic water for RNA cleavage. Substrate alignment and product formation required a second K+ and a third Mg2+, which replaced the first K+ and departed immediately after cleavage. A third transient Mg2+ has also been observed for DNA synthesis, but in that case it coordinates the leaving group instead of the nucleophile as in the case of the RNase H1 hydrolysis reaction. These transient cations have no contact with the enzymes. Other DNA and RNA enzymes that catalyze consecutive cleavage and strand-transfer reactions in a single active site may similarly require cation trafficking coordinated by the substrate.

Keywords: X-ray crystallography, dNTPs, B*acillus halodurans*, cleavage, nucleophile and active site.

Design, Synthesis & Evaluation of small-molecule cyanimide inhibitor (8RK64) serve as a starting point for developing more selective inhibitors for PARK7 which is responsible for cancer and neurodegenerative diseases.

[a, b]Anjani sarvani, Challa* and [b]Ravikiran S. Yedidi*

[a]Department of Biotechnology, Andhra University, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to ASC: challasarvani601@gmail.com and RSY: tcabse.india@gmail.com)

Abstract (Poster presentation):

Parkinson's disease is a brain disorder that causes uncontrollable movements, such as shaking, stiffness, and difficulty with balance and coordination .This occur when nerve cells in the basal ganglia, an area of the brain that controls movement, become impaired and/or die .This appear to be hereditary and a few cases can be traced to specific genetic mutations. Parkinson's disease protein 7 (PARK7/DJ1) is an attractive therapeutic target due to its link with early-onset Parkinson's disease, causes various cancers, and contribution to chemoresistance . A small-molecule cyanimide inhibitor (8RK64) and activity-based probe (8RK59) for the deubiquitinase (DUB) UCHL1 .To gain more insight into the inhibitor binding mode and to guide the design of novel PARK7 inhibitors. Conclusion, developed three novel tools for PARK7: a selective and potent covalent PARK7 inhibitor (JYQ-88), an activity-based probe (JYQ-92) to monitor PARK7 activity in cell lysates , and a FP assay reagent (JYQ-107) to allow for HTS of PARK7 inhibitors. Together, these tools open new avenues to study the biological role of PARK7 activity served by catalytic cysteine rather than its scaffolding function by monitoring PARK7 activity. Further innovative improvements, our probes can also serve as a diagnostic tool, as PARK7 is a well-known biomarker for various cancers.

Keywords: Parkinson's disease, genetic mutations, cyanimide inhibitor, chemoresistance and deubiquitinase.

Sequence homology-based identification of paracetamol metabolizing enzymes in chicken liver homogenates for *in vitro* drug metabolism studies.

Niharikha Mukala* and Ravikiran S. Yedidi*

The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to NM: Niharikhamukala20@gmail.com and RSY: tcabse.india@gmail.com)

Abstract (Oral presentation):

In vitro drug metabolism studies are a crucial part of preclinical drug discovery. The research laboratories need a lot of human liver microsomes to test the metabolism of xenobiotics such as steroids, drugs, and pharmaceuticals by the cytochrome P450 (CYP450) family of enzymes. There is a need for an alternate and reliable source of drug-metabolizing enzymes. Most often the CYP450 assays are expensive and are not affordable by academic laboratories. We want to identify whether the chicken liver extracts can be used as models to test in vitro drug metabolism instead of human liver extracts. In this study, we designed an affordable in vitro assay using the broiler chicken (BCh) liver homogenates/ chicken liver extracts(ChiLEx) as the source of CYP450 enzymes and evaluated the metabolism of a most commonly used non-steroidal anti-inflammatory drug, paracetamol (acetaminophen). Our proton NMR spectra demonstrated that the BCh liver homogenates were able to metabolize paracetamol. Additionally, we performed an extensive sequence homology-based bioinformatics survey and identified BCh homologs that might potentially be involved in the metabolism of paracetamol. Further, the binding profiles of paracetamol in the active sites of the homolog enzymes provided more insights into drug metabolism through our docking studies. Taken together, our studies serve as a prototype for in vitro drug metabolism studies using BCh liver homogenates as a source of metabolizing enzymes in combination with bioinformatics. From this study, our prototype can be used to evaluate the metabolism of various classes of drugs in the future. This assay was performed at a significantly lower cost compared to other standard methods.

Keywords: Drug discovery, Cytochrome P450, non-steroidal drug, anti-inflammatory drugs, acetaminophen, NMR spectra and drug metabolism.

Crystal structure of "The Beta - klotho (5VAN) protein which is an anti-aging single pass membrane protein, a potential therapeutics for aging, chronic kidney diseases and for suppression of signalling by insulin.

Pranavi Satya Lakshmi Appana*

Andhra University College of Engineering, Visakhapatnam, AP, India. (*Correspondence to PSLA: satyalakshmi456@gmail.com).

Abstract (Poster presentation):

Aging is a degenerative phenomenon determined by interactions between the external environment and genes. The Klotho gene is mainly expressed in kidneys and brain. Over-expression of the klotho gene extends life span, demonstrated worms, flies and mainly in mice. I have actually downloaded the 3D structure of 5VAN is used to perform structural analysis using PyMOL. Canonical fibroblast growth factors (FGFs) activate FGF receptors (FGFRs) through paracrine or autocrine mechanisms in a process that requires cooperation with heparan sulfate proteoglycans, which function as co-receptors for FGFR activation. By contrast, endocrine FGFs (FGF19, FGF21 and FGF23) are circulating hormones that regulate critical metabolic processes in a variety of tissues. FGF19 regulates bile acid synthesis and lipogenesis, whereas FGF21 stimulates insulin sensitivity, energy expenditure and weight loss. Endocrine FGFs signal through FGFRs in a manner that requires klothos, which are cell-surface proteins that possess tandem glycosidase domains. Here we describe the crystal structures of free and ligand-bound β-klotho extracellular regions that reveal the molecular mechanism that underlies the specificity of FGF21 towards β-klotho and demonstrate how the FGFR is activated in a klotho-dependent manner. B-Klotho serves as a primary 'zip code'-like receptor that acts as a targeting signal for FGF21, and FGFR functions as a catalytic subunit that mediates intracellular signaling. Our structures also show how the sugar-cutting enzyme glucosidase has evolved to become a specific receptor for hormones that regulate metabolic processes, including the lowering of blood sugar levels. Finally, we describe an agonistic variant of FGF21 with enhanced biological activity and present structural insights into the potential development of therapeutic agents for diseases linked to endocrine FGFs.

Keywords: klotho gene, endocrine, catalytic subunit, fibroblast growth factor, and lipogenesis.

Crystal structure of p38 alpha MAP kinase in complex with a novel isoform selective drug candidate.

[a, b]Manda Jahna Varahallika* and [b]Ravikiran S. Yedidi*

[a]Centre for Biotechnology, Department of chemical engineering, Andhra university college of engineering (A), Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to AKPD: jahnavarahallikamanda@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Alzheimer's disease is the most common cause of dementia and also the best understood Alzheimer's disease is thought to be caused by the formation of abnormal deposits of protein in the brain. Alzheimer's is a type of dementia that affects memory, thinking and behavior. Symptoms eventually grow severe enough to interfere with daily tasks. According to the latest WHO data published in 2020A Alzheimer's and dementia deaths in India reached 126593 or 1.49 % of total deaths, a number of studies have revealed a significant role of p38 MAPK related to Aβ in neuronal cells of AD. Activation of p38 MAPK by Aβ results in increased intracellular calcium, ROS production/accumulation, and mitochondrial stress, all of which have been implicated in the pathology of AD neurons. I downloaded the 3D structure of p38αMAPK using PyMOL to perform structure analysis.Therefore, I successfully performed the secondary structural analysis of p38αMAPK.

Keywords: Alzheimer's disease, dementia, p38, MAP Kinase PyMOL and Structural analysis.

Industrial wastewater treatment with a bioelectrochemical process: assessment of depuration efficiency and energy production.

Sumaiyah Soghra*

M. V. R. Degree College, Visakhapatnam, AP, India. (*Correspondence to SS: lubbu2105@gmail.com).

Abstract (Oral presentation):

Development of renewable energy sources, efficient industrial processes, energy/ chemical recovery from waste are research issues that are quite contemporary. Bio electrochemical processes represent and eco-innovative technology for energy and resources recovery from both domestic and wastewater from industries .The current study was conducted to: Assess bio electrochemical treatability of industrial (diary) wastewater by microbial fuel cells (MFCs); Determine the effects of the applied organic loading rate (OLR) on Microbial fuel cells performance and Identify factors responsible for reactor energy recovery loses (over potential). For this purpose, an Microbial fuel cell was built and continuously operated for 72 days during which the anodic chamber was fed with dairy waste water and the cathodic chamber with an aerated mineral solution. The study demonstrated that industrial effluents from agri-food facilities can be treated by bio electrochemical systems with greater than 85% average organic matter removal, recovering power at an observed maximum density of 27 watts. Outcomes were better than in previous analogous experience, and the demonstration of this type of process could be successfully used for dairy waste water with several advantages.

Keywords: Renewable energy, microbial fuel cells, organic loading rate (OLR) and chemical recovery.

An eye lens protein – Water structure: 1.2 revolution structure of gamma B – crystallin at 150K.

[a, b]Phaneendra Gorrupotu and [b]Ravikiran S. Yedidi

[a]Centre for Biotechnology, Department of chemical engineering, Andhra university college of engineering (A), Visakhapatnam, AP, India. [b]The center for Advanced-Applied Biological Sciences and Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*correspondence to GP: phaniprasad6411@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Gamma Beta-crystallin is a structural protein of the eye lens with a role in the maintenance of an even distribution of protein and water over distances around the wavelength of light, preserving lens transparency. The structure of the 174-residue bovine protein has already been determined at room temperature to 1.47 A resolution. By flash freezing the protein crystals, data have now been collected to a nominal resolution limit of 1.2 A as radiation damage was essentially eliminated. The protein-water model has been refined against this data using the program RESTRAIN converging to an R factor of 18.5% with all data. Atomic positions are clearly indicated in the electron-density maps. Discrete bimodal disorder has been visualized for a few side chains. Out of a total of 498 water molecules present in the crystal asymmetric unit, 394 have been modeled and refined at unit occupancy. The solvent structure is extremely well ordered with an average B value of 23.4 A(2). Partially occupied sites have been identified where disorder in the protein induces concomitant disorder in the local solvent structure. The solvent structure covers 97% of the solvent-exposed surface of the protein in the crystal. 126 water molecules are distributed in second and higher hydration shells. There are networks of hydrogen-bonded solvent extending up to 64 molecules in a network, comprising trimers and tetramers as well as five- and six-membered water-ring structures. The hydration of the protein surface is dominated by arginine and aspartate side chains. Extensive cages of highly ordered solvent molecules are also observed around exposed non-polar groups.

Keywords: Gamma Beta-crystallin, bovine program, R factor and protein crystals.

Discovery and Development of TMPRSS6 Inhibitors Modulating Hepcidin Levels in Human Hepatocytes which is responsible for iron deficiency.

[a, b]Rachana Garikipati* and [b]Ravikiran S. Yedidi*

[a]Department of Biotechnology, Andhra University, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences and Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to RG: rachanagarikapati@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Iron deficiency anemia (IDA) is the most common worldwide anemia with important clinical consequences 1, caused by inadequate iron availability for hemoglobin production due to different factors. The lack of dietary iron, the insufficient uptake of iron and chronic bleeding are the most frequent causes.Iron overload disorders are characterized by the body's inability to regulate iron absorption and its storage which can lead to organ failures. Accumulated evidence has revealed that hepcidin, the master regulator of iron homeostasis, is negatively modulated by TMPRSS6 (matriptase-2), a liver-specific type II transmembrane serine protease (TTSP). Here, we report that treatment with a peptidomimetic inhibitor affecting TMPRSS6 activity increases hepcidin production in hepatic cells. Moreover, similar effects were observed when using non-peptidic inhibitors obtained through optimization of hits from high-throughput screening. Using HepG2 cells and human primary hepatocytes, we show that TMPRSS6 inhibitors block TMPRSS6-dependent hemojuvelin cleavage and increase HAMP expression and levels of secreted hepcidin.

Keywords: Iron deficiency anemia (IDA), Anemia, hemoglobin and peptidomimetic inhibitor.

Role of polyarginine in inhibiting aggregation of p53

[a, b]Gangadhar katchala* and [b]Ravikiran S. Yedidi*

[a]Centre for Biotechnology, Department of chemical engineering, Andhra university college of engineering (A), Visakhapatnam, AP, India. [b]The center for Advanced-Applied Biological Sciences and Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*correspondence to GK: gangadhark2000@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

p53 is a tumor suppressor protein. Under stressful conditions, p53 tightly regulates cell growth by promoting apoptosis and DNA repair. When p53 becomes mutated, it loses its function, resulting in abnormal cell proliferation and tumor progression. Depending on the p53 mutation, aggregation of p53 leads to negative gain of function of protein. 50% of cancers have p53 mutation and several of them are prone to aggregation associated cancers. polyarginine analogues and designer peptides for inhibiting p53 aggregation and tumor growth gives further encouragement in treating cancer as a protein aggregation disease. We classify anticancer molecules with anti aggregation properties into four categories: thiol alkylating agents, designed peptides, agents with chaperone-based mechanisms that inhibit p53 aggregation. Arginine, a cationic amino acid, is known to stabilize proteins under harsh conditions. It is widely used to stabilize protein aggregation, and to correct protein folding during protein production. polyarginine, and polyornithine inhibits p53 conserved peptide aggregation, and the cell proliferation of p53 mutant cancer cells.

Keywords: p53, mutation, cancer, chaperone-based mechanisms and tumor progression.

Design and Evaluation of Crystallographic structure of "human Lysosomal beta-Hexosaminidase A" and its association with Tay-Sachs Disease.

[a, b]P R Ruby Elizabeth* and [b]Ravikiran S. Yedidi*

[a]St. Joseph's College for Women, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Rajahmundry, AP, India. (*Correspondence to PRE: 20ah982bbcruby@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Tay-Sachs disease is a genetic disorder caused by the absence of an enzyme that helps break down fatty substances called gangliosides. PDB ID: 2GJX shows the crystallographic structure of human beta-Hexosaminidase A. The crystal structure of β-hexosaminidase A (Hex A) reveals alpha strands, beta sheets, heterodimer, with each subunit having a functional active site. Only the alpha-subunit active site can hydrolyze GM2 gangliosides due to a flexible loop structure whereas the loop is removed post-translationally from beta. The loop structure is involved in binding the GM2 activator protein. Lysosomal β-hexosaminidase A (Hex A) is essential for the degradation of GM2 gangliosides in the central and peripheral nervous system. Accumulation of GM2 leads to severe neurodegeneration that is associated with Tay-Sachs disease. Using PyMOL the protein structure was analyzed. The ligands NAG(N-Acetyl-D-Glucosamine) and sulfate ion were identified. NAG has four hydrogen bonds and SO4 has three hydrogen bonds. The secondary structure of protein is performed successfully.

Keywords: β-hexosaminidase A, GM2 activator protein, PyMOL and structural analysis.

Design of "Cystic Fibrosis" novel topology of interactions between intracellular nucleotide-binding domains (NBDs) and the intracellular regulatory (R) domain.

[a, b]Mythili Akella* and [b]Ravikiran S. Yedidi*

[a]St. Joseph's College for Women, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Rajahmundry, AP, India. (*Correspondence to MA: mythili3002@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Cystic fibrosis is the most common autosomal recessive disorder. The mutated gene encodes a defective chloride channel in epithelial cells-named cystic fibrosis transmembrane conductance regulator (CFTR) protein. The CFTR protein helps to maintain the balance of salt and water on many surfaces in the body, such as the surface of the lung. When the protein is not working correctly, chloride, a component of salt becomes trapped in cells. The CFTR protein is made up of 1,480 amino acids. Once the CFTR protein chain is made, it is folded into a specific 3-D shape. CFTR is a single polypeptide containing an N-terminal, two transmembrane domains (TMDs), and two nucleotide-binding domains (NBDs). Distinct from other ABC transporters, CFTR also contains an ~200-residue cytoplasmic regulatory (R) domain that regulates the activity of CFTR. Using PyMOL, the structure of protein was analysed, and it is found that they are in total of five ligands, that is Magnesium ions (2), cholesterol (2), ATP's (5), N-(3-carbamoyl-5,5,7,7-tetramethyl-4,7-dihydro-5H-thieno[2,3-c]pyran-2-yl)-1H-pyrazole-3-carboxamid e (1), (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl2-(trimethylammonio) ethyl phosphate (5). In the PyMOL it was found that they are approximately 36 hydrogen bonds. Secondary structure of the protein is performed successfully.

Keywords: Cystic fibrosis, epithelial cells, CFTR protein, PyMOL and structural analysis.

Design of "Crystal Structure" of tyrosinase from *Bacillus megaterium* with L-DOPA in the active site, Determination of tyrosinase substrate-binding modes with type-3 copper proteins.

[a, b]Reshma Kuncham* and [b]Ravikiran S. Yedidi*

[a]St. Joseph's College for Women, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Rajahmundry, AP, India. (*Correspondence to RK: reshmakuncham73@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Albinism is an autosomal recessive disorder i.e.; a genetic condition occurs when the child inherits one mutated copy of a gene from each parent. The term albinism typically refers to oculocutaneous albinism where there is little or no production of the pigment melanin. Seven forms of Albinisms are recognized till date- OCA1, OCA2, OCA3, OCA4, OCA5, OCA6 and OCA7. Every Oculocutaneous albinism (OCA) form causes different kinds of albinism. The pigmentation of our skin is due to Melanin pigment. Melanin pigment is produced in the Melanocytes and stored in Melanosomes. Tyrosinase enzyme helps in production of Melanin. Melanin gives skin, hair, and eyes their color. By using PyMOL the protein structure was analyzed clearly in which 2 Ligands were found, Zn+2 ion and DAH (3,4-DIHYDROXYPHENYLALANINE). Polar contacts and interaction of the ligand with the number of Water molecules. 1st DAH ligand - 3 polar contacts; 2nd DAH ligand - 7 polar contacts; 3rd DAH ligand - 2 polar contacts; 4th DAH ligand - 7 polar contacts. Secondary structure of protein is performed successfully.

Keywords: Albinism, Melanocytes, Tyrosinase enzyme, PyMOL and structural analysis.

Evaluation of X-ray crystallographic structure of myoglobin and oxygen binding site [PDB ID: 3RGK].

[a, b]Sai Rupa Rajam* and [b]Ravikiran S. Yedidi*

[a]St. Joseph's College for Women, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Rajahmundry, AP, India. (*Correspondence to SR: rajamsairupa@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Myoglobin is a protein located primarily in the striated muscles of vertebrates. Myoglobin belongs to the globin superfamily of proteins. The body uses it as an oxygen storage protein in muscle. MB is the gene encoding myoglobin in humans. The expression of the MB gene has also been reported in various tumor cell lines such as breast carcinoma, colon carcinoma, acute leukemia, desmoplastic small round cell tumors, and non-small cell lung cancer. Myoglobin is a single polypeptide chain of 154 amino acids. The chain consists of eight α-helices connected in loops. The molecule contains a heme prosthetic group, which includes a porphyrin ring iron ion. The heme-bound Fe cation can exist in the 2+ (reduced) or 3+ (oxidized) states. The iron ion itself interacts with six different ligands, one of which serves as the binding site for oxygen. This binding site can also function to bind other potential molecules, including CO and NO.Myoglobin has no cooperative binding. As a result, myoglobin's oxygen saturation curve is hyperbolic. The primary function of myoglobin is to supply oxygen to the muscle. It does this by releasing its oxygen supply to the mitochondria that make up the respiratory chain, helping the myocytes to meet their high energy demands. Myoglobin serves as a buffer of intracellular oxygen concentrations and as an oxygen reservoir in muscle. Myoglobin facilitates oxygen diffusion. Myoglobin has also been shown to have enzymatic functions. It is necessary for the decomposition of bioactive nitric oxide to nitrate. In order to understand the structure and function of protein, myoglobin 3 D analysis was done using computational biology tools. In the Protein Data Bank that is PDB myoglobin structure was found with PDB ID: 3RGK. Now the details regarding structure were clearly analyzed and downloaded in PDB format and opened in PyMOL. Sequence of protein, 8 alpha helices, binding site of oxygen were clearly analyzed using PyMOL software. In this way the secondary structure of the protein that is analysis on myoglobin was done successfully.

Keywords: Myoglobin, carcinoma, Protein Data Bank, PyMOL and structural analysis.

Role of infestin – 4 in inhibition of blood coagulation factor – f XIIa.

[a, b]Akhila Bhutala* and [b]Ravikiran S. Yedidi*

[a]Centre for Biotechnology, Department of chemical engineering, Andhra university college of engineering (A), Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to AB: akhilabvr@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Blood coagulation is an important process in haemostasis. Blood coagulation, also known as blood clotting, is the process by which blood changes from a liquid to a gel, forming a blood clot. Blood clotting occurs by several factors there are over a dozen blood clotting factors.they interact in a complicated series of reactions that numerically generate thrombin.coagulation factor XII a is a serine protease plays a central role in initiating the intrinsic cascade of blood coagulation. For inhibiting blood coagulation some substrates act as inhibitors of blood coagulation.A specific thrombin inhibitor called infestin – 4 cloned from midgut of *Triatoma infestans*, was fused recombinant human albumin (rHA). It is a member of non classical kazal- type serine protease inhibitor of fXII a, plasma and factor 10 a.rHA -infestin-4 is a competitive inhibitor of fXIIa with slow and off rate constant binding it can block fXIIa. Mutations like f6t and n8r arise in infestin increase binding efficiency with fXIIa gives good inhibition. At last it confirmed that inhibition ofXIIa by rHA-infestin-4 can produce strong antithrombotic efficacy while preserving haemostasis.

Keywords: Blood coagulation, Haemostasis, Blood clotting, *Triatoma infestans* and antithrombotic efficacy.

Design , Structure & Evaluation of "A3 Domain of von williebrand Factor" responsible for mediating platelet adhesion by binding both collagen of damaged bold vessel and to glycoprotein in BLOOD CLOTTING.

[a, b]RamyaSaiSree Janjam* and [b]Ravikiran S. Yedidi*

[a]Centre for Biotechnology, Department of chemical engineering, Andhra university college of engineering (A), Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to RSSJ: ramyajanjam@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

The Collagen binding protein, Von Willebrand factor (VWF) mediates platelet adhesion to injured vessels by sequestering platelets from blood flow and depositing them to collagen and other exposed subendothelial matrix proteins. This process of capturing platelets to facilitate formation of platelet plugs occurs through transient interactions with platelet glycoprotein Ibα via the VWF A1 domain which also binds collagen. The von williebrand factor in humans helps in blood clotting along with the blood vessels. The binding protein forms a bridge between collagens within connective tissue exposed upon damage of the blood vessel and the platelet membrane glycoprotein lb (GPlb). Bleeding from a damaged blood vessel is stopped by the formation of a platelet plug. The multimeric plasma glycoprotein, Von Willebrand factor (VWF), plays an essential role in this process by anchoring blood platelets to the damaged vessel wall under conditions of high shear stress. This factor mediates platelet adhesion by binding both to collagen of the damaged blood vessel and to glycoprotein Ib on the platelet membrane. The A3 domain of vWF allows it to bind to collagen types I and III present in the perivascular connective tissue of the damaged vessel wall. To gain insight into the mechanism of collagen binding by vWF, we have determined the crystal structure of the human vWF A3 domain.. The structural analysis is done by downloading the PyMOL structure from the protein data bank.

Keyword: College binding protein, Von Willebrand factor (VWF), glycoprotein lb (GPlb), Protein Data Bank, PyMOL and structural analysis.

Narcotics And Its Constituents.

Anand Sai Sahini and Anil Kumar Budi*

Aditya Degree College, Gopalapatnam, Visakhapatnam, AP, India. (*Correspondence to AKB: budianilkumar2003@gmail.com).

Abstract (Oral presentation):

The term “Narcotic” comes from the Greek word “stupor”, also known as “opioids”.A drug that relieves pain and induces drowsiness, stupor and insensibility. Narcotic refers to opium, opium derivatives and their semi-synthetics such as methadone and pethidine as well as cannabis and coca leaf. A drug(such as opium or morphine) that in moderate doses dulls the senses,relieves pain,and induces profound sleep but in excessive doses causes stupor,coma or convulsions. Narcotics Anonymous (NA), founded in 1953, describes itself as a "nonprofit fellowship or society of men and women for whom drugs had become a major problem”. To achieve public health goals, drug prevention should focus not only on preventing all use of drugs which is unlikely to be a realistic goal in most settings but also on preventing or reducing problematic use and the harms of drug use.Evaluations of prevention programs suggest strongly that the content of educational programs should be based on formative research that clarifies the particular reality of initiation of drug use and factors influencing continued and problematic use.

Keywords: Narcotics, Opioids, morphine.

Crystal Structure Of The Ga Module From "*F. magna*".

[a, b]Siri Hanuma Vidadala* and [b]Ravikiran S. Yedidi*

[a]Centre for Biotechnology, Department of chemical engineering, Andhra university college of engineering (A), Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to SHV: sirihanumavidadala2643@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

The anaerobic bacterium *Peptostreptococcus magnus* is a human commensal and pathogen. Previous work has shown that strains of P. magnus isolated from patients with gynecological disease (vaginosis) frequently express an immunoglobulin (Ig) light chain-binding protein called protein L. Gynecologic diseases in general are diseases that involve the female reproductive tract. These diseases include benign and malignant tumors, pregnancy-related diseases, infection, and endocrine diseases. The albumin-binding domain, or GA module, of the peptostreptococcal albumin-binding protein expressed in pathogenic strains of Finegoldia magna is believed to be responsible for the virulence and increased growth rate of these strains. I have downloaded the 3D structure of 2J5Y and used PyMOL to perform structural analysis.

Keywords: *Peptostreptococcus magnus*, immunoglobulin (Ig), albumin-binding protein, PyMOL and structure analysis.

Edible Oil And Its Constituents.

Dinesh Chandra Ponaganti* and Shyam Prasad Karri

Aditya Degree College, Gopalapatnam, Visakhapatnam, AP, India. (*Correspondence to DCP: ponagantidinesh2003@gmail.com).

Abstract (Oral presentation):

Edible oils constitute an important component of food expenditure in Indian households and the Edible oil industry is one of the most important industries of the agriculture sector in India. Edible oil consists of about 96% triglycerides, composed of different fatty acids. Some other compounds, such as free fatty acids, phospholipids ,phytosterols, other antioxidants or waxes, can be found. Some types of edible oils are Mustard oil, Coconut oil, Corn oil, Cottonseed oil, Olive oil, etc. The constituents of fats Fats and oils are called triglycerides (or triacylglycerols) because they are esters composed of three fatty acid units joined to glycerol a trihydroxy alcohol. If all three OH groups on the glycerol molecule are esterified with the same fatty acid, the resulting ester is called a Simple triglyceride. A typical triglyceride obtained from naturally occurring fats and oils contains two or more different fatty acid components and is thus termed as mixed triglyceride. The saturation of the fats and oil are often used to describe the fats or oils obtained from the foods. The physical properties of Pure fats are colorless, odorless and tasteless.The chemical properties of Fats and oils can participate in variety of chemical reactions- for example because triglycerides are esters, they can be hydrolyzed in presence of an acid, a base, or specific enzymes are known as lipases.

Keywords: Triglycerides, phospholipids, phytosterols.

A spotlight on host-microbiome interactions and their therapeutics.

Niharikha Mukala and Pola Sudhakar*

Department of Biotechnology, Andhra University, Visakhapatnam, AP, India. (*Correspondence to SP: drpola@gmail.com).

Abstract (Oral presentation):

The crucial role of microbiota in the human body is regulating various physiological functions and pathological conditions of the body. The pursuit is to understand the connection between the microbiome and health conditions like infections, cancer, neurological disorders, COPD. To provide a broader scientific approach, we must identify the answers to some lead questions like how it alters diversity and composition from one person to another, how the accumulation of microbiomes over the years can be beneficial for an individual, and how we approach the contributing factors for the development of microbiota. The cross-talk between the host and microbiota, among the microbiota, might help analyze the signaling molecules mediating the biological mechanisms for immune responses. The changes in the composition of the intestinal microbiota may negatively impact the function of the lung, kidneys, and brain through systemic immunological effects. Some potential therapies to improve the microbiome or target a specific microbiota are phage therapy, FMT, prebiotics, probiotics, and synbiotics. In recent times, the modulation of the neonatal microbiome has been one of the challenging goals to increase efficacy. However, much more research is required to engineer microbiome therapeutics. This presentation gives an overview of existing challenges and strategies to make the necessary modifications to restore the naive gut.

Keywords: Microbiota, immune responses, probiotics and therapeutics.

Design of Nitric Oxide – Releasing prodrug of 5 HMF for the treatment of Sickle Cell Disease (SCD).

[a, b]Sai Mounika Papala* and [b]Ravikiran S. Yedidi*

[a]Centre for Biotechnology, Department of chemical engineering, Andhra university college of engineering (A), Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to SMP: saimounika289@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Sickle cell disease (SCD) is the most common inherited blood disorder in the United states. People with SCD are born with it. SCD occurs as a result of single point mutation in β chain Glu 6 in normal Hemoglobin (HbA) to Val6 in Sickle Haemoglobin (HbS). Sickle cell disease is caused by polymerisation of deoxygenated sickle hemoglobin (HbS) in its T state forms into fibers that distort red blood cells into characteristic sickle shape. Polymer is initiated by a primary interaction between the mutation β2 Val6 from one HbS molecule and a hydrophobic acceptor pocket formed by the residues β1Ala70, β1Phe75 & β1Leu88 of an adjacent located HbS molecule. This hydrophobic contact initiates the polymerisation process & is augmented by an adjacent hydrogen bond interaction between β2Thr4 & β1Asp73. This polymerisation leads to occlusion of rigid sickle RBCs in capillaries and small blood vessels and obstructing blood flow (vaso-occlusion), haemolytic anemia, hypoxia, stroke and organ damage. One of the reasons for SCD is Nitric oxide (NO) deficiency, so for the treatment we synthesis a NO-Releasing prodrug of 5HMF (5HMF-NO) which forms an adduct with Hb and increases Hb affinity for oxygen and decreases HbS polymerisation and RBC sickling which automatically reduces haemolysis.

Keywords: Sickle cell disease, Vaso-occlusion, Hemoglobin and Val6.

The Paradox In Cancer Progression And Immunotherapy.

[a, b]Charles Babuji Kancherla* and [b]Ravikiran S. Yedidi*

[a]Centre for Biotechnology, Department of chemical engineering, Andhra university college of engineering (A), Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to CBK: charliekancherla@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Cancer is a large group of diseases that can start in almost any organ or tissue of the body when abnormal cells grow uncontrollably, go beyond their usual boundaries to invade adjoining parts of the body and/or spread to other organs through metastasis. Cancer is a genetic disease—that is, it is caused by errors that occur as cells divide, or by damage caused to DNA by harmful substances in the environment, such as the chemicals in tobacco smoke and ultraviolet rays from the sun. Tumor necrosis factor (TNF) is an adipokine and a cytokine. As an adipokine, TNF promotes insulin resistance, and is associated with obesity-induced type 2 diabetes. As a cytokine, TNF is used by the immune system for cell signaling. If macrophages detect an infection, they release TNF to alert other immune system cells as part of an inflammatory response. TNF signaling occurs through two receptors: TNFR1 and TNFR2. TNFR1 is constitutively expressed on most cell types, whereas TNFR2 is restricted primarily to endothelial, epithelial, and subsets of immune cells. TNFR1 signaling tends to be pro-inflammatory and apoptotic, whereas TNFR2 signaling is anti-inflammatory and promotes cell proliferation. Suppression of TNFR1 signaling has been important for treatment of autoimmune disease, whereas TNFR2 signaling promotes wound healing.

Structural Characterization Of Keratin-Degrading M32 Carboxypeptidase From *Fervidobacterium Islandicum* Aw-1.

[a, b]Lakshmi Meghana Munagala* and [b]Ravikiran S. Yedidi*

[a]Centre for Biotechnology, Department of chemical engineering, Andhra university college of engineering (A), Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to LMM: 320106206005@andhrauniversity.edu.in and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Epidermolysis bullosa simplex (EBS) is a group of rare predominantly autosomal dominant genetic skin diseases affecting approximately 1:25000–50 000 live births of the population. EBS is the first identified and best studied variant of keratin disorders and has become the prototype for understanding disease pathology and genotype–phenotype correlations within a broad spectrum of keratin disorders. In EBS, two major subtypes have been defined: suprabasal and basal EBS. Keratin is a protein that helps form hair, nails and your skin's outer layer (epidermis). It helps support your skin, heal wounds and keep your nails and hair healthy. It provides support and protection in your body. EBS is a disease group in which your skin is delicate and develops blisters easily. Keratin gene mutations are most often the cause of EBS. I have downloaded the 3D structure of 5E3X and used PyMOL to perform structural analysis.

Keywords: Epidermolysis bullosa simplex (EBS), basal EBS, PyMOL and structural analysis.

Agro Friendly Microbes.

Swapna Tangi*, Dakshayani Matta and Kamaladevi Vidhyadhara.

M. V. R. Degree College, Visakhapatnam, AP, India. (*Correspondence to ST: tangiswapna123@gmail.com).

Abstract (Poster presentation):

Recent years for man are greatly adapted to used chemicals in farming either in the form of chemical fertilizers or in the form of chemical pesticides. In due course of time, these chemicals are accumulating into the food chain and causing many genetic and biochemical changes both in humans and animals. Many of the people irrespective of age suffer from different types of cancers, hormonal imbalances, autoimmune diseases. If this continues, the human population may be affected a lot. To avoid these adverse conditions, there should be concentration on alternate sources to be used as fertilizers and pesticides. The best alternative source is microbial population. Many types of microorganisms can be used as biofertilizer, biopesticides. This poster is designed to explain about different types and groups of microorganisms to be used as fertilizer and pesticides, their production and marketing procedures and skills.

Keywords: autoimmune disorders, fertilizers, pesticides, micro organisms, biofertilizers and biopesticides.

Effects Of Drinking Water In Anakapalli.

Sai Ganesh Dunna*

M. V. R. Degree College, Visakhapatnam, AP, India. (*Correspondence to SGD: saiganesh222003@gmail.com).

Abstract (Oral presentation):

The two most important resources blessed by nature to mankind are land and water. Undoubtedly, these gifts have to be conserved and maintained with unflinching efforts from every one of us for an effective environmental and ecological balance. The efforts and energy of water resources engineers and conservationists are going in this direction to conserve these precious resources of nature. The present study is an attempt to develop suitable methodology to facilitate decision makers to conserve the resources and also reflects the cause mentioned above has been presented here. The main focus of this study is to identify the critical prone areas for soil erosion and computation of sediment yield in a small basin using Universal Soil Loss Equation and Modified Universal Soil Loss Equation (MUSLE) respectively. It indicated that the water in the municipality is contaminated with pathogenic bacteria and is unfit for drinking. Open defecation, water-logging environment, poor drainage facilities and unscrupulous dumping of domestic waste resulted in deterioration of water quality. That large-scale waterborne diseases are prevalent in this area. Since quality of water is critical in disease prevalence, the water sources used for drinking should be monitored regularly to reduce epidemics, said the study 'Physico-chemical and microbial analysis of water samples in Anakapalle Municipal Corporation' (saradha river). The study was carried out at some selected sampling sites within the municipality. During the study period, all the five water samples showed the presence of the nine pathogenic bacteria such as *Escherichia coli*, *Klebsiella pneumoniae*, *Pseudomonas aeruginosa*, *Salmonella typhi*, *Shigella dysenteriae*, *Staphylococcus aureus*, Group D *Streptococcus*, *Vibrio cholerae* and *V. parahaemolytics*.

Keywords: Universal soil loss equation, Water-logging environment, waterborne diseases and pathogenic bacteria.

Crystal structure of the cytoplasmic actin capping protein Cap32_34 from *Dictyostelium discoideum*.

[a, b]Jayasurya Nakka and [b]Ravikiran S. Yedidi*

[a]Centre for Biotechnology, Department of chemical engineering, Andhra university college of engineering (A), Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to JN: jayasuryanakka@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Dictyostelium discoideum is present in foods such as grain, milk, meat and fish contaminated with this fungus due to poor storage conditions. The AFB 1 is a potent hepatotoxin and carcinogen and it represents a significant cancer threat, especially in developing countries. It is a social amoeba i.e professional phagocyte that can rapidly ingest and degrade bacteria for nutrients. Sentinel cells in *Dictyostelium discoideum* are phagocytic cells responsible for removing toxic material from the slug stage of the social cycle. Because many of its genes are homologous to human genes, yet its lifecycle is simple, *Dictyostelium discoideum* is commonly used as a model organism. It can be observed at organismic, cellular, and molecular levels primarily because of their restricted number of cell types and behaviors, and their rapid growth. It is used to study cell differentiation, chemotaxis, and apoptosis, which are all normal cellular processes. The Social Amoeba *Dictyostelium discoideum* is highly resistant to polyglutamine aggregation. I have downloaded the 3D structure of 4AKR and used PyMOL to perform structural analysis.

Keywords: *Dictyostelium discoideum*, hepatotoxin, carcinogen, 4AKR, PyMOL and structural analysis.

Biofuel - An alternative source of energy for the present and future.

Soniya kumari*, Madhulatha Gorle and Gayathri Purimetla.

M. V. R. Degree College, Visakhapatnam, AP, India. (*Correspondence to SK: sk1915149251@gmail.com).

Abstract (Poster presentation):

Biofuel is a fuel that is produced over a short period of time span from biomass. This can be used as an alternative energy source and this is the ultimate energy source which can be produced in less cost effective methods. The two forms of biofuels i.e Biothermal and biodiesel are currently in usage since 2019, worldwide. Biofuel production provided 3% of the world's fuel for road transport, and a very small amount of aviation biofuel. The international energy agency wants biofuel to make up 64% of the world demand for transportation of fuels by 2018 in order to reduce petroleum microalgae, which have long been considered as a promising feedback for biomass production. Recently microalgae have been discussed to be used as renewable feed stocks. The selection is based on lipids and fatty acids content of the cell wall or the particular species. The microalgae cultivation can be done in an open culture system called ponds. After algae growth, there are many methods for harvesting microalgae. After harvesting this can be converted into biodiesel.

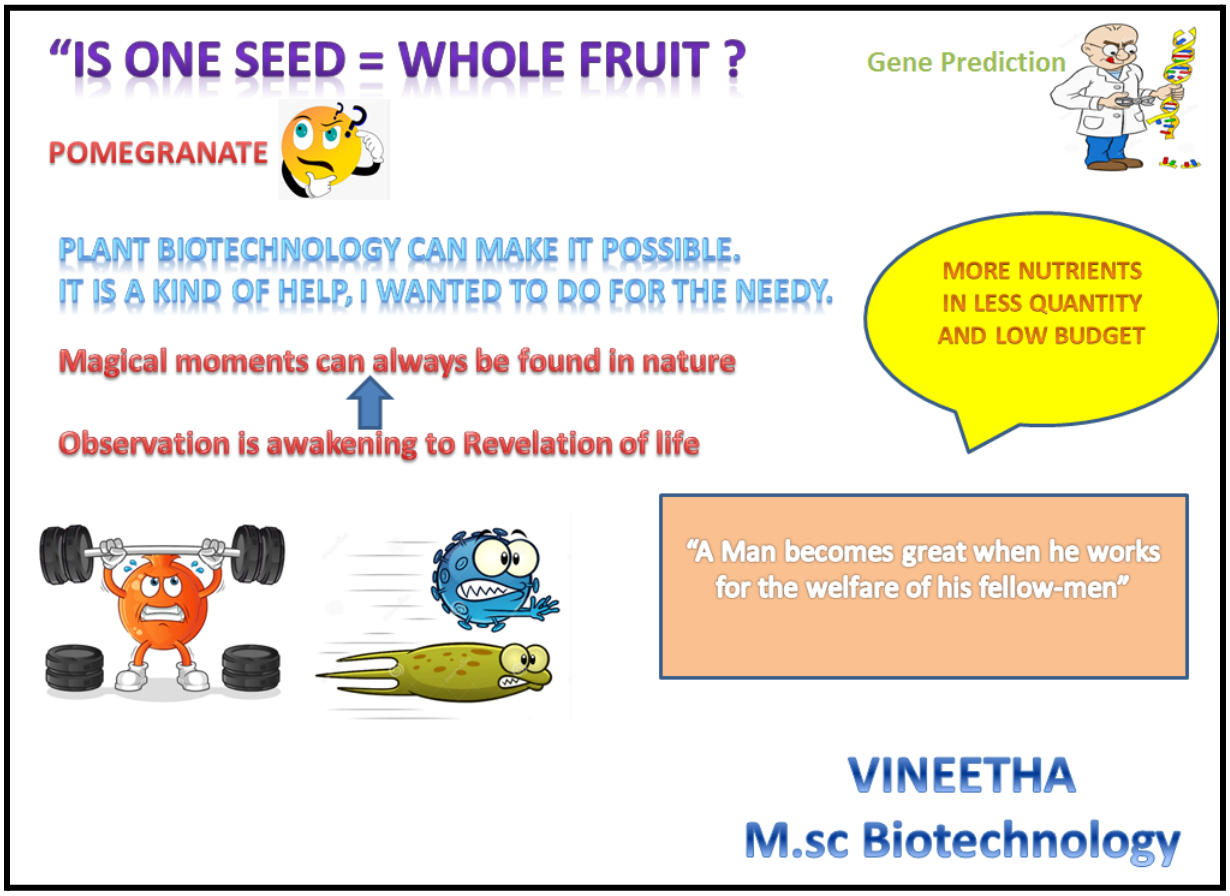
Keywords: Biofuel, microalgae, cell wall, biomass and open culture system.

Is one seed = one fruit?

Vineetha Lenka*

Department of Biotechnology, Andra University, Visakhapatnam, AP, India. (*Correspondence to VL: 721210304053@andhrauniversity.edu.in).

Abstract (Poster presentation):



Keywords: Plant biotechnology, nutrients and cost effective.

Biophysical Approach For Treating Esophageal Squamous Cell Carcinoma With The Help Of Protein Liquid Liquid Phase Condensates.

Manikanta Sodasani* and Ravikiran S. Yedidi*

The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to MS: mani81314821@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Oral presentation):

Esophagus cancer is one of the most casualties causing problem nowadays, because it can only be detectable during the third stage of the cancer. The National Institute of Cancer Biology and Word Health Organization collectively calculated the number of cases and the deaths that are caused by this type of cancer and is about 1 to 2 million per year irrespective of geographical categorization. There are two types of cancers in this category: Esophageal Adenocarcinoma (EAC) and Esophageal Squamous Cell Carcinoma (ESCC). One of the causes of this disease is by negative regulation of the p53/p21 signaling pathway with the help of Long non-Coding RNA BCAR4 which aggravates cell proliferation. Knocking down of lncRNA BCAR4 induces cell apoptosis and G1/S arrest. Mechanistically, lncRNA BCAR4 sponged with mir-139-3p to upregulate ELAVL1, thereby inhibiting the p53/p21 signaling pathway in ESCC. In conclusion, lncRNA BCAR4 promotes ESCC tumorigenesis via regulating cell signaling pathway and develops a brand-new biomarker and medicinal target for ESCC. As a treatment for the cancer as a miRNA therapy, the required miR-139-3p is delivered by a novel bio physical carrier which is Liquid Liquid Phase Condensate caused by Protein Phase Separation.

Keywords: Esophageal Adenocarcinoma (EAC), Esophageal Squamous Cell Carcinoma (ESCC), Long non-Coding RNA BCAR4 (breast cancer antiestrogen resistance 4), Liquid Liquid Phase Condensate Protein Phase Separation.

The crystal structure of COVID-19 main protease in complex with an inhibitor N3.

Afeez Unnisa* and Ravikiran S. Yedidi*

The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to AU: afeezz786@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

SARS-CoV-2 is responsible for the outbreak of viral pneumonia in 2019-2020. They focused on identifying the drug that leads to target the main protease (Mpro) of SARS-CoV-2: Mpro is a key enzyme of coronaviruses which has a vital role in mediating viral replication and transcription. Due to this it becomes an appealing drug target for SARS-CoV-2. We identified a mechanism-based inhibitor (N3) by computer-aided drug design, and then determined the crystal structure of Mpro of SARS-CoV-2 in complex with this compound. Few of those compounds that have been assayed exhibited promising antiviral activity in cell-based assays.

Keywords: SARS-CoV-2, protease, drug target, crystal structure, antiviral activity and cell-based assay.

Comparative Evaluation of Wheat Protein Extract from Natural and Commercial Wheat Flour.

[a]Nandhini Perla*, [a]Prasanthi Cheekurumelli, [b]Prema Kumari, [c]Anjali Devi, [c]Valisha, [a]Jaya Lakshmi, [a]Nooka Bhavana, [a]Roshini, [a]Sri Harshitha and [a]Bhuvaneshwari.

[a]Department of Microbiology, [b]Department of Botany, [c]Department of Chemistry, St. Ann's college for women, Malkapuram, Visakhapatnam, AP, India. (*Correspondence to NP: perlanandini2003@gmail.com).

Abstract (Oral presentation):

Wheat and wheat products play an important role for food industries, comprising among all other cereal products wheat occupy the first position due to its nutritional values. There was a huge scientific challenge today to develop an easily biodegradable wheat protein. The use of excess proteins, lipids and polysaccharides in commercially available wheat flour have thus been disturbing the human health which would bring the acute health issues. The present study is aimed to check the biodegradability of wheat protein by using E.coli as these bacterial cells are beneficial and symbiotic in their nature of digestion. The wheat protein content varies from 114.4gm/500gm - 34.5gm/500gm. The highest wheat protein extract was observed in commercially available wheat flour when compared with naturally grinded wheat flour. The wheat protein Gluten was insoluble in water, alkaline and also acid due to its polymeric nature. The test for polymer presence showed negative results.

Keywords: Wheat protein, Gluten, biodegradability, E.coli and Polymer.

Synergistic effects of Aq. Theobroma Extract and Doxorubicin on Therapeutic Resistant Cervical Cancer Cells.

Prasanthi Chittineedi* and Santhi Latha Pandrangi.

Onco-Stem Cell Research Laboratory, Department of Biochemistry & Bioinformatics, GITAM School of Sciences, GITAM Deemed to be University, Visakhapatnam, AP, India. (*Correspondence to PC: pchittin@gitam.in).

Abstract (Oral presentation):

Doxorubicin (Dox) is one of the potent antineoplastic drugs currently used as a chemotherapeutic agent for several cancers. Numerous studies suggested that multiple chemotherapeutic cycles with Dox might lead to the development of drug resistance and cardiotoxicity in patients leading to poor prognosis and survival outcomes. The present study aims to lower the drug dosage of Dox without altering its antitumor potential. Aqueous Theobroma Extract (ATE) has been reported previously to have several anti-tumor properties and is known to be used as a traditional medicine in the treatment of various diseases without any adverse effects like cardiotoxicity and hepatotoxicity. In the present study, we demonstrate that ATE, when combined with Dox, exhibited a synergistic antitumor effect and sensitizes therapeutic resistant cervical cancer cells thereby reducing both the dosage and adverse side effects imposed by this chemotherapeutic drug. Gene expression analysis, flow cytometry studies, cell cycle and apoptosis analyses were performed to confirm antitumor effects of ATE.

Keywords: Doxorubicin (Dox), Aqueous Theobroma Extract (ATE), cancer, cardiotoxicity, flow cytometry.

Preparation and comparison of herbal sanitizer with different extracts- anti microbial activity and phytochemical activity.

Vasantha Lakshmi Surisetty*.

Department of chemistry, St. Ann's college for women, Malkapuram, Visakhapatnam, AP, India. (*Correspondence to VLS: lakshmivasantha34@gmail.com).

Abstract (Oral presentation):

'Hygiene' is a key to a healthier body and sanitizer plays a key role in hygiene of the body, where hands act as a door for the microbes or fungal things to enter into the body. We the people subjected to use synthetic sanitizer in covid era without knowing its drawbacks such as skin irritation, altering the pH level of skin, damaging the skin moisture, leaving the stains, allergies, some respiratory issues, etc. Upon the consideration of above mentioned issues. We came up with an idea of preparing herbal sanitizer which is free from all toxic hindrances. This herbal sanitizer involves the preparation of 5 plant extracts and additives selected on the basis of antimicrobial and antifungal activities along with a few reagents such as Mayer's reagent, Wangle's reagent and Hager's reagent. Where the mixture of extracts such as neem-ethanol and camphor-ethanol showed higher antibacterial and antifungal activity against *Klebsiella Pneumonia, Staphylococcus* & *Eschiorichia Coli*. The potency of this herbal sanitizer was also checked on the people having sensitive skin and meets the international standards of texture and odor, effective at killing germs as chemical cleaners. It plays a huge success in eradicating the problems faced by using chemical sanitizers.

Keywords: Herbal Sanitizer, antimicrobial and antifungal activities, plant extracts.

Analysis On Various Cancers Causing Protein :Tumor Protein 53 (Tp53).

[a, b]Haradeep Bhaskar Katta* and [b]Ravikiran S. Yedidi*

[a]Centre for Biotechnology, Department of chemical engineering, Andhra university college of engineering (A), Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to HBK: haradeepj@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Proteins control many important Functions like cell growth. Genetic mutations can affect the function of the proteins. Some types of proteins change the healthier cells to become cancerous. The most common mutated gene in people with cancer is Tumor Protein 53 or TP53. P53 is a tumor suppressor gene whose activation induces apoptosis, cell cycle arrest or senescence, in response to distinct stimuli including DNA damage.Loss of functional P53, which makes cells unable to engage apoptosis after exposure to cellular stress, contributes to tumor formation causing breast, colorectal, liver, lung and ovarian cancers. Too much of P53 suppresses cell cycle progression, causing cell death, premature aging and even cancer. Mutation of TP53 causes Primary leukemia, Sarcoma, testicular cancer, malignant melanoma and cervical cancer.

Keywords: P53, Cancer mutations, Suppressor, Mutation, Rescue.

The Crystal Structure of the Human Hepatitis B Virus Capsid.

[a, b]Chamanthi Paidi* and [b]Ravikiran S. Yedidi*.

[a]Department of Biotechnology, Andhra University, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to CP: chamanthipaidi@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Hepatitis B is a small enveloped DNA virus that poses a major hazard to human health. The crystal structure of the T = 4 capsid has been solved at 3.3 Å resolution, revealing a largely helical protein fold that is unusual for icosahedral viruses. The monomer fold is stabilized by a hydrophobic core that is highly conserved among human viral variants. Association of two amphipathic α-helical hairpins results in formation of a dimer with a four-helix bundle as the major central feature. The capsid is assembled from dimers via interactions involving a highly conserved region near the C terminus of the truncated protein used for crystallization. The major immunodominant region lies at the tips of the α-helical hairpins that form spikes on the capsid surface.

Keywords: Hepatitis B, icosahedral viruses, capsid, crystallization.

Structural analysis of apo bovine alpha-lactalbumin complexed with La3+ ion that acts cytotoxic against cancer cells.

[a, c]Geetika Priya Sajja, [b]Padmasree R and [c]Ravikiran S. Yedidi

[a]Centre for Biotechnology, [b]Department of chemical engineering, Andhra university college of engineering (A), Visakhapatnam, AP, India. [c]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to HBK: geetikapriya5926@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Cancer remains one of the biggest threats to human life. The most common type of cancer on the list is breast cancer in which cells in the breast grow out of control. There are massive demands for compounds to selectively kill cancerous cells. A modification in bovine α-lactalbumin(whey protein) made lethal to tumor cells (BAMLET) was done so that it becomes more cytotoxic against cancer cells. The natural Ca binding site of bovine α-lactalbumin is replaced by lanthanum(III) ion which exhibits greater anticancer activity against breast cancer cells. We examined and analyzed the structure of this compound by downloading it from PDB with the PDB Id: 6IP9 and viewing it using PyMOL software. It has only chain A with sequence length 123. There are three binding sites for sulfate ion, lanthanum ion and glycerol. It also consists of a drug which is attached to the compound by hydrogen bonds. Secondary structure analysis of apo bovine α-lactalbumin complexed with lanthanum(III) ion was performed and a mutant was designed which is yet to be synthesized and evaluated in future.

Keywords: Cancer, 6IP9, La3+ion, PDB, PyMOL, La3+ bovine alpha-lactalbumin.

Crystal Structure Of ROR-γt With Ligand C46d Bound HIV-1 Integrase Catalytic Core Domain (A128T).

[a, b]Ramya Tamarala* and [b]Ravikiaran.S Yedidi*

[a]Department of Zoology, Andhra University, Visakhapatnam, AP, India. [b]The Center For Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to RT: tamaralaramya@gmail.com and RSY : tcabse.india@gmail.com)

Abstract (Poster presentation):

HIV is caused by a virus . It can spread through sexual contact, illicit injuction drug use or sharing needles, contact with infected blood, or from mother to child during pregnancy. HIV destroys CD4-T Cells, white blood cells cause loss of command on our own body immune system. 6LOC - Crystalline structure of ROR Gammat with ligand C46D bound belongs to nuclear protein found in man. This is identified by X-RAY diffraction. The 6LOC integrase catalytic core domain consists of 1 protein molecule. Domain families: SPECIFIC HITS - NR - LRD - ROR - LIKE, SUPER FAMILIES: NR - LRD chemical and non-standard biopolymers (1 molecule)-6 cyclobutyl oxy-9 ethyl~(N)-(4-methylsulfonyl phenyl)methyl carbazole-3 carboxamide citing MMDB-Madej T,Lanczyki CJ,Zhang D, Thiessen PA. MMDB and VAST tracking structural similarities between macromolecular complexes.

Keywords: Human immunodeficiency virus **(**HIV), CD4-T Cells, 6LOC.

Human Melanoma Inhibitory Activity (Mia) Protein: role in tumor progression and the metastasis of Melanoma by modulating integrin activity.

[a, b]Neelima Devi Akula* and [b]Ravikiran S. Yedidi*

[a]Department of Microbiology, Andhra University, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to NDA: neelimadeviakula@gmail.com and RSY: tcabse.india@gmail.com)

Abstract (Poster presentation):

The MIA gene controls the expression of the MIA protein. This protein may play a role in the development and spread of melanoma.Melanocytes are the skin cells responsible for producing melanin, which provides the skin with pigment. In people with melanoma, abnormal melanocytes start growing uncontrollably. Without treatment, these cells can spread throughout the body and have serious health consequences. Melanoma inhibitory activity (MIA) is a small secreted protein that interacts with extracellular matrix proteins like fibronectin, laminin and tenascin and masks their binding sites with integrins situated on the melanocytes membrane. In this way, MIA induces a decrease by 30–50% of the attachments between malignant melanocytes and detaches them from the matrix, and promotes tumor cell invasion and migration. I have downloaded Pdb 1HJD and analyzed in PyMOL MIA is a secreted single-domain protein of 12kDa that contains an antiparallel beta-sheet and two disulfide bonds. MIA appears to be the first extracellular protein adopting an Src homology 3 (SH3) domain-like fold. Elevated levels of MIA linked to late stage Melanoma, the higher the level the greater the odds that the Melanoma has metastasized.

Keywords: fibronectin, laminin, tenascin, pdb, protein, SH3, detach, matrix, integrins, Melanoma.

Structure of Rheumatoid arthritis MHC, complexed with human type II collagen.

[a, b]Hemasri Mallavalli* and [b]Ravikiran S.Yedidi*

[a]Department of Biotechnology, Andhra University, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Science & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to HM: hemasrimallavalli321@gmail.com and RYS:tcabse.india@gmail.com)

Abstract (Poster presentation):

Rheumatoid arthritis is an autoimmune condition, which means it's caused by the immune system attacking healthy body tissue. If you have rheumatoid arthritis, your immune system mistakenly sends antibodies to the lining of your joints, where they attack the tissue surrounding the joint. The susceptibility allele for rheumatoid arthritis MHC is HLA-DR1 (DRB1*0101). The expressional changes in this allele causes rheumatoid arthritis disease. To study its function, the three dimensional crystallographic structure of HLA-DR1 is complexed with a RA autoantigen, the human type II collagen peptide CII. The binding sites of MHC and CII peptide have significant roles in causing disease. Participation of DRB1-Arg is significant because it is part of the shared epitope expressed by DR alleles associated with RA susceptibility. One prevailing hypothesis is that the RA-associated HLA-DR molecules present self-antigens to auto aggressive T cells, which subsequently induce an inflammatory response that leads to development of arthritis.

Keywords: Rheumatoid arthritis, autoimmune, HLA-DR1, RA autoantigen, human type II collagen peptide CII.

SHANK3 an autism spectrum disorder (ASD)-associated gene involved in pathogenesis and neuropathology of ASD.

[a, b]Pravallika Sandipamu* and [b]Ravikiran S. Yedidi*

[a]Department of Zoology, Andhra University, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to SP: pravallika.sandipamu@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

SHANK3 is a synaptic scaffolding protein enriched in the postsynaptic density of excitatory synapses and plays important roles in the formation, maturation, and maintenance of synapses. Haploinsufficiency of the SHANK3 gene causes a developmental disorder, 22q13.3 deletion syndrome (known as Phelan-McDermid syndrome), that is characterized by severe expressive language and speech delay, hypotonia, global developmental delay, and autistic behavior. Since several SHANK3 mutations have been identified in a particular phenotypic group in patients with autism spectrum disorder (ASD), the SHANK3 is strongly suspected of being involved in the pathogenesis and neuropathology of ASD. Five CpG-islands have been identified in the SHANK3 gene, and tissue-specific expression of SHANK3 is regulated by DNA methylation in an epigenetic manner. Cumulative evidence has shown that several SHANK3 variants are expressed in the developing rodent brain and that their expression is regulated by DNA methylation of intragenic promoters Autism spectrum disorders (ASD) are developmental disorders with a multiple genetic background. Many genes have been shown to be associated with ASD, including genes coding for cell-adhesion molecules. These molecules are important in developmental processes, such as brain development.

Keywords: SHANK3, 22q13.3 deletion syndrome, autism spectrum disorder (ASD), DNA methylation.

Purification, crystallization and preliminary X-ray diffraction analysis of an oomycete-derived Nep1-like protein, a common toxin fold mediates microbial attack and plant defense for NECROSIS.

[a, b]Kamalakumari Gadigoyala* and [b]Ravikiran S. Yedidi*

[a]Department of Zoology, Andhra University, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to KG: gkamalakumari18@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Many plant pathogens secrete toxins that enhance microbial virulence by killing host cells. Usually, these toxins are produced by particular microbial taxa, such as bacteria or fungi. In contrast, many bacterial, fungal and oomycete species produce necrosis and ethylene-inducing peptide 1 (Nep1)-like proteins (NLPs) that trigger leaf necrosis and immunity-associated responses in various plants. We have determined the crystal structure of an NLP from the phytopathogenic oomycete *Pythium aphanidermatum* to 1.35A resolution. The protein fold exhibits structural similarities to cytolytic toxins produced by marine organisms (actinoporins). Computational modeling of the 3-dimensional structure of NLPs from another oomycete, *Phytophthora parasitica*, and from the phytopathogenic bacterium, *Pectobacterium carotovorum*, revealed a high extent of fold conservation. NLP mutant protein analyses revealed that identical structural properties were required to cause plasma membrane permeabilization and cytolysis in plant cells, as well as to restore bacterial virulence. In sum, NLPs are conserved virulence factors whose taxonomic distribution is exceptional for microbial phytotoxins, and that contribute to host infection by plasma membrane destruction and cytolysis. We further show that NLP-mediated phytotoxicity and plant defense gene expression share identical fold requirements, suggesting that toxin-mediated interference with host integrity triggers plant immunity-associated responses. Phytotoxin-induced cellular damage-associated activation of plant defenses is reminiscent of microbial toxin-induced inflammasome activation in vertebrates and may thus constitute another conserved element in animal and plant innate immunity.

Keywords: Phytotoxins, (Nep1)-like proteins (NLPs), X-ray diffraction, mutant protein analyses.

Structural Foundation for SARS-COV 2 Nucleocapsid Protein Identification by Antibody C 2 with single-domain.

[a, b]Sathvika Geddam* and [b]Ravikiran S. Yedidi*

[a]Department of Zoology, Andhra University, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to SG: sathvika71999@gmail.com and RSY: tcabse.india@gmail.com)

Abstract (Poster presentation):

The growing threat of new & potentially most dangerous infection of twentieth century is covid-19 Pandemic caused by SARS-Cov-2 belongs to family Coronaviridae. The novel coronavirus is an enveloped, non-segmented, positive sense single stranded RNA which uses RdRP (RNA dependent RNA polymerase) for its genomic replication. Among various types of proteins present, Nucleocapsid proteins shows NTD (N-terminal disorder region), and CTD (C-terminal dimerization domain), which can bind RNA cooperatively to promote RNA packaging and chaperoning. However effective vaccines against novel virus has been developed, new method was adopted for detecting active SARSCov-2 infection the crystal structure of three llama derived single domain antibodies have been used as they show high binding affinity, where one recognizes N-terminal RNA binding domain and one recognizing C-terminal dimerization domain which results in RNA-binding affinity & Nucleocapsid separation by Liquid-Liquid phase separation which helps to develop diagnostic tests to detect SARS COV-2 variants.

Keywords: Chaperoning, dimerization, phase separation, RDRP.

RNA Dependent RNA Polymerase of Dengue 3 NS5 Bound with RK-0404678 Compound in the Context of Developing Antiviral Drug.

[a, b]Gayathri Pemmadi* and [b]Ravikiran S.Yeddi*.

[a]Department of Biotechnology, Andhra University, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Andhra University, Visakhapatnam, AP, India. (*Correspondence to GP: nakshtthra.pemmadi@gmail.com and RSY: tcabse.india@gmail.com)

Abstract (Poster presentation):

Dengue virus belongs to the genus Flavivirus within the Flaviviridae family. Dengue caused by 4 different serotypes DENV-1-4. Dengue is a mosquito borne viral infection, mainly occurs in tropical and subtropical areas. Mild infection causes dengue fever and severe infection causes Dengue hemorrhagic fever and Dengue shock syndrome. There is no vaccine and drug to prevent and treat Dengue viral infection. NS5 is the largest non-structural protein (900kDa). It bears enzymatic activity. Its N-terminal encodes dual N7 and 2-OMethyltransferase(MTase), and possibly guanylyl transferase (GTase) while the C-terminal encodes with RNA dependent RNA polymerase (RdRp). RdRp and MTase activities are well characterized structurally and functionally. MTase protects the viral genome by RNA capping while RdRp is responsible for replication of viral RNA which acts as an effective target for drug development. RK-0404678($C_9H_6O_4S$) is an organic compound with EC 50 value of 6.0µm for DENV-2 is selected based on cellular antiviral and cytotoxic assays. Crystallographic analysis reveals 2 unique binding sites within RdRp, inhibiting the RdRp activity. No resistant virus emerged after the serial passage of dengue virus with RK-0404678.nearly 16240 small molecule compounds were screened for their capability to inhibit DENV RdRp activity which provides a new framework for antiviral drug development.

Keywords: Dengue hemorrhagic fever, Dengue shock syndrome, Serotypes, cellular antiviral, Cytotoxic.

Lysine 53 Acetylation of Cytochrome c in Prostate Cancer: Warburg Metabolism and Evasion of Apoptosis.

[a, b]Yathiraj Chigilipalli* and [b]Ravikiran S. Yedidi*

[a]Department of Zoology, Andhra University, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to YC: ch.yathiraj@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Prostate cancer is the second leading cause of cancer-related death in men. Two classic cancer hallmarks are a metabolic switch from oxidative phosphorylation (OxPhos) to glycolysis, known as the Warburg effect, and resistance to cell death. Cytochrome c (Cytc) is at the intersection of both pathways, as it is essential for electron transport in mitochondrial respiration and a trigger of intrinsic apoptosis when released from the mitochondria. However, its functional role in cancer has never been studied. Our data show that Cytc is acetylated on lysine 53 in both androgen hormone-resistant and -sensitive human prostate cancer xenografts. Cytochrome c oxidase (COX) activity analyzed with purified Cytc variants showed reduced oxygen consumption with acetyl mimetic Cytc compared to the non-acetylated Cytc (WT), supporting the Warburg effect.K53Q Cytc had significantly lower caspase-3 activity, suggesting that modification of Cytc K53 helps cancer cells evade.

Keywords: Prostate cancer, Warburg effect, Cytochrome c, Cytochrome c oxidase (COX), acetylation.

HIV capsid is a tractable target for small molecule Therapeutic Intervention.

[a, b]Mahalakshmi Voleti* and [b]Ravikiran S. Yedidi*

[a]Department of Zoology, Andhra University, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to MV: mahimsd5950@gmail.com and RSY: tcabse.india@gmail.com)

Abstract (Poster presentation):

HIV capsid is a tractable target for small molecule Therapeutic Intervention. Despite a high current standard of care in antiretroviral therapy for HIV, multidrug-resistant strains continue to emerge, underscoring the need for additional novel mechanism inhibitors that will offer expanded therapeutic options in the clinic. A new class of small molecule antiretroviral compounds that directly target HIV-1 capsid (CA) via a novel mechanism of action. The compounds exhibit potent antiviral activity against HIV-2, and inhibit both early and late events in the viral replication cycle. The mechanistic studies indicate that these early and late activities result from the compound affecting viral uncoating and assembly, respectively. The Amino acid substitutions in the N-terminal domain of HIV-1 CA are sufficient to confer resistance to this class of compounds, identifying CA as the target in infected cells. A high resolution co-crystal structure of the compound bound to HIV-1 CA reveals a novel binding pocket in the N-terminal domain of the protein. Our data demonstrate that broad-spectrum antiviral activity can be achieved by targeting this new binding site and reveal HIV CA as a tractable drug target for HIV therapy.

Keywords: HIV capsid, multidrug-resistant, antiretroviral compounds, small molecules.

Structural Basis Of Epilepsy-Related Ligand-Receptor Complex Lgi1-Adam22.

[a, b]Naga Prathyusha Gundubogula* and [b]Ravikiran S. Yedidi*

[a]Department of Human Genetics, Andhra University, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to NPG: prathyushagn1@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Epilepsy is a common brain disorder throughout history. Epilepsy-related ligand-receptor complex, LGI1-ADAM22, as their mutations and acquired LGI1 autoantibodies cause epileptic disorders in humans. The crystal structure of the human LGI1-ADAM22 complex, revealing a 2:2 heterotetrameric assembly. The hydrophobic pocket of the C-terminal epitempin-repeat (EPTP) domain of LGI1 binds to the metalloprotease-like domain of ADAM22. The N-terminal leucine-rich repeat and EPTP domains of LGI1 mediate the intermolecular LGI1-LGI1 interaction. Resolution: 1.78 ÅThe high-resolution structures of the LGI1 EPTP–ADAM22 ECD complex and LGI1 LRR allowed us to interpret the 7.13-Å-resolution map and obtain the information of the intermolecular interactions between LRR and EPTP and that between LRR and ADAM22 ECD in the 2:2 heterotetrameric LGI1–ADAM22 complex.

Keywords: Epilepsy, LGI1-ADAM22, crystallization, intermolecular interactions.

Thermally stable structure of ZIKA Virus (5IZ7) helps to reduce the spread of the virus.

[a, b]Roopini Garbhapu* and [b]Ravikiran S. Yedidi*

[a]Department of Biochemistry, Andhra University, Visakhapatnam, AP, India. [b]The center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS - E), Visakhapatnam, AP, India.
(*Correspondence to MA: sravanijyothi38@gmail.com and RSY: tcabse.india@gmail.com)

Abstract (Poster presentation):

Zika virus (ZIKV) is one of the diseases formerly neglected. But recent studies states that it has been associated with microcephaly in fetuses and Gillian Barre syndrome in adults. Here we can see the 3.7 Å resolution structure of ZIK, it is similar to that of other flaviviruses. By comparing sequence and structure of ZIKV envelope (E) protein shows resemble with other neurovirulent West Nile and Japanese encephalitis viruses and some are similar to dengue virus (DENV).The virus particle structurally stable even incubated at 40 ℃ in sharp contrast to the less thermally stable DENV. This structural stability of the virus may help to survive in harsh conditions of semen, saliva and urine. Antibodies that destabilize the structure may reduce the spread of virus.

Keywords: Zika virus (ZIKV), microcephaly, Gillian Barre syndrome, dengue virus (DENV).

Effect Of Apoe Epsilon- 4 Genotype In Alzheimer's Disease.

[a, b]Sasi Prathyusha Puripanda* and [b]Ravikiran S. Yedidi*.

[a]Department of Human Genetics, Andhra University, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to SPP: and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Apolipoprotein E (apoE) is an important lipid-transport protein in human plasma and brain. It has three common isoforms (apoE2, apoE3, and apoE4). ApoE is a major genetic risk factor in heart disease and in neurodegenerative disease, including Alzheimer's disease. The interaction of apoE with heparan sulfate proteoglycans plays an important role in lipoprotein remnant uptake and likely in atherogenesis and Alzheimer's disease. The resolution of the structure is 2.0 Å identified by its high affinity for the N-terminal domain of apoE4, this oligosaccharide was determined to be an octasaccharide of the structure DeltaUAp2S(1→[4)-alpha-D-GlcNpS6S by nuclear magnetic resonance spectroscopy, capillary electrophoresis, and polyacrylamide gel electrophoresis. From the X-ray crystal structure of the N-terminal apoE4, we predicted that binding of the octasaccharide at this site would result in a change in intrinsic fluorescence.

Keywords: Apolipoprotein E (apoE), octasaccharide, DeltaUAp2S, nuclear magnetic resonance (NMR), X-ray crystallography.

The Role Of Gpcr In The Pathology Of Alzheimer's Disease.

[a, b]Nombuso Lolo Fakudze* and [b]Ravikiran S. Yedidi*

[a]Centre for Biotechnology, Department of chemical engineering, Andhra university college of engineering (A), Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to NLF: lolonombusofakudze@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Alzheimer's disease commonly known as AD is the most emerging dementia in the elderly and its increasing prevalence presents treatment challenges. Despite a better understanding of the disease, the current mainstay of treatment cannot modify pathogenesis or effectively address the associated cognitive and memory of deficits. Emerging evidence suggests adenosine G protein-coupled receptors (GPCRs) are promising therapeutic targets for Alzheimer's disease. The adenosine A1 and A2 receptors are expressed in the human brain and have proposed involvement in the pathogenesis of dementia. Targeting these receptors preclinically can mitigate pathogenic beta-amyloid and tau neurotoxicity whilst improving cognition and memory. However currently there are no available medicines targeting these receptors approved for treating dementia. There are strategies that are used to increase drug discovery and enhance the therapeutic response.

Keywords: Alzheimer's, adenosine G protein-coupled receptors (GPCRs), beta-amyloid and tau neurotoxicity.

Cobalt myoglobin studies provide insight into the stereochemistry of bound oxygen molecules and ligand binding sites.

[a, b]Pravallika Lankapalli* and [b]Ravikiran S. Yedidi*

[a]Department of Biochemistry, Andhra University, Visakhapatnam, AP, India. [b]The center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to PL: valliniharika@gmail.com & RSY: tcabse.india@gmail.com)

Abstract (Poster presentation):

The structures of the deoxy, oxy, and aquomet forms of native sperm whale myoglobin reconstituted with cobalt protoporphyrin IX have been determined by X-ray crystallography. Cobalt myoglobin closely resembles native iron myoglobin in overall structure, especially in their respective aquomet forms. In the cobalt oxymyoglobin structure, the Nepsilon of distal histidine 64 lies within hydrogen bonding distance to both the oxygen atom directly bonded to the cobalt and the terminal oxygen atom, in agreement with previous EPR and resonance Raman studies. The metal atom in cobaltous myoglobin does show a small 0.06 Å out of porphyrin plane displacement when moving from oxy to deoxy state. In the case of native iron-containing myoglobin, the oxy to deoxy transition results in a larger 0.16 Å displacement of the metal farther out of the porphyrin plane, attributed to an increase in spin from S = 0 to S = 2. The small displacement in cobalt myoglobin is due to a change in coordination geometry, not spin state (S = 1/2 for both cobalt deoxy- and oxymyoglobin).

Keywords: Aquomet, cobalt protoporphyrin IX, Nepsilon, X-ray crystallography.

An Analysis Of BRCA1 Gene Taking Breast Cancer Into Account.

[a, b]Hanisha Penta* and [b]Ravikiran S. Yedidi*

[a]Department of Microbiology, Andhra University, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to HP: hanisha1401@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Oral presentation):

Breast cancer develops in the epithelial lining of the glandular tissue's ducts or lobules. It can subsequently spread through blood vessels and lymph vessels, leading to metastasis. Breast cancer is the most common disease in the world, affecting 7.8 million people as of the end of 2020. The name "BRCA" is an abbreviation for "BReast CAncer gene". Breast cancer risk is influenced by two different genes, BRCA1 and BRCA2. Contrary to what their names would imply, BRCA genes do not result in breast cancer, rather play a big role in preventing breast cancer. They aid in repairing DNA damage that can cause cancer and the unchecked growth of malignancies. The BRCA genes are hence referred to as tumor suppressor genes. One in 400 individuals have mutant BRCA1 or BRCA2 genes. A BRCA gene mutation may reduce the gene's capacity to repair DNA damage, which might lead to cancer. The breast cancer susceptibility gene contains at its c terminus two copies of a conserved domain that was named BRCT for BRCA1 C terminus (95AA). BRCT domains have been implicated in phosphorylation independent protein interactions. To analyze the three-dimensional structure, the structure is downloaded from the Protein Database and opened in the PyMOL software. The peptide ATRIP interacts with the protein BRAC via nine hydrogen bonds to form a dimeric protein that has two identical monomers. The average hydrogen bond length of 2.9 Angstrom explains why there is a considerable binding affinity between them.

Keywords: Breast cancer, BRCA, tumor suppressor, ATRIP, BRCT domain.

Structural analysis of TP53 in association with different ligands in the context of Cancer.

[a, b]Srividya, Inemella* and [b]Ravikiran S. Yedidi*

[a]Department of Pharmaceutical Biotechnology, Andhra University College of Pharmaceutical Sciences, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to SI: vidyasivani229@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Oral presentation):

Cancer is a disease caused by uncontrolled division of abnormal cells. Somatic TP53 mutations occur in almost every type of cancer at rates from 38%–50% in ovarian, oesophageal, colorectal, head and neck, larynx, and lung cancers and to about 5% in primary leukemia, sarcoma, testicular cancer, malignant melanoma and cervical cancer. TP53 (Tumor Protein) is a protein coded by the TP53 gene that acts as tumor suppressor by regulating cell division. TP53 protein structure was secured from RCSB PDB and secondary structure analysis was done by using PyMOL software. Using the zinc database different ligands were searched and selected based on activity. The two-dimensional structures were downloaded and converted to three-dimensional structures by chemsketch, later by using PyMOL, they were transformed to pdb files, by utilizing autodock tools. Pdb files were converted to pdbqt files. The docking score of different ligands was obtained through autodock vina, finest score ligands were chosen and out of which best pose was analyzed using PyMOL.

Keywords: TP53, cancer, ligands, RCSB PDB, PyMOL, chemsketch, pdbqt, autodock tools, vina.

A Radical Solution for Human health.

[a, b]Jahnavi Chintalapati* and [b]Ravikiran S. Yedidi*

[a]Department of Biochemistry, Andhra University, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to JC: janu2001bg@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Oral presentation):

The fact that the number of microbial genes in our body is greater than our own genes signifies the plausible impact of microbiome on humans. The diverse human microbiome plays a myriad of roles in health and wellness, several of which have been proved. Yet there is much more to be cognizant of in terms of how it can be applied to have a healthy lifestyle, as microbiome is the key interface between the body and the environment. Furthermore, several other fields of science could be utilized to bring in advancements benefiting society.

Keywords: Human Microbiome, health, lifestyle.

Structural analysis of Dystrophin-Actin binding amino terminal domain (ABD1).

[a, b]SaiTejaSri Meka* and [b]Ravikiran S. Yedidi*

[a]Department of Human Genetics, College of Science and Technology, Andhra University, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to STM: saitejasrim@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Dystrophin is a cytoskeletal multidomain protein which is an essential component that keeps muscle cells intact as it supports muscle fiber strength. It is responsible for connecting the cytoskeleton of each muscle fiber to the underlying basal lamina through a protein complex i.e., dystrophin associated glycoprotein (DAG) complex containing many subunits. Its N-terminal domain binds to F-actin (ABD1) and its C-terminal binds to the DAG complex in the membrane. ABD1 contains two calponin homology domains. At the sarcolemma, dystrophin binds to dystroglycan, which in turn acts as a receptor for multiple ECM ligands. The Structural Analysis of N-terminal actin binding domain of Human Dystrophin protein (PDB ID: 1DXX) is performed using PyMOL Software. Pathogenic Mutations result in Duchenne or Becker muscular dystrophy (DMD or BMD).

Keywords: Dystrophin, ABD1, Structural Analysis, PyMOL.

Structural analysis of Rev protein in association with different ligands in context of HIV.

[a, b]Raviteja Kolluru* and [b]Ravikiran S. Yedidi*

[a]Department of Pharmaceutical Biotechnology, Andhra University College of Pharmaceutical Sciences, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India. (*Correspondence to RK: ravitejakolluru98722@gmail.com and RSY: tcabse.india@gmail.com).

Abstract (Oral presentation):

HIV is a Human Immunodeficiency virus that attacks the body's immune system. REV is a transactivating protein that is coded by the REV gene, which is essential to the regulation of HIV-1 protein expression. It mediates the export of unprocessed HIV-1 RNAs to cytoplasm leading to production of viral progeny. The REV protein was obtained from RCSB PDB and secondary structure analysis was done by using PyMOL software.Using zinc databases different ligands were searched and selected. The two-dimensional structures were downloaded and converted to three-dimensional structures by chemsketch, later by using PyMOL, it was transformed to .pdb files. By utilizing autodock tools .pdb files were converted to .pdbqt files.The docking score of different ligands was obtained through autodock vina, finest score ligands were chosen and out of which best pose was analyzed using PyMOL.

Keywords: Human Immunodeficiency virus (HIV), REV, PyMoL, ChemSketch, Autodock vina.

Regulation of cell proliferation, survival and death by casein kinase II.

[a, b]Sowjanya Viyyapu* and [b]Ravikiran S. Yedidi*

[a]Department of Human Genetics, Andhra University, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E). (*Correspondence to SV: and RSY: tcabse.india@gmail.com).

Abstract (Poster presentation):

Casein Kinase II is a multifunctional protein kinase which is a hetero tetramer having two alpha catalytic subunits and two beta regulatory units, Beta subunit has a truncated form of a C-Terminal structure which has been determined by X-Ray Crystallography (1.7Å resolution). It has ligand interactions with Mg+2 and Zn+2. CK2 is found in both Nucleus and cytoplasm. CK2 regulates several cellular processes such as Cell Growth, Proliferation, death, Cell signaling, transcription and maintenance of Cell viability. CK2 is responsible for Phosphorylation of Substrates and it has apoptotic function which allows cancer cells to escape cell death. It also had its role in Viral infections. CK2 mediated phosphorylation ensures the survival of tumor cells and it is an important target for antitumor therapy.

Keywords: Casein Kinase II, X-Ray Crystallography, Cancer, antitumor therapy.

Autism spectrum disorder.

Nandini Tamada*

M. V. R. College, Visakhapatnam, AP, India. (*Correspondence to NT: nandinitamada01@gmail.com).

Abstract (Poster presentation):

Autism is a development disorder that manifests itself in early childhood. Autism is characterized by having difficulties with social interaction, displaying problems with verbal and non verbal communication exhibiting repetitive behaviors and having narrow obsessive interests. These behaviors can range in impact from mild to disability In the last 40 years, there has been a huge increase in autism genetics research and a rapidly growing number of discoveries. Recent studies have shown that genetic mutations occur in the majority of individuals with autism which cause a variety of disorders. AD is a constellation of neurodevelopmental presentations with high heritability and both phenotypic and genetic heterogeneity. There is currently no cure for autism, drugs are used for treating irritability associated with autism. No drug therapies currently target the underlying causes or core manifestations of autism.

Keywords: Autism, genetic heterogeneity, genetic mutations.

Autoimmune disorder - myositis.

Dhanalakshmi Thedlapu*

M. V. R. College, Visakhapatnam, AP, India. (*Correspondence to DT: thedlapudhana1@gmail.com).

Abstract (Poster presentation):

The autoimmune disorders are idiopathic inflammatory myopathies; they are characterized by inflammation of skeletal muscle and organ involvement to identify genetic risk factors and to increase our understanding of disease pathogenesis. These associative genes are involved in both the innate and adaptive immune response while identifying variants in autoimmune disorder gene expression studies from individuals and confirmed the role of interferon signaling and other dysregulated pathways and also identified cell type specific signatures. The most common cub types of autoimmune myositis are dermatomyositis, immune mediated necrotizing myopathy l, these all are rare diseases specific autoantibodies associated with unique clinical phenotypes may be used for diagnostic and prognostic purposes. Diagnosing the specific subtypes of autoimmune myopathy can be achieved by combining relevant features of history.

Keywords: Autoimmune disorders, autoantibodies, myopathy.

Lumpy skin disease in cattle.

Chandrika Kona*

Andhra University, Visakhapatnam, AP, India. (*Correspondence to CK:chandrikakona17@gmail.com).

Abstract (Oral presentation):

As per the literature scanned, outbreaks of LSD in cattle and Buffalo have been reported in certain pockets of the world (endemically). Outbreaks of LSD have been reported in late 2019 (as per OIE report) in India. Recently, the outbreaks have been documented in certain parts of Maharashtra. Therefore, it was found pertinent to publish a review article, highlighting the recent updates of this disease. A brief description of a viral disease called LUMPY SKIN DISEASE (LSD). Lumpy skin disease is an emerging bovine viral disease, which is endemic in most African countries and some Middle East ones, and the elevated risk of the spread of disease into the rest of Asia and Europe should be considered. The recent rapid spread of disease in currently disease-free countries indicates the importance of understanding the limitations and routes of distribution. The causative agent, Capripoxvirus, can also induce sheeppox and goatpox. The economic significance of these diseases is of great concern, given that they threaten international trade and could be used as economic bioterrorism agents. The distribution of capripox viruses seems to be expanding due to limited access to effective vaccines and poverty within farming communities. This is largely due to the economic effects of the Covid-19 pandemic and the imposition of crippling sanctions in endemic regions, as well as an increase in the legal and illegal trade of live animals and animal products, and also global climate change. The present review is designed to provide existing information on the various aspects of the disease such as its clinicopathology, transmission, epidemiology, diagnosis, prevention and control measures, and the potential role of wildlife in the further spread of disease.

Keywords: Lumpy skin disease **(**LSD), bovine viral disease, endemic.

Basics of biofloc technology and its importance in aquaculture.

Khadem Hussain Saeedii*, Chandrasekhar A. & Manjulatha C.

Department of Zoology, Andhra University, Visakhapatnam. (*Correspondence to KHS: khadem.saeedi@gmail.com).

Abstract (Oral presentation):

Currently, Biofloc technology (BFT) has attracted the attention of many researchers and farmers. Constantly the demands of aquatic animals are tremendously increasing, and the natural or old pond culture system will not fulfill worldwide demands. The primary role of biofloc technology is to shift from a normal culture system to an intensive or extensive culture system which at least cope with some demands. BFT enhances and facilitates the management of pond water for prawn and fish. The biofloc technology helps in converting nitrogenous waste which is being produced from water of cultured animals or added feed, into microbial proteins. To make ponds healthier and decrease the cost of consumption, it is one of the big challenges in the current era of aqua farming. Biofloc is one of the suitable alternatives in decreasing the feed cost and increases the immunity of cultured organisms against pathogens and disease and may act as probiotic as well. At present, there are few approaches to develop biofloc for new initiating ponds. The current scenario, approaches, gaps and existing problems will be described in this paper. In addition, the role of different microorganisms in biofloc will also be discussed.

Keywords: Biofloc technology, Pond culture, probiotics, microorganisms, and pathogens.

Photocatalytic Degradation of Indigo Carmine Dye using $CuBi_2O_4$ Nanocatalyst and Effect of Various Operational Parameters.

[a]B.B.V Sailaja,* and [b]Ch Jagadeesh

[a]Department of Chemistry, Andhra University, Visakhapatnam, AP, India. [b]Department of Chemistry, Welfare Institute of Science Technology and Management, Andhra University, Visakhapatnam, AP, India. (*Correspondence to BBVS: sailajabbv.chem@gmail.com).

Abstract (Oral presentation):

Visible light responsive $CuBi_2O_4$ nanocatalyst (NPs) has been successfully synthesized by Co-precipitation method at 300 ºC. The photocatalytic degradation of Indigo Carmine (IC) dye has been investigated over $CuBi_2O_4$ (NPs) photocatalyst. The structural and morphological studies were carried out by using X-ray diffraction (XRD), Scanning Electron Microscope (SEM), Energy Dispersive Spectroscopy (EDS) and Fourier Transform Infrared (FT-IR) spectra showing the single phase monoclinic structure. The X-ray diffraction (XRD) analysis confirmed a single phase monoclinic crystal. The EDS plots revealed the existence of no extra peaks other than constituents of the taken up composition. $CuBi_2O_4$ nanocatalyst was found to be an efficient catalyst for the degradation of dye and 94% degradation was observed in 120 min. Effect of various operational parameters such as amount of catalyst (0.1–0.25 g/L), initial concentration of dye (5 ppm–25 ppm) and pH (3–11) of dye solution on the rate of dye degradation was studied. The optimum operational parameters for the degradation of IC were observed at pH 4.0, at 20 ppm concentration and at a catalyst loading of 1 g/L. Moreover, hydroxyl radicals have been detected in the photocatalytic reaction mixture by using Terephthalic acid photoluminescence probing technique.

Key words: Photocatalysis; Indigo Carmine (IC); $CuBi_2O_4$; Terphthalic acid.

Increase in the predicted mRNA stability of certain SARS CoV-2 mutant spike proteins compared to wild type may pose potential risk to vaccines.

[a, b]Abhinav V. K. S. Grandhi* and [b]Ravikiran S. Yedidi*

[a]Koringa School of Pharmacy, Korangi, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E), Visakhapatnam, AP, India.

Abstract (Oral presentation):

Emergence of mutant variants in severe acute respiratory syndrome coronavirus-2 (SARS CoV-2) has been evident in the past two years (2019 to 2021). Irrespective of the origin of mutations, these mutant variants caused a great liability to human life with high morbidity rates across the world. Minute changes in the surface topology of the viral spike protein may cause significant changes in its epitope and may contribute to the failure of the current vaccines. In this study, we generated mutations in a systematic way throughout the receptor binding domain (RBD) of the spike protein and calculated the corresponding mRNA stability of the mutants. Our results indicate that more than 15 mutant variants have higher mRNA stability when compared to the wild type spike protein mRNA. By taking the predicted stability of mRNA as a guide we accessed the potential risk of epitope changes in such mutants that may cause risk to the existing vaccines. Our findings suggest that there is a potential risk for epitope changes that has to be evaluated in the future.

Keywords: SARS CoV-2, Vaccines, mutants, COVID-19, bioinformatics, mRNA stability.

Drug Utilization Evaluation of Anticancer Drugs at Tertiary care Hospital in East Godavari.

Ratnapriya Geddam* and Abhinav Grandhi*

Koringa School of Pharmacy, Korangi, AP, India.
(*Correspondence to RG: geddamratnapriya@gmail.com and AG: 2402abhinav@gmail.com).

Abstract (Poster presentation):

The present study aimed to evaluate the trends and pattern of prescribing of anticancer drugs. The objectives of the study were to assess the rational use of anticancer drugs, to identify various types of cancer and to estimate the distribution of anticancer drugs. An observational, prospective study was conducted on 304 patients in the oncology department. Data were collected from case reports, prescriptions and medication charts in specially designed forms. The usage of drugs was found to be rational and most of the drugs used were from the hospital formulary. The prescribing habits were appropriate and were in accordance with World Health Organization guidelines. The present study appeared to support best prescribing practices in order to promote treatment and better health care delivery.

Keywords: Anticancer, chemotherapy, oncology, prescribing pattern.

Inhibiting Matrix Metalloproteinases by the Tissue Inhibitors of Metalloproteinases in intimal thickening and atherosclerotic plaque rupture.

[a, b]Hemsai Yadav Palla* and [b]Ravikiran S. Yedidi*

[a]Department of Biotechnology, Andhra University, Visakhapatnam, AP, India. [b]The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E). (*Correspondence to HYP: hemsai.yadav@gmail.com and RSY: tcabse.india@gmail.com)

Abstract (Oral presentation):

Atherosclerosis is the buildup of fats, cholesterol and other substances in and on the artery walls. This buildup is called plaque. The plaque can cause arteries to narrow, blocking blood flow. It all starts when the artery wall gets damaged which leads to plaque formation and the blood flow gets narrowed decreasing the oxygen supply to myocardium, if the plaque gets uprooted it may cause severe heart stroke which leads to death. Intimal thickening,the accumulation of cells and extracellular matrix within the inner vessel wall, is a physiological response to mechanical injury, increased wall stress, or chemical insult (e.g., atherosclerosis). If excessive, it can lead to the obstruction of blood flow and tissue ischemia. Together with expansive or constrictive remodeling, the extent of intimal expansion determines final lumen size and vessel wall thickness. Plaque rupture represents a failure of intimal remodeling, where the fibrous cap overlying an atheromatous core of lipid undergoes catastrophic mechanical breakdown. Plaque rupture promotes coronary thrombosis and myocardial infarction, the most prevalent cause of premature death in advanced societies. The matrix metalloproteinases (MMPs) can act together to degrade the major components of the vascular extracellular matrix. All cells present in the normal and diseased blood vessel wall upregulate and activate MMPs in a multistep fashion driven in part by soluble cytokines and cell-cell interactions. Activation of MMP proforms requires other MMPs or other classes of protease. MMP activation contributes to intimal growth and vessel wall remodeling in response to injury, most notably by promoting migration of vascular smooth muscle cells. A broader spectrum and/or higher level of MMP activation, especially associated with inflammation, could contribute to pathological matrix destruction and plaque rupture. Inhibiting the activity of specific MMPs or preventing their upregulation could ameliorate intimal thickening and prevent myocardial infarction. Elevated levels of MMP-1 MMP-2, MMP-3, MMP-7, MMP-9, MMP-11, MMP-12, MMP-13 , MMP-14, and MMP-16 are all found in human atherosclerotic plaques, especially at the macrophage-rich shoulder regions. Enhanced MMP-1 overexpression is located with areas of increased circumferential tensile stress in the fibrous cap (148) where ruptures are likely to occur. MMP-7 and lesser amounts of MMP-12 are confined to the borders between the lipid core and the macrophage-rich shoulder regions. MMP expression is prominent in macrophages but also present in VSMC, lymphocytes, and EC,. TIMP-1 levels are unchanged or elevated in atherosclerotic plaques. TIMP-2 is also abundant in plaques and TIMP-3 is clearly increased because it is a product of inflammatory macrophages Upregulation of MMPs-1, -2, -3, and -9 is readily detected in models of lipid-induced atherosclerosis in rabbits and MMPs-3, -11, -12, and -13 are also upregulated in mouse plaques Upregulation of MMPs is an early event in fatty streak formation in rabbits and mice and is therefore associated with plaques at all stages, not just in the late events of plaque instability. In cholesterol-fed rabbits, the levels of TIMP-1 and TIMP-2 clearly rise in plaques, and this partly

compensates for the increase in MMP activity . In particular, it was suggested that this confines MMP activity to the pericellular region, stabilizes the base of the lesions, and may prevent plaque penetration into the media. so i conclude that if we downregulate the MMPs by inhibiting them by timps the plaque rupture can be prevented which can stop heart strokes.

Keywords: Atherosclerosis,Plaques, matrix metalloproteinases (MMPs), TIMP's.


The Center for Advanced-Applied Biological Sciences & Entrepreneurship (TCABS-E)
Danavaipeta, Rajahmundry; Tel./WhatsApp: 8660301662; Email: tcabse.india@gmail.com
TCABS-E