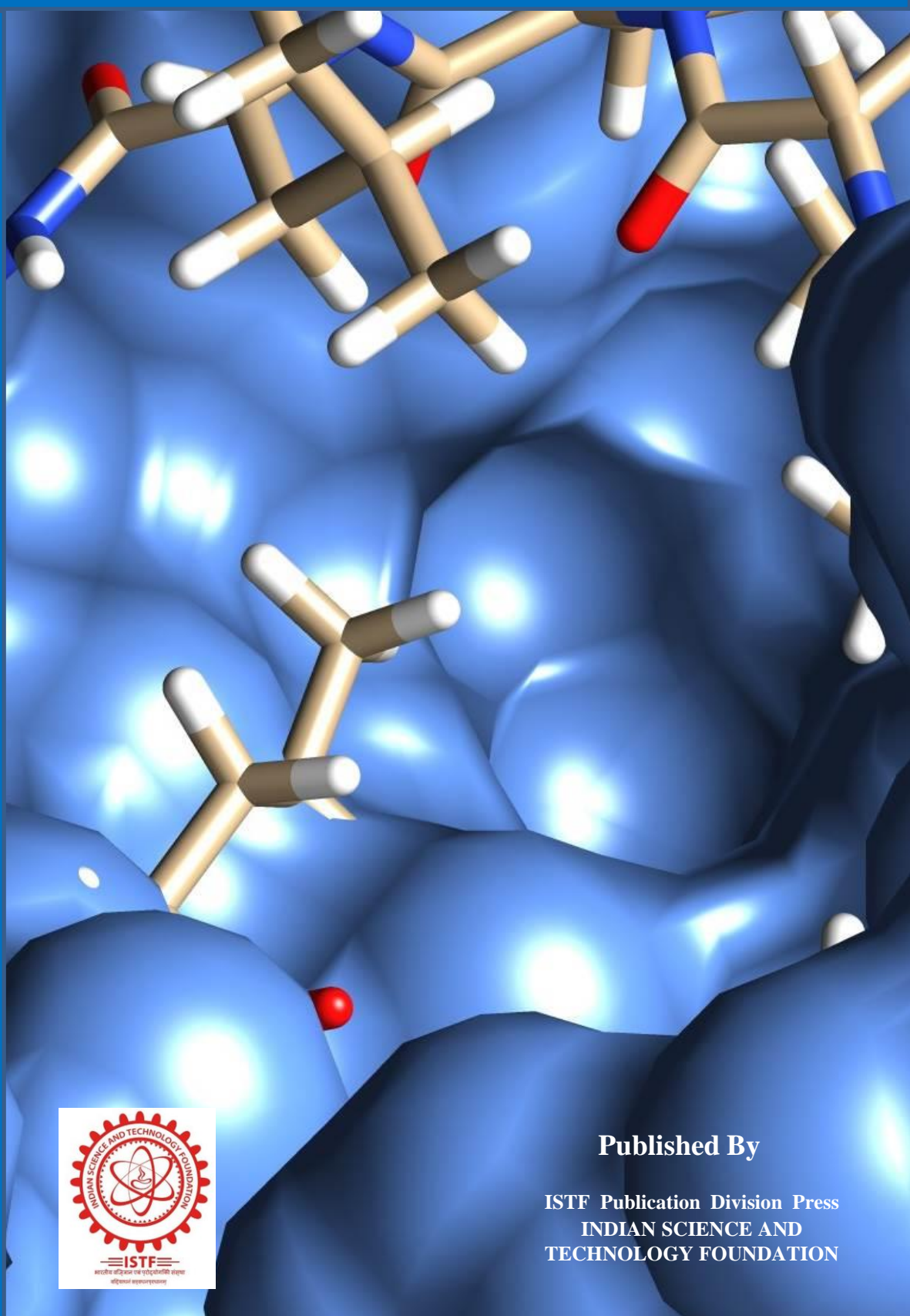


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Journal of Science (JoS, <http://istf-jos.com>) is a scientific journal of Indian Science and Technology Foundation (ISTF, [www.isto-india.org](http://www.isto-india.org)). The Journal publishes peer reviewed original research articles and scientific reviews. The Journal of Science (JoS) aims principally at publishing articles resulting from original research whether pure or applied in the various aspects of academic Endeavour broadly classified as Science (Physical, Biological and Chemical) and Technology.

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# 1<sup>st</sup> Virtual International Conference on Biotechnology and Bioinformatics (ICBB-2022)

On 26<sup>th</sup>-27<sup>th</sup> February 2022

Organized by:

Insight BioSolutions, France

In technical collaboration with

Indian Science and Technology Foundation, India



The Insight Biosolutions, (IBS), France in technical collaboration with Indian Science and Technology Foundation (ISTF), India organized a 1<sup>st</sup> Virtual International Conference on Biotechnology and Bioinformatics (ICBB-2022) on 26<sup>th</sup>-27<sup>th</sup> of February 2022. The conference aim was to provide platform for students, research scholars, post docs, scientists, academicians as well as industrial professionals from all over the world in the field of Biotechnology and Bioinformatics. The ICBB invited abstracts for Oral/Poster presentation **on the following topics (but not limited to)** to provide a Platform Opportunity for exchange of ideas and dissemination of knowledge among scholars from across the globe.

Biotechnology	Bioinformatics
Agriculture Biotechnology	Artificial Intelligence in Bioinformatics
Animal Biotechnology	Bioinformatics & Computational Biology
Biomedical Engineering & Applications	Bio-inspired computing
Bioprocess Engineering	Big data analytics in healthcare
Bioremediation and Biodegradation	Biological network reconstruction and analysis
Bio-Safety and Bioethics	Cheminformatics and QSAR
Environmental Biotechnology	Clinical databases and information systems
Enzyme and Protein Engineering	Computational proteomics
Fermentation Technology	Computational systems biology
Food Processing Technology	Combinatorial optimization in molecular biology
Genetic Engineering	Database Development in Bioinformatics
Genomics	Data-driven healthcare
Industrial Biotechnology	Data mining, machine learning, and artificial intelligence
Marine Biotechnology	DNA, RNA and protein sequence analysis
Medical Biotechnology	Drug Discovery
Microbial Biotechnology	Genome analysis
Molecular Biology	Gene expression analysis
Microbiology	Health informatics
Nano Biotechnology	Next-generation and Third-generation sequencing
Next generation sequencing (NGS)	Modeling and simulation of biological processes, pathways
Pharmaceutical Biotechnology and Drug Design	Machine Learning in Bioinformatics
Pharmacogenomics	Medical and biomedical informatics
Plant Biotechnology	Molecular evolution and phylogeny
Protein Biochemistry	Proteomics for Bioinformatics
Protein Sequencing & Molecular Interactions	Parallel and distributed computing for life science
Protein Structure	Software and Tool Development in Bioinformatics
In vitro Toxicological Science	Structural bioinformatics and computational biochemistry
Advanced Cell Culture Technology & Applications	Systems Biology
Current Cell and Tissues Based In vitro Models and Applications	Structural Biology

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## Study Affinities of Chemical Compounds with Hepatic Transporter BSEP Protein Using In-Silico Approach

<sup>1</sup>Abira Dey, <sup>1</sup>Ritushree Biswas, <sup>1</sup>Sarra Akermi, <sup>2</sup>Sunil Jayant, <sup>3</sup>Jean Bernard Idiope (✉)

<sup>1</sup>Indian Science and Technology Foundation, New Delhi, India

<sup>2</sup>Annotation Analytics Pvt. Ltd., 36, Ward no-14, Biswa, Amanpura, Gurgaon-122001, Gurgaon, India

<sup>3</sup>Insight Biosolutions (IBS), Rennes, France

(✉)Corresponding author: email: [jean.idiope@insight-biosolutions.com](mailto:jean.idiope@insight-biosolutions.com)

Transporters are proteins which transports the drugs to target cells and also removes the unused or toxic particles of the drug outside the body (1). BSEP is an efflux transporter protein present in the hepatocytes membrane that plays important role in flow of bile acid from hepatocyte cell into the bile canaliculi (2,3). Impaired BSEP activity due to drug interaction leads to accumulation of bile acid within the hepatocyte cells and results in cholestasis liver injury (DILI) (4). However, there is no detail information about interaction of compounds with BSEP. Therefore, in our work we will study affinities of chemical compounds with Hepatic Transporter BSEP proteins using in-silico approach. The 3D structure of the BSEP protein (6LR0) was obtained from RCSB databank. The FDA approved compounds were selected from literature and docked against the BSEP structure using PATCHDOCK (PD) and HADDOCK(HAD). The post docking complex was analyzed in order to evaluate the affinity of compounds with BSEP. Molecular docking shows that Cyclosporin A (IC<sub>50</sub>: 0.70μM, PD score: 9502, HAD score: -65.7 +/- 0.7), Cetorelix acetate (IC<sub>50</sub>: 1.47μM, PD score: 9922, HAD score: -65.9 +/- 1.3) and Valinomycin (IC<sub>50</sub>: 1.56μM, PD score: 9966, HAD score: -69.0 +/- 1.2) produced higher affinity for BSEP. Drugs such as Imatinib (IC<sub>50</sub>: 26.10μM, PD score: 6526, HAD score: -49.5 +/- 0.5) and Rifabutin (IC<sub>50</sub>: 26.70μM PD score: 8164, HAD score: -44.8 +/- 2.1) produced medium affinity for BSEP, while drugs such as Omeprazole (IC<sub>50</sub>: 99.00μM, PD score: 4970, HAD score: -24.6 +/- 5.3) and

Testosterone (IC<sub>50</sub>: 105.00μM, PD score: 4520, HAD score: -21.1 +/- 4.0) produced poor affinity for BSEP. Our *in-silico* approach provides deep insight about interaction of compounds with the BSEP protein. Therefore, our *in-silico* approach may be helpful to design *in-vitro* experiments using BSEP in order to predict precisely the role of compounds in hepatotoxicity.

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## Fluorometric Sensing of Hexavalent Chromium in waste water and living cells by C dot decorated biocompatible FeOOH nanoparticles

<sup>1</sup>Bidisha Ghosh,<sup>1</sup> Shubham Roy,<sup>1</sup>Souravi Bardhan,<sup>1</sup>Sukhen Das,<sup>1</sup>Kaustuv Das (✉)

<sup>1</sup> Department of Physics, Jadavpur University, Kolkata-700032, India

(✉)Corresponding author: email: [kaustuv12@gmail.com](mailto:kaustuv12@gmail.com)

Phone no: 9433116177

Chromium is accounted as one of the most recognized carcinogenic heavy metal. It is found in nature as trivalent chromium Cr (III) and hexavalent (VI)[1]. Cr (VI) has many deleterious effects in the body and has been seen to cause defects in RBC formation [2]. The present work focuses on using *in-situ* synthesized carbon quantum dots into the goethite ( $\alpha$ -FeOOH) nano-matrix and then fluorometric detection of hazardous hexavalent chromium Cr (VI) in wastewater and Cr (VI) contaminated live cells is being performed the nano-hybrid has a potential for identifying the of chromium contamination levels in various types of water samples. This fluorometric probe is extremely sensitive to hexavalent chromium having a LOD 81nM making it a specialized chromium sensor. Furthermore, the sensing process has been evaluated using Stern-equation Volmer's and fluorescence lifetime studies, which revealed that photoinduced electron transfer and the inner filter effect occur simultaneously. This chromium sensor has also been used to determine the level of pollution in actual industrial effluent. The sensing performance of the probe when tested in a real-world wastewater sample is pretty impressive. This biocompatible fluorometric sensor has also been utilized to demonstrate Cr (VI) sensing in HeLa cells *in vitro*. Theoretical docking simulations have been used to validate the

rapid detection mechanism of hexavalent chromium in real cells. This fluorometric sensor material can be assumed to open up new possibilities in wastewater monitoring and biomedical applications in the future.

**Keywords:** Hexavalent Chromium, Fluorometric sensor, Stern- Volmer plot, Molecular docking.

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## Applications of Bacterial Isolates in Agriculture and Pharmaceuticals from Manipur, India

Debananda S. Ningthoujam\*, Rakhi Khunjamayum and Yurembam Rojiv Singh

Microbial Biotechnology Research Laboratory (MBRL)

Department of Biochemistry

Manipur University, Canchipur-795003 (Manipur), India

\*(e-mail: [debananda.ningthoujam@gmail.com](mailto:debananda.ningthoujam@gmail.com)) Phone no.: 9862027271)

It is imperative to search for new and more effective antimicrobial compounds for applications in medicine and agriculture. The promise of new microbial metabolites from terrestrial sources has become almost exhausted. However, the rise of resistant pathogens dictates the search for novel metabolites from different bacterial sources especially endophytes. Endophytes associated with medicinal plants have great potential to produce unique secondary metabolites that may be exploited for beneficial applications in agricultural, pharmaceutical and other sectors [1]. Our laboratory, MBRL, has been investigating PGP properties of rhizospheric and endophytic bacteria especially actinobacteria on rice. Under nethouse conditions, *chakhao* (unique black rice variety of Manipur) plants treated with endophytic strain *O. intermedium* (AcRz3) exhibited significant increases in root and shoot lengths, and number of leaves over the control. The strain significantly increased the number of filled grains per plant over the control. Another 8 endophytic bacterial isolates [*Streptomyces* sp. AcRz3\*, *Streptomyces* sp. AcRz21, *Paenibacillus* sp. CcS9, *Bacillus* sp. PtL11, *Bacillus* sp. TgIb4, *Bacillus* sp. TgIB5, *Priestia* sp. TgIb12 and *SxL10* (a putative *Streptomyces* sp.)] significantly increased the growth of traditional rice cultivars and decreased the disease lesions caused by *Rhizoctonia solani*. A keratinolytic bacteria, *Amycolatopsis* sp. MBRL40, could increase the germination percentage of rice seedlings and could

significantly enhance their growth. A keratinase from MBRL 40 isolate has also shown promising potential in digesting amyloid fibres generated from lysozyme under *in vitro* conditions and may be developed as a therapeutic candidate for amyloid diseases such as Alzheimer's disease (AD).

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## Binding affinity prediction between FDA approved drugs and plant metabolites against Transglutaminase 2 to target Human Hepatocellular Carcinoma

<sup>1</sup>Jasbir kaur Simak, <sup>1</sup>Anshul Nigam, <sup>2</sup>Ashwani Sharma (✉)

<sup>1</sup>Amity Institute of Biotechnology, Amity University Mumbai, Mumbai - Pune Expressway, Bhatan Post - Somathne, Panvel, Mumbai, Maharashtra 410206, India

<sup>2</sup>Indian Science and Technology Foundation, Delhi, 110053, India

(✉)Corresponding author: email: [director@isto-india.org](mailto:director@isto-india.org)

Hepatocellular carcinoma (HCC) also known as malignant hepatoma is a severe illness occurring in patients suffering from chronic hepatitis B and hepatitis C. FDA approved drugs for the treatment of HCC including sorafenib, regorafenib, levatinib, cabozantinib, and ramucirumab come with inevitable side effects ranging from diarrhea, fatigue, hand-foot skin reactions, hypertension, blurred vision, and numbness [1]. Other major challenges that aid in the development of prevalent HCC are resistance to FDA approved drugs and diagnosis of HCC at a later stage. Thus, the development of potential markers and drug alternatives is necessary.

Studies have shown that Cepharanthine, a natural compound extracted from *Stephania cepharantha* Hayata has the potential in the treatment of HCC [2]. Accordingly, Transglutaminase 2 (TGM2) has shown to be a potential biomarker besides Alpha-fetoprotein (AFP) as it is present in AFP deficient cells and in tumor tissues with low levels of serum AFP [3]. Our docking results using AutoDock Vina showed that cepharanthine has a good binding affinity of -9.2kcal/mol against Transglutaminase 2. The use of plant metabolites like Cepharanthine has the potential to treat HCC with low or negligible side effects.

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## Bioactivity of medicinal plant and insect associated microbiota

Nikena Khwairakpam<sup>1</sup> and Debananda S. Ningthoujam<sup>1</sup>(✉)

<sup>1</sup>Microbial Biotechnology Research Laboratory, Department of Biochemistry, Manipur University, Canchipur - 795003, Manipur

(✉)Corresponding author: email: [debananda.ningthoujam@gmail.com](mailto:debananda.ningthoujam@gmail.com)

Phone no: 7085965023

The worsening global challenges such as climate change and increased population are leading to agricultural stress and antimicrobial resistance (AMR), necessitating the search for novel sources of microbial diversity [1]. Microbial diversity remains an unparalleled source of bioactive molecules and, of late, symbiotic microbes associated with plants and insects have been proposed as promising sources [3]. The present study was targeted at accessing selected ethno-medicinal plants and insects in Manipur, India for isolating bacterial symbionts and screening their promising bioactivities.

As soil microbiota have been overexploited for bioactive molecules, bioprospecting of endophytic microorganisms inhabiting plants especially medicinal plants and symbiotic microbes associated with insects holds great promise.

A total of 321 bacterial strains were isolated from 6 ethnomedicinal plant (*Blumeopsis flava*, *Pholidota graffithii*, *Alocasia indica*, *Vangueria spinosa* Linn., *Curcuma aromatica* Salisb, *Celtis timorensis* Linn) and 6 insect samples (putatively identified as *Oecophylla smaragdina*, *Oxya sp.*, *Apis cerana*, *Thysia wallichii tonkinensis*, *Crematogaster sp.*, and an as-yet unidentified black ant species). Thirty-eight (38) of the 321 bacterial symbiont isolates showed antibacterial activity against one or more of the 3 test organisms (*Micrococcus luteus*, MTCC 106; *Bacillus subtilis*, MTCC 121 and *Escherichia coli*, MTCC 739). Thirty-seven (37) isolates showed biocontrol activity against one or more of the 5 fungal test organisms (*Rhizoctonia solani*, MTCC 4633, *Pyricularia oryzae*, MTCC 1477, *Fusarium*

*oxysporum* MTCC 284, *Aspergillus niger*, MTCC 432, and *Curvularia oryzae*, MTCC 2605). All the 67 bioactive bacterial symbiont isolates were screened for Plant Growth Promoting (PGP) traits, of which 19 were found positive for phosphate solubilization and 11 for siderophore production. 12 isolates have been selected for characterization as they were found to have broad spectrum antibacterial or antifungal activity. Interestingly, 2 insect associated bacterial isolates (D4IN-8 and D3N-1) showed both phosphate solubilization and siderophore production traits. Further screening of these isolates for other PGP traits are currently underway. The study indicates that bacteria associated with ethnomedicinal plants and insects in Manipur have potential antimicrobial activities and can be exploited as biocontrol and plant growth promoting (PGP) agents for agricultural applications and pharmaceutical use.

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## Quantification and comparison of the content of indigo in different parts of in vitro cultured *Strobilanthes cusia* Nees (Kuntz) by using UV-Vis spectrophotometry

<sup>1</sup>Rajkumari Lunphasana Devi <sup>2</sup>K Sanatombi. ([lunpha25@gmail.com](mailto:lunpha25@gmail.com))

<sup>1,2</sup>Department of biotechnology, Manipur University, Canchipur, India  
([lunpha25@gmail.com](mailto:lunpha25@gmail.com)) phone no. 9856855790

### Abstract:

*Strobilanthes cusia*(Nees.) Kuntze is indigo dye yielding plant used in the Meitei community of North Eastern India and other Asian countries from ancient time for dyeing of fabrics and clothes [1]. With the advancement in science and technology, synthetic dyes occupy main position in textile industry but it has adverse harmful effect to the environment and human health which draw the attention back towards the natural products. The dye is mainly extracted from leaf in the traditional way which leads to mass destruction of the plant from the natural habitat. For overcoming its mass exploitation and utilizing its different parts for dyeing purpose an in vitro protocol is developed for mass production. From the in vitro grown plant, different parts i.e. root, stem, leaf and callus cell culture is compared for its indigo content and determination of most efficient parts for indigo production and utilization for dyeing purpose. The test of indigo content is done in different water extracts of the plant parts by using UV-Vis spectrophotometer [2]. It is then analyzed and compared for the most productive part to be used in future with less harmful effect to the environment.

**Keywords:** *Strobilanthes cusia*(Nees.)

Kuntze, UV-Vis spectrophotometry, indigo

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## Prediction of binding affinity of Chemical preservatives on Fibronectin protein of *Staphylococcus aureus* using Molecular Docking: Analyzing safety for Skin care products

<sup>1</sup>Sarra Akermi<sup>#\*</sup>, <sup>1</sup>Ritushree Biswas, <sup>2</sup>Sagarika Sahoo, <sup>1</sup>Abira Dey, <sup>3</sup>Jean Bernard, <sup>4</sup>Sunil Jayant<sup>\*</sup>

<sup>1</sup>Indian Science and Technology Foundation (ISTF), C-1/131, Yamuna Vihar, New Delhi.

<sup>2</sup>Amity University Mumbai, Bhatan Post - Somathne, Panvel, Mumbai, Maharashtra 410206, India

<sup>3</sup>Insight Biosolutions, Rennes, 35000, France

<sup>4</sup>Annotation Analytics Pvt. Ltd. 36, Ward no -14, Biswa, Amarpura, Gurgaon-122001 Haryana India

<sup>#</sup> Presenting Author, <sup>\*</sup>Corresponding Author, email : [sarahakermi221@gmail.com](mailto:sarahakermi221@gmail.com)

Skin Care products contain several chemical ingredients such as organic & inorganic compounds, fragrances, natural plant extracts and big volume of water, therefore it is always requiring prevention from the microbial contamination. Cosmetics producers add some chemical preservatives in the cosmetics formulation to increase shelf-life of skin care products (1). However, it is also particularly important to pre-evaluate the safety assessment of these preservatives on human skin to guarantee consumer's safety. In-vitro methods are available to understand effect of these preservatives on microbes and to predict their skin sensitization on human (1,2). However, it is still unknown about how these preservatives effect on the microbes? and these in-vitro methods are expensive and time consuming. Therefore, we proposed a proof of concept using computational molecular docking-based approach to understand effect of preservatives on *Staphylococcus aureus* growth by analyzing affinity of these chemicals with Fibronectin virulence protein. Later, safety assessment of these chemicals is analyzed for Skin irritation and Skin sensitization potency by QSAR. Our docking study revealed that chemical preservative Benzalkoniumchloride (Docking energy -10 kcal/mol) produced strong affinity with Fibronectin protein, however predicted irritant and sensitizer by QSAR. Chemicals

Triclosan (Docking energy – 6.00 kcal/mol, irritant and non-sensitizer) and Triclocarban (Docking energy – 6.20 kcal/mol, non-irritant and sensitizer) produced medium affinity with Fibronectin protein. Glycerol (Docking energy – 3.50 kcal/mol, non-irritant and non-sensitizer) produced low affinity with Fibronectin protein. Therefore, our docking and QSAR approach may be able to understand mechanism of inhibition on growth of *Staphylococcus aureus* by analyzing affinity with Fibronectin virulence protein and safety of these compounds by QSAR method. Our in-silico study will help the cosmetic ingredients producers and formulators for designing finished products formulations with safer preservatives to prevent microbial contamination.

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## DNA barcoding of edible freshwater gastropods and bivalves found in Nagaland

<sup>1</sup>Lanusangla Imsong, <sup>2</sup>Dr.M.Murali.

<sup>1</sup>Research Scholar, St.Joseph University, Zoology Department, Dimapur-797112, Nagaland, India

<sup>2</sup>Assistant professor, St.Joseph University, Zoology Department, Dimapur-797112, Nagaland, India

(✉)Corresponding author: email: [sangtila9436@gmail.com](mailto:sangtila9436@gmail.com)

Phone no: 9774915620

Freshwater gastropods and bivalves of phylum Mollusca are extensively distributed in various freshwater habitats of Nagaland. Molluscs are considered to be ecologically important and highly favored as traditional food item because of its nutrition, medicinal properties and low cost. This reflects the need of proper identification and documentation. However, the identification based on morphological characters is challenging due to the existence of cryptic species that shows similar morphology which can lead to erroneous identification of species. The primary objective of this study is to identify the edible mollusc species in Nagaland by DNA bar coding technique using a fragment of cytochrome oxidase I (COI) gene. Genomic DNA of the species was successfully isolated from the tissues and the primers used for forward and reverse amplification process are LCO (5' GGTCAACAAATCATAAAGATATTGG 3') and HCO (5' TAAACTTCAGGGTGACCAAAAAATCA 3'). The sequence was analyzed with those available in GenBank and uploaded in NCBI to obtain accession number. The molecular identification was consistent with the identification of species based on shell and teeth morphology. The molecular method helped identify 4 species of bivalves and 3 species of gastropods. The name of the species with the NCBI accession number is as follows- *Lamellidens marignalis* (MT490309), *Parreysia* (*Parreysia*) *corrugata* (OM074301), *Indonaia subclatharata* (OM075118), *Radiatula caerulea* (OM076974), *Filopaludina*

*bengalensis* (MT089706), *Paludomus* (*Paludomus*) *siamensis* (OM078498), *Brotia costula* (OM056887).

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## Molecular Identification of edible insects of Nagaland using DNA barcoding technique

<sup>1</sup>Lipoktola Tzudir <sup>2</sup>Dr. M. Murali.

<sup>1</sup> Research Scholar, St. Joseph University, Department of Zoology, Dimapur- 797115, Nagaland, India

<sup>2</sup> Assistant Professor, Department of Zoology, Dimapur-797115, Nagaland, India

(✉)Corresponding author: Lipoktola Tzudir email: [tzudir\\_lipok@yahoo.com](mailto:tzudir_lipok@yahoo.com) Phone no: +91 8974425604

Entomophagy practices should rely on proper identification of insects, which are usually classified relying on morphological keys and traditional knowledge practices. This may lead to misidentification of edible insects. Hence, the recent study, DNA barcoding was used to identify and documentation of edible insects. In the primary study 5 edible insects were collected and identification by performed by morphological studies and confirmed by DNA barcoding method and the species level was confirmed through phylogenetic tree analysis using BLAST. COI gene sequence was submitted to Gene Bank under the accession number *Choroedocus violaceipus* (JQ301451) *Chondracris rosea* (MN829822), *Samia ricini* (MN829823), *Yunnanites coriacea* (JQ301463) and *Vespa affinis* (MN820554)

**Keywords:** COI gene sequences, DNA barcode, edible insects.

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## Persimmon peel as a potential source of bioactive components

<sup>1</sup>NADIRA ANJUM, <sup>2</sup>ANJU BHAT. Corresponding author (✉): NADIRA ANJUM

<sup>1</sup> Division of Food Science and Technology, Sher-e-Kashmir University of Agricultural Sciences and Technology (SKUAST) Jammu, Chatha-180009

<sup>2</sup> Division of Food Science and Technology, Sher-e-Kashmir University of Agricultural Sciences and Technology (SKUAST) Jammu, Chatha-180009

(✉)Corresponding author: email: nadiraanjum1736@gmail.com

Phone no: +919622731073

Persimmon peel considered as waste, is receiving much attention because of its chemical composition [1]. It contains high levels of antioxidants, including vitamin C, total phenolics, total flavonoids and total carotenoids, are also present. Among the phenolic compounds, caffeic acid, *p*-coumaric acid, ferulic acid, and gallic acid are present in large quantities. The level of total carotenoids in persimmon peel is very high (about 340 mg/100 g of dried peels as  $\beta$ -carotene equivalents) as compared to the peels of other fruits like banana and apple [2]. The quantity of bioactive compounds (biologically active components), especially carotenoids and polyphenols, is greater in the peel compared to the pulp. Hence, persimmon peel should be consumed by individuals and used for industrial processing. Several studies reported that a 2-week intake of persimmon peel supplemented diet considerably reduces food intake, blood glucose, total cholesterol, and plasma triglycerides level in diabetics. Persimmon peel rich in high level of antioxidant and fiber with antidiabetic properties may be characterized as a possible nutritional supplement for improving diabetic complications and hyperglycemia [3].

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## Phytochemical Screening and Estimation of Total Phenolics, Flavonoids and Triterpenoids content in *Clematis napaulensis* DC.

Pangwan M. Konyak<sup>1</sup>, Moaakum<sup>1</sup>, Z. Heise<sup>2</sup>, S. Lakshmana Prabu<sup>3</sup>, K. Ruckmani<sup>3</sup>, V. Heise<sup>1</sup>, T. Ajungla<sup>4</sup>, H.S. Rathore<sup>5</sup>

<sup>1</sup>Department of Botany, Nagaland University, Lumami Nagaland – 798627, India

<sup>1</sup>Department of Botany, Kohima Science College, Jotsoma Nagaland – 797002, India

<sup>2</sup>Department of Science & Technology - Nagaland Science & Technology Council, Govt. of Nagaland, Kohima-797001, India.

<sup>3</sup>Department of Pharmaceutical Technology, University College of Engineering (BIT Campus), Anna University, Tiruchirappalli – 620 024, India

<sup>1</sup>Department of Botany, Kohima Science College, Jotsoma Nagaland – 797002, India

<sup>4</sup>Department of Botany, Nagaland University, Lumami-798627, India

<sup>5</sup>Department of Biotechnology, School of Engineering and Technology, Nagaland University, Dimapur- 797112

Corresponding author email: [moaakumjamir@gmail.com](mailto:moaakumjamir@gmail.com)

Phone no: +919436077729

### ABSTRACT

In the Indian subcontinent, medicinal plants are having good economic value and also provide different therapeutic values. The usage of plants for medicinal purposes is as old as human civilization. Phytochemicals in the medicinal plants are non-nutritive but have disease protective properties in human beings. *Clematis napaulensis* DC. belongs to the family Ranunculaceae which is being used by the Chakesang tribe of Nagaland as traditional medicine for the treatment of Rheumatoid Arthritis. Preliminary phytochemical screening and determination of the bioactive phytochemical in medicinal plants is considered as a valuable key step in isolation and to discover a new chemical moiety with the better efficiency. Earlier studies about the genus of *Clematis* reported to have several bioactive compounds with different pharmacological activities. The aim of the present study is to identify, understand the bioactive phytoconstituents of the leaf extracts and quantification of important secondary metabolites like flavonoids,

triterpenoids and phenolic compounds from the solvent extract. Analysis for the presence and absence of important secondary metabolites have indicated positive for phenolic compounds, alkaloids, glycosides, flavonoids, saponins, tannins, triterpenoids, gums, proteins and reducing sugar but negative for non-reducing sugars. Quercetin, Oleanolic acid and Gallic acid were used as standard references for the determination of total flavonoid content, total triterpenoid content and total phenolic content respectively. According to the literature, this is the first report on phytoconstituent screening, total phenolic content, total flavonoid content and triterpenoid content of from the extract of *Clematis napaulensis*. The generated phytochemical data from extract of *Clematis napaulensis* have shown that the plant is an important natural source of various types of phytoconstituents with varied chemical structure and can potentially be used as therapeutic agent against various diseases.

Keywords: Phytochemical screening, TPC, TFC, TTC, *Clematis napaulensis* DC.

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## In Silico Analysis of Candidate Drugs Against BSEP and MRP2 for their Roles in the Development of DILI

Suparna Dey<sup>1</sup> and Ashwani Sharma<sup>2,\*</sup> (✉)

<sup>1</sup> Department of Biotechnology, St. Xavier's College (Autonomous), Kolkata, West Bengal, India

<sup>2</sup> Indian Science and Technology Foundation (ISTF), New Delhi, India

\*(✉)Corresponding author: email: [director@isto-india.org](mailto:director@isto-india.org)

Hepatocytes are polarized cells that have specialized transport systems in the canalicular/apical and sinusoidal/basolateral membrane to maintain hepatic bile acid homeostasis and detoxify endogenous and xenobiotic toxins. Under physiologic conditions, the bile salt export pump (BSEP) and Multidrug resistance-associated protein 2 (MRP2), are the two proteins that mediate an ATP-dependent export of xenobiotic drug conjugates and conjugated bilirubin across the canalicular membrane into bile, where they can form micelles with other bile components such as phospholipids or cholesterol. Owing to their central role in the hepatic excretion of bile acids and toxins, functional impairment of BSEP and MRP2 has been hypothesized to play a role in the development of liver injury often as a side effect of drug therapy. While several experimental studies have confirmed the potential drug inhibitors of BSEP, the lack of an experimentally validated structure of MRP2 in the Protein Data Bank limits the scope of extensive ligand binding studies with the protein. Consequently, in silico approaches in combination with homology modelling have unveiled the identity of several candidate drug inhibitors for the two liver transporters for a comparative analysis. Studies in the same line have also supported the hypothesis that the risk of Drug Induced Liver Injury (DILI) may be even greater if a compound inhibits not just one but both the hepatic bile acid transporters BSEP and MRP2. Therefore, if the compound under study is a BSEP inhibitor, the inhibitory

potency on MRP2 should also be evaluated to improve the correlation with liver injury compared with inhibition of BSEP Or MRP2 inhibition alone. In this work, we have attempted to find a correlation between the experimentally determined IC<sub>50</sub> values of four drugs namely pioglitazone, cyclosporine A, papaverine and acyclovir, and their respective in silico binding affinities to BSEP and MRP2. Molecular docking studies showed that the drugs with lower IC<sub>50</sub> values (cyclosporine A and pioglitazone) had more negative binding energies when compared to the ones with higher IC<sub>50</sub> values (papaverine and acyclovir). Since the binding energies tie in with the magnitude of inhibition, further experimental mutation studies are required to confirm the in silico findings.

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## PGP Potential of Ethnomedicinal Plant Endophytic Bacteria from Manipur, India on Traditional Rice Cultivars

**Rakhi Khunjamayum, Debananda S. Ningthoujam, Wahengbam Pusparani Chanu, Yurembam Rojiv Singh and Nikena Khwairakpam**

Microbial Biotechnology Research Laboratory (MBRL)  
Department of Biochemistry  
Manipur University, Canchipur-795003 (Manipur), India  
(e-mail: [debananda.ningthoujam@gmail.com](mailto:debananda.ningthoujam@gmail.com) Phone no.: 9862027271  
[rakhikhunjamayum@gmail.com](mailto:rakhikhunjamayum@gmail.com) Phone no.: 9774101970)

With the continually burgeoning world population, the global necessity to boost agricultural production has placed considerable strain on our agro ecosystems. The increasing demand for organic agriculture warrants the search for plant growth promoting (PGP) agents that can be deployed as biostimulants (BS), biofertilizers (BFs) and biocontrol agents (BCAs) for enhancing crop yields with no/less inputs of synthetic agrochemicals [1]. In the present study, 167 endophytic bacteria were isolated from nine (9) indigenous medicinal plants of Manipur. Twenty-nine (29) endophytic bacterial isolates exhibiting potent antifungal and promising PGP activities were selected for seed vigor tests on rice. 4 isolates (*Streptomyces* sp. AcRz3\*, SxL10 (a putative *Streptomyces* sp.), *Paenibacillus* sp. CcS9 and *Bacillus* sp. TgIb4) with highest vigor indices were further assayed for rice (*Drum Phou*) plant growth promotion under *Rhizoctonia solani* challenged conditions in small-scale field trials. All 4 endophytic bacterial isolates significantly increased the growth of traditional rice cultivars and decreased the disease lesions caused by *Rhizoctonia solani*. These 4 most promising endophytic bacteria (AcRz3\*, CcS9, SxL10 and TgIb4) associated with medicinal plant

could be exploited for application as biocontrol and biofertilizing agents for rice production.

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## ***In silico* identification and characterization of patatin-related phospholipase A (pPLA) gene family in *Sorghum bicolor***

<sup>1</sup>Reshma Parveen, <sup>1</sup>Divya Gupta and <sup>1</sup>Mahesh Kumar Basantani (✉)

<sup>1</sup>Faculty of Biosciences, Institute of Biosciences and Technology, Shri Ramswaroop Memorial University, Lucknow Deva Road, Barabanki, 225003, Uttar Pradesh, India

(✉) Corresponding author: e mail: [mkbasantani@gmail.com](mailto:mkbasantani@gmail.com) Phone no: +91 9839534061

Patatin-related phospholipase A (pPLAs) are involved in a wide range of physiological and metabolic activities in plants, from normal growth to the management of biotic and abiotic stresses. Cell elongation, gravitropism, defense signaling, phosphate metabolism, flower and seed development, and jasmonic acid production are all functions that pPLAs play in plants [1]. The presence of a catalytic center comprised of an esterase box GTSTG and an anion-binding element DGGGXRG distinguishes patatin-related proteins in plants. Based on sequence similarities, plant pPLAs are divided into three groups: Group I, II, and III. The catalytic dyad in Group I and II pPLAs consists of a conserved aspartic acid in the patatin domain and a typical serine hydrolase motif of GX SXG. The hydrolase motif sequence of GXGXG is found in Group III pPLAs [2].

In the current study, bioinformatics identification and characterization of pPLA gene family were carried out in an agriculturally important crop viz *Sorghum bicolor*. It is usually called sorghum or jowar belongs to poaceae family. There were some information about the presence of pPLA gene family in this crop, and the whole genome sequences of the crop were accessible [3]. The pPLA gene family has been characterized in *Vigna radiata*, *vigna angularis* and *Glycine max* [4], *Brassica napus* [5], grapevine [6], rice [7], *Arabidopsis thaliana* [8], etc. In the study different bioinformatics approaches were used to

characterize these pPLAs. The identification of pPLAs in *S. bicolor* was validated using pPLAs from *A. thaliana* as the query sequence. In *S. bicolor*, a total of 21 pPLA genes were discovered. NCBI Batch CD Search verified the domain organization of pPLAs. In the identified pPLA proteins, the conserved patatin domain was located towards the N-terminus. There were total 1 pPLA in Group I, total 12 pPLAs in Group II, and total 8 pPLAs in Group III. By subcellular localization prediction, Group I pPLAs were identified in plasma membrane, Group II pPLAs in cytoplasm, mitochondria, peroxisome, and chloroplast, and Group III pPLAs were located in chloroplast and nucleus. The number of amino acids ranged from 97 to 1338, the pI was 5.58 to 10.07, and the molecular weight was 10.35 to 147.47 (kDa). The gene organization of the pPLAs was consistent with the canonical gene architecture of the pPLA gene family. The existence of significant conserved motifs in the pPLA proteins was discovered using the Multiple Expectation Maximization for Motif Elicitation (MEME) method. According to their classification, the pPLAs were clustered into three groups (I, II, and III) using phylogeny analysis. The pPLA gene family of this crops was found to be identical to that of *A. thaliana*, rice, and grapevine, with the pPLA genes of Group II were highest in number, followed by pPLA genes of Group III and Group I and the length of the pPLA-I, II, and III proteins is identical to previous studies such as *A. thaliana*, *Vigna*

*radiata*, *vigna angularis* and *Glycine max*.  
The current study's findings will be important  
in the molecular and functional  
characterization of this gene family.

**Key-words:** Bioinformatics, Phospholipase,  
Patatin-related phospholipase A (pPLA),  
*Sorghum bicolor*

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## Prediction of patients at high risk and associated risk factors in Mucormycosis using Artificial Intelligence based methods

<sup>1</sup>Shradha Jain and <sup>1</sup>Yatender Kumar. (✉)

<sup>1</sup> Department of Biological Sciences & Engineering (BSE), Netaji Subhas University of Technology (NSUT), Dwarka Sector-3, New Delhi - 110078

(✉)Corresponding author: email: [yatender.kumar@nsut.ac.in](mailto:yatender.kumar@nsut.ac.in)

Phone no: +91-9718936319

Mucormycosis is a rare fungal disease that has proven to be fatal in most cases. It was first detected in the year 1847 and its increase in cases has created havoc in India and many other parts of the world with the onset of COVID19. In India, especially during the second wave of COVID, mucormycosis cases dramatically saw a rise proving to be of high mortality rate in many instances. The patients of mucormycosis before coming in contact with COVID19 displayed a high mortality rate of 54% and even an higher mortality rate of 96% for disseminated mucormycosis[1]. Initially, there are symptoms or no symptoms in patients having mucormycosis and it quickly spreads to other areas such as the eyes, and brain leaving the person dead, if not treated early. Nearly, 50% of cases of mucormycosis are said to have diagnosed in the post-mortem only, owing to the difficult diagnosis [2]. Early diagnoses of mucormycosis is crucial for mucormycosis detection in patients for timely treatment and improved survival rate [3]. Here, we present an artificial intelligence-based model to predict the patients at high risk and associated high-risk factors in mucormycosis since it is crucial that patients at high risk can be warned in advance. The model assesses COVID-associated mucormycosis also so that patients suffering from COVID19 or patients who have even recovered from COVID19 can benefit from the same. We have performed an extensive literature search in electronic databases like Google Scholar and PubMed and obtained the data of patients who have suffered from mucormycosis. The results

suggest that the presence of comorbidities affects the condition of mucormycosis. Among the various comorbidities present, Diabetes was most prevalent. Reports of rhino cerebral mucormycosis were also higher followed by pulmonary mucormycosis.

World Health Organization has stressed that the early diagnosis and recognition of mucormycosis is crucial to improve mucormycosis outcomes [4]. Thus, the early prediction of mucormycosis will serve as a crucial factor in diagnosis of Mucormycosis.

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## Antifungal screening, plant growth promoting activities, characterization and analysis of rice seed vigor index of rhizobacteria isolated from the rhizospheric soils of Chakhao Angangbi and Chakhao Wairi

Sajida Sultana, Debananda S. Ningthoujam,

Microbial Biotechnology Research Laboratory (MBRL), Department of Biochemistry, Manipur University, Canchipur – 795003 (Manipur), India.

E-mail: [sultanamakakmayum@gmail.com](mailto:sultanamakakmayum@gmail.com) Phone no. 6009031984

**Key Words:** Chakhao, characterization, antifungal, PGP traits, rhizospheric isolates.

Rhizospheric bacteria, having plant growth-promoting ability by colonizing the plant roots, are known as PGPR (Kloepper and Schroth 1978). PGPRs are potentially useful in stimulating plant growth and increasing crop yields (Sayyed et al. 2010). PGPR not only provide essential nutrients for plant growth promotion, but they are also important in biocontrol of pathogens; they also improve soil health in the long term and, can potentially reduce the use of chemical fertilizers and chemical pesticides (Lugtenberg and Kamilova 2009). Black rice is mainly cultivated in limited areas in Manipur as the yield is poor. Therefore, the focus of the present work is isolation of bacteria from rhizospheric soils of Chakhao Angangbi and Chakhao Wairi and screened their PGP potential.

In our present study, 93 rhizobacteria strains were isolated from the rhizospheric soils of **Chakhao Angangbi** and **Chakhao Wairi**, screened for their antifungal activity against *Rhizoctonia solani* (MTCC4633), *Fusarium oxysporum* (MTCC287), *Curvularia oryzae* (MTCC2605), *Pyricularia oryzae* (MTCC1477) and *Aspergillus niger* (MTCC1344). The bacterial[ cultures showed potent antagonistic activities in dual culture assay. 21 antagonistic isolates were tested for their plant growth promoting (PGP) traits, extra cellular enzyme production, salt

and pH tolerance. Two isolates mentionably CR12 and CW11 were most effective which may be useful as biofertilizers, they may enhance the growth of chakhao rice and other rice plants due to the production of ammonia, IAA, HCN, phosphate solubilization, siderophore production and acc deaminase production and also having antifungal activity against phyto pathogenic fungi. Their vigor indices in rice seeds have been performed and the results are significant. Molecular characterization of CR12 and CW11 have also been done.

These rhizobacterial isolates can be promising candidate biocontrol agents for development of rice cultivation. A rhizospheric isolate of **Chakhao Wairi**, CW11 showed 194µg/ml at pH 3.20 of phosphate solubilisation on quantitative estimation which is in between the phosphate solubilisation index of 30-246 µg/ml in liquid broth (Shumaila Batool et al.. 2019). Again an isolate from rhizospheric soil of **Chakhao Angangbi**, CR12 produce siderophore of around 73.15% in nutrient broth media that is almost considerable comparing with the previous documented bacteria (Swapan Kumar et al. 2015). Moreover, these cultures showed potential plant growth promoting traits. The pot trial and field trial of CR12 and CW11 are currently underway.

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## Computational insights into GST gene family identification and characterization in *Coffea canephora*

Swati Vaish<sup>1</sup>, Divya Gupta<sup>1</sup> and Mahesh Kumar Basantani<sup>1\*</sup>

<sup>1</sup>Faculty of Biosciences, Institute of Biosciences and Technology, Shri Ramswaroop Memorial University, Lucknow Deva Road, Barabanki, 225003, Uttar Pradesh, India

<sup>1\*</sup>Corresponding author: Dr. Mahesh Kumar Basantani, Institute of Bioscience and Technology, Shri Ramswaroop Memorial University, Lucknow-Deva Road, Barabanki, 225003, Uttar Pradesh, India Tel: +91 9839534061 [mkbasantani@gmail.com](mailto:mkbasantani@gmail.com)

Glutathione S-transferases are a multifunctional protein super family that is involved in diverse plant functions such as defense mechanisms, signaling, stress response, secondary metabolism, plant growth and development [1]. GSTs are classified into three distinct superfamilies namely cytoplasmic, mitochondrial and microsomal. Cytoplasmic and mitochondrial GSTs are soluble; and microsomal GSTs (MAPEGs) are membrane associated proteins involved in eicosanoid and glutathione metabolism. Soluble plant GSTs are further categorized into 14 different classes based on sequence similarity, genomic organization, immunological cross reactivity and functions viz. tau (U), phi (F), theta (T), zeta (Z), lambda (L), Dehydroascorbate reductase (DHAR), Tetrachloro-hydroquinone dehalogenase (TCHQD), Elongation factor 1B $\gamma$  (EF1B $\gamma$ ), microsomal prostaglandin E synthase type 2 (mPGES2), Glutathionyl hydroquinone reductase (GHR), iota, hemerythrin, metaxin and Ure2p [2]. GST gene family have been identified and characterized in various plant species such as 39 GSTs in *Cucumis melo* var. *saccharinus* [3], 92 GSTs in *Medicago truncatula* [4], 32 GSTs in *Cucurbita maxima* [5], 330 GSTs *Triticum aestivum* [6], 82 GSTs in *Raphanus sativus* [7], 51 GSTs in chickpea [8] and 31 GSTs in *Vigna radiata* [9].

Although the coffee whole genome sequence is available but the distribution of GST genes on coffee chromosomes, their subcellular localization, gene structure, their evolutionary relation with each other, conserved motifs and their roles are still unknown. A total of 71 GST genes with the canonical thioredoxin fold have

been identified belonging to nine GST classes namely tau, phi, theta, zeta, lambda, DHAR, EF1G, mPGES2 and GHR. Tau and theta GST genes were highest in number. The 71 GST genes were distributed into 10 coffee chromosomes. The physicochemical features showed most of the CGST proteins as highly stable and hydrophilic protein, majorly localized in the cytoplasm. Gene architecture showed the conservation of exon numbers in each GST classes. MEME analyses revealed few class specific motifs and many motifs were found in all the GST classes. Multiple sequence alignment of coffee GST revealed the Ser and Cys as conserved catalytic residue. Gene duplication analyses showed both the tandem and segmental duplication as a driving force for GST gene family expansion in coffee. The phylogenetic analyses of coffee GST with angiosperm (*Arabidopsis* and rice), gymnosperm (*L. kaempferi*) and bryophyte (*P. patens*) revealed that the evolution of plant GSTs might be earlier than their division into individual groups such as bryophyte, pteridophyte, gymnosperm and angiosperm and also the each GST classes have diverged prior to the division of monocot and dicot. Additionally, the numbers of each class of GSTs expanded in a species specific manner independently and irrespective of their genome size. Cis-regulatory element analyses showed the dominance of light responsive element followed by stress and hormone responsive element. The comprehensive and organized studies of CcGST genes family provides groundwork for further functional analyses of CcGST genes in coffee at molecular level and further for plant breeding approaches.



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## Effect of sucrose concentration on *in vitro* microrhizome production in *zingiber zerumbet*

Sanasam Thoibi and K. Sanatombi

Department of Biotechnology, Manipur University, Canchipur, Imphal, 795003, Manipur, India

(✉)Corresponding author: [sanasamthoibi@gmail.com](mailto:sanasamthoibi@gmail.com)

Phone no: 8974844712

*Zingiber zerumbet* popularly known as shampoo ginger is a traditional medicinal plant belonging to Zingiberaceae family and locally known as “singkha” in Manipur (1). The plant is propagated through rhizomes but the rhizome cannot be stored for a longer period of time as it is susceptible to fungal diseases, which affect the quality of the propagules (2). Moreover, the plant is also grown in the wild environment which limit the availability of this plant. The present study will give a simple protocol for *in vitro* microrhizome production of *Zingiber zerumbet* which can be used an alternate source for mass propagation of this plant and also studied effect of different concentration of sucrose on the microrhizome formation in *Zingiber zerumbet*. *In vitro* microrhizomes of *Zingiber zerumbet* were produced from *in vitro* derived microshoots upon transfer to Murashige and Skoog (MS) medium containing various concentration of sucrose (3-9%) with 5 mg/l BAP cultured under 16 hours photoperiod at 25±2°C after twelve weeks of culture. 6% sucrose was found to be most effective concentration of sucrose in the induction of microrhizome in *Zingiber zerumbet* by giving highest mean (8.33±1.33) number of shoots per explant and also give highest mean (0.435±0.05 g) weight of microrhizome.

Keywords: *Zingiber zerumbet*, Zingiberaceae, microrhizome, Murashige and Skoog medium, microshoots.

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## Quantifications of Endogenous Formaldehyde Levels in Mouse Organ Tissues through Two-Photon Fluorescence Bioimaging

<sup>1</sup>Uttam Samanta, <sup>1</sup>Subhankar Singha (✉)

<sup>1</sup>Centre for Interdisciplinary Sciences, JIS Institute of Advanced Studies and Research, JIS University, Kolkata, 700091, India

(✉)Corresponding author: email: [subhankar@jisiasr.org](mailto:subhankar@jisiasr.org)

Phone no: (91)-9330430247

Formaldehyde (HCHO) is known to be associated with various biological functions and produced endogenously in the body with the help of various demethylase and oxidase enzymes. To investigate formaldehyde biology in more details, it is utmost necessary to observe the variation of formaldehyde levels in different tissues depending upon the organs or body parts. For such purpose, two-photon fluorescence detection and fluorescence bioimaging is highly advantageous [1]. Accordingly, in this study, a probe has been used to perform the two-photon excitable ratiometric fluorescence bioimaging of formaldehyde in various organ tissues (brain, lung, liver, kidney, and colon) of mouse [2]. The probe, upon interaction with endogenous formaldehyde, allows the ratiometric fluorescence imaging necessary to estimate the endogenous formaldehyde levels in different mouse organs. Upon the incubation of the tissues with the probe, followed by initial collection of two-photon microscopic fluorescence images at two separate emission channels and further processing of those images to convert pixel-to-pixel ratiometric images, finally provides the quantified values of formaldehyde levels in various tissues, such as, 190  $\mu\text{M}$  in colon; 430–600  $\mu\text{M}$  in brain, lung, and kidney; 850  $\mu\text{M}$  in liver. This imaging technique was further applied to investigate formaldehyde levels in intestinal organoids (villi and crypts) and the result shows a high level of formaldehyde around the crypts region of small intestine ( $\sim 500 \mu\text{M}$ ). Moreover, it is known that the crypts of small intestine contain Paneth cells which protects stem cells

and epithelial cells by releasing various antimicrobial defensins [3]. In that respect, the results of the study here are suggesting the possible protective role of formaldehyde (in association with Paneth cells) in the small intestine crypts.

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