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Andhra Bio-Summit Symposium Poster Abstracts.

Expression, Purification and Crystallization of mutant receptor binding domain of coronavirus spike protein.

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Coronavirus disease-2019 (COVID-19) has generated a pandemic in recent years due to lack of appropriate vaccinations and antiviral agents. Majority of lives were lost due to the unavailability of treatment options on time. Many different strategies were explored for COVID-19 vaccine design such as the mRNA vaccine, etc. However, new variants of coronavirus emerged quickly and caused the second wave of pandemic due to the severe failure of vaccines. In this study we hypothesize that new variants of coronavirus may have mutations in their spike proteins causing altered epitopes. In order to verify this hypothesis, we chose to study the T150I mutant receptor binding domain (RBD) of the spike protein that was previously shown to cause major structural deviations in the epitope. The T150I substitution was generated by PCR site-directed mutagenesis using mutagenic primers and the mutant plasmid was used to express the T150I RBD. Ni-NTA affinity column purification was performed. NaCl and $(NH_4)_2SO_4$ grid screens were used to obtain preliminary crystallization hits for the T150I mutant. X-ray diffraction will be performed in future.

Small molecule therapeutic identification for inhibiting CXCL10 protein on beta cells of pancreas.

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Diabetes is one of the major medical issues across the globe. Type 1 diabetes, also known as insulin-dependent diabetes or juvenile-onset diabetes, is a chronic condition that affects the insulin-producing cells of the pancreas. Type 1 diabetes is an autoimmune disease. The body's immune system mistakenly attacks and destroys the beta cells in the pancreas, which are responsible for producing insulin. As a result, the pancreas cannot produce enough insulin. Insulin is a crucial hormone that allows sugar (glucose) to enter cells, providing energy for various bodily functions. Here we identified hit molecules from the ZINC database by taking the CXCL10 protein present in the membranes of the pancreatic beta cells. The small molecules identified in this study show promising binding affinities that can be evaluated further *in vitro* and *in vivo* to test their activity. Further, the toxicity profiles are yet to be evaluated to assess the safety.

Unveiling the molecular ballet: Computational exploration of MCL1 protein interactions for leukemia therapeutics.

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Leukemia is a group of blood cancers that usually begin in the bone marrow and result in high numbers of abnormal blood cells. There are four main types of leukemia, acute lymphoblastic leukemia (ALL), acute myeloid leukemia (AML), chronic lymphocytic leukemia (CLL) and chronic myeloid leukemia (CML) as well as a number of less common types. The myeloid cell leukemia 1 (MCL1) protein is a crucial member of the B-cell lymphoma 2 (BCL-2) family playing a pivotal role in regulating apoptosis. MCL1 is primarily located in the outer mitochondrial membrane where it governs the intrinsic apoptotic pathway by controlling the release of Cytochrome c and other pro-apoptotic factors. The active site of the MCL1 protein was screened using ligands from the ZINC database. We identified a hit molecule with promising binding affinity close to -10 kcal/mol. This compound is yet to be synthesized and evaluated in future.

Structural insights into migraine: rational design and target-specific development of potential therapeutics.

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Migraine is a genetically influenced complex neurological disorder characterized by episodes of moderate-to-severe headache, most often unilateral and genetically associated with nausea and light and sound and sensitivity. Migraine is believed to be caused by a mixture of environmental and genetic factors that influence the excitation and inhibition of nerve cells in the brain. The blood protein responsible for

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migraine is DKK1 (PDB ID: 3S8V). Increased levels of DKK1 protein has been linked to cause stress on the trigeminal nerve that causes migraine. Using the ZINC database, compounds that can affect the said protein are listed out and further Swiss-dock (online website for virtual screening) is performed. The small molecule with highest binding is chosen and is then visualized in 3D using a software program Chimerax, to find the highest binding site of the protein-small molecule complex. This orientation of the complex is downloaded and overlaid on the protein using PyMOL to find the number of hydrogen bonds. The binding affinity of the hit compound is -8.08 kcal/mol., forming one hydrogen bond. This compound is yet to be evaluated *in vitro* and *in vivo*.

In silico evaluation of the CPEB4 protein as a potential drug target to identify lead compounds for the treatment of autism.

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Autism, formally called autism spectrum disorder (ASD) or autism spectrum condition (ASC) is a neurodevelopmental disorder marked by impaired social communication and restricted, repetitive patterns of behavior. Clinically autism is regarded as a spectrum disorder i.e., it can manifest differently in each person. Cytoplasmic polyadenylation element binding proteins 1-4 (CPEB1-4) regulate the translation of specific mRNAs by modulating their poly(A)-tails and thereby participate in embryonic development and synaptic plasticity. CPEB binds the transcripts of ASD risk genes. Imbalances in the transcript isoforms of CPEB have been confirmed in the brains of affected people. In this study, the CPEB4 protein was chosen as the drug target to screen the ZINC database. We identified hit compounds with promising binding affinity values that are yet to be synthesized and evaluated in future for both the *in vitro* and *in vivo* activity of the lead compound. The toxicity profile also needs to be tested further using appropriate animal models.

Proton NMR spectral analysis of the small molecule, phenytoin extracted from the tablets to assess the quality.

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Nuclear magnetic resonance (NMR) spectroscopy is a powerful technique that can be used to analyze the structure of both small and macromolecules in solution. The ^{1}H-NMR spectrum detects only the protons (hydrogen atoms), their presence, location within the surrounding chemical space and distribution. Hence this is referred to as single dimensional NMR. One can also perform 2D (^{1}H-^{15}N, ^{1}H-^{13}C) and 3D (^{1}H-^{15}N-^{13}C) NMR spectra that are mostly used for protein. In this study we performed the ^{1}H-NMR spectroscopy to determine the purity of phenytoin extracted from the tablets and assess the quality of tablets available in the market. Raw data was deconvoluted using TopSpin software. The expected aromatic protons were seen between 7-8 ppm concluding the presence of phenytoin which contains two benzene rings and no aliphatic protons. Additional peaks were also found in the spectrum indicating that the sample was not completely pure suggesting that a better method of extraction should be used in the future.

Virtual screening of compounds to identify leads for the inhibition of SARS CoV-2 spike protein for COVID-19 treatment.

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SARS-CoV-2 belongs to the beta-coronavirus genus lineage-B, alongside SARS-CoV-1. Coronaviruses are enveloped, single-stranded RNA viruses characterized by club-like spikes projecting from their surface and an unusually large RNA genome. The SARS-CoV-2 genome encodes four major structural proteins: the spike (S) protein, nucleocapsid (N) protein, membrane (M) protein and the envelope (E) protein each of which is essential to compose the viral particle. The SARS-CoV-2 spike glycoprotein is a type I membrane protein which forms a trimer, anchored to the viral membrane by its transmembrane segment, while decorating the virion surface with its large ectodomain. It binds to the receptor angiotensin-converting enzyme-2 (ACE-2) on a host cell and undergoes large structural rearrangements to promote membrane fusion. The structure of SARS CoV-2-Receptor binding protein is retrieved from the Protein Data Bank. The compounds that can be effective targets are listed out from the Zinc database and are docked using Swiss-dock. The resultant compound with highest binding and the site is chosen using Chimerax and further visualized in PyMOL for the identification of hydrogen bonds. The highest binding affinity of the compound is -8.24 kcal/mol and it forms 5 hydrogen bonds with the protein.

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Whole genome sequencing, variant identification and lineage Analysis of SARS CoV-2 isolates from COVID-19 patients of the current wave.

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COVID-19 is a worldwide public health crisis caused by the SARS-CoV-2 virus. Continuous monitoring of genomic data has revealed changes and mutations in the virus's genome, leading to the emergence of new lineages. Some of these variants are of concern or interest as they can enhance the virus's ability to spread, cause more severe illness, or evade immunity. This study conducted using samples from Kerala, aims to identify any genetic variations and mutations in SARS-CoV-2. Also, the study seeks to analyze the lineages of these isolates due to the variations and mutations in the virus's genome. Six swab samples that tested positive for SARS-CoV-2 used for study. Viral RNA was extracted to create the cDNA, which was then used to perform RT-PCR. After partially digesting the cDNA, a library created by adapter-ligating it and then quantified. Then the template was generated by diluting it and sequenced using the Ion GeneStudio S5 System. The Torrent Software was used to analyze the results and identify variants and mutations. The PANGOLIN COVID-19 software used to identify lineages. CoVSurver from GISAID was used to analyze the mutations. Analysis of the samples revealed genetic variations in SARS-CoV-2 isolates, which included changes in the lineage and amino acid composition. Variants were detected in both the structural and non-structural proteins, as well as the accessory proteins. There were multiple amino acid changes and mutations in the spike protein and several non-structural proteins within the ORF1ab gene. Lineage analysis confirmed that patients were infected with the Omicron variant (XBB.1.16 & XBB.2.3.11 and XXB.1.16.1lineages). It has been revealed that the virus is a member of XBB lineage, which was the most common lineage during that period. By using NGS techniques researchers have gained valuable insights into the virus's evolution and adaptability. This has revealed the emergence and spread of new variants.

Structural analysis of amyloid beta protein precursor of Alzheimer's disease for designing potential therapeutics.

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A crucial membrane protein found in many neuronal synapses, called amyloid-beta precursor protein (APP). This is a cell surface receptor that is also known to regulate iron export, neuronal plasticity, synapse formation, and antibacterial activity. This is most recognized as the precursor molecule that produces amyloid beta, the main constituent of amyloid plaques in Alzheimer's disease patients' brains being its amyloid fibrillar form. This is also observed to have few positive effects in the body like antimicrobial activity which plays a role in the brain's defense against pathogens, this also can act as iron export etc. The structure of Alzheimer's Amyloid Beta-Protein Precursor was chosen from PDB (PDB ID: 1AAP). PyMOL software is used for 3D visualization. The structural analysis is done using Chimera to identify the binding pockets to bind the ligand on the target. The docking is done by SwissDock and the molecules with best binding affinities were observed. Out of 4 compounds identified with top hits, the best compound was found with -6.33 kcal/mol. This compound should be further analyzed using *in vivo* and *in vitro* experiments.

Virtual screening of compounds to identify potential therapeutics against neurophysin II for the treatment of hereditary hypophyseal diabetes insipidus.

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Neurophysin II is a carrier protein for vasopressin, the antidiuretic hormone (ADH) that is produced by the hypothalamus. The most rare form of central diabetes insipidus (DI) is familial nephrogenic diabetes insipidus, this form of DI is due to an inherited mutation of the arginine vasopressin-neurogenic II (AVP-NPII) gene inherited in an autosomal dominant manner. ADH controls the water content in the body. Abnormalities in the ADH gene can disrupt the water balance that can damage the kidney. Previously, inhibitors of ADH receptors were designed and tested with limited success. In this study, neurophysin II was chosen as a drug target to test the hypothesis whether the inhibition of the ADH molecule itself can produce similar outcomes. Virtual screening was performed using the ZINC database. The binding affinities of hit molecules were found by using the SwissDock. The molecule with the highest binding affinity was found to be -8.5366374 (kcal/mol), this was compared with the protein using the Chimerax at the specific site where it binds. The drug with the lowest binding affinity was found to be -7.6529393 kcal/mol. The hit molecule has to be

synthesized and evaluated *in vitro* and *in vivo* in future in order to understand its effect.

Structural insights into mycobacterial protein, serine-threonine kinase: implications for designing therapeutics for tuberculosis.

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Mycobacterium tuberculosis bacterium possesses Serine-Threonine kinase proteins which play crucial roles in various cellular processes and are also essential for the survival and virulence of *M. tuberculosis*, making them potential targets for drug development against TB. The genome of *M. tuberculosis* contains 11 serine threonine protein kinases (STPK) genes among which, PknJ and Pknl genes are unique to pathogenic *M. tuberculosis*. The Pknl gene in the *M. tuberculosis* has been shown to phosphorylate the downstream STPKs and could serve as valuable drug targets. In this study, we screened the ZINC database by using the STPK as the docking receptor and identified hit molecules with promising binding affinity values. The highest binding affinity of the compound is -8.98 kcal/mol. This hit compound shows 4 hydrogen bonds with the protein. This hit compound should be further synthesized and evaluated *in vitro* and *in vivo* in future.

Identification of potential therapeutics against pituitary homeobox 2 protein for the treatment of stroke.

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Stroke is a medical disorder in which inadequate blood flow to the brain results in cell death. It is sometimes referred to as a cerebrovascular accident (CVA) or brain assault. There are two primary types of stroke: hemorrhagic (results from bleeding) and ischemic (results from a reduction in blood flow). Pituitary homeobox protein 2 (PITX2) is a transcription factor expressed in the neural crest, encoding transcription activators and interacting with FOXC1, which may increase the risk of stroke. The structure of the Pituitary homeobox 2 (PITX2) is retrieved from the Protein Data Bank. Small molecules that are effective on the protein are listed out from the Zinc database. Using Swiss-dock the protein is docked with the small molecules and the highest binding compound is analyzed using the Chimerax software to identify the site of binding. The protein-compound complex is 3D visualized using PyMOL to identify the number of hydrogen bonds. The resulting compound binding affinity is -8.24 kcal/mol, forming two hydrogen bonds.

Virtual screening of compounds to identify potential therapeutics for the treatment of osteoporosis.

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Osteoporosis is a skeletal disorder characterized by low bone mass, micro-architectural deterioration of bone tissue leading to bone sterility and consequent increase in fracture risk. This is more likely to occur in people who have low calcium intake. There is a related gene observed for causing osteoporosis called SPARC (Secreted Protein Acidic and Rich in Cysteine). This gene was chosen as the drug target. The Protein chosen from PDB was SPARC-Collagen Complex of PDB ID: 2V53. The structure is analyzed in 3D using a software, PyMOL. The related drug compounds that target this protein were chosen from Zinc DataBase and are docked against the protein chosen, which is analyzed by a tool called Chimerax. The potential drug was chosen and is overlayed with the protein to estimate the binding site. After the docking is done the results were obtained from the Swiss Dock, where the highest binding affinity was observed to be -8.01kcal/mol and there are three hydrogen bonds formed with the protein. This hit compound should be further synthesized and evaluated *in vitro* and *in vivo* in future.

Human blood genomic DNA extraction and purification using spin columns for high quality for forensic analysis.

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The Extraction of DNA is done to separate the genetic material from the rest of the cell components such as proteins, RNA, cell membrane etc. This extracted DNA can be used further for studying individual genes, sequence the genome, modify sections of DNA etc. This procedure is done using prep spin columns in three steps: adsorption of DNA to the membrane, removal of residual contaminants and elution of pure genomic DNA. The collection of blood is done in sterilized conditions at room temperature. Proteinase K is

added followed by addition of lysis solution and prepared for binding. Once these procedures are done the lysates are loaded in prep Spin Columns and centrifuged followed by prewash and then final wash which will be collected in the collection tube. The DNA is eluted with an elution buffer, after a certain time of incubation the final DNA concentration in the eluate significantly. The temperatures should be taken care while storing DNA. Agarose gel electrophoresis confirmed a very high quality of genomic DNA that can further be used for forensic analysis.

Identification of inhibitors of HPV viral oncoprotein, E6 that is responsible for causing cervical cancer by using computational biology approach.

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Cervical cancer is due to the abnormal growth of cells that have the ability to invade or spread to other parts of the body. This cancer is caused by the virus called Human papillomavirus. HPV contains 2 main oncoproteins that are involved in the cancer are E6 and E7. These oncoproteins affect the regulation of the host cell cycle by interfering with P53. The oncoproteins also adversely affect the normal function of the host cell by binding to their signaling proteins. E6 oncoprotein is a potential target for cervical cancer and is retrieved from the Protein data bank (PDB ID: 4GIZ). The molecular structure of the E6 protein is analyzed using the PyMOL software. From the Zinc database, a list of compounds that are effective on the protein are retrieved. Dock the compounds onto the protein using Swiss-dock and the highest binding affinity compound is visualized in Chimerax. Using the said software, the binding site is retrieved and is visualized in PyMOL, where the compound is overlaid on the protein to identify the hydrogen bonds. The highest binding affinity obtained from this procedure is -8.4kcal/mol, forming three hydrogen bonds with the protein.

In silico approaches to identify promising therapeutic candidates against *chlamydia psittaci.*

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Psittacosis, caused by the bacterium *Chlamydia psittaci*, is a disease transmitted to humans from infected birds belonging to the Order Psittacine. I aimed to utilize computational biology tools to identify and design a potential drug for psittacosis. I have employed the Swiss Model software to predict the protein structure of a protein associated with the disease. Its structure is visualized using PyMOL software. I utilized the Zinc database in order to identify potential ligands for the target protein. Next, molecular docking experiments were performed using the Swiss Docking method to investigate the interactions between the target protein and various ligands. Finally, I have successfully identified a promising therapeutic candidate that displayed high binding affinity and promising interactions with the target protein. My research work presents a computationally designed promising frontier for psittacosis, providing a novel approach for the development of anti-psittacosis therapeutics. Further experimental validation and refinement of the designed drug candidate are essential to progress towards clinical trials. The findings of my research contributes to the field of drug design for infectious disease.

Novel integrated approach to harvest electricity in conjunction with waste water treatment process.

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My model addresses concerns surrounding the treatment of sewage and wastewater by proposing a solution for the recovery, treatment, and sustainable use of water resources. The initial step in the treatment process involved the segregation and transfer of liquid wastes through a gravity channel equipped with bar screens to remove coarse solids. The receiving chamber utilized a diluted air flotation system (DAF) to eliminate suspended solids from the wastewater, effectively reducing biochemical oxygen demand (BOD). Alum and polyaluminium chloride were utilized to enhance the treatment process. The pre-treated water is directed to second chamber with microbial fuel cell (MFC) for sewage treatment. The MFC harnessed the metabolic activity of microorganisms known as electrogenic bacteria to generate electrical energy by transferring electrons from organic matter in sewage. The third chamber incorporated trickling filters eliminates pollutants. A Biofilm layer is formed when water passes through it making it non-toxic. It is then collected and used for domestic purposes. My model demonstrates efficiency in achieving complete treatment of wastewater. Furthermore, the treated water produced will be suitable for consumption, effectively removing microplastics, pollutants. Additionally, this allows in Generation of electricity which can be used for domestic purposes boosting the economy.

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Targeting the mineralocorticoid receptor with an inhibitor to control the renovascular hypertension in chronic kidney disease patients.

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Chronic kidney disease (CKD) is a condition where the kidneys lose their ability to filter blood. Because of this, excess fluid and waste from blood remain in the body and may cause other health problems, such as heart diseases and stroke due to Reno-vascular hypertension. Mineralocorticoid is a nuclear membrane receptor when bound to a ligand such as aldosterone results in a signal transduction affecting specific gene expression in the nucleus which is responsible for the maintenance and regulation of proteins, ionic molecules like sodium, potassium and water transport between the blood vessels and the nephrons. By inhibiting the mineralocorticoid receptor from binding with the aldosterone can terminate the reabsorption of sodium and water back into the blood and increases the absorption of proteins from urine which reduces proteinuria and blood pressure. Based on our virtual screening using ZINC database, the substance with the highest binding efficiency of -8.37 kcal/mol is bound to the 5th and 7th helix of the active site through hydrogen bonding in the mineralocorticoid receptor protein which competitively inhibits the aldosterone from binding at the active binding site of the receptor.

Targeting the desmoglein-3 protein to inhibit the action of autoantibodies against it in the disease *pemphigus vulgaris*.

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Pemphigus vulgaris (PV) is an autoimmune disease that results in blisters on cutaneous and mucosal surfaces. It is caused by autoantibodies that target keratinocyte proteins, desmogleins. It has been found in patients with PV, the presence of autoantibodies against desmoglein 1 (Dsg1) and desmoglein 3 (Dsg3). Desmogleins are transmembrane glycoproteins that are an integral part of desmosomes, which in part is required for cell-cell adhesion. The most common targets on desmoglein for IgG antibodies are the extracellular cadherin domains, which can result in loss of desmosome adhesive properties, signaling pathways that trigger endocytosis, depletion and direct inhibition of Dsg 3 trans-interactions. I took 5 ligands from the ZINC database and performed docking using SwissDock. Among others, one of the ligands showed the highest binding affinity of -11.21 kcal/mol. This molecule is evaluated by using chimera and analyzed for hydrogen bonds in PyMOL. I found that the ligand makes 5 hydrogen bonds with the protein.

Analysis of *Helicobacter pylori* urease subunit beta protein involved in gastric cancer.

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Helicobacter pylori, the causative bacterium of various gastroduodenal diseases, produces a large amount of urease that neutralizes gastric acid by producing ammonia for the survival of the bacteria. The crystal structure of *H. pylori* urease shows a 1.1 MDa spherical assembly of 12 catalytic units with an outer diameter of ~160 angstroms possibly adapted for acid-resistance. In this study, we used the urease as the drug target and performed virtual screening using the ZINC database. Retrieved relevant structural data from PDB, Molecular visualization was done with the help of PyMOL, Swissdock is used for the docking, structural analysis was done with the help of Chimerax. Among the top 7 compounds, the highest binding affinity is -10.02 kcal/mol. This hit compound showed two hydrogen bonds with the protein suggesting that its affinity is due to van der Waals interactions rather. In future, this hit compound will be synthesized and evaluated *in vitro* and *in vivo* to understand its efficacy.

Analysis of human thyroglobulin protein: insights into structure, function and implication for thyroid health.

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Thyroid makes hormones that control many activities in our body, including the heart rate and how fast we burn calories from food. The protein Thyroglobulin (TG) is a precursor of the thyroid hormones triiodothyronine (T3) and Tetraiodothyronine (T4). The synthesis of T3 and T4 from TG proceeds in the thyroid gland by iodination and coupling of pairs of tyrosine residues positioned closely on TG. The process of iodination is catalyzed by the enzyme Thyroid

peroxidase (TPO). TG is a homodimer of glycoproteins. Its structure was recently resolved by cryo-electron microscopy: PDB ID: 6SCJ. The structural data is retrieved with help of PDB and the chemical compounds were taken from the zinc database. The molecular structure of the thyroglobulin was visualized with the help of PyMOL. Swissdock software is used for the docking. Chimerax is used for molecular analysis. In ten compounds one compound has the highest binding affinity that is -9.60 kcal/mol. It forms three hydrogen bonds. This compound should be further analyzed in future.

Network analysis and target identification for structure-based drug design for stroke research.

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Ischemic strokes are frequently caused by disorders such as atherosclerosis, which occurs when fatty deposits (plaque) develop in the arteries, narrowing them and reducing blood flow. Other risk factors for ischemic stroke include high blood pressure, diabetes, high cholesterol, smoking, obesity, and sedentary behavior. In this study, we used the STRING database to create a protein interaction network focused on ischemic stroke, which includes 25 important proteins involved in its pathogenesis. We analyzed this network in Cytoscape and included reference pathways such as long-chain fatty acid import regulation and synaptic transmission to contextualize the molecular causes of ischemic stroke. This technique provides insights into the complicated biological mechanisms that underpin the illness, allowing for prospective therapy strategies. The potential drug targets identified in this study will be further validated by cross checking the individual pathways in order to finalize one target. The final drug target will then be used for small molecule therapeutic design.

Targeting the Dengue viral NS5 protein *in silico* for identification of potential antiviral therapeutics.

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Flaviviruses include important human pathogens, such as dengue virus and Zika virus. NS5 is a nonstructural protein essential for flavivirus RNA replication with dual MTase and RdRp enzyme activities and thus constitutes a major drug target. Insights into NS5 structure, dynamics, and evolution should inform the development of antiviral inhibitors and vaccine design. The 3D crystal structure of NS5 protein was downloaded from the protein data bank and was used as the drug target to virtually screen compounds from the ZINC database. Eleven compounds were shortlisted based on their binding affinity ranking. Out of the 11 compounds, the hit molecule with highest binding affinity (-15.96 kcal/mol.) was chosen for further structural analysis. This molecule will be synthesized and evaluated *in vitro* and *in vivo* in future.

Analysis of BST-2/Tetherin ectodomains reveals an evolutionarily conserved design to inhibit virus release.

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Bone marrow stromal antigen-2 (BST-2)/Tetherin is a host antiviral molecule that functions to potently inhibit the release of enveloped viruses from infected cells. BST-2 traps budding virions by using two separate membrane anchoring regions that incorporate into the host and viral membrane. This extended coiled-coil structure with inherent plasticity is necessary to accommodate the dynamics of viral budding while ensuring separation of the anchors. In this study we screened for small molecules from the ZINC database to bind BST-2 and control the viral budding. Data is retrieved from PDB, Chemical compounds taken from zinc database, Molecular Visualization was done with the help of PyMOL, Swissdock software is used for the docking, Structural analysis was done using Chimerax. A hit molecule was identified that is yet to be synthesized and evaluated further.

Targeting tau: inhibiting the hyper phosphorylation sites to attenuate Alzheimer's progression.

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Alzheimer's disease is a brain disorder that slowly destroys memory and thinking skills and, eventually, the ability to carry out the simplest tasks. People with Alzheimer's also experience changes in behavior and personality. Alzheimer's disease is not a normal part of aging. It's the result of complex changes in the brain that start years before symptoms appear and lead to the loss of brain cells and their

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connections. Tau protein in Alzheimer's undergoes hyperphosphorylation at the sites Ser202/Thr205, Thr212, Ser214, Thr217, Ser262 and Ser422. I used the structure of Tau protein to perform virtual screening for small molecules from the ZINC database and identified a hit compound. The hit compound that I have docked to Tau protein binds near ser285 and ser293. The drug blocks the site of hyperphosphorylation so that the Tau does not move away from the membrane of the microtubule which stops the death of neurons to some extent. This compound has to be synthesized and evaluated *in vitro* and *in vivo* in future.

Evaluating the antibacterial activity of marine algal extracts.

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Antimicrobial susceptibility testing (AST) is a laboratory procedure performed by medical technologists to identify which antimicrobial regimen is specifically effective for individual patients. Susceptibility testing is used to determine whether antimicrobials will inhibit the growth of the bacteria or fungi causing a specific infection. AST is important in clinical surveillance analysis for resistance patterns due to mutation in the bacterial DNA. The common susceptibility testing includes diffusion method and minimum inhibitory concentration (MIC) for phenotypic identification of susceptibility. The experimental design includes preparation of LB-Agar medium for mini culture, broth microdilution with various concentrations of antibiotics, spreading of the mini culture onto the antibiotic containing media, overnight incubation and observation of susceptibility and resistance property of the sample. In this analysis, growth of bacterial colonies was observed in 30 mcg of antibiotic media and no bacterial growth was observed in 150 mcg of antibiotic media suggesting that the 150 mcg is the MIC of the extracts.

Qualitative analysis of raw and purified proteins using SDS-PAGE.

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Sodium Dodecyl Sulphate – Polyacrylamide Agarose gel Electrophoresis (SDS-PAGE) is a broadly used laboratory technique for separation of proteins based on their molecular weight. This has a wide range of uses like assessing protein purity by the bands formed, identifying protein expression, determining the molecular weight of the proteins, monitoring protein purification by checking the presence and purity of protein of interest. In this study, we analyzed the purity of horseradish peroxidase by using SDS-PAGE. The samples from before and after purification were loaded onto the gel and electrophoresis was performed. Once the electrophoresis is done, the gel was stained with Coomassie blue and destained. The obtained results are compared to the ladder added and the protein is known. The purified protein was assessed to be >90% pure after affinity chromatography column purification. This qualitative analysis helped us to understand the purity of the enzyme which dictates its activity.

Pairwise alignment of the CD9 protein using NCBI BLAST-Global align algorithm.

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Analyzing two or more protein sequences to find areas of overlap and divergence is known as protein sequence alignment. The purpose of this alignment is to verify the proteins' structural characteristics, functional roles, and evolutionary links. This report provides analysis of CD9 protein products. This sequence alignment is obtained using the Needleman-Wunsch algorithm which is a tool for doing global alignment, by maximizing the similarity score which is calculated by using match, mismatch and gap penalties for each pair of amino acids. The sequence used is Query_ 2478671 and the data is produced. There is a good match of amino acids which means there is almost 89% of similarity between them and this shows a common ancestor and they are being conserved. They also show the functional similarities. There are very few gaps found which give a result of very few mutations or evolutionary changes which are done depending on various facts like their location, size etc. Further analysis is to be done in order to know the protein product better.

Reverse transcriptase polymerase chain reaction for cDNA synthesis and cDNA amplification.

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RT-PCR is a modified version of PCR. This is a two step process where the RNA strand is first reverse transcribed to complementary DNA (cDNA) by the enzyme reverse transcriptase and the resulting cDNA is amplified by the traditional PCR. In RT-PCR a pair of primers are used which are complementary to a defined sequence on each of the two strands of the cDNA. These primers are then extended by a DNA polymerase and a copy of the strand is made after each cycle which leads to the exponential amplification. It is a very sensitive method and is used to generate large cDNA libraries from very small amounts of mRNA and in gene expression studies. The purpose of converting mRNA to cDNA is mainly for the analysis of the template mRNA because DNA is much more stable than RNA. Once mRNA is converted to cDNA, the cDNA can be used for RT-PCR, as a probe for expression analysis and for cloning of the mRNA sequence.

Restriction digestion of pUC19 plasmid using EcoRI endonuclease and qualitative analysis using agarose gel electrophoresis.

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Restriction Digestion is a process in which DNA is cut at specific sites with the help of restriction endonucleases. This results in the formation of blunt and sticky ends and is evaluated by Gel electrophoresis. The plasmid that is being digested in this process is pUC19. This is helpful in Molecular Cloning, RFLP, AFLP, STRP etc. The process includes two major steps, the first one being digestion of plasmid with EcoRI and next one is analysis which is done through a 1% agarose gel electrophoresis. Initially the reaction mixture is prepared by mixing the lambda DNA with EcoRI, buffer and deionized water to makeup the volume to 25 ul. followed by incubation at 37 ℃ for 1 hour. Then the samples are brought to room temperature and loading dye is added to the sample. The samples are set to run the gel along with the ladder. The samples are run and analyzed under UV transilluminator. Multiple bands were obtained when compared to the uncut plasmid.

Comparative analysis of biophysical methods to evaluate hormonal content in raw milk.

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Milk obtained from cattle injected with artificial hormones for increased milk production was observed to have a significant increase in the amount of hormones present in it. The different types of hormones identified in milk were prolactin, insulin like growth factor-1 (IGF-1), prostaglandins and steroid hormones including glucocorticoids, androgens, progesterone, estrogens etc. Several studies have reported that the presence of such hormones can affect both male and female by provoking breast tissue, prostate tissue, endometrial tumors, PCOS and other hormonal-related cancers. Different methods are proposed regarding the filtering out hormones from the milk in that two methods are very effective. Fabric Phase Sorptive Extraction method (FPSE) and second one by using Protein-based Nanoparticles. FPSE is a novel and green sample preparation technique that uses a natural or synthetic fabric substrate that has been chemically coated with a sol-gel sorbent. FPSE has emerged as a powerful analytical technique for the extraction of emerging pollutants from complex aqueous matrices. It is considered a green alternative to traditional extraction methodologies. In this work, the FPSE technique was evaluated to perform the simultaneous extraction of 15 steroid hormones from raw milk. In future we plan to work on proposing a simpler technique regarding filtering out hormones from milk(which is eco-friendly and don't cause any harm or side effects as it is based on green synthesis).

Restriction Fragment Length Polymorphism analysis.

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Restriction Fragment Length Polymorphism (RFLP) is the difference in homologous DNA sequences that can be detected by the presence of fragments of different lengths after digestion of the DNA samples with specific restriction endonucleases. In RFLP analysis, DNA samples are digested into fragments by one or more restriction enzymes and resulting fragments are then separated by gel electrophoresis

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according to their size. The similarities and differences of the patterns generated by RFLP can be used to differentiate species from one another. In this study, we used the lambda phage DNA and digested this DNA with either EcoRI or HindIII by adding the enzyme to the DNA along with the appropriate buffer. The reactions were incubated at 37 ℃ for one hour to achieve complete digestion as suggested by the manufacturer. Agarose gel electrophoresis revealed different banding patterns of the digested lambda DNA suggesting that a similar pattern would be obtained with different DNA samples.

Small scale fermentation of wheat for the production of fermented beverages.

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Fermentation is a process whereby yeast converts glucose to ethyl alcohol and carbon dioxide gas (CO_2) giving the fermented beverages, the alcohol content and carbonation. The market demand for alcoholic beverages is rising these days making it a profitable business. Typically the composition of alcoholic beverages such as beer include water, malt, hops, yeasts. The process involves different steps such as malting, mashing, lautering, boiling, cooling, fermentation, conditioning, carbonation and packaging. Benefits include vitamins, minerals, flavonoids, low risk of coronary heart disease, helps produce good cholesterol, reduce sensitivity to insulin. Downsides include damage of organs and risk of cancer, heartburn, high blood pressure. In this study we performed a small scale (100 ml) of fermentation using wheat as the starting material and complete the process within two weeks.

Expression of glutathione-S-transferase (GST) gene in *E. coli* using an IPTG-inducible promoter.

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Gene expression is the process by which the information encoded in a gene is turned into a function. This process mostly occurs via transcription of RNA molecules that code for proteins or non-coding RNA molecules that serve other functions. Plasmids that are used to carry foreign genes into a specific host are referred to as cloning vectors. It is important that a gene be inserted into the plasmid in the proper reading frame to ensure that the correct protein will be expressed. If the foreign genes are to be expressed in *E. coli*, one must use bacterial expression vectors. These expression vectors contain inducible promoters which can be controlled by the addition of an inducer such as IPTG, most commonly used. In this study we expressed the glutathione-S-transferase (GST) gene using IPTG induction. The protein expression was verified by SDS-PAGE by comparing the sample with and without IPTG induction. Thick band was seen from the sample containing IPTG and light band can be seen from the sample in which the IPTG is absent indicating leaky expression.

Phytoremediation: synergetic use of plants and bacteria to clean up the environment.

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Phytoremediation is a relatively new approach to removing contaminants from the environment. It may be defined as the use of plants to remove, destroy or sequester hazardous substances from the environment. Unfortunately, even plants that are relatively tolerant of various environmental contaminants often remain small in the presence of the contaminant. To remedy this situation, plant growth-promoting bacteria that facilitate the proliferation of various plants especially under environmentally stressful conditions may be added to the roots of plants. These bacteria have been selected to lower the level of growth-inhibiting stress ethylene within the plant and also to provide the plant with iron from the soil. The net result of adding these bacteria to plants is a significant increase in both the number of seeds that germinate and the amount of biomass that the plants are able to attain, making phytoremediation in the presence of plant growth-promoting bacteria a much faster and more efficient process.

Unmasking cystic fibrosis: a journey to better breathing.

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Cystic fibrosis is an autosomal recessive genetic disease caused by CFTR (cystic fibrosis transmembrane conductance regulator) gene defect. The CFTR gene expresses the production of CFTR protein. CFTR protein helps to maintain the balance of salt and water on many surfaces in the body such as the lung surface. CFTR protein is also referred to as "ion channel" because it aids in transfer of chlorides from inside to outside the cell. When there is a mutation in CFTR gene the CFTR protein is produced in reduced quantity or not at all produced. We built the homology models of 5 different mutants of CFTR using SWISS MODEL. These models were further used for molecular dynamics (MD) simulations to evaluate their trajectories. Due to the massive size of CFTR protein in addition to the membrane, the simulations were slow on gaming laptop. Currently these MD simulations are ongoing and will be available soon for analysis.

Breaking the silence: progress in Alzheimer's disease with APOE3.

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Alzheimer's disease (AD) is a progressive, neuro-degenerative disorder that causes degeneration of the cells in the brain and it is the main cause of dementia, which is used to describe loss of memory, language, problem solving, and other thinking abilities. Common symptoms include: memory loss, paranoia, depression, anger, aggression, anxiety, apathy, loneliness, and psychosis. These symptoms vary from person to person. Additionally, several risk factors such as increasing age, genetic factors, head injuries, vascular diseases, infections, and environmental factors play a role in the disease. We performed a network analysis using the STRING database. We identified the APOE3 protein standing out in our network analysis. Molecular dynamics simulations showed that the overall trajectory of APOE3 is indeed different compared to the other APOEs confirming its role in AD.

Predict protein structure using alpha fold AI model.

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AlphaFold is an AI model from DeepMind used to predict the 3D shapes of proteins. It is pre trained using various protein structures to make these predictions to unlock the secrets of life at a molecular level. So, in a nutshell, AlphaFold is like a protein puzzle-solving champion. Here we demonstrate how to take an amino acid sequence and run it using AlphaFold AI model and predict the structure of protein.

What are genes? NCBI database.

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The National Center for Biotechnology Information (NCBI) offers a lot of resources on retrieving information regarding various genes not only from the human genome but also from any other organisms including viruses. Here we demonstrate how one can use the NCBI database to retrieve the information regarding genes and their nucleotide sequences with ease using a laptop.

Understanding molecular interactions in docking.

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In our poster presentation, we delve into the world of molecular interactions during docking. Using advanced computational methods, our research focuses on understanding how molecules interact with each other. By studying the binding process, energy changes, and structural movements, we aim to uncover the essential factors that influence successful docking. Our findings not only contribute to the scientific understanding of these processes but also hold potential applications in drug discovery and design. The poster provides a comprehensive overview of our methods, results, and their implications, emphasizing the importance of unraveling molecular interactions in docking for advancements in various scientific fields. We have outlined the process of analyzing various molecular interactions such as hydrogen bonding, van der Waals, etc. by using the HIV-1 capsid protein and a small molecule drug. These analyses shed light on how different drugs have different binding affinities against the same drug target.

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PCR-based molecular diagnosis of genetic abnormalities in SPINK1 gene using gastric cancer patient samples.

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Gastric cancer is one of the leading cancers that causes global human health issues. Besides the conventional way, infections such as *Helicobacter pylori* add fuel to this burning problem. While the H. pylori infection rates are skyrocketing, the antibiotic-resistance is making this problem worse. In addition to counteracting the bacterial infections, one needs to understand more about the underlying reasons for gastric cancer. In this study we evaluated the genetic polymorphisms in gastric cancer patients focused on the SPINK1 gene. Twenty one samples were used to PCR-amplify the previously reported domain of SPINK1 gene with specific primers. Qualitative analysis of PCR products using agarose gel electrophoresis revealed that 12 samples yielded a PCR product out of the 21 samples. These results suggest major genetic rearrangements in the patients' genomic DNA at the SPINK1 gene locus. Further DNA sequencing analysis should be performed in order to confirm this finding.

Molecular genetics and bioinformatics analysis of breast cancer patient samples focused on the RING domain of BRCA1 gene.

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Breast cancer (BC) is one the leading global causes for human morbidity. While the early detection can prevent BC, it is challenging to detect the BC early due to lack of biomarkers in certain cases such as triple negative BC. The BRCA1 gene containing various domains such as the RING domain, BRCT domains, etc. has been identified to play a critical role with respect to the oncogenic mutations that cause BC. In this study, we evaluated the presence or absence of mutations such as substitutions, deletions and insertions in the RING domain of the BRCA1 gene by using an integrated approach of Molecular Genetics and Bioinformatics. Twenty four patient samples were obtained through a research collaboration with the local hospital with appropriate ethical approvals. Genomic DNA was isolated and used as a template for PCR-amplification of the BRCA1-RING domain. Followed by the qualitative analysis using agarose gel electrophoresis, the patient samples were further sequenced. One deletion mutation was identified among the 24 samples. In future, the consequences of this mutation causing frameshift will be analyzed at the protein level.

In silico repurposing of HIV-1 aspartyl protease inhibitors as Renin aspartyl protease inhibitors to treat hypertension.

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The post COVID-19 era has encountered a significant number of human deaths due to sudden cardiac arrests due to various unforeseen conditions. Hypertension and diabetes have been considered as the predisposed primers towards such sudden cardiac arrests. Today's stressful life is not making these conditions easy. Different types of antihypertensive drugs are widely used for patients. However, the drug side effects are not very pleasant. Hence new antihypertensive drugs are needed. In this study we repurposed *in silico*, the HIV-1 aspartyl protease inhibitors as inhibitors of human renin, an aspartyl protease. Our molecular docking and molecular dynamics simulations showed promising results with six inhibitors, amprenavir, darunavir, indinavir, lopinavir, nelfinavir and saquinavir. The binding affinity values and overall MD profiles suggest nelfinavir, darunavir and lopinavir as possible candidates that are yet to be evaluated *in vitro* and *in vivo* in order to further confirm our *in silico* findings. These findings will not only help hypertension patients but also lead to a new avenue of dual purpose drugs.

Repurposing ricin as antimicrobial agent.

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Ricinus communis is most widely used in India for castor oil that has multiple domestic and industrial applications. Ricin is a lectin, a carbohydrate binding protein and a highly potent cytotoxin that is synthesized in the endosperm cells of maturing seeds of *R. communis*. Ricin A chain acts as a glycosidase that removes a specific adenine residue from an exposed loop of the 28S rRNA (A4324 in mammals), leading

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to rRNA breakage. Ricin B chain binds to beta-D-galactopyranoside moieties on cell surface glycoproteins and glycolipids and facilitates the entry into the cell of the A chain. The disulfide linkage between the chains is broken, and the A chain travels through the cytoplasm, inactivating 1500 ribosomes per minute and ultimately killing the cell. Ricin clips off a single adenine base at the tip of the sarcin/ricin loop that is essential for interaction with the elongation factors and inactivates the ribosome permanently. Our preliminary studies showed some antibacterial activity against *E. coli* cells *in vitro*. However the mechanistic details of this antibacterial activity are yet to be dissected in the future.

An overview on various *in vitro* and *in vivo* models of Alzheimer's disease.

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Alzheimer's disease is an age related neurodegenerative disorder. The main symptom of Alzheimer's is loss of memory. Various studies have been carried out to find therapeutic approaches for Alzheimer's disease. But the proper treatment option is not available. Natural therapy including herbs & medicinal plants has been used in the treatment of Alzheimer's disease. The plants includes Ashwagandha, Lavender, *Ginkgo biloba*, *Melissa officinalis*, Saffron, Brahmi, Gotu kola, Glycyrrhiza glabra, Shankhpushpi, *Aloe vera*, Neem, Hibiscus, etc. The different parts of plants having different chemical constituents which are responsible to treat Alzheimer's disease. The root part of ashwagandha, Brahmi, *Glycyrrhiza glabra,* etc. The leaves part of *Ginkgo biloba, Melissa officinalis*, Brahmi , Gotu kola, Shankhpushpi, Neem, etc. The flower part of Lavender, Saffron, Brahmi, Shankhpushpi, Hibiscus, etc. The resin part of *Aloe vera,* etc. These parts of plants having various chemical constituents like Withanolide -A , alkaloids, linalool, flavonoids, terpenoids, phenols , saponins, steroids, etc.. These chemical constituents are responsible to relieve oxidative stress and decrease the beta amyloid plaques in brain by using mice.

Molecular Docking & Dynamic Simulation Studies as a Strategy for Identifying New Potential Bio-Fungicide against 1,3-beta-Glucan Synthase of *Magnaporthe oryzae*.

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Magnaporthe oryzae also known as Rice blast fungi is the most prevalent rice fungal Disease across rice growing regions of the world. Among all the factors resulting in reduced yield in rice, infection with rice blast fungus is a significant factor affecting the yield. Hexaconazole is widely used fungicide for controlling *Magnaporthe oryzae*, however alternative natural molecules which acts as good fungicide against this disease is the need of the hour considering potential harmful effects of the synthetic molecules. In silico repurposing is a technique to discover potential molecules against diseases and it also cuts Research and Development cost and time. 1, 3 Beta Glucan Synthase is present in phospholipid bilayer of fungal cell membrane. It is mainly responsible for the production of Beta D Glucans which are Building Blocks of the fungal cell wall. Blocking of 1, 3 Beta Glucan Synthase will disrupt the formation of fungal cell wall which makes it a potential candidate for targeting. 1, 3 Beta Glucan Synthase of *Magnaporthe oryzae* amino acid sequence was taken from UNIPROT database ID L7JF68_MAGOP and a 3-D model was constructed by Using PHYRE 2 Server. The model was validated by ERRAT and Procheck. Quality of the protein sequenced was validated by using ERRAT software. Glob plot analysis was done to identify conserved domains which revealed the presence of TransMembrane region and Cytochrome B 450. After docking studies, we conclude that two bio active compounds Anonaine from *Annona squasoma* out of studied compounds shows strongest binding affinity to 1, 3 Beta Glucan Synthase of *Magnaporthe oryzae*. Further molecular dynamic Simulation studies revealed the Stability of the Complex. Followed by a bioassay using Anonaine & Nimbolin-B will help in Conformation for control of *Magnaporthe oryzae* in large scale Screening.

Climate change-sustainability by compostable plastics.

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The most disquieting situation scaring the Environmental Sustainability is Climate Change. It is more subtle, cruel and cumulative. Our current actions don't just exacerbate the situation—they compound it and it is one of the greatest challenges of the present time by affecting social and environmental determinants of health. One of the decisive factors is the release of greenhouse gases on burning fossil fuels, which are a major cause of Global warming leading to long-term climate change. And now it's time to focus on the finest adaptation strategy - to conserve non-renewable resources and mitigate climate change by making resources more efficient and resilient to climate change. We all know what plastic does to our environment and thus replacing

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petroleum-based plastics with Compostable plastics could reduce industrial greenhouse gas emissions by 25%. Compostable plastic bags are also made using plant materials that revert to base organic components when processed. In addressing this, the production of such compostable plastics using cellulose (common natural polymer non toxic gases are released into the environment on decomposition) extracted from corn husk-an abundant byproduct obtained from corn processing. Corn Plastic is a non-petroleum material made by converting corn into a resin called poly lactic acid (PLA). And then by using Sorbitol, starch, and chitosan as the plasticizer, matrix, and preservative respectively corn plastic is produced. It can also be made from sugarcane, tapioca root, cassava and sugar beet. Compostable plastics production requires 65% less energy and Emits 68% fewer greenhouse gases than traditional petroleum-based plastics, unlike natural gas or crude oil that's a finite resource, corn is available, functional and renewable. Hence by Substituting compostable bioplastics for conventional plastics reduces climate emissions by reducing carbon footprint. Thus compostable plastics are a viable and valuable solution for a more sustainable and inclusive future and thus contributes to climate change mitigation.

Why algae as an alternative for the production of biofuels rather than plant-based biofuels.

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Biofuels are fuels that are biomass-derived from plants, animals or waste depending on which type of biomass is used, they could lower CO2 emissions by 20-80% compared to conventional jet fuel. With the evolution going on, there are many ways possible to produce biomass out of which one of the ways was found to be through Algae. Recent studies through various articles have shown that genetically modified microalgae can be used to increase the biofuel production. It is found that the components like microalgae, wastewater, flue gas, certain metabolites formed from detoxification of metals may together help in production of algal biofuels by cultivating the algae in an open pond system which could be a bioprospecting aspect. The CO2 emission occurring during the burning of biofuel is equal to that consumed by algae which also helps in maintaining a carbon neutral system hence may not cause any imbalance in the nature.

Lateral transfer of ampicillin-resistance gene between bacteria to gain insights into the human gut microbiome.

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Horizontal or lateral gene transfer is generally defined as exchange of genetic information between contemporary organisms. Horizontal transfer is distinct from vertical transfer by which genetic information is passed from parent to offspring. A special case of the horizontal transfer involves the transfer of DNA between chloroplast or mitochondrial and nuclear genomes. In addition to entire genes, parts of genes, such as exons or introns, may also be transferred in this way. Although horizontal transfer is more likely to be successful between closely related than distantly related species, it does occur between species as divergent as those found in different domains of life. Lateral transfer of ampicillin-resistance gene among bacteria provides valuable insights into the dynamics of the human gut microbiome. Through this transfer mechanism, bacteria can rapidly adapt to antibiotic pressures, posing challenges for clinical interventions. Understanding the mechanisms and frequency of gene transfer enhances our ability to devise strategies for managing antibiotic resistance and preserving the balance of the gut microbiome. Further research into the intricate interplay of bacterial communities and the transfer of resistance genes is crucial for developing effective therapeutic interventions and safeguarding public health.

Antibacterial evaluation of marine algal extracts using the laboratory *E. coli* DH5-alpha strain.

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Antibacterial assays play a crucial role in evaluating the efficacy of potential antimicrobial agents. Continued research should focus on expanding the spectrum of tested microorganisms, exploring synergistic effects of combinations, and investigating the mechanisms of action. Our antibacterial assays involving marine algal extracts (MAEs) focus on exploring the potential of compounds derived from marine algae to combat bacterial infections. Among the six MAEs that we tested in this study, we identified that MAE-B has potential antibacterial activity at a concentration <150 ug/ml. Hence we have determined the minimum inhibitory concentration (MIC) as 150 ug/ml. Our current studies involve further investigation of LC-MS profile for MAE-B in order to understand the chemical

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components and metabolites that might show the antibacterial activity. Additionally, assessing the toxicity and potential resistance development is essential for the practical application of these agents.

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