

CRITERION-III

EVIDENCE(S), AS PER SOP

METRIC No. 3.7.1	Number of collaborative activities with other institutions/ research establishment/industry for research and academic development of faculty and students per year
1	cuments indicating the collaboration/related documents indicating the boration and activities year-wise



School of Studies in Anthropology Pt. Ravishankar Shukla University, Raipur (C.G.)

Dr. Ashok Pradhan Professor & Head

No. 4337 /Anth/2022

E-mail: pradhan.akp@gmail.com Mobile No. : 94255-11967

Raipur, Dated : 19/07/2022

No. Date: 14 July 2022

To, **Mr Job Zachariah** Chief Field Office UNICEF Chhattisgarh

Sub: Request for releasing funds for the first quarter

Dear Mr Zachariah,

With reference to the letter dated 12 July, 3044/KS/2022 from Dr Keshari Lal Verma, Vice Chancellor, Pt. RSU assigned me as the nodal officer of the proposed partnership between Pt RSU and UNICEF.

We request you to release the first tranche of funds for Rs. 16,48,000.00 for the period 15 July to 14 October 2022 related project titled "Augmenting Mission Indradhanush 4.0: Engage, sensitise media, religious & tribal leaders and other key influencers to promote RI in CG".

Please find below bank details for transferring funds:

Payee: RSU General Fund Registrar Pt RSU Account # 10049590033 Bank: State Bank of India, RSU Branch, Raipur

The budget is attached for your reference.

Thanking you,

1416120

(Dr. Ashok Pradhan)

(Dr. Ashok Pradhan) Professor & Head SoS in Anthropology Pt. Ravishankar Shukla University Raipur (C.G.)

In vitro Propagation of *Curcuma caesia* Roxb. via Bud Culture Technique and ISSR Profiling of the Plantlets for Genetic Homogeneity

Anjum Afreen, Singh Vikram, Adil Smriti and Quraishi Afaque*

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Abstract

An in vitro propagation protocol has been developed for Curcuma caesia Roxb., an endangered medicinal plant by Foundation for Revitalisation of Local Health Traditions and Central Forest Department of India. The plant bears poorly germinated seeds and produces two-storage organs: rhizomes and multiple root tubers. Only rhizomes have medicinal-economic values. They serve as propagules too, which results in a shortage of planting material. Therefore, a complete one-year production cycle of C. caesia has been standardized through in vitro propagation including explants establishment (one month), subculture cycles (seven months), rooting (one month) followed by primary hardening (one month) and secondary hardening (two months).

Dormant shoot buds on rhizome served as explants for culture initiation on Murashige and Skoog (MS) medium supplemented with different concentrations of 6-benzyladenine (BA) and kinetin (KIN) in combination with citric acid (CA), adenine sulfate (AdS) and indole-3-acetic acid (IAA). Maximum bud break (70%) was obtained on MS with 8 mg L^{-1} BA, 8 mg L^{-1} KIN, 100 mg L^{-1} CA, 200 mg L^{-1} AdS and 2 mg L^{-1} IAA (standard medium). Shoot production potential continued on this medium during the subsequent seven-month-long subculture cycle. The in vitro raised shoots rooted best on $\frac{1}{2}$ -strength MS containing 1 mg L^{-1} indole-3-butyric acid. Plantlet survival rate was >95% after acclimatization. The genetic homogeneity of plantlets with the mother plant was analyzed using Inter Simple Sequence Repeats which generated a monomorphic banding pattern to confirm the uniformity of in vitro raised plantlets of C. caesia.

Keywords: Meristem culture, Kali Haldi, Subculture, Rooting, Acclimatization.

Introduction

Curcuma caesia Roxb., popularly known as 'Kali Haldi' ('Black Turmeric' in English), is a perennial, tuberous rhizomatous herb belonging to the family Zingiberaceae²⁸. It is an endangered plant native to Central and North-East India²³ where it is used as a spice and in food preservation. The rhizome is rich in camphor curcuminoids, phenolics, flavonoids, certain proteins, amino acids, essential oil and alkaloids³⁰. Sesquiterpenes and monoterpenes from the extract of *C. caesia* rhizomes have good antioxidant, antiinflammatory and tumor cell inhibitory activities^{2,6,10,20}. The essential oil from leaves of *C. caesia* also possesses the potential and biologically important activity and can be used as natural antioxidants, anti-inflammatory and antimicrobial agents in pharmaceutical industries⁷.

The Central Forest Department of India has declared this species an 'endangered herb' due to biopiracy²¹. It is categorized as a critically endangered species of Central India¹⁴. C. caesia bears seeds that are poorly germinated¹⁰. Therefore, the plant is commonly propagated through underground rhizomes only⁴. Medicinal and economic values reside in these rhizomes. Moreover, the plant produces many underground root tubers too. These root tubers have no market value. Thus, due to the production of two storage organs, the yield of the desired part- rhizome becomes low during its cultivation. The harvested rhizomes, after cultivation, are sold for the recovery of cultivation cost and profit-making. Hence, lower yields of the rhizomes create a shortage of the propagules for cultivation resulting in very high costs for its saplings¹⁶. Low rhizome productions result in the propagule unavailability for cultivations.

Hence, to fulfil the demand, it is directly harvested from the forests pushing the plant into endangered status²². *In vitro* culture technique facilitates the production of planting materials to propagate species²⁷. Reports are there for plantlet regeneration of *C. caesia* via meristem culture^{3,4,5,29,35} or via callus too^{31,37}. However, all these reports neither examine the regeneration efficiency during subculture cycles nor analyze the genetic fidelity of the regenerants. The present study reports a complete one-year *in vitro* production cycle and genomic template stability of the plantlets of *C. caesia*.

Material and Methods

Healthy rhizomes of *C. caesia* were collected from the National Center for Natural Resources, Pandit Ravishankar Shukla University, Raipur (India) in June 2019. Rhizomes were first washed with running tap water to remove soil particles followed by treatment with surfactant tween-20 for 5 to 10 min and a fungicide solution containing 0.1% (w/v) Bavistin 50WP (BASF India Ltd., Mumbai, India) and 0.25% (w/v) Carbendazim 50WP (Hindustan Insecticides Ltd., Bathinda, India) for 20 minutes. The dormant shoot buds (explants) on the rhizome were chopped off; the surface

GENETICS & EVOLUTIONARY BIOLOGY - ORIGINAL ARTICLE



Screening of a new candidate tree legume- *Pithecellobium dulce* (Roxb.) Benth., for lead remediation

Satyam Kumar Kumbhakar¹ · Ravishankar Chauhan^{1,2} · Vikram Singh¹ · S. K. Jadhav¹ · Afaque Quraishi¹

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Abstract

A fast-growing, leguminous tree species- *Pithecellobium dulce* (Roxb.) Benth., was screened in vitro against Pb-stress for the first time. In the current study, Pb toxicity affected the seedlings growth, lipid peroxidation, hydrogen peroxide production, antioxidant enzymes activity, proline content, and genomic template stability in a dose-dependent manner. The plant showed a high Pb tolerance, uptake and accumulation (> 2300 mg Kg⁻¹). Citric acid application could mitigate Pb-stress in the seedlings exhibited by the examined morphological, biochemical, and molecular parameters, including remarkably enhanced Pb uptake by the roots. Citric acid addition to the Pb solution reduced lipid peroxidation and ROS production in the seedlings roots, stem, and leaves. Citric acid also induced the antioxidant enzymes activities in the seedlings that were reduced by Pb exposure. Citric acid-mediated recovery under Pb-stress was evidenced by the growth and development of the seedlings, higher chlorophyll pigments, lower proline content and maximum tolerance index. The Pb exposure altered the genomic template stability that was also recovered by citric acid. Thus, after further field studies, *P. dulce* with citric acid mitigation may prove suitable for Pb remediation from contaminated sites.

Keywords Antioxidant enzymes \cdot Genomic template stability \cdot Lipid peroxidation \cdot Pb-stress \cdot Pb-accumulation \cdot Phytoremediation

1 Introduction

Globally, lead (Pb) contamination in soils is a growing concern (Wang et al. 2021). Pb is highly toxic, non-biodegradable and long half-life heavy metal that is present in abundance (Frank et al. 2019; Latif et al. 2020). It can cause severe damage to ecosystems as well as human health (Cano-Ruiz et al. 2020). Excessive use of paints, mining, sludge, industrial waste, and agricultural activities are mainly responsible for Pb contamination of the environment (Frank et al. 2019; Samreen et al. 2021; Raju et al. 2021). Patra et al. (2020) stated that Pb contamination of agricultural land is a major environmental concern. Pb may enter the human body through ingestion and inhalation, this first one being directly linked with the food chain and can

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² National Center for Natural Resources, Pt. Ravishankar Shukla University, Raipur 492010, India cause severe diseases (Iheanacho et al. 2017; Vladimirovich et al. 2021). Pb toxicity showed a negative relationship with nutrient uptake, antioxidant activity, and photosynthesis in plants. In response to metal-induced toxicity, Plants have evolved defense mechanisms including synthesis of antioxidant enzymes (Giannakoula et al. 2021) such as SOD, CAT, and APX that help to maintain cellular redox homeostasis. This redox equilibrium may be disturbed due to the excess generation of reactive oxygen species under Pb-stress (Giannakoula et al. 2021). ROS induces oxidative stress and lipid membrane peroxidation that damages the biological molecules and alters normal metabolic pathway resulting in cellular destruction (Pourrut et al. 2011).

Presently, several phytotechnologies are available to treat contaminated areas due to their low cost and environmentally friendly nature (Yan et al. 2020). Trees due to their long life cycle, huge biomass, and extensive root system are considered more suitable for the purpose than the grasses or other plants (Kaur et al. 2019). An ideal tree candidate must be fast-growing, multiple stress-tolerant, able to grow on poorly nutrient soils combined with high toxicant tolerance, uptake, and accumulation. *Pithecellobium dulce*

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Contents lists available at ScienceDirect

Plant Stress

journal homepage: www.sciencedirect.com/journal/plant-stress

Gamma radiation: A potential tool for abiotic stress mitigation and management of agroecosystem

ABSTRACT

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Context: Being sessile, it is impossible for the plants to evade from the unfavourable environmental conditions prevailing due to various abiotic stresses like heat, salinity, drought, flood, heavy metals, and high radiance amongst many others. These abiotic stresses disrupt plant growth and limit crop productivity to a large extent globally. Crop plants need to acclimatize themselves in these unsuitable environmental and edaphic conditions utilizing their inherent biological mechanisms. Massive amount of pertinent researches have been done in the last few decades regarding utilization of gamma rays for improvement in traits, and management of agroecosystem by developing superior quality crops/ germplasms. It has been well established that the gamma rays promotes abiotic stress tolerance in plants at low doses (50–100 Gy). Gamma rays are also being widely used as mutation techniques in an attempt to raise abiotic stress tolerance and, disease resistant crop varieties. Furthermore, a better understanding of tolerance mechanisms induced by gamma rays will help in improving crop productivity under stress conditions. However, the potential mechanisms involved in this are still indefinable. This review illustrates general information about gamma ray, its dose dependant responses; beneficial effects and lethality, and also the potential mechanism(s) underlying the tolerance induction and performance enhancement of plants growing under various abiotic stress conditions.

Objective: To elucidate the role of gamma rays as a potential tool for stress mitigation and management of agroecosystem.

Methods: Gamma rays have been used quite differently by various researchers for alleviation of abiotic stress imposed responses in plants.

Results and conclusions: Application of gamma radiation has popularly been noticed to enhance nutrient uptake, modulate biosyntheses of numerous secondary key metabolites and osmolytes, and regulate various metabolic activities to engender tolerance against environmental stresses.

Significance: In most of the developing and under developed nations, owing to limited development in agromanagement systems, abiotic stresses are seen to cause potential threats to growth and productivity of crops. Therefore, it is essentially to explore novel cost effective possibilities like use of low dose of gamma rays in crop plants for improvement in their performance during these rapidly changing climatic conditions.

1. Introduction

Crop plants encounter various abiotic stresses in their life span owing to global warming and climatic abnormalities which majorly limits their growth and productivity. Drought, temperature extremes, salinity and acidity of soil, light intensity, submergence, and anaerobiosis are dominant abiotic stresses amongst others, and are hostile to farming and the ecosystem (Wania et al., 2016). Crop plants of approximately 90% of cultivable area are facing one or several of the above stresses (dos Reis et al., 2012), which results in approximately 70% losses in the yield of major food grains *viz.*; *Oryza sativa, Triticum aestivum* and *Zea mays,* and hence affecting food security (Tigchelaar et al., 2018). As per the report of FAO (2007), merely 3.5% land area has left untouched by any of the environmental constrain.

Amongst the enlisted abiotic stresses, salinity becomes the most stubborn one by escalating the salt concentration in the arable land

Abbreviations: Reactive Oxygen Species, ROS.

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Reactive oxygen species

Keywords:

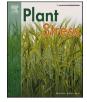
Gamma ravs

Abiotic stress

Antioxidants

Mutation

Review





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A comparative study of (Response surface methodology) RSM and (Artificial Neural Network and Genetic Algorithm) ANN-GA for optimization of biohydrogen production by *Pseudomonas aeuroginosa* SBT-Pa 092

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Abstract:

This communication discusses the optimization of carbon and nitrogen sources for the enhanced bio-hydrogen production from rice mill effluent. Three critical factors, concentrations of glucose (10-20 g/l), yeast extract (1-5 g/l) and Ammonium per sulphate (1-2 g/l) were optimized by response surface methodology (RSM) with central composite design (CCD) for better production. The hydrogen produced by *Pseudomonas aeuroginosa* SBT-Pa 092 was enhanced after using RSM. The value of R² obtained by ANN after training (75%) are 14 samples, validation (15%) are 3 samples and testing (15%) are 3 samples were 0.86976, 0.78299, and 0.94523 for bio hydrogen production. The value of R² obtained by ANN after training (40%) = 10 samples, validation (25%) = 5 samples and testing (25%) = 5 samples were 0.79317, 0.8596 and 0.90984 respectively, for biohydrogen production. The % error for ANN and RSM were 0.0016 and 0.01 for biohydrogen production, which showed the authority of ANN in exemplifying the non-linear behaviour of the system. Thus, ANN/RSM together successfully identify the substantial process conditions for Biohydrogen production. The results obtained indicate that use of both RSM and ANN with appropriate experimental design can be used to optimize culture conditions for enhancement of hydrogen production.

Key words: Biohydrogen, Pseudomonas aeuroginosa SBT-Pa 092, RSM, CCD and ANN.

Introduction:

To meet the energy requirements of the society the world economy is completely dependent upon the fossil fuel. The rising cost and harmful effect of fossil fuels on the environment has resulted in the development of eco-friendly and alternative source of energy. Hydrogen is considered as an environment friendly and clean source of energy as it does not produce any of the green house gases during combustion [Wang et al 2014; Jiang et al 2014]. Also it is having high energy content (142 kJ/g) which is 2.75 times higher than the fossil

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Biocatalysis and Agricultural Biotechnology

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Bacterial consortia mediated induction of systemic tolerance to arsenic toxicity *via* expression of stress responsive antioxidant genes in *Oryza sativa* L.



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ARTICLE INFO

Keywords: Antioxidative enzymes Arsenic Bacterial consortia Gene expression Oxidative stress Plant growth promotion

ABSTRACT

Arsenic (As) is a toxic metalloid which pollutes soil and water, and negatively affects the growth and development of plants at different levels. This study investigated the effects of As-resistant and plant growth promoting (PGP) bacterial consortia on the germination and growth attributes of two cultivars (Swarna and MTU 1010) of rice (Oryza sativa L.) under As-flooded environment. The consortium consisted of five bacterial strains; Bacillus nealsonii strain ARP2, Pseudomonas nitritireducens strain ARP3, Exiguobacterium aestuarii strain ARRP3, Bacillus tequilensis strain ART2 and Microbacterium paraoxydans strain ADT5, which were isolated from different regions of Chhattisgarh, India. Soils inoculated with the bacterial consortia and supplemented with As(V)/As(III) were used to grow rice seeds under in vitro conditions. The results ascertained that the seedlings inoculated with the bacterial consortia grew well even in the presence of As, which was marked by increased shoot and root length, biomass, and total chlorophyll content. Further, inoculation of bacterial consortia reduced the oxidative stress to a significant level by up-regulating the expressions of protective genes encoding antioxidant enzymes. This consortium could decrease the As accumulation in plants upon successful colonization in the rhizosphere, suggesting possible exploitation of it for enhanced growth of plants and in the remediation of As-contaminated soils.

1. Introduction

Arsenic (As) is a toxic and non-essential metalloid for plants, leading to different phytotoxic effects (Yoon et al., 2015). It exists primarily as inorganic arsenate [As(V)] and/or arsenite [As(III)], which are the dominant species in soil environments, and their chemical behaviour is heavily influenced by the striking redox reactions of soil (Ascar et al., 2008). Although arsenic occurs naturally in the environment, irrigation with As-contaminated water has increased the risk of this metalloid being transferred and accumulating in subsequent food chains (Jablońska-Czapla et al., 2020). It is a potent carcinogen and mutagen, which raises potential hazard and concern for both public health and the environment (Kapaj et al., 2006). Having similarity with phosphate (PO_4^{-3}), As(V) easily enters into the plant cell *via* high-affinity phosphate transporters, while As(III) is incorporated by aquaporin channels (Allevato et al., 2019). Both these result in severe toxicity, which is marked by the disturbances in various physiological and biochemical processes and genetic stability (Talukdar, 2011).

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Abstract: The solubilization capacity of a series of sustainable phenylalanine-derived surface-active ionic liquids (SAILs) was evaluated towards polycyclic aromatic hydrocarbons-naphthalene, anthracene and pyrene. The key physico-chemical parameters of the studied systems (critical micelle concentration, spectral properties, solubilization parameters) were determined, analyzed and compared with conventional cationic surfactant, CTABr. For all studied PAH solubilization capacity increases with extension of alkyl chain length of PyPheOCn SAILs reaching the values comparable to CTABr for SAILs with n = 10-12. A remarkable advantage of the phenylalanine-derived SAILs PyPheOC_n and PyPheNHC_n is a possibility to cleave enzymatically ester and/or amide bonds under mild conditions, to separate polycyclic aromatic hydrocarbons in situ. A series of immobilized enzymes was tested to determine the most suitable candidates for tunable decomposition of SAILs. The decomposition pathway could be adjusted depending on the choice of the enzyme system, reaction conditions, and selection of SAILs type. The evaluated systems can provide selective cleavage of the ester and amide bond and help to choose the optimal decomposition method of SAILs for enzymatic recycling of SAILs transformation products or as a pretreatment towards biological mineralization. The concept of a possible practical application of studied systems for PAHs solubilization/separation was also discussed focusing on sustainability and a green chemistry approach.

Keywords: surface-active ionic liquids (SAILs); enzymatic decomposition; biodegradability; sustainability; solubilization; polycyclic aromatic hydrocarbons (PAHs)

1. Introduction

Ionic liquids (ILs) have been widely used in many industries [1–3] and are one of the core focuses of research over the past two decades [4,5]. ILs are proposed as more desirable than conventional volatile solvents in many physical and chemical processes, often referred as "green" solvents [6]. They can be of natural origin and be prepared by a "benign by design" approach [5,7]. Designing ILs that lead to a reduction in the losses of solvents as well as less damage to the environment is an important aspect in green chemistry [6]. Ionic liquids in general fulfil many of the 12 criteria as a green solvent related to the availability, price, recyclability, synthesis, toxicity, biodegradability, performance, stability, flammability, storage, and renewability [8]. Ionic liquids can offer a better alternative to volatile solvents, which has led to its massive use in industrial applications such as separation and purification, and as chemical catalysts, biorefinery concepts [3], extractions [1] and others [9–12]



Citation: Kapitanov, I.V.; Sudheer, S.M.; Yadav, T.; Ghosh, K.K.; Gathergood, N.; Gupta, V.K.; Karpichev, Y. Sustainable Phenylalanine-Derived SAILs for Solubilization of Polycyclic Aromatic Hydrocarbons. *Molecules* **2023**, *28*, 4185. https://doi.org/10.3390/ molecules28104185

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Article Mixed Oxime-Functionalized IL/16-s-16 Gemini Surfactants System: Physicochemical Study and Structural Transitions in the Presence of Promethazine as a Potential Chiral Pollutant

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Abstract: The increasing concern about chiral pharmaceutical pollutants is connected to environmental contamination causing both chronic and acute harmful effects on living organisms. The design and application of sustainable surfactants in the remediation of polluted sites require knowledge of partitioning between surfactants and potential pollutants. The interfacial and thermodynamic properties of two gemini surfactants, namely, alkanediyi- α , ω -bis(dimethylhexadecyl ammonium bromide) (16-s-16, where s = 10, 12), were studied in the presence of the inherently biodegradable oximefunctionalized ionic liquid (IL) 4-((hydroxyimino)methyl)-1-(2-(octylamino)-2-oxoethyl)pyridin-1ium bromide (4-PyC8) in an aqueous solution using surface tension, conductivity, fluorescence, FTIR and ¹H NMR spectroscopic techniques. The conductivity, surface tension and fluorescence measurements indicated that the presence of the IL 4-PyC8 resulted in decreasing CMC and facilitated the aggregation process. The various thermodynamic parameters, interfacial properties, aggregation number and Stern-Volmer constant were also evaluated. The IL 4-PyC8-gemini interactions were studied using DLS, FTIR and NMR spectroscopic techniques. The hydrodynamic diameter of the gemini aggregates in the presence of promethazine (PMZ) as a potential chiral pollutant and the IL 4-PyC8 underwent a transition when the drug was added, from large aggregates (270 nm) to small micelles, which supported the gemini:IL 4-PyC8:promethazine interaction. The structural transitions in the presence of promethazine may be used for designing systems that are responsive to changes in size and shape of the aggregates as an analytical signal for selective detection and binding pollutants.

Keywords: mixed surfactant system; ionic liquid; gemini surfactants; chiral pollutants; promethazine; dynamic light scattering

1. Introduction

The increasing concern about chiral pharmaceutical pollutants is connected to environmental contamination causing both chronic and acute harmful effects on living organisms. It is a problem of direct importance to detect chiral compounds [1], including chiral pollutants of different natures [2]. Using surfactants for increasing analytical signals and, consequently, reducing the detection concentration of the pollutants is one of the attractive strategies in chemical analysis [3,4] since it may ensure selective binding of one of the components, providing more reliable detection in the cases when the structurally similar compounds are present in the mixture. For example, dimeric (gemini) surfactants were reported to exhibit selectivity toward the binding of calixarenes modified with different



Citation: Pandya, S.J.; Kapitanov, I.V.; Banjare, M.K.; Behera, K.; Borovkov, V.; Ghosh, K.K.; Karpichev, Y. Mixed Oxime-Functionalized IL/16-s-16 Gemini Surfactants System: Physicochemical Study and Structural Transitions in the Presence of Promethazine as a Potential Chiral Pollutant. *Chemosensors* **2022**, *10*, 46. https://doi.org/10.3390/ chemosensors10020046

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Science of the Total Environment

journal homepage: www.elsevier.com/locate/scitotenv

Chemical fractionation of particulate-bound metal(loid)s to evaluate their bioavailability, sources and associated cancer risk in India



Archi Mishra^a, Shamsh Pervez^{a,*}, Madhuri Verma^a, Carla Candeias^b, Yasmeen Fatima Pervez^c, Princy Dugga^a, Sushant Ranjan Verma^a, Indrapal Karbhal^a, Kallol K. Ghosh^a, Manas Kanti Deb^a, Manmohan L. Satnami^a, Kamlesh Shrivas^a, Aishwaryashri Tamrakar^a

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^c Government Dr. Waman Wasudev Patankar Girls PG College, Durg, Chhattisgarh, India

HIGHLIGHTS

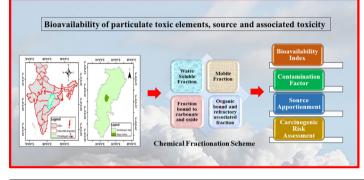
GRAPHICAL ABSTRACT

- Chemical fractionation of 11 metal(loid)s in Indian ambient fine and coarse particulates
 PM_{2.5} metal(loid)s bioavailable fractions
- $^{\circ}$ PM_{2.5} metal(fold)s bloavallable fractions are 2.4-fold higher than those for coarse mode.
- Mn has shown highest bioavailable fraction in both fine and coarse particulate mode.
- Source apportionment of fine and coarse particulate metal(loid)s bioavailable fractions
- Bioavailable index, contamination factors and Carcinogenic risks were estimated.

ARTICLE INFO

Editor: Philip K. Kopke

Keywords: Chemical fractionation Bioavailable fraction Source apportionment Cancer risk Health risk index Source markers



ABSTRACT

Eleven potentially toxic metal(loid)s (Al, As, Cd, Co, Cr, Cu, Fe, Mn, Ni, Pb, and Zn), proven source markers of mineral based coal-fired industrial emissions and vehicular exhausts, were analysed using the four steps sequential extraction method to evaluate metal(loid)s concentration, in total and fractions of bioavailable and non-bioavailable for fine (PM_{2.5}) and coarse (PM_{10-2.5}) particulate modes. A total of 26-day-wise samples with three replications (total number of samples = 78) were collected in January–December 2019 for each PM₁₀ and PM_{2.5} at an urban-residential site in India. In both the coarse and fine particulate modes, Pb and Cr have respectively shown the highest and lowest total concentrations of the measured metal(loid)s, indicating the presence of coal-fired power plants and heavy vehicular activities near to study area. In addition, Mn has shown highest bioavailable fraction for both coarse and fine particulate modes. More than 50 % of metal(loid)s concentration, in total to a bioavailable fraction (BAF) were observed in case of As, Cd, Cr, Co, Mn, Ni, and Pb of PM_{2.5}. Mn and Zn have shown similar behaviour in the case of coarse particulate mode. Source apportionment of metal(loid)s bioavailable fractions using positive matrix factorization (PMF 5.0) has found three significant sources: crustal and natural dust (30.04 and 39 %), road traffic (49.57 and 20 %), and industrial emission (20.39 and 41 %) for coarse and fine particulate mode, respectively. Cancer risk through the inhalation pathway was high in total concentration but lower in BAF concentration in both age groups (children and adults).

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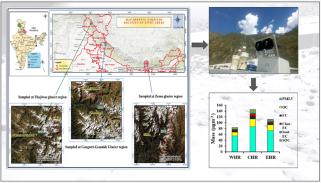
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Atmospheric Abundance of PM_{2.5} Carbonaceous Matter and Their Potential Sources at Three High-Altitude Glacier Sites over the Indian Himalayan Range

Sushant Ranjan Verma, Shamsh Pervez,* Papiya Mandal, Judith C. Chow, John G. Watson, Syed Muzaffarali Andrabi, Madhuri Verma, Princy Dugga, Noor Afshan Khan, Yasmeen Fatima Pervez, Archi Mishra, Manas Kanti Deb, Indrapal Karbhal, Suresh Tiwari, Kallol K. Ghosh, Kamlesh Shrivas, and Manmohan Lal Satnami



ABSTRACT: This study inspects the concentrations of fine particulate matter ($PM_{2.5}$) mass and carbonaceous species, including organic carbon (OC) and elemental carbon (EC), as well as their thermal fractions in the Indian Himalayan glacier region at the western Himalayan region (WHR; Thajiwas glacier, 2799 m asl), central Himalayan region (CHR; Gomukh glacier, 3415 m asl), and eastern Himalayan region (EHR; Zemu glacier, 2700 m asl) sites, throughout the summer and winter periods of 2019–2020. Ambient $PM_{2.5}$ samples were collected on quartz fiber filters using a low-volume sampler, followed by carbon (OC and EC) quantification using the IMPROVE_A thermal/optical reflectance methodology. Different seasonal variations in $PM_{2.5}$ and carbonaceous species levels were found at all three sites



investigated. Averaged PM_{2.5} mass ranged 55–87 μ g m⁻³ with a mean of 55.45 ± 16.30 μ g m⁻³ at WHR, 86.80 ± 35.73 μ g m⁻³ at CHR, and 72.61 ± 24.45 μ g m⁻³ at EHR. Among the eight carbon fractions, high-temperature OC4 (evolved at 580 °C in the helium atmosphere) was the most prevalent carbon fraction, followed by low-temperature OC2 (280 °C) and EC1 (580 °C at 2% oxygen and 98% helium). Char-EC representing incomplete combustion contributed to 56, 67, and 53% of total EC, whereas soot-EC contributed to 38, 26, and 43% of total EC in WHR, CHR, and EHR, respectively. The measured OC/EC ratios imply the presence of secondary organic carbon, whereas char-EC/soot-EC ratios suggested that biomass burning could be the predominant source of carbon at CHR, whereas coal combustion and vehicular emission might be dominant sources at WHR and EHR sites. KEYWORDS: *PM*_{2.5} *Himalayan glacier aerosol, carbonaceous matters, char-EC and soot-EC, secondary organic aerosol, biomass burning*

1. INTRODUCTION

Carbonaceous aerosols, including organic and elemental carbon, are important components of suspended particulate matter (PM), especially in the respirable fraction with aerodynamic diameters less than 2.5 μ m(PM_{2.5}).¹ These carbonaceous aerosols work as climate forcing² agents and contribute to glacier retreat via interactions with solar radiation in the atmosphere.^{3,4} The Himalayan glacier contains the most extensive glacial area outside the polar regions and is also known as the "Third pole".⁵ Severe glacier retreat in the Himalayan region has the potential to disrupt water availability to billions of residents living in the Indo-Gangetic plain.^{5–11} Because of lower population density and minimal industrial activities, the Himalayan region is considered to be one of the most pristine region, alongside the Arctic and Antarctic.

However, the emergence of atmospheric brown clouds (ABCs) over south Asia raised environmental concerns.^{12–14}

Numerous studies have suggested that long-range transport of pollutants from the Indo-Gangetic plain to the Himalayan region during premonsoon is the vital factor.^{15,16} In addition, local sources from low lands of the Himalayan region also contribute to air pollution.¹⁷ Most of studies were conducted in the foothills^{18–20} rather than high altitudes of the Himalayan region.^{21–23} This study measures ambient PM_{2.5} and carbonaceous matter (OC and EC) over three subregions of Himalayan glacier locations to evaluate associated spatiotem-

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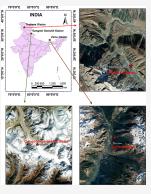
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Optical Properties of Fine Mode Aerosols over High-Altitude Himalayan Glacier Regions

Sushant Ranjan Verma, Shamsh Pervez,* Judith C. Chow, John G. Watson, Syed Muzaffarali Andrabi, Papiya Mandal, Noor Afshan Khan, Suresh Tiwari, Umesh Chandra Dumka, Rajan K. Chakrabarty, Madhuri Verma, Yasmeen Fatima Pervez, Archi Mishra, Aishwaryashri Tamrakar, Hulivahana Nagaraju Sowmya, Manas Kanti Deb, Kallol K. Ghosh, Vikas Kumar Jain, Indrapal Karbhal, Kamlesh Shrivas, and Manmohan Lal Satnami

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ABSTRACT: During the summer and winter periods of 2019–2020, we conducted sampling of fine mode ambient aerosols in the western Himalayan glacial region (WHR; Thajiwas glacier, 2799 m asl), central Himalayan glacial region (CHR; Gomukh glacier, 3415 m asl), and eastern Himalayan glacial region (EHR; Zemu glacier, 2700 m asl). We evaluated the aerosol optical properties, which included the mass absorption coefficient, mass absorption efficiency, mass scattering efficiency, absorption angstrom exponent, single scattering albedo, as well as their simple radiative forcing efficiencies. We observed the highest absorption in the near ultraviolet–visible wavelength range (200–400 nm), with CHR showing the highest absorption compared to the other two sites, WHR and EHR, respectively. Across the wavelength range of 200–1100 nm, the overall contribution of black carbon to light attenuation was greater than that of brown carbon. However, brown carbon dominated the absorption in the near UV–visible wavelengths, providing evidence of its non-trivial presence over the Himalayan region. Additionally, we observed a positive radiative forcing (W/g), which leads to net warming at these sites. The findings of this ground-based study contribute to our understanding of the light-absorbing nature of carbonaceous aerosols and their impact on the Himalayan glacier regions.



KEYWORDS: light-absorbing aerosols, carbonaceous matters, radiative forcing, Himalayan glacier, brown and black carbon

1. INTRODUCTION

The Himalayas, often called the "Third Pole" or the "Asian water tower," have witnessed excessive glacier melting in recent decades.¹ Carbonaceous aerosols of anthropogenic origin significantly contribute to glacier melting.² Aerosols deposited on the glacier surface reduce its albedo (reflectivity) and accelerate the melting process. Glacier melting has far-reaching implications, including climate change, water resource availability for downstream communities, and alterations in river flow patterns. Carbonaceous aerosols are primarily generated by natural sources like volcanic eruptions and sea spray, as well as human activities such as fossil fuel combustion and biomass burning. During the pre-monsoon period, the primary driver of carbonaceous aerosol abundance over the Himalayas is the long-range transport from the Indo-Gangetic plains.^{3,4} In addition to long-range transport, local sources such as cooking and heating activities also contribute a significant amount of carbonaceous aerosols to the nearby atmosphere.

The major components of carbonaceous aerosols include organic carbon (OC), elemental carbon (EC), sulfate, mineral dust, and nitrate. OC and EC, also known as brown carbon (BrC) and black carbon (BC), respectively, due to their lightabsorbing nature toward solar radiation, play a crucial role in climate forcing by influencing the radiative balance and cloud formation.⁵ BC is known to warm the atmosphere by absorption of solar radiation, whereas OC shows strong scattering behavior across the broad range of the solar spectrum.^{6,7} However, recent studies have observed that OC exhibits strong absorption in the near ultraviolet wavelengths of the shortwave spectrum.^{8–11} Smoldering or low-temperature combustion of biomass burning is a major source of BrC.^{8,9,12–14} Previous studies examining light absorption by OC and EC have shown that OC has lower absorption than BC in the ambient atmosphere, from the near infrared to UV–visible spectrum.¹⁵ However, OC can have mass emissions that is 3–12 times larger than that of BC, making it important to study the light absorption properties of BC and OC component wise.^{16,17}

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Environmental Research

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Using functionalized asphaltenes as effective adsorbents for the removal of chromium and lead metal ions from aqueous solution

<u>Mohammad Nahid Siddiqui</u>^a <u>∧</u> <u>∧</u>, <u>Shamsh Pervez</u>^b <u>∧</u>, <u>Indrapal Karbhal</u>^b, <u>Princy Dugga</u>^b, <u>Saravanan Rajendran</u>^c, <u>Yasmeen Fatima Pervez</u>^d

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Highlights

- Functionalized asphaltene was prepared and applied for the removal of Cr and Pb
- The maximum adsorption capacity for Cr was 833.3 mmolg⁻¹ and for Pb 22.42 mmolg⁻¹ at 4.5 pH
- Thermodynamic studies shows that the adsorption is spontaneous and endothermic.

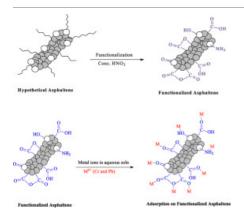
Abstract

For the first time, functionalized asphaltene has been designed, synthesized, and used for the removal of heavy metals from the water. Asphaltene was separated from the crude oil with the addition of n-alkanes. Asphaltene having a complex chemical structure including multilayered and clustered aromatic fused rings bearing aliphatic chains. Asphaltene also contains heteroatoms like N, S, and O atoms along with Ni and V as prominent trace metals. On functionalization of asphaltene with <u>nitric acid</u>, the aliphatic chains and some of the naphthenic rings broke down and developed -COOH, -C=O, C-O, and other oxygen functional groups which are playing key roles as surface-active agents in the removal of the heavy metals via <u>chemisorption</u>. The study was conducted using different parameters such as dose, time, pH, and concentration. The adsorption efficiency for this material at pH 4 is excellent for the removal of chromium and lead. The Langmuir, Freundlich and Temkin adsorption isotherm models as well as Lagergren pseudo second-order kinetic model were investigated. The positive enthalpies Δ Hs confirm that the adsorption process is endothermic and the negative free energies Δ Gs confirm the spontaneity of the process. The good efficiency of the adsorption implies the efficacy in the removal of the heavy <u>metal ions</u>, as well as

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Using functionalized asphaltenes as effective adsorbents for the removal of chromium and lead metal ions from aqueous solu... the good efficiency in desorption, which implies the excellent recovery of the adsorbent. The effective reusability of this adsorbent makes it applicable for industrial water treatment from contaminants.

Graphical abstract



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Introduction

The consumption of crude oil increased dramatically in the last decades. About 70% of the heavy crude oil residue is drilled out and a very small amount is being used without significant process (Speight, 1990).

One of the fractions that are considered as the most troublemaker is the asphaltenes in the refinery and cracking processing of the petroleum, that's due to the precipitation of the asphaltenes can reduce the flow of the oil and also can lead to blockage problems in several types of equipment (Cimino et al., 1995). Moreover, these compounds can form sludges and can deactivate the hydro-desulfurization and hydro-cracking catalysts which lead to a reduction in conversion efficiency for the two processes (Bartholomew, 1994; Miyauchi and de Wind, 1994).

The structure of these compounds was very difficult to study due to their chemical complexity & composition, it was reported that this material is composed of poly-aromatic groups in the center connected with alicyclic and aliphatic groups along with some heteroatoms and some metal ions (Hasan et al., 1988; Shirokoff et al., 1997).

The contamination of water by heavy metal ions is a very serious issue, the source of these metals are different industries such as mining, battery, and other chemical industries. Small concentrations of these heavy metal ions can cause dangerous diseases such as anaemia, cancer, renal and kidney failure, mental retardation, and other serious diseases (Nordberg et al., 2014).

These metal ions are non-biodegradable that's why they need to be removed from the water. There are many methods available for the removal of these materials such as hydroxide or sulfide precipitation, ion exchange, flocculation, membrane separation, and adsorption. Among these methods, adsorption is one of the most promising and effective methods due to its eco-friendly, simple, cost-effectiveness, and applicability for the industry.

Many sorbents are used for the removal of these heavy metals such as activated carbon (Rao et al., 2007), fly ash (Ayala et al., 1998), peat (Ho and McKay, 1999), recycled alum sludge (Chu, 1999), peanut hulls (Brown et al., 2000), resins (Diniz et al., 2002), kaolinite (Arias et al., 2002), zeolite (Biškup and Subotić, 2005), biomaterials, carbon nanomaterial (Ekmekyapar et al., 2006; Li et al., 2004), and multi-walled carbon nanomaterial (Rao et al., 2007) Graphene Oxide (Sahoo and Hota, 2019). But there are several drawbacks for metal oxides due to their poor stability and corrosion. On the other hand, carbon-based materials such as graphene oxide (GO), carbon nanotubes (CNTs), and different forms of carbon have been widely used due to their high surface area, stability, and reusability. Moreover, recently the functionalization of carbon-based materials has attracted great attention due to their strong

5/27/24, 2:21 PM Using functionalized asphaltenes as effective adsorbents for the removal of chromium and lead metal ions from aqueous solu... affinity towards metal ions (Shaikh et al., 2021, Siddiqui, 2017, Siddiqui et al., 2020, Siddiqui et al., 2021, Suliman et al., 2020). Functionalization of carbon-based material can generate high surface active sites such as –OH, –COOH, –C ==O, -C-O, –NH₂, and -S- etc resulting in enhanced hydrophilicity and wettability as well as they play key roles for strong interaction with metal ions by complexation, hard-hard or borderline hard and soft interaction. Although, GO and CNTs have been widely used as an adsorbent but due to their limitations and cost-effectiveness, it is needed to develop low cost, reusable and environmentally friendly materials.

Looking to the current scenario, in this work the asphaltenes have been isolated and functionalized as adsorbents for the removal of water pollutants such as some types of heavy metals ions (Cr and Pb). Hexavalent chromium and lead are known to be mutagenic and carcinogenic in nature (IARC 2012). WHO water quality standards recommend permissible limits of hexavalent Cr (0.05 mg.L⁻¹) and Pb (0.01 mg.L⁻¹) for potable water (WHO, 2017). Many industrial effluents including textile industries, metal finishing, leather tanneries and lead acid batteries are known for higher contents of Cr(VI) and Pb(II) ions and contaminate the adjoining natural water streams and soils (Mahato et al., 2016; Singh et al., 2017). Looking in to the advantages of the functionalized asphaltene, different functional group such as –OH, COOH, –NH₂, -S- etc act as chelation centres to bind with metal ions and remove the Cr(VI) and Pb(II) from water via hard-hard or borderline hard and soft interaction (Ravikumar et al., 2016). In cases of most of the environmental samples, Cr(VI) and Pb(II) are found in ionic forms and asphaltene has different functional groups which can bind either with coordinated bond due to presence of lone pair of electron on O, N and C or ion exchange mechanism takes place at certain pH (Xiao and Lin, 2020).

There are several advantages to use functionalized asphaltene such as reusability, low cost, durability, and the presence of surface-active functional groups such as -COOH, -OH, -C=O, -C-O, $-NH_2$, and -S- etc show more promising behaviour to adsorb metal ions. Heavy metal ions could interact with the hydrophilic functional group through H-bonding or complexation and electrostatic interaction and can adsorb more metal ions than non-functionalized (Coughlin and Ezra, 1968; McKay et al., 1985; Yang and Xing, 2010). As functionalized asphaltene is metal-free and has high surface-active agents influencing the adsorption performance and can open the new window to develop sustainable material from the waste.

Section snippets

Asphaltenes separation

About 7.0g of Arabian heavy residue was transferred to a beaker and heated with a very small amount of n-heptane. The solution was mixed properly and transferred to 2L container, then to this solution 700ml of n-heptane was added. The solution was placed in a mechanical shaker with a water bath. To increase the residue solubility in the heptane, it was heated at 90 °C for 2h with continuous stirring. Then the solution was covered using aluminium foil and was stand for cooling overnight. The ...

Functionalized asphaltenes characterization

The functionalized asphaltenes were characterized using different techniques: SEM, FT-IR, Elemental analysis, and EDX.

Fig. 1 represents the IR spectra of AH asphaltene and functionalized asphaltene. The presence of a broad peak at 3450 cm^{-1} is due to the –OH stretching frequency in both samples. After functionalization, the peak appeared at 1720 cm^{-1} , which confirms the presence of the carbonyl (C=O) group compared to the non-functionalized. Moreover, there are other peaks such as at 2925 cm^{-1} ...

Adsorbent regeneration and reuse

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The regeneration and the reusability of the adsorbent were investigated for the two contaminants (Table 5, Table 6(b)), two solutions were used for the regenerate 0.4g of the adsorbent was placed in 30ml of 0.1M sulfuric acid solution and 0.1M hydrochloric acid and the desorption time was from 10min to 24h, as we can see in the table below the Pb ions were almost removed from the adsorbent in hydrochloric solution but it didn't desorb from the adsorbent in sulfuric acid solution, the Cr ions ...

Conclusion

A novel adsorbent from the functionalization of asphaltenes was prepared to form low-cost material with very good yield. The adsorbent was found to have a good removal efficiency for Cr and Pb ions due to the development of functional groups such as -C=0, -COOH, -C-O, and others. These functional groups are responsible for the ion exchange and complexation with the metals. The adsorption process obeyed Langmuir, Freundlich and Temkin isotherm models and, also fitted Lagergren pseudo second-order ...

Author contributions

Mohammad Nahid Siddiqui: Conceptualization, Funding acquisition, Writing – original draft preparation, Supervision. Shamsh Pervez: Conceptualization, Writing – original draft preparation, Supervision. Indrapal Karbhal: Writing – review & editing. Princy Dugga: Writing – review & editing, Saravanan Rajendran: Writing – review & editing. Yasmeen Fatima Pervez: Writing – review & editing....

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper....

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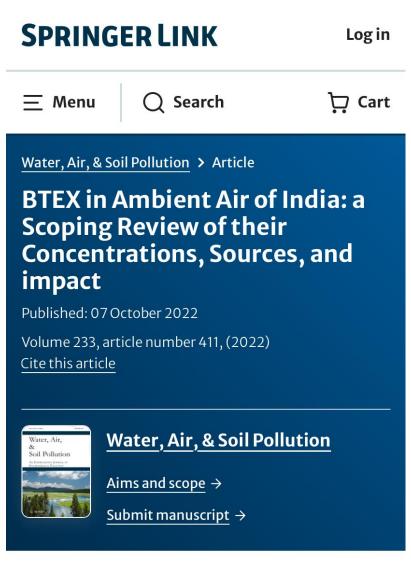
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Chemical fractionation of particulate-bound metal(loid)s to evaluate their bioavailability, sources and associated cancer risk in India

Archi Mishra^a, <u>Shamsh Pervez</u>^a <u>S</u> <u>M</u>, <u>Madhuri Verma^a, <u>Carla Candeias</u>^b, <u>Yasmeen Fatima Pervez</u>^c, <u>Princy Dugga^a,</u> <u>Sushant Ranjan Verma^a, Indrapal Karbhal^a,</u> <u>Kallol K. Ghosh^a, Manas Kanti Deb^a,</u> <u>Manmohan L. Satnami^a, Kamlesh Shrivas^a,</u> <u>Aishwaryashri Tamrakar^a</u></u>

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"Efficiency Enhancement Of Solar Module via MPPT Technology"



A Dissertation Submitted in Partial Fulfilment of the requirements For the degree of

MASTER OF TECHNOLOGY

in

Optoelectronics and Laser Technology Submitted by

ASHISH PATEL

(2110196001)

Under the Guidance of

Supervisor

Mr. Viral Raulji

EPC Head

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Vadodara, Gujrat

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Work carried out at



Mecpower Solutions Limited

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June 2023



Date: 06th May 2023

TO WHOMSOEVER IT MAY CONCERN

This is to certify that **Mr. Ashish Patel**, 2nd year M.Tech. Student of Optoelectronics and Laser Technology at Pt. Ravishankar Shukla university, Raipur Chhattisgarh has undergone project training for his thesis work on "Efficiency Enhancement of Solar Module via MPPT Technology."

During his project work at Mecpower, he has worked hard with sincerity. I wish him a successful and bright career ahead.

For, Mecpower Solutions Limited.



Mr. Viral Raulji

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Chhattisgarh

CERTIFICATE

This is to certify that the dissertation work entitled, "Efficiency Enhancement of Solar Module via MPPT Technology" submitted by Ashish Patel is a credible work carried by him at MECPOWER SOLUTIONS LIMITED, Vadodara during the period July 2022 to May 2023. The work has been presented in a manner suitable to affirm acceptance towards in the partial fulfilment of the requirement for the degree of Master of Technology in Optoelectronics and Laser Technology, Pt. Ravishankar Shukla University, Raipur, Chhattisgarh.

INTERNAL SUPERVISOR Dr. Kavita Thakur Professor & Course Coordinator

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Chhattisgarh

Dissertation Approval For M.Tech

Session 2022-23

This dissertation work entitled, "Efficiency Enhancement of Solar Module via MPPT Technology" submitted by Ashish Patel at MECPOWER SOLUTIONS LIMITED, Vadodara, Gujrat during the period July 2022 to May, 2023 is Approved for the degree of Master of Technology (IVth Semester) in Optoelectronics and Laser Technology, Pt. Ravishankar Shukla University, Raipur, Chhattisgarh

EXTERNAL EXAMINER

Di. Sesha Vempati Assistant Professor Department of Physics Date: The of remology Bbilai G.L.C. Campus, Sejbahar, Differ - 494,015, CrG., India

INTERNAL OF EXAMINER

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DECLARATION

I hereby declare that the dissertation entitled "Efficiency Enhancement Of Solar Module via MPPT Technology" submitted to the School of Studies in Electronics & Photonics, Pt. Ravishankar Shukla University, Raipur, Chhattisgarh for the degree of Master of Technology in Optoelectronics & Laser Technology is an original record of work done by me at MECPOWER Solutions Limited, Vadodara under the guidance of Mr. Viral Raulji, EPC Head, MECPOWER Solutions Limited, Vadodara. I also declare that I have adhered to all principles of academic honesty and integrity.

I further declare that to the best of my knowledge my dissertation does not contain any part of any work which has been submitted for the award of any degree either in this institute or in any other university without proper citation.

Ashish Patel (Roll No: 2110196001) Enrollment No: AG/00431 M.Tech (OELT), IVth Semester

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I would like to express my deep sense of gratitude to my project Supervisor Mr. Viral Raulji, EPC Head at MECPOWER Solutions Limited, Vadodara, Gujrat, who has been guided with the necessary expertise and encouragement throughout. I am extremely exhilarated to have completed this report under his able and inspiring guidance.

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I am immensely indebted and greatly obliged to Mr. Madhu Allalla, Mr. Mohnish Sahu, and, Mr. K. Anil Kumar Guest Lecturer, PRSU, Raipur for their motivation, guidance, advice, and constructive criticisms.

I would also wish to express my sincere thanks to my friends and seniors, who helped me during this work, and extend my gratitude to MECPOWER Solutions Limited.

I extend my gratitude to my friends and batchmates Nilesh, Lokesh, Dibyanchal, Harsh, and all the colleagues of PRSU in all regards and you all have made this journey beautiful and memorable.

Last but not least, I express my thanks to my **parents** for providing me congenial atmosphere during the period of the project report.

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ASHISH PATEL

"Facile preparation of high-performance antifouling PVDF/PEI/ SnO₂ mixed matrix membranes for effective antibiotic removal"



A Dissertation Submitted in Partial Fulfillment for the degree of MASTER OF TECHNOLOGY

In

Optoelectronics and Laser Technology

Submitted by

Mr. Lokesh Kumar Sahu

(2110196004)

Under the guidance of

Supervisor

Prof. Shobha Shukla

Professor, Department of Metallurgical Engineering and Material Science, Indian Institute of Technology, Bombay, M.H. Co-Supervisor

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June 2023



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Place - Mumbai Date 10/cc/2

18/5/2023

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Signature of Supervisor Prof. Shobha Shukla Professor, IIT Bombay



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This is to certify that the dissertation work entitled, "Facile preparation of highperformance antifouling PVDF/PEI/ SnO₂ mixed matrix membranes for effective antibiotic removal" submitted by Lokesh Kumar Sahu is a credible work carried by him at Nanomaterial Engineering and Modeling (NEMO) Laboratory, Department of Metallurgical Engineering and Material Science, Indian Institute of Technology Bombay during the period July, 2022 to June, 2023. The work has been presented in a manner suitable to affirm acceptance towards in the partial fulfilment of the requirement for the degree of Master of Technology in Optoelectronics and Laser Technology, Pt. Ravishankar Shukla University, Raipur, Chhattisgarh.

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Dissertation Approval For M.Tech

Session 2022-23

This dissertation work entitled, "Facile preparation of high-performance antifouling PVDF/PEI/ SnO₂ mixed matrix membranes for effective antibiotic removal"submitted by Lokesh Kumar Sahu at Nanomaterial Engineering and Modeling (NEMO) Laboratory, Department of Metallurgical Engineering and Material Science, Indian Institute of Technology Bombay during the period July 2022 to June, 2023 is Approved for the degree of Master of Technology in Optoelectronics and Laser Technology, Pt. Ravishankar Shukla University, Raipur, Chhattisgarh

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DECLARATION

I hereby declare that the dissertation entitled "Facile preparation of high-performance antifouling PVDF/PEI/ SnO₂ mixed matrix membranes for effective antibiotic removal" submitted to the School of Studies in Electronics & Photonics, Pt. Ravishankar Shukla University, Raipur, Chhattisgarh for the degree of Master of Technology in Optoelectronics & Laser Technology is an original record of work done by me at Nanomaterial Engineering and Modeling (NEMO) Laboratory, Department of Metallurgical Engineering and Material Science, Indian Institute of Technology, Bombay under the guidance of Prof. Shobha Shukla Professor Indian Institute of Technology, Bombay. I further declare that I have adhered to all principles of academic honesty and integrity.

I also declare that to the best of my knowledge my dissertation does not contain any part of any work which has been submitted for the award of any degree either in this institute or in any other university without proper citation.

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ACKNOWLEDGMENT

I would like to express my deep sense of gratitude to my project supervisor **Prof. Shobha Shukla**, Professor at MEMS Department, IIT Bombay for her encouragement, guidance, motivation for providing me with all the required facilities for my project work. I feel proud to have the opportunity to work with such exceptionally experienced professors. Her insightful comments and valuable suggestions have contributed significantly to my work and improved my understanding of the subject matter. Without her encouragement and guidance this project would not have materialized. I am extremely exhilarated to have completed this report under her able and inspiring guidance.

I sincerely wish to express my gratefulness to **Prof. Kavita Thakur** (Professor, SoS in Electronics and Photonics, PRSU, Raipur) for her suggestions, help, coordination and support for giving me her precious time to improve the quality of this project work.

I would also express my sincere thanks to Mr. Dharmveer Yadav, Ms. Triparna Chakraborty, Dr. Chandan Kumar, Dr. Arun Jaiswal, Dr. Rahul Das, Mr. Abhishek Pandey, Mr. Ajinkya Palwe and all the member of NEMO lab for their valuable recommendations, remarkable support, and assistance in carrying out many experimental projects.

I would also wish to express my sincere thanks to faculty of my department, Mr. Naman Shukla, Miss. Sweta Minj, Mr. Mohnish Sahu, Mr. K. Anil, Mr. Madhu Allalla and all my colleagues & friends, who helped me during this work, I also extend my gratitude to the lab coordinators and all technical-non-technical staff of the department for their support. Last but not least, I express my thanks to my parents for providing me congenial atmosphere for me to work on project report.

Lokesh Kumar Sahu

"Design, Optimization and Experimental Investigation of Eco-Friendly Double Perovskite Solar Cell"



A Dissertation Submitted in Partial Fulfillment of the requirements For the degree of MASTER OF TECHNOLOGY

in

Optoelectronics and Laser Technology Submitted by Nilesh Jaiswal (2110196005)

Under the Guidance of

Supervisor Dr. Saurabh Kumar Pandey Associate Professor & Course Coordinator Electrical Engineering Department Indian Institute of Technology, Patna Bihar Co-Supervisor **Dr. Kavita Thakur** Professor & Course Coordinator

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Signature of Sup

Dr. Saurabh K. Pandey Assistant Professor Dr Indian Institute of Technology Patna, Bihar 99 Patna, Bihar 99 Binta, Patna-801 103

Date: 21/04/23 Place: Patron



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CERTIFICATE

This is to certify that the dissertation work entitled, "Design, Optimization and Experimental Investigation of Eco-friendly Double Perovskite Solar Cell" submitted by Nilesh Jaiswal is a credible work carried by him at Sensor & Optoelectronics Research Group, Indian Institute of Technology Patna during the period 13 July 2022 to 10 May 2023. The work has been presented in a manner suitable to affirm acceptance towards the partial fulfillment of the requirement for the degree of Master of Technology in Optoelectronics and Laser Technology, Pt. Ravishankar Shukla University, Raipur, Chhattisgarh.

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Dissertation Approval For M.Tech.

Session 2022-23

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I hereby declare that the dissertation entitled "Design and Performance Optimization of Eco-friendly Double Perovskite Solar Cell" submitted to the School of Studies in Electronics & Photonics, Pt. Ravishankar Shukla University, Raipur, Chhattisgarh for the degree of Master of Technology in Optoelectronics & Laser Technology is an original record of work done by me at Sensor and Optoelectronics Research Group (SORG) Lab, Electrical Engineering Department, Indian Institute of Technology Patna, under the guidance of Dr. Saurabh Kumar Pandey, Associate Professor & M.Tech. Coordinator (VLSI & ES).

I certify that:

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- The work contained in this thesis is original and has been done by me under the guidance of my supervisor.
- The work has not been submitted to any other university/institute for any degree or diploma.
- I have followed the guidelines provided by the university in preparing the thesis.
- I have conformed to the norms and guidelines given in the Ethical Code of Conduct of the university.
- Whenever I have used materials (data, theory, and text) from other sources, I have given due credit to them by citing them in the text of the thesis and giving their details in the reference section.

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ACKNOWLEDGMENT

It has been a great privilege to be an M.Tech. student in the School of Studies Electronics and Photonics, at Pt. Ravishankar Shukla University Raipur. It provides many opportunities for me to learn from courses, books, and people around me. This thesis is a result of two years of work from many persons who have accompanied and supported me. In light of this, I would want to express my heartiest respect and appreciation to them.

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I would also express my sincere thanks to Dr. Kavita Thakur, Head of Department, S.O.S. in Electronics & Photonics PRSU, Raipur, Chhattisgarh, for her support. I am immensely indebted and greatly obliged to Mr. Madhu Allalla, Mr. Mohnish Sahu, and, Mr. K. Anil Kumar, PRSU, Raipur for their motivation, guidance, advice, and constructive criticisms.

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I extend my gratitude to my friends and batchmates Ashish, Lokesh, Dibyanchal, Harsh, and all the colleagues of PRSU in all regards and you all have made this journey beautiful and memorable.

Most importantly, I express my deepest gratitude to my family specially my parents Madhu Jaiswal and Satya Prakash Jaiswal, and brother Nikhil Jaiswal in my life for their endless love, support, and encouragement, this aided me in developing the mental and emotional person I am today.

Last but not least, I want to thank God for providing me with the strength to complete my research assignment.

Nilesh Jaiswal

"Photo performance characteristics of Tradescantia pallida for dye sensitized solar cell"



A Dissertation Submitted in Partial Fulfilment of the requirements For the degree of MASTER OF TECHNOLOGY

in

Optoelectronics and Laser Technology Submitted by Tithi Karmakar (2110196007)

Under the Guidance of

Supervisor Dr. Tejashree Bhave Associate professor

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Department of Applied Physics Government of India



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Signature of Supervisor Dr. Tejashree Bhave Associate Professor DIAT Girinagar Pune

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Dissertation Approval For M.Tech

Session 2022-23

This Thesis work entitled, "Photo performance characteristics of Tradescantia pallida for dye sensitized solar cell" submitted by Tithi Karmakar at DEFENCE INSTITUTE OF ADVANCED TECHNOLOGY, PUNE during the period January 2023 to June 2023, is Approved for the degree of Master of Technology (IVth Semester) in Optoelectronics and Laser Technology, Pt. Ravishankar Shukla University, Raipur, Chhattisgarh.

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I hereby declare that the Thesis entitled "Photo performance characteristics of Tradescantia pallida for dye sensitized solar cell" submitted to the School of Studies in Electronics & Photonics, Pt. Ravishankar Shukla University, Raipur, Chhattisgarh for the degree of Master of Technology in Optoelectronics & Laser Technology is an original record of work done by me at Defence Institute of Advanced Technology, Pune, under the guidance of Dr. Tejashree Bhave, Associate Professor. I also declare that I have adhered to all principles of academic honesty and integrity.

I further declare that to the best of my knowledge my dissertation does not contain any part of any work which has been submitted for the award of any degree either in this institute or in any other university without proper citation.

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ACKNOWLEDGMENT

I would like to express my deep sense of gratitude to my project Supervisor **Dr. Tejashree Bhave Associate Professor Defence Institute of Advanced Technology Girinagar Pune,** who has been more guided with the necessary expertise and encouragement throughout. I am extremely exhilarated to have completed this report under his able and inspiring guidance.

I would also express my sincere thanks to **Dr. Kavita thakur**, **Professor & Head of Department, School of Studies in Electronics and Photonics Pt. Ravishankar Shukla University, Raipur** (C.G.) for his encouragement and valuable discussions in successfully completing myproject work.

I am also obliged to Mr. Mohnish Kumar Sahu, Assistant professor (Guest), Mr.

K. Anil Kumar, Assistant professor (Guest) and Madhu Allalla, Assistant professor (Guest). SOS in Electronics and Photonics, PRSU Raipur (C.G.). for their motivation, course lectures, guidance advice and constructive criticisms.

I would also wish to express my sincere thanks to **My Friends and Co- guide Kalyanee Patil, Akshaya Pisal Deshmukh, Rucha, Kavita, Haritha** who helped me duringthis work. Last but not least, I express mythanks to **My parents** for providing me congenial atmosphere during theperiod of project report.

TITHI KARMAKAR

"LASER-ASSISTED PHOTOACOUSTIC WAVE GENERATION FOR UNDER-WATER COMMUNICATION APPLICATION"



A Dissertation Submitted in Partial Fulfilment of the requirement for the degree of

MASTER OF TECHNOLOGY

in

Optoelectronics and Laser Technology

Submitted by

Vaishali Soni

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Under the Guidance of

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Date 25/03/2023 Place Pune



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Dissertation Approval For M.Tech.

This dissertation work entitled, "Laser-Assisted Photoacoustic Wave Generation for Under-Water Communication Application" submitted by Vaishali Soni, is a credible work carried by her at Advance Laser Laboratory, Department of Applied Physics, Defence Institute of Advanced Technology (DIAT), Pune during the period January 2023 to June 2023. The work has been presented in a manner suitable to affirm acceptance towards the partial fulfilment of the requirement for the degree of Master of Technology in Optoelectronics and Laser Technology, Pt. Ravishankar Shukla University, Raipur, Chhattisgarh.

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DECLARATION

I hereby declare that the dissertation entitled "Laser-Assisted Photoacoustic Wave Generation For Under-Water Communication Application" submitted to the School of Studies in Electronics & Photonics, Pt. Ravishankar Shukla University, Raipur, Chhattisgarh, for the degree of Master of Technology in Optoelectronics & Laser Technology is an original record of work done by me at Advance Laser Laboratory, Department Applied Physics, Defence Institute of Advanced Technology (DIAT), Pune under the supervision of Dr. Devnath Dhirhe, Associate Professor, Department of Applied Physics, I also declare that I have adhered to all principles of academic honesty and integrity.

I further declare that to the best of my knowledge, my dissertation does not contain any part of any work which has been submitted for the award of any degree either in this institute or in any other university without proper citation.

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Vaishali Soni

(Roll. No.: 2110196008) Enrolment No: AE/00644 M.tech. (OELT), IVth Semester

Date: 31/05/2023

DECLARATION FOR PLAIGARISM CHECK

This is to certify the M.Tech thesis titled "Laser-Assisted Photoacoustic Wave Generation For Under-Water Communication Application," submitted by Vaishali Soni under the supervision of Dr. Devnath Dhirhe, Associate Professor, Department Applied Physics, Defence Institute of Advanced Technology (DIAT), Pune, is original research carried out by the candidate.

We have read the provision of DIAT (DU) plagiarism policy, and it is to certify that all the conditions prescribed in the aforesaid policy are complete with respect to above mentioned M.Tech. Thesis.

The thesis has been checked for plagiarism, and a report has been submitted for further processing.

We are aware that any issue related to plagiarism in the future will have to be addressed by the candidate and the supervisor concerned.

Vaishali Soni

Signature:

Date:

Dr. Devnath Dhirhe

Signature:

Date:

ACKNOWLEDGMENT

I would like to deeply express my sense of gratitude to my project supervisor Dr. Devnath Dhirhe, Department of Applied Physics, DIAT, Pune, for his encouragement, guidance, and motivation and for providing me with all the required facilities for my project work. I am proud to record that I had the opportunity to work with an exceptionally experienced professor like him. His comments and suggestions have contributed a lot to my work and improved my understanding of the matter. Without his words of encouragement and guidance, this project would not have materialized. I am extremely exhilarated to have completed this report under his able and inspiring guidance.

I sincerely wish to express my gratefulness to Dr. Kavita Thakur (Professor, SoS in Electronics and Photonics, PRSU, Raipur) for her suggestions, help, coordination, and support for giving me her precious time to improve the quality of this project work.

I would also like to express my sincere thanks to Mr. Sahil Saini (SRF) and Mr. Pankaj Bhujbal (SRF) for their valuable suggestions, ever-encouraging words, and motivation for work. I would also like to thank Miss Madhurima for her important recommendations, remarkable support, and aid in carrying out many experimental projects. I would also like to express my gratitude to all my lab mates for their assistance whenever I needed it.

Vaishali Soni

Subject Dependent and Subject Independent Analysis for Emotion Recognition Using Electroencephalogram (EEG) Signal

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Abstract. Brain signals for the human-computer interface is a research interest in recent years. The brain is the most vital part of our body. It handles and manages all types of activities of the body. Brain signals appear when neurons inside the brain send electrical impulses to communicate and elicit electrical potentials. This electrical activity can be measured by Electroencephalogram (EEG) through electrodes. EEG signals can help to recognize human emotions effectively. It is a non-invasive method to collect brain signals. In this paper, we have studied the subject-dependent and subject-independent analysis for four emotions (happy, sad, fear, and neutral) using the SEED-IV dataset of EEG signals for emotion. The raw EEG signals of the SEED-IV dataset have been preprocessed to remove unwanted signals and noise. 32 statistical features have been extracted from the preprocessed EEG signals and used as input for classifiers. Here, we achieved an average of 95.73% accuracy for 15 subjects for subject-dependent analysis for emotional classification using a cubic support vector machine (SVM). Based on cubic SVM and fine Gaussian SVM, we achieved an average classification accuracy of 78.46% and 83.7% for subject-independent analysis.

Keywords: Electroencephalogram, Support Vector Machine, Emotion

1. Introduction

Complex psychological and physiological states known as emotions can be brought on by both internal and external factors. They are subjective experiences that involve a range of cognitive, behavioral, and physiological responses [1,2]. Some common emotions are fear, anger, happiness, surprise, sadness, love, and disgust. Emotions are also categorized as positive or negative emotions, as they vary in duration and intensity. They are affected by various reasons, including genetics, culture, upbringing, personality, and experiences. Emotions play an important role in communication.

Long Short Term Memory Network based Emotion Recognition using Speech Signals

Abstract. The inherent emotion in human speech plays a key role in effective communication. Human-computer interactions are drastically increasing as more advanced technologies are growing. The state-of-the-art research field in artificial intelligence is to understand human emotion and take decisions according to the input emotions. The emotion recognition-based models can be utilized to develop some improved applications like virtual assistants, interactive video games, entertainment, etc. In the present work, we have proposed an LSTM network-based multiclass emotion detection model using the SAVEE dataset. Fusion of Mel frequency magnitude coefficients (MFMC) and the Mel frequency cepstral coefficients (MFCC) are the features. The performance of the multiclass emotion recognition model is evaluated using a 5-fold data division protocol.

Keywords: LSTM, Speech signal, MFMC, MFCC, Speech emotion recognition

1. Introduction

Speech is the regular way of communication that used to convey the information and sentiment of the speaker to the listener [1]. The inherent sentiments in the speech are plays a key role in the human communication. There are many applications reported based on human machine interaction. Speech emotion recognition (SER) is one of the prominent approaches in human machine interaction. Some emerging applications based on SER are like Smart health services, interactive video games, call center, digital assistant, lie and stress detection etc. [1]. There are various approaches available for emotion recognition like electroencephalogram (EEG), speech, facial image and gesture, text, etc. Among the various approaches, Speech based approach that means SER is the most feasible way of emotion recognition.

2. Related Works

Badshah et al. (2017) reported three convolution layer based SER technique [2]. In this method, the speech signals were converted into spectrogram of seven emotions namely neutral, fear, anger, happy, sadness, disgust and boredom of berlin data set. Two different experiments were performed using CNN. Using new CNN network prediction accuracy more than 50% were achieved for four emotion namely anger, boredom, disgust and sad. In the second experiment a pre-trained Alex Net with transfer learning approaches was utilized. CA improvement was reported using transfer learning for emotion



Arti Parganiha <arti.parganiha@gmail.com>

Your lab has been matched with the PSA Valence-Dominance Study

11 messages

Chris Chartier <cchartie@ashland.edu> To: Arti Parganiha <arti.parganiha@gmail.com> Tue, Jan 9, 2018 at 11:45 PM

Dear Arti,

You signed up to be part of the first Accelerator Data Collection Wave, and you have been selected as a data collection laboratory for this project! We are so happy to have you on board!

The most urgent next step is for all data collection labs to obtain ethics approval. Please start this process as soon as possible. Ethics approval has created the longest hold ups in the past for similar projects (such as Many Labs), so we have set the deadline for each lab's submission as 2 weeks from receiving this email. We have attached the final study proposal here if that helps you get started.

Please update your ethics approval status in this spreadsheet when you have submitted your materials, and again when you have received approval.

The lead authors for this project, Lisa de Bruine and Ben Jones (University of Glasgow), and the PSA Director, Chris Chartier (Ashland University), have submitted their materials for IRB approval, and we will share them when they are approved in the case that their materials may help you prepare yours or that their approval may expedite your own review process.

We anticipate that between 50 and 100 labs will collect data for this project. The included labs were selected based on their data collection capacity as well as geographic location, to allow for an adequate distribution over world regions. We look forward to sharing this exciting journey with you!

All the best,



Dr. Christopher R. Chartier Associate Professor, Psychology Director, Psychological Science Accelerator Ashland University cchartie@ashland.edu

Arti Parganiha <arti.parganiha@gmail.com> To: babita pande <babitatime14@gmail.com> Thu, Jan 11, 2018 at 12:39 PM

------ Forwarded message ------From: **Chris Chartier** <cchartie@ashland.edu> Date: Tue, Jan 9, 2018 at 11:45 PM Subject: Your lab has been matched with the PSA Valence-Dominance Study To: Arti Parganiha <arti.parganiha@gmail.com>

Dear Arti,

You signed up to be part of the first Accelerator Data Collection Wave, and you have been selected as a data collection laboratory for this project! We are so happy to have you on board!

PI	Institution	City	Country	Contributing Lab Members	Email Addresses	Collecting data in 2018?	Likely total N in 2018	Other Planned Contributions	Subject Pool Info	Primary language(s) of data collection	Specialized Equipement, Software, or Other Resources	Subfield (Social, Cognitive, Clinical, etc.)
Denis Cousineau	University of Ottawa	Ottawa	Canada		denis.cousineau@u	Yes for me;	300 yearly;	Based on	No subject	French	Computers; CRT screens	Cognitive; visual
wolf vanpaemel	KU Leuven	Leuven	Belgium	francis tuerlinckx	wolf.vanpaemel@ku	yes (in the fall)	100)	dutch	dutch		cognitive
Niklas Steffens	University of	Brisbane	Australia	together with Kim Peters	n.steffens@uq.edu.	yes	100)	University	English	We have access to labs for	Social, organisational,
Jerome Olsen	University of Vienna,	Vienna	Austria	Jerome Olsen, Martin	jerome.olsen@univi	yes	100)	Pool of	German	tenerus strudies (instrudies	Social
Olivier Klein	Université Libre de	Brussels	Belgium	Nicolas Van der Linden	nivdlind@ulb.ac.be	Yes	I can quite	Translation	First-year	French	For online studies, we use	Social and intercultural
Hause Lin	University of Toronto	Toronto	Canada	Hause Lin, Michael	hause.lin@mail.utor	yes	100)	Mix of		PsychoPy, ePrime, MediaLab,	Social, cognitive,
Daniel Ansari	University of Western	London	Canada	la li e la t	Daniel.ansari@gmai	yes	100)	University	English	E-prime, PsychoPy	Cognitive, Developmental
Lorne Campbell	University of Western	London	Canada	Lorne Campbell,	lcampb23@uwo.ca	yes	100)	Introductor		Qualtrics	
Gorka Navarrete	Universidad Adolfo	Santiago	Chile		gorkang@gmail.co	Yes			University	Spanish	PsychoPy, Limesurvey,	Social & Cognitive
Diego Forero	Universidad Antonio	Bogota	Colombia	Diego Forero, Andrés	diego.forero@uan.e	Yes	200)	University		Devel TeelDev	
William Jimenez Leal	Universidad De Los	Bogota	Colombia	William Jiménez,	w.jimenezleal@unia	yes	200	Data	120.	Spanish	8 networked computers, biopac	Thinking and reasoning,
Darko Loncaric	University of Rijeka	Rijeka	Croatia		dloncaric@uniri.hr	Yes	100	Local	Preschool,	Croatian, English	E-Prime; PsychoPy; LimeSurvey;	Developmental and
Marek Vranka	Charles University	Prague	Czech		vranka.marek@gm	yes	100)	University	Czech, English (non-native)		Social
Kaminski Gwenael	Toulouse university,	Toulouse	France		., gwenael.kaminski@	yes	200	Data analysis	University	French	E-prime, MAtlab, Qualtrics, (Eye	Social and Cognitive
Susann Fiedler	Max Planck Institute	Bonn	Germany		susann.fiedler@gm	yes			University	German	Eye-tracking, PsychoPy, z-tree,	Social Psychology,
Balazs Aczel	Eötvös Loránd	Budapest	Hungary	Marton Kovacs, Peter	 marcikovacs95@g	Yes	In lab - 200,		Undergrad	Hungarian	Qualtrics, Opensesame	Cognitive
MohammadHasan	University of Tehran	Tehran	Iran	Javad Hatami	hasan.sharifian@ut.	yes	···· // ··· 100		University	Persian		Social and Cognitive
Marco Tullio Liuzza	"Magna Graecia"	Catanzaro	Italy		liuzza@unicz.it	Yes	300)	Undergrad	Italian	PsychoPy	Social, Cognitive
Patrizio Tressoldi	Dipartimento di	Padova	Italy		patrizio.tressoldi@u	Yes	100)	<u> </u>	Italian		
David Clarance	Busara Center for	Nairobi	Kenya		david.clarance@bus	yes	~15000		Low	Swahili, English	zTree, oTree, PsychoPI,	Behavioral Economics,
Vilius Dranseika	Vilnius University	Vilnius	Lithuania	Vilius Dranseika	vilius.dranseika@fsf	Yes	100+		Lithuanian		Or an Caracteria Overheiden	Constant Delitical
Steve Janssen	University of	Kuala	Malaysia	Steve MJ Janssen	steve.janssen@notti	Yes	100)		English	E-prime, psychopy	
Humberto Nicolini,	Grupo Medico Carracci	Mexico City	Mexico	Humberto Nicolini, Nuria	nicolini_humberto@	Yes	100)	Mexican	Spanish	EEG, TMS, CANTAB, biological	Clinical, cognitive,
Joanne M. Chung	Tilburg University	Tilburg	Netherlands	H	j.m.h.chung@uvt.nl	Yes	100)	Dutch	Dutch, English	en el la constructión de la Martín el	Developmental,
Dongning Ren	Tilburg University	Tilburg	Netherlands		d.ren@uvt.nl	Yes	100)	 Dutch	Dutch, English		Social
Mark Brandt	Tilburg University	Tilburg	Netherlands		m.j.brandt@tilburgu	yes	150 for any		Includes	English/Dutch	computers/qualtrics/inquisit	social
Gerit Pfuhl	UiT The Arctic	Tromso	Norway		Gerit.pfuhl@uit.no	yes	100 in		2 year	norwegian but fluent in	access to inquisit, matlab,	cognitive, neurocognitive
Janis Zickfeld	University of Oslo	Oslo	Norway	Janis Zickfeld, Thomas	jhzickfeld@gmail.co	Yes	100)	1 year	Norwegian (fluent in English)	E-Prime, Inquisit, Presentation,	Social
Michal Parzuchowski	SWPS University of	Sopot	Poland	Bogdan Wojciszke,	mparzuchowski@s	Yes	>500 for	where	Undergrad	Polish	Inquisit, E-prime, PsychoPy,	Social/Cognitive
Samuel Lins	University of Porto	Porto	Portugal	ихт	samuel.bezerra.lins	yes	maximum		University	Portuguese		Social
Ivan Ivanchei	Russian Academy of	Moscow	Russia		ivancheyii@gmail.co	Yes	100 (00)	undergradu	Russian	E-prime, PsychoPy, Matlab, R,	Cognitive
Vanja Ković	Laboratory for	Belgrade	Serbia	Vanja Ković, Anđela	vanja.kovic@f.bg.ac	yes	100 in		University	Serbian	ERP - Neuroscan, SMI eye-	cognitive, neurocognitive
Iris Zezelj	University of Belgrade	Belgrade	Serbia	<u>Ă vi.</u>	izezelj@f.bg.ac.rs	yes	300	Based on	University	Serbian, Bosnian	Inquisit, OpenSesame, Survey	Social
Gabriel Baník	Institute of	Presov	Slovakia	Gabriel Baník, Ivan	gabriel.banik@gmai	yes	150)	undergradu	Slovak	Manline Ormanian lab with 40	Cognitive, Social,
Miguel Vadillo	Universidad	Madrid	Spain		miguel.vadillo@uam	-	100		Undergrad	Spanish	Matlab, PsychToolbox, PsychoPy	Cognitive
Zoltan Kekecs	Lund University	Lund	Sweden		zoltan.kekecs@psy.	yes	100	Methodologic	no	Swedis, but English may		clinical psychology,
Evie Vergauwe	university of Geneva	Geneva	Switzerland	Kim Uittenhove	Evie.Vergauwe@uni	Yes	maximum	Community	first year	French	e-prime, MAtlab	Cognitive, developmental
Sau-Chin Chen	Tzu-Chi University	Hualian	Taiwan		pmsp96@gmail.co	Yes	400 (50	Anywhere	University	Chinese (Written in	Opensesame, Gorilla	Cognitive
Harry Manley	Chulalongkorn	Bangkok	Thailand		harrisonmanley@g	Yes	100		(~300 1st	Thai / English	Inquisit, PsychoPy, E-Prime	Cognitive / Social
Adil Saribay	Bogazici University	Istanbul	Turkey		adil.saribay@boun.e		100		Introductor		Medialab, DirectRT, E-Prime,	v

Toro Maraball	Brunol Linivoroity	London			Toro Maraball@hrun	1400	100		Introductor	English	oBrimo Qualtrico Inquisit	Social paragraphi
Tara Marshall	Brunel University		UK		Tara.Marshall@brun	·		1. 1	Introductor	English	ePrime, Qualtrics, Inquisit	Social, personality
Gavin Sullivan	Coventry University	Coventry	UK	Chris Day, Vanessa	Ab7809@coventry.a		150 or more -	Indonesia is	University	E se l'al	Matel Device	0
Benjamin Vincent	University of Dundee	Dundee	UK		b.t.vincent@dundee		50 (joint with		University	English	Matlab, PsychoPy	Cognitive
	University of Dundee		UK		b.z.saunders@dund		50 (joint with			English		
Miroslav Sirota	University of Essex		UK		msirota@essex.ac.	yes	100		1st year	English	Qualtrics, Inquisit, (E-prime &	Cognitive/Social
Christopher R.	Ashland University	Ashland	USA	Christopher R. Chartier,	cchartie@ashland.e	yes		Project	Traditional	English	ePrime, MedliaLab, BioCapture	Social, Meta
Brady Wiggins	Brigham Young	Idaho	USA	Brady Wiggins	wigginsb@byui.edu	Yes	100 - 300	Where	Psychology	English	Qualtrics, Matlab, OpenSesame,	Clinical, Theoretical and
Dustin Calvillo	California State	San	USA	Dustin Calvillo	dcalvill@csusm.edu	Yes	~100		Undergrad	English	Computers, Eprime, qualtrics	Cognitive
Nikki Legate	Illinois Institute of	Chicago	USA	Nikki Legate	nlegate@iit.edu	Yes	In lab - 100,		Undergrad	English		
Jack Arnal	McDaniel College	Westminst	USA		Jarnal@mcdaniel.ed	yes	~100		Liberal	English	SuperLab, Qualtrics	Cognitive (but happy to
William Chopik	Michigan State	East	USA	William Chopik	chopikwi@msu.edu	Yes	200		Undergrad	English	Psychopy, Qualtrics, could easily	social, personality,
Randy McCarthy	Northern Illinois	DeKalb	USA		rmccarthy3@niu.ed	yes	200		Introductor	English		Social
Ernest Baskin	Saint Joseph's	Philadelphi	USA	Ernest Baskin	ebaskin@sju.edu	yes	100		Principles	English		
Kathleen Schmidt	Southern Illinois	Carbondale	USA		kathleenschmidt1@	Yes	200-300	Where I'm	Intro	English	ePrime, MediaLab, Qualtrics;	Social Cognitive
Justin Robert Keene	Texas Tech University	Lubbock	USA		justin.r.keene@ttu.e	Yes	200		Mass	English	ePrime, MediaLab, Biopac,	Cognitive
Heather Urry	Tufts University	Medford	USA		heather.urry@tufts.e	yes	100		undergradu	English	E-Prime, Inquisit, Qualtrics,	Affective Science
Gwen Gardiner	UC - Riverside	Riverside	USA		ggard001@ucr.edu	Yes	100		Undergrad	English		Personality
J. Protzko	University of	Santa	USA	J. Protzko	protzko@gmail.com	Yes	60 for 30-		500	English		
Daniel Storage	University of Illinois	Urbana-	USA	Daniel Storage	research@danielsto	yes	100		Undergrad			
Crystal N. Steltenpohl	University of Southern	Evansville	USA	Crystal N. Steltenpohl	cnsteltenp@usi.edu	Possibly	Hopefully 100	Where	Sona	English	Trying to get MediaLab,	Community, social
Nicholas Coles	University of	Knoxville	USA	Deanna Jordan	colesn@vols.utk.ed	Yes	250	Anywhere	Undergrad	English	E-Prime, Qualtrics, Camtasia,	Social/Affective
Mike Mensink	- University of	Menomonie	USA	Desiree Budd, Sarah	mensinkm@uwstout	Yes	100		Undergrad	English	Qualtrics, E-Prime, Biopac, SMI	Cognitive/Social
Henrik Danielsson	Linköping University	Linköping	Sweden		henrik.danielsson@l	Possiby		Methodology	Students	Swedish	· · · · · · · · · · · · · · · · · · ·	Cognitive
Cynthia Fu	University of East	London	UK		c.fu@uel.ac.uk	Possiby		and Data				
Liam Satchell	University of West	Ealing	UK		liam.satchell@uwl.a	Possibly	Perhaps 100		No subject	English	Qualtrics	Forensic (legal and
Tony Buchanan	Saint Louis University	St. Louis	USA		tbuchan7@slu.edu	Possibly			Undergrad	English	E-Prime, Qualtrics, eye tracking,	affective, neuro
Luis H. Favela	University of Central	Orlando	USA		luis.favela@ucf.edu	Possibly				English		Cognitive, perception-
Yarrow Dunham	Yale University	New Haven	USA		yarrow.dunham@yal	Possibly			Undergrad	English	Inquisit, Qualtrics	Social/Cognitive/Develop
Kai Horstmann	Humboldt-Universität	Berlin	Germany	Kai Horstmann	kaitobiashorstmann	No		Methodologic		-		Psychometrics
Anna Szabelska	Queen's University	Belfast	Northern		aszabelska01@qub.		N/A	data		English, Polish	R, Python, SPSS, Microsoft Azure	Cognition
Miguel A. Silan	University of the		Philippines		MiguelSilan@gmail.	No		Methodologic		English, Tagalog, Bisaya		Social / I/O
Hannah Moshontz	Duke University	Durham	USA	Hannah Moshontz	hmoshontz@gmail.c	No		-1	Undergrad		Qualtrics, can likely get access	Social
Melissa Kline	MIT		USA		mekline@mit.edu	No	NA				· · · · · · · · · · · · · · · · · · ·	Developmental, Cognitive
S. Mason Garrison	Vanderbilt University	Nashville	USA	S. Mason Garrison	s.mason.garrison@	No	No	Methodologic		R	R, Mplus, git, computing Cloud,	Quantitive/Differential
Pekka Santtila	NYU Shanghai	Shanghai	China		pekka.santtila@nyu.	Hopefully		-1	University	Chinese		Legal Psychology
Jan Antfolk	Åbo Akademi	Turku	Finland		jantfolk@abo.fi	Hopefully			Population-	Finnish, Swedish		Logarroyonology
Hans IJzerman	Université Grenoble	Grenoble	France		h.ijzerman@gmail.c	Yes	Unknown for		h			social
Michelangelo Vianello	A 1	Padova	Italy				100		Master	Italian	Inquisit	500101
_	-		-		michelangelo.vianell	162	100				Inquisit	
Oscar Oviedo-	Centre for Accident	Brisbane	Australia		oscar.oviedotrespal							
Ryan Perry	University of	Melbourne	Australia		ryanmalkmus@gma				Linder and M	Ca aliah	Madiatala Osciliator Inc. 1975	
Khandis Blake	University of New	Sydney	Australia		k.blake@unsw.edu.				University	English	Medialab, Qualtrics, Inquisit, Eye-	social/evolutionary
Tiago Lim	University of Fortaleza	Fortaleza	Brazil		tiago.souzalima@ho							

Jill A. Jacobson	Queen's University	Kingston	Canada		jill.jacobson@queen						
Bernard	Université du Québec	Montreal	Canada		bernard.paquito@uq	 -					
John R. Vokey	N 84					 					
Patricia Brosseau-	University of	Lethbridge Ottawa	Canada Canada		vokey@uleth.ca						
1. Second	University of Ottawa				pbrossea@uottawa.						
Ravin Alaei	University of Toronto	Toronto	Canada		ravin.alaei@mail.uto						
Julia zhao	Shanxi Normal	Shaanxi	China		18335181126@163.						
Vojtech Zika	Center for Behavioral	Prague	Czech		vojtech.zika@cebex	 					
Andero Uusberg	University of Tartu	Tartu	Estonia		andero.uusberg@ut.						
Eric Karlsson	Fakulteten för	Turku	Finland		epa.karlsson@gmail					Psytools, Soile, Eye-tracking,	Evolutionary, Forensic,
Armand Chatard	Université de Poitiers	Poitiers	France		armand.chatard@un						
Christoph Stahl	Department for	Cologne	Germany		christoph.stahl@uni-						
Benjamin Gagl	Goethe Universität	Frankfurt	Germany		gagl@psych.uni-						
Philipp Kanske	Technische	Dresden	Germany		philipp.kanske@tu-						
Johannes Lutz	Universität Potsdam	Potsdam	Germany		jlutz@uni-						
Bettina Schwörer	University of Hamburg	Hamburg	Germany		bettina.schwoerer@				English, German		Motivation and Self-
Lea Hildebrandt	University of	Wurzburg	Germany		lea.k.hildebrandt@g						
DR Abhijit Das	AMRI Institute of	Kolkata	India		abhijit.neuro@gmail.						
Michael Gilead	Ben-Gurion University	Beersheba	Israel		michael.gilead@gm						
Daniel Lakens	Eindhoven University	Eindhoven	Netherlands Ann	ne Scheel	D.Lakens@tue.nl		Methodologic		Dutch		Meta
Alan KS Nielsen	Max Planck Institute	Nijmegen	Netherlands		alan@languageevol						
Mark Verschoor	University of	Groningen	Netherlands		m.verschoor@rug.nl						
Simon Columbus	Vrije Universiteit	Amsterdam	Netherlands		simon@simoncolum						
Michael Philipp	Massey University	Palmerston	New Zealand		M.Philipp@massey.	≤ 100		university	English	Psychpy, DirectRT, Qualtrics,	
Katarzyna Jasko	Jagiellonian	Krakow	Poland		kasia.jot@gmail.co	 		aturdanta		Disease/A slumanula data /EMO	
Dmitry Lyusin	Higher School of	Moscow	Russia		ooch@mail.ru	 					
Ljiljana Lazarevic	Institute of	Belgrade	Serbia		ljiljana.lazarevic@f.	 					
Taehwan Yoon Ph.D.	ICS, Seoul National	Seoul	South Korea		thyoon93@snu.ac.k	 					
Oskar Flygare	Karolinska Institutet	Solna	Sweden		oskar.flygare@ki.se	 					
Peter Edelsbrunner	ETH Zurich	Zurich	Switzerland		peter.edelsbrunner						
Florian Brühlmann	University of Basel	Basel	Switzerland		florian.bruehlmann						
Tim Böttger	University of St. Gallen	St. Gallen	Switzerland		tim.boettger@unisg.						
Hamza Dincer	Boğaziçi University	Istanbul	Turkey		hamzamustakdincer	 -					
Sami Gulgoz	Koc University	Istanbul	Turkey		sgulgoz@ku.edu.tr	 -					
Anıl Şafak Kaçar	Koç University	Istanbul	Turkey		akacar@ku.edu.tr	 -					
İlker Dalğar	Middle East Technical	Ankara	Turkey		ilkerdalgar@gmail.c						
Vera Kempe	Abertay University	Dundee	UK		v.kempe@abertay.a						
Emily S. Cross	Bangor University	Gwynedd	UK		e.cross@bangor.ac.	 					
Ruth Horry	Swansea University	Swansea	UK		R.horry@swansea.a	 		ļ			
Stephanie Rossit	University of East	Norwich	UK		s.rossit@uea.ac.uk	 					
Zander Crook	University of Edinburgh	Edinburgh	UK		zander.crook@ed.a	 					
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	University of Edinburgh	Edinburgh				 					
Lisa DeBruine	University of Glasgow	Glasgow	UK		lisa.debruine@glasg						

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	University of Glasgow	•	UK	ben.jones@glasgow						
	University of Sheffield		UK	ek.damer@gmail.co						
	University of	Winchester		manuela.thomae@g						
	University of York		UK	cylcia.bolibaugh@yo						
	Boston College		USA	info@l3atbc.org						
Joshua Grubbs E	Bowling Green State	Bowling	USA	GrubbsJ@BGSU.ed						
Jessica Urschel	Eastern Washington	Seattle	USA	jurschel@ewu.edu						
Erica Musser F	Florida International	Miami	USA	Emusser@fiu.edu						
Sue Kraus F	Fort Lewis College	Durango	USA	Kraus_s@fortlewis.						
Katie Corker C	Grand Valley State	Allendale	USA	k.corker@gmail.co						
Brent Donnellan	Michigan State	East	USA	donnel59@msu.edu						
Christopher M.	Nicholls State	Thibodaux	USA	Christopher.castille						
Shelia Kennison C	Oklahoma State	Stillwater	USA	Shelia.kennison@ok						
Natalia Van Doren F	Penn State University	University	USA	nataliavandoren@p						
Brad Wyble F	Penn State University	University	USA	bwyble@gmail.com						
Sean Duffy F	Rutgers university -	Camden	USA	Seduffy@scarletmai						
Uma Karmarkar	ÛCSD	San Diego	USA	ukarmarkar@ucsd.e						
Patrick Forscher U	University of Arkansas	Fayetteville	USA	forscher@uark.edu						
Dan Relihan U	University of California	Irvine	USA	drelihan@uci.edu						
Jacinth Tan L	University of	San	USA	jacinthjx.tan@gmail.						
· · · · · · · · · · · · · · · · · · ·	University of Missouri	Columbia	USA	Jjwzp5@mail.misso						
Doug Markant	University of North	Charlotte	USA	dmarkant@uncc.ed						
Alexander Danvers	University of Oklahoma	Norman	USA	alexander.danvers						
	Vassar College	Poughkeep		Alclifton@vassar.ed						
	Virginia		USA	jjoygaba@vcu.edu						
	Willamette University		USA	millerj@willamette.e						
	Ghent University		Belgium	ernst.koster@ugent.						
	Carleton University		Canada	andrea.howard@car			Varies.		I am currently using smartphone	Developmental and
	University of Manitoba	Manitoba	Canada	M_Soderstrom@um			access to	English		
	University of Western	London	Canada	chahn@uwo.ca				2.19.1011		
	University of Western		Canada	etienne.lebel@gmail						
	York University		Canada	 kayflake@gmail.co		measurement				
	Hubei University		China	qlcactus16@gmail.c		Incasarement				
-	Universidad del		Colombia							
r	Deserie Demeté	•		oliver.muller@urosa						
	Ecole Normale		France	coralie.chevallier@g						
	Freie Universität Berlin		Germany	lars.schulze@fu-						
ι	Johannes Gutenberg University Medical Center	Mainz	Germany	hcp4715@gmail.com						
	University of Hamburg	Hamburg	Germany	wiebke.herrmann@						
Pamei Gairanlu J	Jawaharlal Nehru	New Dehli	India	pameigairan@gmail						
Bastiaan Rutjens	University of	Amsterdam	Netherlands	b.t.rutjens@uva.nl						
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Proposers: Benedict Jones, Lisa DeBruine, Jessica Flake

Title: Does Oosterhof and Todorov's valence-dominance model of social perception of faces generalize across world regions?

Link for demo version: http://faceresearch.org/project?PSAeng&auto

Background. Oosterhof and Todorov (2008 PNAS) found that Principal Component Analysis of trait ratings of face images made by students at a US university produced two components (faces were rated for aggressiveness, attractiveness, caringness, confidence, dominance, emotionalstability, unhappiness, intelligence, meanness, responsibility, sociability, trustworthiness, weirdness). The first component, which they labeled 'valence', was correlated with all traits except dominance and was particularly highly correlated with trustworthiness. The second component, which they labeled 'dominance', was highly correlated with rated dominance, correlated with aggressiveness and confidence, and largely unrelated to the other traits.

Although this two-component model of social judgments of faces has become very influential, the extent to which it applies to trait ratings of faces made in other regions of the world is not yet known (but see Sutherland et al., in press PSPB for a recent replication in China). The proposed project will test whether the model described in Oosterhof and Todorov (2008 PNAS) can (1) be replicated in a new sample of North American raters and (2) can also explain trait-ratings made in other world regions (United Nations Country Grouping: Africa, Asia, Central America, Eastern Europe, European Union, Middle East, North America, Oceania, South America, The Caribbean).

Participant characteristics.Adult participants. No restriction on sex, sexual orientation, or ethnicity necessary. Data on age, sex, sexual orientation, ethnicity, and country of residence would be collected. Only world region of residence (determined from country of residence) would be used in the proposed analyses. The other factors would be made available for further, exploratory analyses.

Participating labs will be expected to collect data from 50-100 participants during 2018 to earn authorship on the resulting manuscript.

Procedure. Each participant would be allocated to rate 102faces (49 female and 53 male faces, diverse ethnicity) for one of 14adjectives (aggressive, attractive, caring, confident, dominant, emotionally stable, unhappy, intelligent, mean, responsible, sociable, trustworthy, weird, old) using a 1 (very low) to 7 (very high) scale. These are the same 13adjectives used by Oosterhof and Todorov (2008), plus 'old' (shown by Sutherland et al., 2013 Cognition to produce a third component). To mitigate potential problems with translating single-word labels, dictionary definitions for each of the 13 original adjectives would also be provided (following Bainbridge et al., 2013 JEP:G; see appendix for their definitions). Although this departs from Oosterhof and Todorov's methods, we have discussed this change with Todorov who agrees it is sensible. Each

participant would rate all 100 faces for one adjective only (which adjective they rated the faces for would be randomly determined). Based on data collected in our lab (UK), the mediantime to complete this task is ~5 minutes (90^{th} percentile = ~8 minutes). Following Oosterhof and Todorov's original paper, we would require a minimumof15 participants from each geographic region to rate the faces for each adjective (i.e., a minimum of 210 raters per region).

Our lab can provide a set of 102faces (49 female, 53 male faces, diverse ethnicity) for the study (https://figshare.com/articles/Face_Research_Lab_London_Set/5047666). We have already made these images open access and they were recently used by Todorov's lab in a replication and extension of their original paper (see Oh et al., 2017 https://psyarxiv.com/fxvcu).

Analysis plan. Analyses would be based on those reported by Sutherland et al. (in press PSPB). These analyses use averaged ratings for each face. Ratings from each world region will be analyzed separately. Countries will be allocated to world regions using the United Nations Country Grouping (Africa, Asia, Central America, Eastern Europe, European Union, Middle East, North America, Oceania, South America, The Caribbean).

First, we would identify how many components (i.e., factors) underpin judgments in each geographic region. This will be done using exploratory factor analysis (i.e., principal axis factoring) with a non-orthogonal rotation. Number of factors will be identified from scree plots, number of factors with eigenvalues greater than one, minimum average partial procedure, and parallel analysis. Differences in the outcome of these methods will be reconciled using a procedure described in Flake et al. (2015 Contemporary Educational Psychology).

Second, for each geographic region, we will identify which traits have strong loadings on each factor, which traits have weak loadings on each factor, and which traits crossload between or among factors. Criteria for strong and weak loadings will be set following Flake et al. (2015).

Publication plan. We suggest submitting to Nature Human Behavior as a registered report in the first instance, with Royal Society Open Science as a backup plan (again as a registered report). This would require a list of participating labs. Importantly, each lab would be required to have ethics approval before submitting the registered report for Stage 1 review.

Equipment required: A computer with Internet connection to access online study.

Appendix. Trait definitions used in Bainbridge et al. (2013 JEP:G). Note that Bainbridge et al. did not include dominance or age in their study. We propose defining dominant as "strong; important" and old as "having greater age; not young". Like the Bainbridge et al. definitions, these are adapted dictionary definitions.

Trait	Definition
aggressive	inclined to behave in a hostile fashion
attractive	appealing to the senses through beauty,
	form, character, etc
caring	feeling or showing compassion
confident	sure of oneself; having no uncertainty
	about ones own abilities
emotionally stable	not subject to emotional instability or
	illness; sane; mentally sound
unhappy	not joyful; sad or depressed
intelligent	having a good understanding or a high
	mental capacity
mean	offensive, selfish, or unaccomodating;
	nasty; malicious
responsible	able to take rational decisions without
	supervision; accountable for ones own
	actions
sociable	friendly or agreeable in company;
	companionable
trustworthy	deserving of confidence; dependable;
	reliable
weird	strange or bizarre

Report On The Workshop "Hands-on Actigraphy" Date: 28th JULY 2022 Venue: LG-1, GMU Organized by Odisha Centre for Geriatrics and Gerontology

Odisha Centre for Geriatrics and Gerontology of Gangadhar Meher University, Sambalpur, Odisha organized a workshop on "Hands on Actigraphy" on 28th July 2022 at LG-1 of GMU. The workshop was organized in collaboration with the Centre for Translational Chronobiology (CTC), Pt. Ravishankar Shukla University, Raipur. In the workshop, Prof. Arti Parganiha, the Coordinator of CTC, was present as a resource person and subject expert.

Importance of Workshop

The Odisha Center for Geriatrics and Gerontology (OCGG) at Gangadhar Meher University (GMU), Sambalpur is the first-ever center in the field of Geriatrics and Gerontology in Odisha. The Center was established in 2020 with financial assistance from the World Bank-funded "Odisha Higher Education Programme for Excellence and Equity" (OHEPEE) which focuses on interdisciplinary research on the social, psychological, and biological aspects of the elderly persons of Odisha.

One of the core objectives of the Center is to determine the sleep quality and cognitive abilities of the elderly population in Odisha. Therefore, the workshop has significant importance to the study of sleep quality measurement for the elderly population. Actigraphy is a non-invasive technique that is used to assess objective sleep variables and the rest-activity cycle of human subjects.

Proceeding of the workshop

The workshop began at 11:00 AM along with the introduction of the theme by Prof. Arti Parganiha.

Prof. Arti Parganiha elaborated in her lecture on the Application of Actigraphy-based output in various groups of subjects, such as seemingly healthy humans, cancer patients, and subjects with obstructive sleep apnea in the study area of Raipur. She also elaborated on the different parameters which are associated with the sleep quality in human subjects. She emphasized the importance of two rhythm parameters, i.e., autocorrelation coefficient at 24 hours (*r*24) and dichotomy index (I<0). She also highlighted the challenges faced during her studies. During the hands-on training session, she explained how to study the sleep-wake rhythms in human subjects using Actiwatch - MotionWatch8. She demonstrated how to configure the MotionWatch8 on a PC for data collection and how to retrieve the data of MotionWatch8 using

the software. She explained in detail the MotionWatch8-derived important sleep variables, Non-Parametric Circadian Rhythm Analysis (NPCRA), and the 24-hour activities of subjects. She explained the uses and operations of MotionWare Software.

During the deliberation, Prof. Parganiha suggested some points to incorporate into the OCGG study. The points are:

- a) To check the normality and homogeneity of data,
- b) To make a protocol that includes a selection of area, subjects, inclusion and exclusion criteria for Actigraphy study,
- c) Only trained persons should operate the MotionWatch8.

Participants

28/07/22 01:08 PM

In the workshop, the participants were PI, Co-PI, Research Associate, Research Assistant, and Office Assistant of OCGG and other faculties from the School of Anthropology and School of Botany.



Some Photographs during the Workshop

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Curr Drug Metab. 2022;23(9):757-780. doi: 10.2174/1389200223666220627110049.

Advances in Hybrid Vesicular-based Drug Delivery Systems: Improved Biocompatibility, Targeting, Therapeutic Efficacy and Pharmacokinetics of Anticancer Drugs

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Abstract

Anticancer drugs and diagnostics can be transported in nanoscale vesicles that provide a flexible platform. A hybrid nanoparticle, a nano assembly made up of many types of nanostructures, has the greatest potential to perform these two activities simultaneously. Nanomedicine has shown the promise of vesicular carriers based on lipopolymersomes, lipid peptides, and metallic hybrid nanovesicle systems. However, there are significant limitations that hinder the clinical implementation of these systems at the commercial scale, such as low productivity, high energy consumption, expensive setup, long process durations, and the current cancer therapies described in this article. Combinatorial hybrid systems can be used to reduce the above limitations. A greater therapeutic index and improved clinical results are possible with hybrid nanovesicular systems, which integrate the benefits of many carriers into a single structure. Due to their unique properties, cell-based drug delivery systems have shown tremendous benefits in the treatment of cancer. Nanoparticles (NPs) can benefit significantly from the properties of erythrocytes and platelets, which are part of the circulatory cells and circulate for a long time. Due to their unique physicochemical properties, nanomaterials play an essential role in cell-based drug delivery. Combining the advantages of different nanomaterials and cell types gives the resulting delivery systems a wide range of desirable properties. NPs are nextgeneration core-shell nanostructures that combine a lipid shell with a polymer core. The fabrication of lipid-polymer hybrid NPs has recently undergone a fundamental shift, moving from a two-step to a one-step technique based on the joint self-assembly of polymers and lipids. Oncologists are particularly interested in this method as a combinatorial drug delivery platform because of its two-in-one structure. This article addresses various preparative methods for the preparation of hybrid nano-vesicular systems. It also discusses the cellular mechanism of hybrid nanovesicular systems and describes the thorough knowledge of various hybrid vesicular systems.

Keywords: Anticancer hybrid vesicular; biocompatibility; cellular mechanism; nanomedicines; preparative method; specific targeting.

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Review article

Non-viral nucleic acid delivery approach: A boon for state-of-the-art gene delivery

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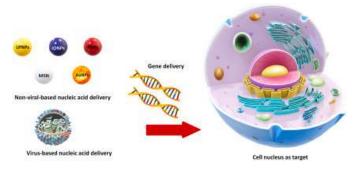
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Abstract

An increasing number of gene therapy applications necessitate the use of delivery methods that are risk-free, highly effective, highly targeted, and do not cause any threat to the recipient. Due to their modifiable nature with a variety of physicochemical characteristics, <u>nanostructures</u> for nucleic acid (NA) delivery provide an unparalleled possibility to overcome conventional delivery disadvantages. Because nanomaterials are easy to work with, they can be easily designed to interact with any biomolecules or moiety for selective targeting. The expression of DNA and RNA can be altered using <u>NA</u> therapeutic methods like DNA, mRNA, and <u>siRNA</u>, and this area of study has received a significant amount of research attention. Combining gene therapies with nanoscale delivery technologies has greatly increased the number of ways these molecules can be used in medicine and biology, such as for bioanalysis, vaccinations, replacing proteins, and turning genes off. This article provides an overview of <u>NA</u> delivery methods and technologies for molecular diagnostics and treatment for various disorders that urge gene-based therapy. It also describes the design concerns of NA nanodelivery, their amazing attributes, and the significance of these nanomaterials in biological systems and diseased cells and tissues. Further, it explains the limitations that NA nanodelivery poses along with the clinical and technical challenges that it has to overcome to extend this state-of-the-art delivery technology.

Graphical abstract



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Introduction

Gene therapy is a specialized field of medicine that focuses on changing the genes of cells to have therapeutic benefits or to treat a disorder by repairing or improving damaged genes [1]. It has the ability to treat and even cure a range of medical conditions, including cancer, HIV/AIDS, diabetes, heart disease, cystic fibrosis, hemophilia, and so forth [2,3]. NAs have been garnering a growing amount of interest as a result of recent findings such as RNAi and CRISPR-based genetic modification [4]. In addition, current worldwide efforts to elucidate the human genome have also contributed to this trend. Gene therapy is the manipulation of the expression of a specific gene or the modification of the biological features of live cells in order to treat a patient's condition. In recent years, numerous regulatory organizations have given their efforts to multiple gene treatment modalities so that they can be utilized for a variety of purposes. The approval of mRNA vaccines as a means of combating the COVID-19 epidemic is maybe the most instructive illustration of this principle [4,5].

The field of gene therapy can be broken down into three primary subfields. The first method involves utilizing the CRISPR–Cas technology to modify mutated genes in order to create a gain or loss of function [6]. Second, an increase in the level of gene expression may be accomplished by inserting a functioning gene copy that is intended to be expressed. This can be done with molecules such as pDNA, mcDNA, synthetic syn–mRNA, circular RNA, and saRNA. In the last step, substances such as siRNA, ASOs, and shRNA are utilized to inhibit the production of miRNA [4,7,8].

When compared to traditional medicines, NAs provide a number of beneficial features. In contrast to the latter, the action mechanism and huge specificity of NAs provide a prospective therapy pathway for viral infections, different malignancies, and untreatable genetic illnesses with unmet clinical needs [9,10]. This is because NAs have a significant therapeutic potential, which is clearly obvious in the form of patents registered in the previous 50 years all over the world (Fig. 1, Supplementary 1). In addition, according to one line of thought, a single dose of the genetic payload may be sufficient to have a long-lasting and maybe even curative impact [11]. But it can be hard to get NAs to where they need to be in the cell because they don't last long in biological systems and are quickly degraded by the host outside of cells. NAs further have trouble getting across the cellular membrane as a result of their high molecular weight, negative charge, and hydrophilicity [12]. Besides this, DNA and RNA do have many issues in common when it comes to delivery issues. For instance, the payload and delivery carrier toxicity is more of a concern while delivering RNA molecules, which often have short-term effects and don't stay in the cell long enough, so they need to be given frequently [13]. On the other hand, the activity of DNA in the nucleus adds up problems related to inappropriate nuclear transportation, which leads to different design principles for the delivery mechanism than for RNA molecules. In addition to problems that are specific to the molecule being given, the main problem is that it is hard to make individualized systems that make it easier for NA to get into target cells [14,15]. Once inside the cell, the carrier must be able to get past both intracellular and extracellular barriers, protect their payload from nuclease operations in the bloodstream, increase cellular absorption, and help endosomal escape [16].

The gene delivery systems are often categorized as either viral or non-viral, and their development may be traced back over the previous few decades (Fig. 2). It is possible to use viruses to deliver a gene of interest to a target cell

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Non-viral nucleic acid delivery approach: A boon for state-of-the-art gene delivery - ScienceDirect

by inserting the gene into the genome of the viral host, which is then accompanied by cell transfection and genetic expression [17]. Adenoviruses, retroviruses, parvoviruses, lentiviruses, and adeno-associated viruses, which have high DNA transfection efficiencies, have been utilized for a very long time to treat diseases like cancer, HIV, muscular dystrophy, and so on [18]. Even though viral gene delivery systems are very good at getting genes into cells, there is still leeway in biomedical research and clinical practice for other ways to deliver genes. This happens because viral gene delivery systems can be quickly cleared out of the body because of antibodies that are already there, the production of neutralizing antibodies against the vector, the small size of the vector (generally less than 7kb), and possible side effects. Because of this, scientists have tried to make non-viral methods of delivering genes based on peptides, lipids, polymers, and inorganic substances [19].

With the help of new technologies, gene delivery carriers have made a lot of progress in clinical investigations. But there are still many questions that need their answer on how effectively these carriers are purported to direct a certain NA to a certain type of cell [20,21]. As a result, the search for a formulation platform that is universally applicable ought to be reconsidered. This method is shown to be relevant to the genetic payload when findings from methods that are comparable provide outcomes that are startlingly different from one another. The "CVnCoV" mRNA lipid nanoparticles (LNPs) vaccine named CureVac made against COVID-19 was a viable candidate because it used an LNP formulation similar to the successful vaccines that Pfizer and Moderna had made [22]. Tragically, CVnCoV two-dose vaccination demonstrated just 47% efficiency at averting the illness. A possible explanation for these findings might be the distinction between the modified mRNA payloads utilized by Pfizer and Moderna and the unmodified mRNA payload utilized by CureVac, as well as the requirement to tailor the particle for the particular RNA sequence [23].

Therefore, the integration of material qualities, NA intracellular activity, its alterations, and disease traits should be covered by next-generation gene delivery techniques. To handle and analyze massive data sets of effective delivery cargoes, advanced robotic high-capacity screening techniques and algorithms for artificial intelligence (AI) are being created [24]. This will allow the procedure to be specifically optimized for a certain target, resulting in accurate gene therapy, exact clinical outcomes, and time and effort savings.

The goal of this article is to pay attention to the various ways that nanomaterials can be used to deliver NAs. It highlights the important considerations taken during the development of delivery platforms and prospective manufacturing methodologies, including the testing of numerous delivery platforms, including LNPs, liposomes, polymeric and inorganic NPs [[25], [26], [27], [28], [29]]. The review includes several methods for evaluating the characteristics of nanomaterials, data analysis, and downstream biological significance. Through pertinent examples, the main uses of NA-NPs are outlined and illustrated, comprising bioanalysis, gene silencing, gene editing, nano-barcoding and, vaccinations, and immunotherapy. The prognosis and perspective for the future are also discussed, highlighting the significant problems that the scientific community will face over the next ten years.

Section snippets

Need for chemical modification and nanocarrier-based approaches for delivery of nucleic acid

One of the biggest problems with delivering NAs is that they don't stay stable for very long. In fact, non-modified NAs don't act like drugs very well, they are unstable in the blood, and nucleases in extracellular fluids and serum can break them down right away [30]. Aside from encapsulating NAs in nanocarriers, chemical modification to nucleotides, such as modifications to their backbones, bases, and sugars, can increase chemical stability and minimize the immunological repercussions of NAs [...

Nanocarrier architecture and design considerations

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Lipid-based NPs, polymeric NPs (PNPs), and inorganic NPs are the leading non-viral nanocarriers for transporting NAs. This section of the article will discuss the most important parts of designing and making NPs, along with the most common ways to modify them. Fig. 3 illustrates the different potential means of gene delivery....

Synthesis concern, surface functionalization and characterization of NA delivery carrier

Although it is well-established that NP properties play a significant influence on the biological response, the precise method through which NP characteristics interact with biological systems remains unclear [106]. In this section, we have covered the concern and significance of nanomaterials involving synthesis and characterization of nanocarriers based on the physicochemical aspects, as well as how these qualities might alter the biological response. Here, Table 1 summarizes the different...

Application of nanocarrier in gene therapy

NA-based therapies are changing the world of medicine because they can target the genes that cause diseases instead of the proteins that are made as a result [4]. This means they can treat many difficult conditions for a long time or even cure them (Table 2). In this section, it was discussed how nanomaterials-based NA delivery could be utilized in some important areas and provided some concrete examples....

Replicability and cloud hosting

Recent years have witnessed significant efforts to create standards for data deposition, experiment record accuracy, and nanomaterial design. However, their application is still difficult. There are a number of crucial elements that need to be carefully considered in order to increase data repeatability and provide transparency.

Nano-engineered materials will be utilized to get around the many biophysical and physiological problems caused by the complex cellular microenvironment [193]. Designing ...

Limitations of NA nanocarriers and ways to improve

The translational problem of efficient gene delivery for medicinal applications still exists. Oligonucleotides are typically bulky, polyanionic molecules that take time to traverse the plasma membrane. These NAs must also evade the reticuloendothelial system, renal clearance, and nuclease destruction *in vivo* in order to reach their target. To get over these restrictions, viral and non-viral nanocarriers have been anticipated. The majority of the cancer gene treatments that are currently...

Clinical and other technical challenges

The deployment of alliance in the scientific community, especially on investigational and reporting standards, as well as the emergence of ambitious NA delivery techniques, will further push the science and technology, and clinical hurdles for nanomedicine. In this section, we take a closer look at the most important challenges that the scientific community will face in the next ten years and discuss potential solutions....

Conclusion

Recent advances in gene delivery and modification point to the arrival of a powerful new way to treat diseases in people. Even though a lot of work has been done by academic institutions and industrial researchers, it is still hard to turn this important molecular biology discovery into effective medicines that can be used in the real world. Even though gene-based medicines confront various obstacles addressed in this study, such as targeting issues, data repeatability, and expensive production ...

Declaration of competing interest

None....

Acknowledgments

The authors acknowledge their affiliated institutions and organizations for the resources and assistance....

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Original article

Tanshinone-I for the treatment of uterine fibroids: Molecular docking, simulation, and density functional theory investigations



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Keywords: Uterine fibroids Molecular modelling Tanshinone-I Progesterone blocker Docking

ABSTRACT

Uterine fibroids (UF), most prevalent gynecological disorder, require surgery when symptomatic. It is estimated that between 25 and 35 percent of women wait until the symptoms have worsened like extended heavy menstrual bleeding and severe pelvic pain. These UF may be reduced in size through various methods such as medical or surgical intervention. Progesterone (prog) is a crucial hormone that restores the endometrium and controls uterine function. In the current study, 28 plant-based molecules are identified from previous literature and docked onto the prog receptors with 1E3K and 2OVH. Tanshinone-I has shown the best docking score against both proteins. The synthetic prog inhibitor Norethindrone Acetate is used as a standard to evaluate the docking outcomes. The best compound, tanshinone-I, was analyzed using molecular modeling and DFT. The RMSD for the 1E3K protein-ligand complex ranged from 0.10 to 0.42 Å, with an average of 0.21 Å and a standard deviation (SD) of 0.06, while the RMSD for the 20VH protein-ligand complex ranged from 0.08 to 0.42 Å, with an average of 0.20 Å and a SD of 0.06 showing stable interaction. In principal component analysis, the observed eigen values of HPR-Tanshinone-I fluctuate between -1.11 to 1.48 and -1.07 to 1.25 for PC1 and PC2, respectively (1E3K), and the prog-tanshinone-I complex shows eigen values of -38.88 to -31.32 and -31.32 to 35.87 for PC1 and PC2, respectively (20VH), which shows Tanshinone-I forms a stable protein-ligand complex with 1E3K in comparison to 2OVH. The Free Energy Landscape (FEL) analysis shows the Gibbs free energy in the range of 0 to 8 kJ/mol for Tanshinone-I with 1E3K and 0 to 14 kJ/mol for Tanshinone-I with the 20VH complex. The DFT calculation reveals ΔE value of 2.8070 eV shows tanshinone-I as a stable compound. 1E3K modulates the prog pathway, it may have either an agonistic or antagonistic effect on hPRs. Tanshinone-I can cause ROS, apoptosis, autophagy (p62 accumulation), up-regulation of inositol requiring protein-1, enhancer-binding protein homologous protein, p-c-Jun Nterminal kinase (p-JNK), and suppression of MMPs. Bcl-2 expression can change LC3I to LC3II and cause apoptosis through Beclin-1 expression.

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1. Introduction

Tumors of the uterine lining, sometimes called leiomyomas (UFs), are frequent benign gynecological tumors that develop from the proliferation of smooth muscle cells in the uterus (Fig. 1A) (Okesola et al., 2022). It's estimated that 70–80% of women will be affected by them at some point in their lives and vast majority of those cases will show no symptoms at all (Don et al., 2022). Abnormal bleeding, pelvic discomfort, menorrhagia, infertility, miscarriages, and other obstetric difficulties are all clinical indications of UF that contribute to poor quality of life (Keizer et al., 2022; Piriyev and Römer, 2023; Yudha Pratama Putra et al., 2021).

Although the precise origin of UF is unknown, several variables have been linked to its pathogenesis, including genetics, cytokines, growth factors, hormones including estrogen and prog and/or their receptors, the environment, epigenetics, and the overproduction of extracellular matrix (ECM) (Al-Hendy et al., 2021; Czarnik et al., 2023).

There are several therapies that may be employed, i.e., pharmacological, surgical, and radiological techniques, including uterine embolization or magnetic resonance targeted ultrasound. Hysterectomy, meanwhile, continues to be the standard, one-sizefits-all approach for fibroids. Nevertheless, numerous women require a successful substitute to a hysterectomy due to numerous reasons, namely quicker healing and the preservation of reproductive ability. As a result, conservative solutions are required, and secure and efficient pharmacological intervention is one of them.

Tranexamic acid, oral contraceptives, oral and injectable prog, Prog-releasing intrauterine systems, antiprogesterone, gonadotropin-releasing hormone (GnRH) agonists and antagonists, selective prog receptor modulators (SPRMs), selective oestrogen receptor modulators (SERMs), aromatase inhibitors, danazol, and gestrinone are some of the medical interventions currently available. The majority of these treatments do not particularly target UF; rather, they are employed to regulate irregular UF. Prog. is among those employed most frequently.

Prog is a vital hormone, regulates uterine function, principally involved in the restoration of the endometrium. Prog interaction with the human prog receptor (HPR), comes under the nuclear hormone receptor superfamily, represents the joint functions of PR-A and B. Upon ligand binding, these may affect cellular physiology and alter gene expression through two methods: (i) PRs act as ligand-activated transcription factors to directly interact with DNA promoter transcription and modulate the downstream genes expression (ii) PRs interact through Src tyrosine kinases and trigger MAPKs, which affect gene functioning (Boonyaratanakornkit et al., 2001; Boonyaratanakornkit and Edwards, 2007; Leonhardt et al., 2003; Patel et al., 2015).

It has been shown that Prog promotes UFs growth by increasing the number of cells, size as well as ECF amount. Proteins called PR-A and PR-B were also found to be higher in fibroids than in healthy myometrium. Both Prog and growth factor are linked to several processes, such as cell growth and death (apoptosis) (Fig. 1). Therefore, Prog blockers may play an effective role in the treatment of UFs. Phyto-constituents possess enormous potential in the management of life threatening diseases. Many phytoconstituents e.g., curcumin, quercetin, rutin etc are reported to possess anticancer potential.

Therefore, the present study has been designed to explore the potential of 28 phytochemicals from different plants to block the human prog receptor as a therapy for uterine fibroids using insilico methods. Fig. 2 shows the schematic illustration of the present study for the discovery of potential prog receptor inhibitors.

CAM therapy may turn out to be a good way to treat UF. Literature shows that Gui Zhi Fu Ling Tang, *Ramulus cinnomomi*, and *Poriae cocos* decoction, *Danshen Gegen* decoction (*Salviae Miltiorrhizae* Radix, *Purariae Lobatae*, Radix decoction), Genistein, Green Tea (*Camellia sinensis*), and Tanshinone-I are effective against UF.

Tanshinone-I is obtained from *Salviae miltiorrhizae* and employed in the treatment of atherosclerosis, downregulation of adhesion molecules, and enhancement of microcirculation by stimulating endothelium-dependent vasodilatation (EDVD) in coronary arterioles through the neuromodulators endothelial nitric oxide synthase (eNOS) and angiotensin II. Interestingly, it also stops the growth of vascular smooth muscle cells (VSM) and thins the intima. It does this by cleaving caspase-3 to promote cell death and blocking the PI3K/AKT/mTOR pathway to cause autophagy (Ansari et al., 2021; Dalton-Brewer, 2016).

2. Materials and methods

2.1. Molecular docking study

The molecular docking studies of the identified compounds were performed on a 5950 X 16-Core Processor (3.40 GHz); AMD Ryzen-9; Windows 10 (64-bit); and 64-GB RAM.

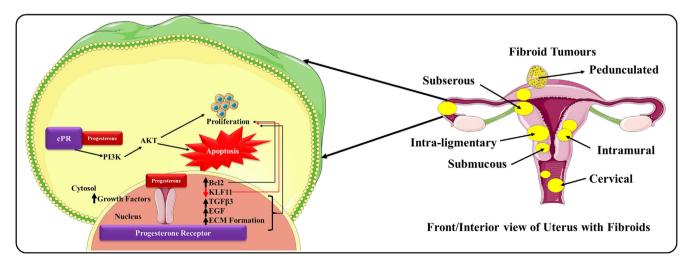


Fig. 1. Interrelation of Prog and growth factors in fibroid management.

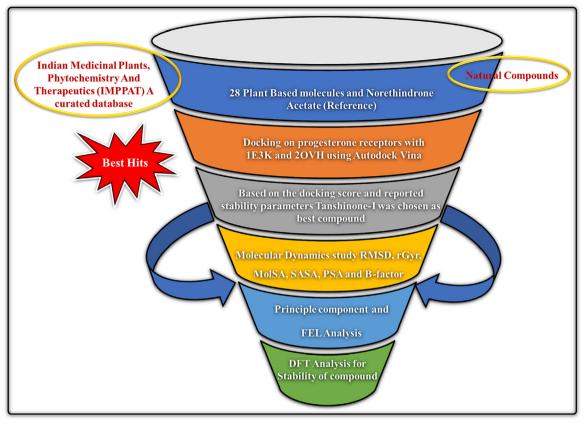


Fig. 2. Schematic illustration of the present study for the discovery of potentialprog receptor inhibitors.

2.2. Selection and protein receptors from PDB:

We have collected all reported structures from PDB (https:// www.rcsb.org) and compared them to one another in order to explore the variability in the ligand binding patterns in different crystal structures of human PR. Their receptors were thoroughly examined as well. In order to examine SPRMs and human PRs, we have selected two PDBs i.e., 1E3K and 20VH from the RCSB database. Protein preparation was carried out using the Autodock Wizard by deleting attached water molecules, bound heteroatoms or ligands, adding polar hydrogens, Kollman charges, spreading charge equally over all atoms, and checking for missing atoms on residues. The PDB files were then converted to the PDBQT format for executing the next step. Table 1 shows the details of all human prog receptor structures retrieved from the PDB 2 database (Saritha et al., 2023).

2.3. Molecular docking procedure

2.3.1. Grid generation

For carrying out docking between prepared receptors and ligands, grid was generated by taking the center on the attached ligand. The grid dimensions are given in Table 2.

2.3.2. For PDB 1E3K

The crystallographic 3D structure of the Human Prog Receptor (HPR) Ligand Binding Domain in complex with the ligand metribolone (R1881) was accessed from Protein Data Bank (PDB ID code 1E3K) with unit cell (Å) a = 58.402, b = 65.011, c = 71.181, and angles (°) α = 90, β = 95.65 and γ = 90 respectively. The resolution of the X-Ray Diffraction (XRD) structure of this model enzyme is 2.80 Å. After optimizing hydrogen bonds, OPLS-2005 was used as

Table 1Human prog receptors from PDB 2 database.

Category	PDB	Ligand	Resolution (A ⁰)
GROUP-1	2W8Y	Mifepristone (MT)	1.8
Steroidal antagonist	4A2J	Asoprisnil (AS)	2.0
	40AR	Ulipristal acetate (UA)	2.41
	20VH	Asoprisnil	2.0
	20VM	Asoprisnil	2.6
GROUP-2	4APU	A2K	1.9
(Non-steroidal SPRM)	3G80	30X	1.90
	3ZR7	OR8	1.65
	3HQ5	GKK	2.1
	3KBA	WOW	2.0
GROUP-2	1A28	PROGESTERONE (STR)	1.8
Steroidal Agonist	1E3K	Metribolone (R18)	2.8
	1SR7	Mometasone furoate	1.46
	3D90	Levonorgestrel	2.26
GROUP-2	1ZUC	Tanaproget (T98)	2.0
Non-steroidal Agonist			

Tabl	e 2
Grid	Parameters

S. No.	Parameters	1E3K	20VH
1)	Exhaustiveness	8	8
2)	center_x	28.6348	30.6727
3)	center_y	-7.7984	0.7615
4)	center_z	9.5311	28.3292
5)	size_x	16.0747	16.0146
6)	size_y	16.1977	16.1716
7)	size_z	16.1712	16.1487

the force field to refine the structure minimization to an RMSD constraint value of 0.3 Å. Grid box dimensions were 16.0747 X 16.1977 X 16.1712 (all in Å) with a 0.375 Å grid point spacing.

Protein residues that include ligand-restricting sites are logically expected to contain certain ligands that can bind reversibly. The correct orientation for other protein-affirming amino acid residues was provided.

2.3.3. For PDB 20VH

Protein Data Bank (PDB ID code 20VH) provided access to the crystallographic 3D structure of the prog receptor with bound Asoprisnil and a peptide from the co-repressor SMRT, with unit cell (a) = 87.475, b = 87.475, c = 90.599, and angles (°) α = 90, β = 90, and γ = 120, respectively. This model enzyme's XRD structure has a resolution of 2.00 Å. After optimizing hydrogen bonds, the structural reduction was further refined using the OPLS-2005 force field to achieve the 0.20 Å RMSD constraint value. The grid box measures 16.0146 × 16.1716 × 16.1487 (all in Å) with a grid point spacing of 0.375 Å. It stands to reason that certain ligands with reversible binding capabilities would be present in protein residues with ligand-restricting sites. Other protein-affirming amino acid residues were given the proper orientation.

2.4. Selection and preparation of phytoconstituents

28 phytochemicals are selected on the basis of a review of the literature from search engines and the IMPPAT 2.0 database, which provides extensive information with 100 books and 7000 + research articles on Indian medicine. The phytoconstituents are selected on the basis of their antitumor effects. In order to virtually test the ability of phytoconstituents to bind to specific proteins, this database provides information regarding phytochemicals, medical applications, as well as 2D and 3D chemical structures. Table 3 shows the phytoconstituents selected for the study with their IMPPAT-ID (https://cb.imsc.res.in/imppat/). All the phytoconstituents were downloaded in SDF format from PubChem, their energy reduced by the MMFF94 Force Field, and then opened in the PyRx program, which converted them to PDBQT format. The LigPrep application (the trial version of Schrödinger) was used to prepare the ligands. Energy optimization for all ligands was done using the OPLS 2005 force field, but the 0.01 Å RMSD cut-off was not reached. At the desired pH of 7 \pm 2, Epic was used to produce tautomers, all conceivable ionization states, and low energy ring conformations for each ligand. The output format of the Schrodinger Maestro was used to save the prepared ligands.

2.5. Docking and visualization of results

Docking was used to collect a set of ligand-binding site conformations and orientations. PyRx, AutoDock-Vina scoring-functionbased analysis of binding sites, and docking runs of target proteins with ligands. Each ligand's conformations were analyzed, and the ones with the highest binding affinities were selected. Maestro Visualizer was used to generate the 3D and 2D interaction diagrams.

2.6. Molecular dynamics simulations

The Desmond tool from Schrödinger's suite was used to do molecular dynamics simulations on the ligand-protein combination (Bowers et al., 2006). The best chemical from those that passed screening was chosen for MD simulations using criteria including the number of hydrogen bonds, binding energy, and glide score. Tanshinone-I, the best docked chemical, was chosen for simulation analysis in this investigation. We neutralized the charge and adjusted the salt content to 0.15 M of Na⁺ and Cl⁻ ions to create the physiological condition of the simulation box. Aligning the major axes of the solute along the box vectors or the diagonal reduces the volume of the simulation box. Proteins, protein complexes, protein–ligand complexes, proteins embedded in a membrane bilayer, etc. make up the solute in the solvated system. By doing a 100 ps low-temperature (100⁰K) Brownian motion MD simulation (NVT ensemble), we were able to remove steric conflicts in the complex and reduce the energy of the ligand–protein interaction. From the MD tab's work space, we loaded the preprocessed ligand protein complex, and then we adjusted the temperature to 300⁰ K and the pressure to 1.01325 bar in the NPT ensemble. The ligand–protein complex's trajectory was measured at 4.8 ps after 100 ns of simulations, which were run after the model system was relaxed. The conformational behaviour and stability of the complex were examined by calculating and analyzing energy, ligand–protein RMSD, RMSF, protein–ligand interactions, and ligand characteristics throughout the course of a 100 ns simulation.

2.7. Analysis of simulation data

After analyzing the MD trajectories, the root-mean-square deviation (RMSD), root-mean-square fluctuation (RMSF), and other measures for the distance between residues and inhibitors were computed using the VMD (version: 1.9.1) or in-house Perl scripts.

2.8. Principal component analysis (PCA)

The large-amplitude movements were analyzed with a principal component analysis (PCA). The eigenvalues and eigenvectors were analyzed with the covariance matrix that was constructed from the diagonalized covariance matrix. The principal components (PCs), also known as eigenvectors, reveal the motional orientation of the ligand and receptor atoms, while the corresponding eigenvalues characterize the mean square fluctuations of the complex. Using calculations and graphs, PC1 and PC2 were used to validate their motions (Dalal et al., 2021).

2.9. FEL analysis

The FEL along the PC was postulated in order to better understand the energy distribution of the protein folding route during molecular dynamics. The formula for calculating the free energy of a protein is (Eq. (1):

$\Delta \boldsymbol{G} = \boldsymbol{\Sigma} - \boldsymbol{K} \boldsymbol{T} \boldsymbol{B} \, \boldsymbol{l} \boldsymbol{n} \, (\boldsymbol{P} \boldsymbol{A} - \boldsymbol{P} \boldsymbol{B}) \tag{1}$

-where \triangle G represents the Gibbs energy landscape, TB is the gas constant, and K is the equilibrium constant. PA and PB represent the two protein probabilities along the dynamic pathway. Using the eigenvector values obtained from the PCA, 3D FEL plots of protein–ligand complexes were created. To analyze the maximum and minimum energy of drug complexes, a FEL plot with different contour maps of various color patterns, such as red, yellow, green, orange, and blue, was generated (Dalal et al., 2021).

2.10. Density functional theory (DFT) analysis

The phytochemical reactivity was analyzed with DFT. The analysis used the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) energies. The expression was used to figure out the band energy gap. All of these labels come straight from the calculations of quantum physics. This formula was used to determine the HOMO–LUMO energy difference (Eq. (2):

$$\Delta \mathbf{E} = \mathbf{E}_{LUMO} - \mathbf{E}_{HOMO} \tag{2}$$

The HOMO and LUMO energies to get the chemical potential (μ) (Eq. (3), chemical hardness (η) (Eq. (4) and chemical softness (σ) (Eq. (5) of the system:

Table 3

Phytochemicals isolated	from fruits and vegetable	es for Fibroid treatment	and their mechanisms of action.

S. No.	Name	IMPPAT ID	Biological sources	Uses	References
1.	Apigenin	IMPHY004661	Lonicera gracilipes var. glandulosa	Anticancer	(Si et al., 2009; Wu et al., 2005)
2.	Equol	IMPHY005820	Pueraria mirifica and Cordyceps militaris	Cancer	(Axelson et al., 1982; Setchell et al., 2005; Wang et al., 2014)
3.	Daidzein	IMPHY004566	Pueraria mirifica and Cordyceps militaris	Anti-oxidant, anti- carcinogenic	(E. Kim et al., 2015; Sakamoto et al., 2016)
4.	Genistein	IMPHY004643	Flemingia vestita	Anticancer	(Choi et al., 2020; Hwang et al., 2020; Lian; et al., 2018)
5.	Catechin	IMPHY014854	Camellia sinensis	Anticancer	(Alshatwi, 2010; Cheruku et al., 2018; Waffo-Téguo et al., 2001)
6.	Myricetin	<u>IMPHY005471</u>	Tibouchina paratropica	Antimicrobial	(Jinwal et al., 2009; Phillips et al., 2011; Semwal et al., 2016; Tzeng et al., 1991; Xu et al., 2016)
7.	Isorhamnetin	IMPHY008724	Pollen typhae	Anti-cancer	(Hu et al., 2015; Kim et al., 2011)
8.	Fisetin	IMPHY005433	Galeditsia triacanthos	Antioxidant, Anticancer, Neuroprotection	(S. C. Kim et al., 2015; Mukhtar et al., 2015
9.	Eriocitrin	IMPHY012252	Citrus limon	Anticancer	(Wang et al., 2016)
10.	Tanshinone-I	IMPHY010828	Salvia miltiorrhiza	Anticancer	(Su and Chiu, 2016; Xie et al., 2015; Zhang et al., 2016)
11.	Naringenin	IMPHY010550	Aglaia duperreana	Anticancer	(Saponara et al., 2006)
12.	Taxifoline	IMPHY011967	Silybum marianum	Anticancer	(Angelis et al., 2016; Ren et al., 2020)
13.	Myricetin	<u>IMPHY005471</u>	<u>Myrica nagi</u> Thunb.	Anti-oxidant, anticancer, antidiabetic and anti-	(Du et al., 2012)
14.	(-) Gallocatechin	IMPHY011735	Saxifraga cuneifolia, Quercus dentata	inflammatory Antioxidant, anti-obesity activity	(Waffo-Téguo et al., 2001)
15.	(-)-Epicatechin	IMPHY014854	Camellia Sinensin	Anticancer	(Nogueira et al., 2011; Shay et al., 2015; Wang et al., 2015)
16.	(-)-Epigallocatechin	IMPHY011735	Camellia Sinensin	Anticancer	(Chung and Vadgama, 2015; Lee and Tan, 2015; Waffo-Téguo et al., 2001)
17.	(–)-Epicatechin 3- gallate	IMPHY011874	Camellia Sinensin	Anticancer	(Takizawa et al., 2003; Wang et al., 2013)
18.	(–)-Epigallocatechin 3-gallate	IMPHY011671	Camellia Sinensin	Anticancer	(Chiou et al., 2012; Ignasimuthu et al., 2019 Kannen et al., 2013)
19.	Flavone		Apium graveolens, Petroselinum crispum, artichoke Cynara scolymus	Anticancer, Antioxidant	(Kellis and Vickery, 1984)
20.	Dihydrodibenzoxepin	IMPHY006809	Bauhinia variegate	Anti-cancer	(Lee et al., 2010)
21.	Glicentin	MPHY015706	Monoclonal anti-glucagon	Stimulation of insulin secretion, inhibition of gastric acid secretion	(Raffort et al., 2017)
22.	Kaemferol	IMPHY004388	Lotus ucrainicus	Antitumor	(An and Kim, 2015; Luo et al., 2012, 2011 Shin et al., 2015)
23.	Quercentin	IMPHY004619	Camellia sinensis	Anti-oxidant Atherosclerosis	(Liu et al., 2020; Navarro-Núñez et al., 2010) Yang et al., 2015)
24.	Cyanidin	IMPHY008945	Rhododendron cv.	Anticancer	(Cheng et al., 2009; Kannan and Kolandaivel, 2018; Lee et al., 2013)
25.	Pelargonidin	IMPHY003437	Philodendron	Anticancer	(Khandelwal and Abraham, 2014)
26.	Norethindrone Acetate	<u>IMPHY013743</u>	Synthetic second-generation progestin	Heavy periods, Breast cancer	(Cheng and Wolfe, 1983; Muneyyirci-Dela and Karacan, 1998)
27.	Eriodictyol	IMPHY004038	Eriodictyon californicum	Anticancer	(Zhang et al., 2020)
28. 29.	Quercitrin Gnetol	IMPHY015054 IMPHY000794	Citus families, berries Genus gnetum	Anticancer Anticancer (tyrosinase inhibitor)	(Vafadar et al., 2020) (Ohguchi et al., 2003)

$$\mu = \frac{E_{LUMO} - E_{HOMO}}{2e} \tag{3}$$

$$\eta = \frac{E_{LUMO} - E_{HOMO}}{2} \tag{4}$$

$$\sigma = \frac{1}{\eta} \tag{5}$$

The electron affinity (A) is equal to the LUMO energy level, while the ionization potential (I) is defined as the – E_{HOMO} energy level. The following equations can be used to determine the electronegativity (χ) (Eq. (6), electrophilicity (ω) (Eq. (7),

maximum charge transfer (Eq. (8), and nucleophilia (Eq. (9) of a substance:

$$\chi = \frac{\mathbf{I} + \mathbf{A}}{2} \tag{6}$$

$$\omega = \frac{\mu^2}{2\eta} \tag{7}$$

$$\Delta \mathbf{N}_{\max} = \frac{\chi}{\eta} \tag{8}$$

$$(\mathbf{N}) = \mathbf{E}_{LUMO} - \mathbf{E}_{HOMO(TCE)}$$
(9)

Table 4

Molecular Docking Results.

S. No.	Binding Af (kcal/mol)	finity	Compound Name
	1E3K	20VH	
1.	-9.2	-8.8	Apigenin
2.	-9.4	-8.9	Equol
3.	-9.5	-8.9	Daidzein
4.	-8.9	-9	Genistein
5.	-8.5	-8.5	Catechin
6.	-8.3	-8.7	Myricetin
7.	-8.3	-8.8	Isorhamnetin
8.	-9.3	-8.5	Fisetin
9.	-10.2	-9.9	Tanshinone-I
10.	-9	-8.7	Naringenin
11.	-8.9	-9	Eriodictyol
12.	-8.8	-8.8	Taxifoline
13.	-8.3	-8.9	Quercitrin
14.	-8.3	-8.7	Myricetol
15.	-8	-8.4	(+)-Gallocatechin
16.	-8.5	-8.5	(–)-Epicatechin
17.	-8	-8.4	(–)-Epigallocatechin
18.	-4.3	-9.5	(–)-Epicatechin 3-gallate
19.	-3.7	-9.2	(–)-Epigallocatechin 3-gallate
20.	-9	-8.6	Flavanone
21.	-8.1	-7.6	Dihydrodibenzoxepin
22.	-9	-8.8	Glycitein
23.	-8.8	-8.6	Kaemferol
24.	-8.3	-8.9	Quercetin
25.	-8.7	-8.6	Cyanidin
26.	-8.5	-8.4	Pelargonidin
27.	-8.1	-7.6	Gnetol
28.	-8.5	-7.8	Pterostilbene
29.	-10.7	-10.1	Norethindrone Acetate

3. Results

3.1. Docking results

The docking results are shown in Table 4. The docking interaction of 1E3K showed Tanshinone-I is the best docked compound when compared with the standard drug, as shown in Figs. 3 and 4. Other compounds like Equol, Fisetin, Genistein, Myrecetin, and Apigenin have showed good results and illustrated in the supplementary file Fig. 1a–5a. Table 5 shows the interacting amino acids with 1E3K, whereas Table 6 shows the interacting amino acids with the 20VH receptor protein. The docking interaction of 20VH showed Tanshinone-I is the best docked compound when compared with the standard drug, as shown in Figs. 5 and 6. Other compounds like (-)-Epicatechin 3-gallate, (-)-Epigallocatechin 3-gallate, Eriodictyol, Genistein, and Quercetin have shown good results and are shown in the supplementary file Fig. 6a–10a. Fig. 10a. 3d&2d- Docking interaction on 2OVH with Genistein has been showed below (Tiwari et al., 2022).

3.2. Prediction of ADMET analysis

The Swiss ADME software (https://www.swissme.ch) was used to estimate each ADME analysis (physicochemical properties, water solubility, lipophilicity, pharmacokinetics, and drug similarity). The results of the physicochemical properties of some phytochemicals are shown in supplementary table 1a. The results of lipophilicity, water solubility, pharmacokinetics, and druglikeness are shown in supplementary tables 2a, 3a, 4a, and 5a, respectively, and included in the supplementary files. The lipophilic properties were put into three main groups: fragmental (based on fragments, wLog P), topological (based on descriptors, mLog P), and 3D physics-based (iLog P and xLog P, based on solvent free energy in octanol). The pink area represents the optimal range for each property (lipophilicity: MLOGP less than 4.15, XLOGP between -0.7 and + 5.0, size: MW between 150 and 500 g/mol, polarity: TPSA between 20 and 130 Å2, solubility: log S not higher than 6, saturation: the fraction of carbons in the sp3 hybridization not less than 0.25, and flexibility: no more than 9 rotatable bonds). From these results, the compound can be predicted not to be orally bioavailable, but to be too flexible and polar. Figs. 7-9 depict the protein-ligand RMSD, RMSF, and secondary structure of proteins, Ligand RMSF, and Protein Ligand Contacts for 1E3K and Figs. 10-12 for 20VH, respectively. Results of (a) principal component analysis (b) FEL 3D, are shown in Fig. 13 for 1E3K and Fig. 14 for 2OVH. Fig. 15 depicts the HUMO and LUMO analyses of Tanshinone-I.

Results of Principle compnent analysis and FEL 3D for IE3K

3.3. Results from DFT analysis

The energy gap ΔE (eV) between EHOMO (eV) and ELUMO (eV) and other parameters are shown in Table 7.

4. Discussion

The development of synthetic prog ligands with either prog receptor (PR) agonist (progestins) or mixed agonist/antagonist action has been stimulated by the apparent, if uncertain, contribution of prog lead to the formation of fibroids. It has been

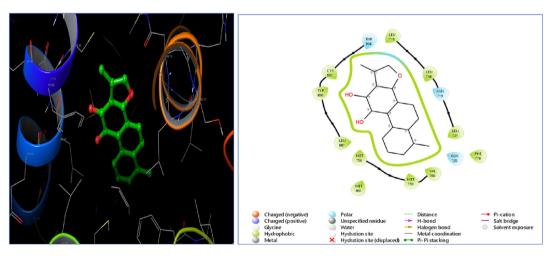


Fig. 3. 3d-&2d Docking interaction on 1E3K with Tanshinone-I.

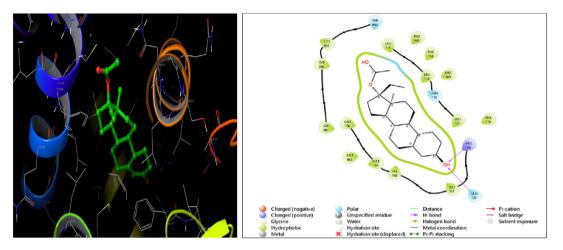


Fig. 4. 3d&2d- Docking interaction on 1E3K with Norethindrone Acetate.

demonstrated that prog and PR complexes decrease apoptosis and encourage fibroid cell growth. hPR-A and hPR-B are the two main isoforms of PRs. By means of two distinct promoters, the same gene can produce both isoforms. Another PR isoform, PR-M, is assumed to contribute to cellular respiration and provide shielding from apoptosis. It has nongenomic action. Recently, it was discovered that the fibroid edge has higher levels of PR-M expression and mitochondrial density than the myometrium. Thus, a nongenomic progestin-induced rise in cellular respiration may play a significant role in the development of fibroid.

Norethindrone acetate is used for menorrhagia associated with fibroids at a dose of 5–15 mg/day, which has been taken as the standard drug for the study. This belongs to the class of progestins and works by stopping the uterine lining from growing and stopping proliferation. This drug is associated with numerous side effects, namely irregular vaginal bleeding or spotting, menstrual flow modifications, enlarged/tender breasts, nausea, blood clots,

Table 5

Hydrophobic and polar bond interaction of selected phytoconstituents with 1E3K Protein.

S. No.	Compound names	Hydrophobic bond	Polar bond
1.	Tanshinone-I	Val760; Met759; Met756; Met801; Leu887; Tyr890; Cys891; Leu715;	Gln725; Asn719;
		Leu718; Leu721	Thr894
2.	Norethindrone	Leu763; Val760; Met759; Met756;	Gln725;
	Acetate	Met801; Leu887; Tyr890; Cys891;	Asn719;
		Leu715; Phe905; Phe794; Leu718; Met909	Thr894
3.	Equol	Leu763; Met759; Phe794; Tyr890;	Asn719;
		Leu715; Leu718,	Thr894;
			Thr716
4.	Fisetin	Phe778; Leu763; Val760; Met759;	Asn719;
		Met801; Met756; Leu887; Tyr890;	Thr894;
		Cys891; Val903; Leu715; Leu718;	Thr716
		Leu721; Polar Charged Arg719,	
		Gln725	
5.	Genistein	Leu763; Met801; Phe778; Met756;	Asn719;
		Met759; Leu887; Val760; Met759;	Thr894;
		Tyr890, Cys891, Met756; Leu715;	Thr716
		Val903; Leu718; Leu721	
6.	Myrecetin	Leu763; Met801; Phe778; Met756;	Asn719;
		Met759; Leu887; Tyr890; Cys891;	Thr894;
		Met756; Leu715; Val903; Leu715;	Thr716
		Leu718; Leu721	
7.	Apigenin	Leu763; Met759; Met756; Leu887;	Asn719
		Tyr890; Cys891; Leu715; Leu718;	
		Leu721; Tyr890	

vomiting, difficulty falling asleep, acne, brown patches on the face, hair loss and growth of hair on the face, etc. It works at the molecular level. Progestins like norethisterone affect target cells by binding to prog receptors, which change target genes. The reproductive system, the breast, the pituitary gland, the hypothalamus, the skeleton, and the central nervous system all have cells that are targets. Norethisterone also causes the endometrium to change in ways that make it unsuitable for implantation, such as shrinking, irregular secretion, and slowed growth. Tanshinone-I, which comes from plants, can be used instead of a synthetic standard drug.

The molecular docking studies revealed the promising potential of Tanshinone-I among the 28 docked compounds. The binding affinity of Tanshinone-I on 1E3K and 2OVH was found to be -10.2 and -9.9, respectively, which is comparable with that of standard Norethindrone Acetate on 1E3K and 2OVH, which is -10.7 and -10.1, respectively. Further, PCA and FEL data analysis of Tanshinone-I on the 1E3K receptor revealed a stable and strong interaction with the receptor, proving its promising role in the treatment of uterine fibroid.

Table 6

Hydrophobic and polar bond interaction of selected phytoconstituents with 20VH Protein.

- Totem			
S. No.	Compound names	Hydrophobic bond	Polar bond
1	Epicatechin-3-	Leu715; Leu718; Leu721; Leu726;	Asn719; Gln725
	gallate	Trp755; Met759; Val760; Leu763; Phe778; Leu 887; Tyr 890; Leu 797; Cvs891	GIN/25
2	Eriodictyol	Leu721; Leu763; Phe778; Val760;	Thr894:
		Met759: Met756: Met801: Leu887:	Asn719;
		Tyr 890; Leu797;Cys891	Gln725
3	Genistein	Leu715; Leu718; Leu721; Phe778;	Thr894;
		Met759; Met801; Leu763; Leu797	Asn719;
			Gln725
4	Myricetol	Leu715; Leu718; Leu721; Leu763;	Thr894;
		Phe778; Val760; Met759; Met801;	Asn719;
		Leu887;Tyr890; Leu797;Cys891	Gln725
5	Norethindrone	Leu718; Leu721; Leu763; Val760;	Thr894;
	Acetate	Met759; Met801; Leu797; Leu887;	Asn719;
		Cys891	Gln725
6	Quercentin	Leu715; Leu718; Leu721; Leu763;	Thr894;
		Phe778; Val760; Met759; Met756;	Asn719;
		Met801; Leu887; Tyr890; Leu797;	Gln 725
7	Tanshinone-I	Thr890; Cys891	Thr894:
/	Tansninone-i	Leu718; Leu721; Leu763; Phe778;	,
		Val760; Met759; Met756; Met801; Leu887; Tyr890; Leu797; Cys891	Gln725

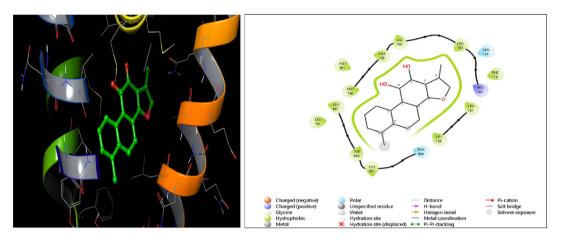


Fig. 5. 3d &2d- Docking interaction on 20VH with Tanshinone-I.

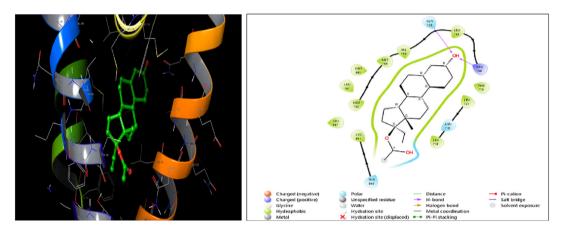


Fig. 6. 3d & 2d- Docking interaction on 20VH with Norethindrone Acetate.

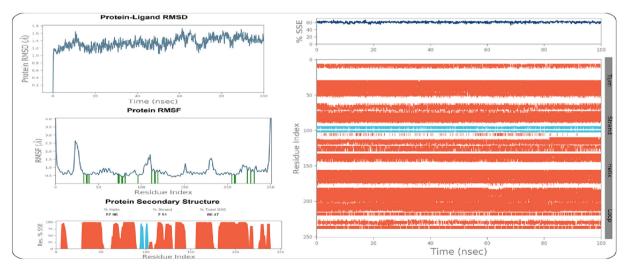


Fig. 7. Protein Ligand RMSD, RMSF, secondary structure of protein, % SSE and residue Index with 1E3K.

Tanshinone-I is virtually docked with 1E3K protein with a docking score of -10.2 kcal/mol and 13 rotatable bonds and affinities with amino acids like Val 760; Met 759; Met 756; Met 801; Leu 887; Tyr 890; Cys 891; Leu 715; Leu 718; Leu 72 (hydrophobic), Gln 725; Asn 719; Thr 894 (polar). This drug has shown a comparable docking score with the standard drug Norethindrone Acetate of -10.7 kcal/mol; 16 rotatable bonds and affinities with amino acids like Leu 763; Val 760; Met 759; Met 756; Met 801; Leu 887; Tyr 890; Cys 891; Leu 715; Phe 905; Phe 794; Leu 718; Met 909 (hydrophobic) and Gln 725; Asn 719; Thr 894 (polar). Similarly, with 20VH, Tanshinone-I with a docking score of –9.9 kcal/mol is comparable to the standard, Norethindrone Acetate, (-10.1 kcal/mol); 16 rotatable bonds and affinities with amino acids such as Leu 718, Leu 721, Leu 763, Phe 778, Val 760,

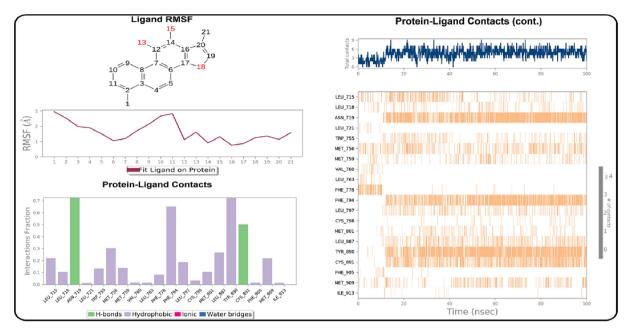


Fig. 8. Ligand RMSF and Protein Ligand Contacts for 100 ns with 1E3K protein.

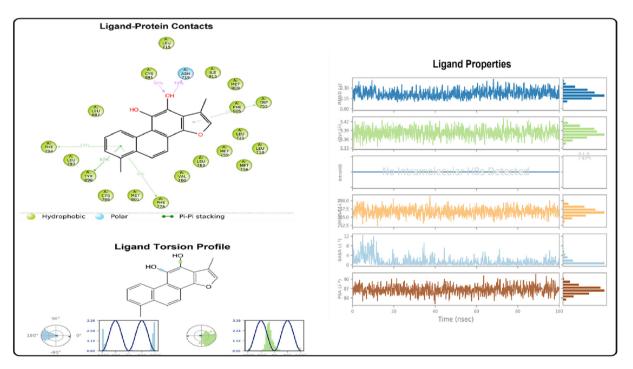


Fig. 9. Ligand-Protein contact with 1E3K and interaction with different amino acids, Tanshinone-I torsion profile and Properties (PSA, SASA, MolSA, rGyr and RMSD).

Met 759, Met 756, Met 801, Leu 887, Tyr 890, Leu 797, Cys 891 (hydrophobic) and Thr 894; Asn 719; Gln 725 (polar) (Si et al., 2009; Wu et al., 2005).

4.1. Molecular dynamics simulation

It is the best method to validate the docking score. Tanshinone-I was found to be the most potent drug against receptor 1E3K and 20VH and showed the maximum docking score (-10.2 kcal/mol and -9.9 kcal/mol). The complex of protein with ligand has been

simulated for 100 ns and found stable (Basu et al., 2020; El Ouafy et al., 2022).

RMSD and RMSF estimations have been performed to assess the trajectory generated following simulation, as shown in Fig. 7. The RMSD of the protein–ligand complex attained a minimum value of 0.10 Å and a maximum value of 0.42 Å with an average value of 0.21 Å between 100 ns and a standard deviation of 0.06. Rad gyration (rGyr) was found to be 3.33 Å with a mean value of 3.38 Å, and a standard deviation of 0.02 (Fig. 8). RMSF values have been estimated to assess the residue's mobility for conformational

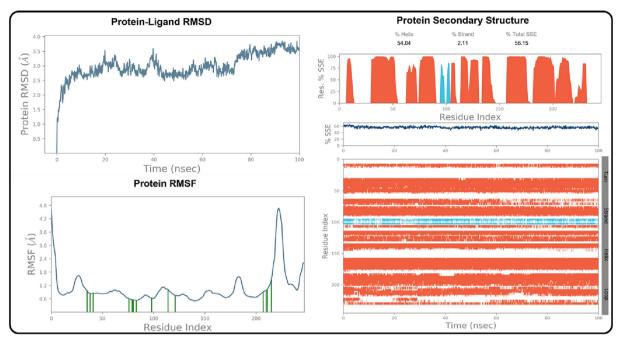


Fig. 10. Protein Ligand RMSD, secondary structure of protein % SSE and residue Index with 20VH.

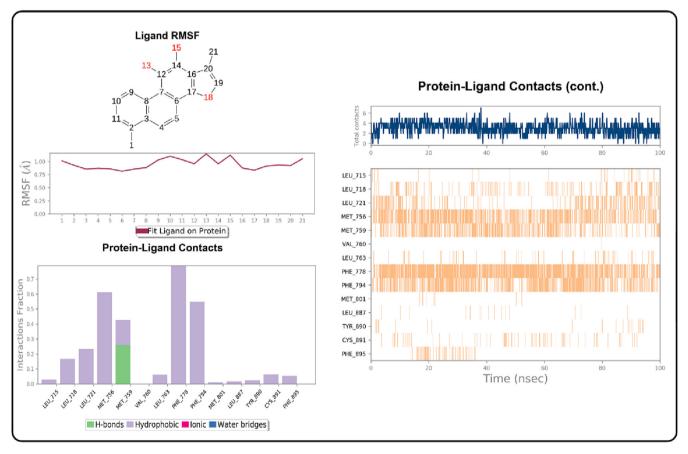


Fig. 11. Ligand RMSF and Protein Ligand Contacts with 20VH.

alterations in complex-ligand interaction. The Vander Waals surface area (MolSA) was found to be 252.36 Å² with an average value of 256.70 Å² and a standard deviation of 1.20. The solvent accessible surface area (SASA) was found to be 12.34 Å² with an average

value of 1.26 $Å^2$ and a standard deviation of 1.79. The molecular polar surface area (PSA) was found to be 82.10 $Å^2$ with an average value of 86.60 Å2 and standard deviation of 1.33. On the basis of the above analysis, the docked protein–ligand composite of 1E3K

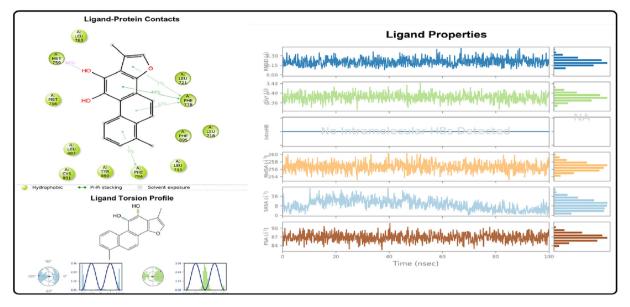


Fig. 12. Ligand-Protein contact with 20VH and interaction with different amino acids, Tanshinone-I torsion profile and Properties (PSA, SASA, MolSA, rGyr and RMSD).

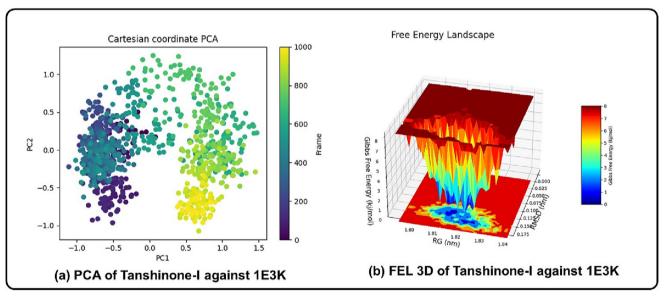


Fig. 13. Results of (a) Principle compnent analysis (b) FEL 3D for 1E3K.

with Tanshinone-I was found to be stable, and the docking result might be validated (Fig. 9). The protein secondary structure shows 57.96 % helix, 2.51 % strand, and 60.47 % protein secondary structure elements (SSE) (Fig. 7). Asn 719 and Cys 891 have shown the most hydrogen bonding, while Phe 794, Tyr 890, Arg 841 and Asp 855 had shown the most hydrophobic bonds. H-bonds have a mean value of 4.382 with a standard deviation of 0.974. There was no ionic or intramolecular hydrogen bond interaction. The torsion profile of ligands is shown in Fig. 9. This shows that there is no bond that can rotate at 3600 angles (Basu et al., 2020; El Ouafy et al., 2022).

Similarly, RMSD and RMSF calculations of Tanshinone-I with 20VH are shown in Fig. 10. The RMSD of the protein–ligand complex was as low as 0.08 Å and as high as 0.42 Å, with an average value of 0.20 Å and a standard deviation of 0.06. rGyr was found to be 3.33 Å, with a mean value of 3.38 Å and a standard deviation

of 0.02. (Fig. 11). RMSF values have been calculated to figure out how easily the residue can change shape if the complex and ligand interact. The average value of the MolSA was 256.62 Å2, and the standard deviation was 1.15. The average value of SASA was 8.83 Å2, and the standard deviation was 4.31. The average value of PSA was 86.84 Å2, and the standard deviation was 1.33. Based on the above analysis, the docked protein-ligand complex of 20VH with Tanshinone-I was found to be stable, which means that the docking result could be confirmed (Fig. 12). There is 54.04% helix, 2.11% strand, and 56.15% SSE in the protein's secondary structure (Fig. 10). Most hydrophobic bonds were made by Phe778, Phe794, Leu721, and Leu718. Most hydrogen bonds were made by MET 759. There was no interaction between ions and molecules through hydrogen bonds. Fig. 11 shows the ligands' torsion profiles. This proves that there is no bond that can turn 3600 degrees (Basu et al., 2020; El Ouafy et al., 2022; Miar et al., 2021).

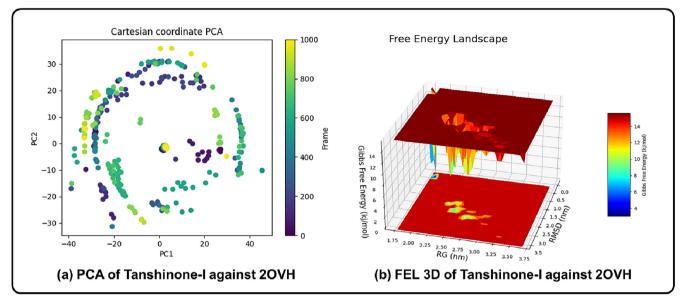


Fig. 14. Results of (a) Principle compnent analysis (b) FEL 3D for 20VH.

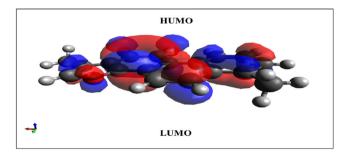


Fig. 15. Energy gap between HUMO and LUMO for Tanshinone-I.

Table 7

S. No.	Calculation (eV)	Tanshinone-I (eV)
1.	Е _{номо}	-5.9400
2.	E _{LUMO}	-3.1330
3.	ΔE	2.8070
4.	μ	-4.5365
5.	N	1.4035
6.	σ	0.7125
7.	I	5.9400
8.	Α	3.1330
9.	χ	4.5365
10.	ω	7.3316
11.	ΔNmax	3.2323
12.	Ν	3.4286

4.2. Results of PCA analysis

The PCA reveals an overall increase in protein during the simulation; consequently, differences in dynamics were produced along each of the 1002 eigenvectors. PCs are responsible for a significant portion of the global motion of a protein. Two-directional movements of PCs, also known as the first eigen vector (PC1) and the second eigen vector (PC2), were investigated. In Fig. 13A, it can be observed that the eigen values of HPR-Tanshinone-I fluctuate between -1.11 to 1.48 and -1.07 to 1.25 for PC1 and PC2, respectively (1E3K), and in Fig. 14A, the prog-tanshinone-I complex shows eigen values of -38.88 to -31.32 and -31.32 to 35.87 for PC1 and PC2, respectively (20VH). Overall, PCA results affirm that binding of the Tanshinone-I to 1E3K forms the most stable pro-

tein-ligand complex in comparison to Tanshinone-I to 20VH (Dalal et al., 2021).

4.3. Results of FEL analysis

Tanshinone-I complexes show a higher number of stable conformations, as shown in Fig. 13B and 14B. Additionally, the Tanshinone-I to 1E3K complex showed Gibbs free energy in the range of 0 to 8 kJ/mol and the Tanshinone-I to 20VH complex showed 0 to 14 kJ/mol. Moreover, 3D plots of free energy of Tanshinone-I to 1E3K and Tanshinone-I to 20VH complexes were generated to determine the RMSD and RG for favorable conformations of the complexes. As shown in Fig. 13B and 14B. Tanshinone-I to 1E3K complex exhibits lesser RMSD and RG as compared to Tanshinone-I to 20VH (Dalal et al., 2021).

4.4. DFT analysis

During molecular interactions, both the LUMO and the HOMO absorb electrons. The energy of the LUMO is related to the electron affinity (EA), while the energy of the HOMO is related to the ionization potential (IP). The HOMO-LUMO energy gap is helpful for figuring out how molecules can move electricity because it shows how the final charge transfer happens inside the molecule. A high orbital gap (HOMO-LUMO energy gap) means that it is energetically unfavorable to add an electron to the high-lying LUMO in order to remove electrons from the low-lying HOMO. This makes the molecule less reactive and more stable. Compounds that are more stable, like those with a large HOMO-LUMO energy gap, are less likely to change chemically than those with a smaller gap. Table 7 and Fig. 15 show that tanshinone-I ($\triangle E = 2.8070 \text{ eV}$) is a stable compound (Miar et al., 2021).

4.5. Possible mechanisms of selected best compound Tanshinone-I

Tanshinone I can cause ROS, apoptosis, autophagy (p62 accumulation), up-regulation of inositol requiring protein-1, enhancer-binding homologous protein, and p-c-Jun N-terminal kinase (p-JNK), and suppression of MMPs. B-cell leukemia/ lymphoma-2 (Bcl-2) expression can change LC3I to LC3II and cause apoptosis through Beclin-1 expression (seven mechanisms as shown in Fig. 16). It also induced Aurora A-p53, and surviving, sig-

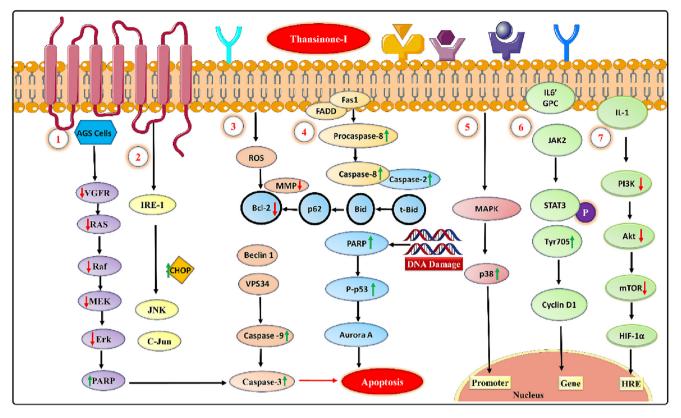


Fig. 16. Possible mechanism of Selected drug.

naling pathways lead to upregulation of PARP, which further stimulates p53 expression and reduces the Aurora A kinase level. Along with this, it also regulates caspase-3 and caspase-9, which in turn induce apoptosis in colorectal cancers. It also dissociates the procaspase-8 and suppresses the Bid, while t-Bid stimulates caspase-2. Through the downregulation of PI3K/Akt/m-TOR, breast cancer triggers apoptosis. It also acts through the MAPK pathway, which induces p38 to act as a promoter in the nucleus. Another pathway reported is JAK2, which further effects the gene through cyclin D1 and further stimulates the Tyr 70S. Another pathway involved is the downregulation of Bcl2 and MMP, which further promotes the degradation of nucleic acids in tumor cells (Naz et al., 2020; Taylor and Leppert, 2012; Pang et al., 2016; Gao et al., 2012; Kakisawa et al., 1969; Ma et al., 2015; Jang et al., 2003; Xu et al., 2018).

5. Conclusions

The present this research explores 28 phytochemicals and two different types of medicines were coupled to the 1E3K and 2OVH proteins. Tanshinone-I has demonstrated the highest level of activity for both of the proteins. Tanshinone-I has also been demonstrated through MD simulation research to form stable interactions with the receptors. In addition, the DFT study demonstrated that the molecule is not unstable. In general, these findings suggest that tanshinone-I might be useful as a medication in the treatment of fibroids. 1E3K is a steroidal agonist that modulates the prog pathway and can have an agonist or antagonistic effect on hPRs. Strong binding with 1E3K shows that it works to reduce the size of fibroid tumors instead of reducing heavy menstrual bleeding. Tanshinone-I with that of different ligands that bind to PR, such as full agonists and SPRMs. Even small changes to the structure of the parent molecule can make a big difference in how the derivative works. Non-steroidal SPERMs are being made all the time, like the recently reported 3-aryl indoles. Due to the fact that it works in different ways against different types of cancer, this drug has the potential to solve the problem either on its own or in combination with other drugs. Tanshinone-I may be the focus of future drug development strategies for fibroids.

CRediT authorship contribution statement

Abhishek Tiwari: Writing – review & editing, Writing – original draft, Software, Conceptualization. Varsha Tiwari: Writing – original draft, Software, Conceptualization. Ajay Sharma: Software. Deependra Singh: Writing – original draft. Manju Singh Rawat: Writing – original draft. Manish Kumar: Writing – review & editing. Abdulsalam Alhalmi: Writing – review & editing. Tarun Virmani: Writing – review & editing. Girish Mittal: Writing -review & editing. Resu Virmani: Writing - review & editing. Ramzi A.Mothana: Writing – review & editing. Omar M. Noman: Writing -review & editing. Mohammad Alali S: Writing -review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jsps.2023.05.002.

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Exploration of crystal structure, and luminescence behaviors of Terbium-activated CaWO₄ phosphor

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ABSTRACT

This manuscript includes structural, optical, photoluminescence, and thermoluminescence behaviors of Terbium incorporated CaWO₄ samples with nominal compositions of Ca_{1-x}Tb_{2x/3}WO₄ (x = 0.01, 0.02, 0.03, 0.04, 0.05) prepared by the traditional solid-state reaction route. Results found from the Rietveld refinements of X-ray diffraction patterns confirmed that all the samples have tetragonal crystal structures with 14₁/a space group. The variation of unit cell volume with the compositions shows an anomaly at x = 0.03 Band gap energy values of these synthesized samples are found from the UV-Visible absorbance spectra with increasing order. Photoluminescence behaviors, as well as the FWHM values, are analyzed from the excitation along with the emission spectra. Critical quenching concentration at x = 0.03 with a critical energy transfer distance of ~ 20 Å caused by the dipole-dipole interactions is found in these spectra. CIE Chromaticity coordinates are indicated the green emission color of all the prepared samples with high color purity, correlated color temperature, color rendering index, and luminous efficiency of radiation values. Quantum efficiency of the material with x = 0.03 The output does is described as the lower UV dosimetry and second-order kinetics of the material.

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1. Introduction

Over the last few decades, phosphors having luminescent nature are used in the light emitting diodes rather than the conventional lighting . They have good luminescence properties, different types of devices colors of emission, considerable efficiencies, excellent operating conditions, fewer pollutions, low power utilization, wide uses in lighting applications, and many more important features . Therefore, several pieces of research are going on by scientists to synthesize phosphors with improved luminescence properties. Material scientists are involved to explore these types of phosphors like nitrates, molybdates, silicates, aluminates, oxides, and tungstates with enhanced pho-. It has been studied that metal tungstates toluminescence behaviors with scheelite structures have wide emission ranges, good efficiencies, and self-activating behaviors and can be utilized in the lighting devices such as LEDs, FEDs, and display screens and all the metal tungstates, Calcium tungstates have prominent properties in photoluminescence and thermoluminescence spectroscopy, blue emission color with extensive emission range in UV Visible region, a great/value in color purity & quantum efficiency, less optical loss, appropriately correlated color temperature value —. Hence Calcium tungstate acts as a suitable host material for the light emitting diodes —. Moreover, past investigations are revealed that doping of different rare earth materials with CaWO₄ can be improved luminescence properties by producing various paths for energy transfer and reducing the critical quenching concentration of the material

Photohuminescence behaviors with orange-red emission color of Sm doped CaWO₄ are discussed extensively by Kam et al. Du et al. explained the yellow emission color of Dy doped CaWO₄ and also then optical behaviors. Zhang et al. prepared En and D doped CaWO₄ phosphors and investigated that they have red as γ of as group emission colors respectively. However, the reason the bound code γ can be

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Type Ia supernovae SN 2013bz, PSN J0910 + 5003, and ASASSN-16ex: similar to 09dc-like?

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ABSTRACT

We present optical photometric and spectroscopic studies of three supernovae (SNe): SN 2013bz, PSN J0910 + 5003, and ASASSN-16ex (SN 2016ccj). UV-optical photometric data of ASASSN-16ex obtained with the Swift Ultraviolet/Optical Telescope (UVOT) are also analysed. These objects were initially classified as 09dc-like type Ia SNe. The decline-rate parameters $(\Delta m_{15}(B)_{true})$ are derived as 0.92 ± 0.04 (SN 2013bz), 0.70 ± 0.05 (PSN J0910 + 5003), and 0.73 ± 0.03 (ASASSN-16ex). The estimated B-band absolute magnitudes at maximum, -19.61 ± 0.20 mag for SN 2013bz, -19.44 ± 0.20 mag for PSN J0910 + 5003, and -19.78 ± 0.20 mag for ASASSN-16ex, indicate that all three objects are relatively bright. The peak bolometric luminosities for these objects are derived as $\log L_{bol}^{max} = 43.38 \pm 0.07$, 43.26 ± 0.07 , and $43.40 \pm 0.06 \, \mathrm{erg \, s^{-1}}$, respectively. The spectral and velocity evolution of SN 2013bz is similar to that of a normal SN Ia, hence it appears to be a luminous, normal type Ia supernova. On the other hand, the light curves of PSN J0910 + 5003 and ASASSN-16ex are broad and exhibit properties similar to 09dc-like SNe Ia. Their spectroscopic evolution shows similarity with 09dc-like SNe: strong CII lines are seen in the pre-maximum spectra of these two events. Their photospheric velocity evolution is similar to SN 2006gz. Further, in the UV bands, ASASSN-16ex is very blue, like other 09dc-like SNe Ia.

Key words: techniques: photometric -- techniques: spectroscopic -- supernovae: general -- supernovae: individual: SN 2013bz -supernovae: individual: PSN J0910 + 5003-supernovae: individual: ASASSN-16ex.

1 INTRODUCTION

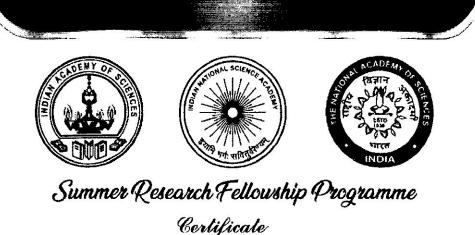
Thermonuclear supernovae are an important class of supernovae (SNe): the progenitors are low-mass stars found in elliptical as well as spiral galaxies. They are commonly known as Type Ia SNe (SNe Ia) and populate the brighter side of the luminosity distribution of SNe. Most SNe Ia, referred to as 'normal SNe Ia', display uniform spectral and light-curve properties. Their luminosity is correlated with the width of their light curve (Phillips 1993; Phillips et al. 1999) and hence they are considered standardizable candles. This uniformity and high luminosity make them a vital probe for studying cosmic evolution (Riess et al. 1998; Perlmutter et al. 1999). SNe Ia are the primary source of iron-group elements (IGEs) and hence play an important role in enriching the interstellar medium (ISM) with IGEs (Matteucci & Greggio 1986; Matteucci et al. 2009; Nomoto, Kobayashi & Tominaga 2013).

Our understanding of the progenitor and explosion mechanism giving rise to these events still needs to be completed. From the theoretical and observational work, it is inferred that thermonuclear disruption of a carbon-oxygen (C/O) white dwarf (WD) in a binary system results in a Type Ia explosion (Hoyle & Fowler 1960; see Maoz, Mannucci & Nelemans 2014; Jha, Maguire & Sullivan 2019

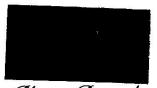
* E-mail: shrutikatiwari7@gmail.com (ST): nkchakradhari@gmail.com (NC); dks@iiap.res.in (DS)

for reviews). There are two possible progenitor models suggested for a WD to explode. In the first one, a WD accretes matter from a non-degenerate star, known as the single-degenerate (SD) model (Whelan & Iben 1973). In the double-degenerate (DD) model, the explosion results from the merger of two WDs (Iben & Tutukov 1984; Webbink 1984). Most SNe Ia are considered to be an explosion of a Chandrasekhar-mass WD (Mazzali et al. 2007) via delayed detonation (Khokhlov 1991). However, if the accumulated material is He-rich, the explosion can occur at a sub-Chandrasekhar mass through double detonation. With sufficiently rapid He accretion on the surface of a C/O WD, a detonation is first initiated within the helium layer. The emanating shock wave propagates through the WD and triggers carbon detonation at the centre of the WD (Woosley & Weaver 1994; Woosley & Kasen 2011; Ruiter et al. 2014; Tanikawa, Nomoto & Nakasato 2018). The donor star could be either a nondegenerate He star (SD channel), another C/O WD with He in the outer layer, or a He WD (DD channel). This mechanism can explain normal and fast-declining SNe Ia of different brightness distributions (Pakmor et al. 2013). Currently, it is difficult to identify which SN results from which channel (see Livio & Mazzali 2018; Wang 2018; Soker 2019; Ruiter 2020, for reviews).

With the increasing number of well-studied SNe Ia, it became clear that there is a considerable spread in the luminosity of SNe Ia. There are objects populating both the higher and lower luminosity end of normal objects (Li et al. 2011). Some have extreme properties



This is to certify that Mr Nand Kumar Ghakradhari worked on a project entitled "Study of Type Ia Supernova SN 2018bz" during June- August 2022 as a Summer Research Fellow under the supervision of Lrof. D. K. Sahu, Indian Institute of Astrophysics, Bengaluru. The Summer Research Fellowship Lrogram is jointly sponsored by IASc (Bengaluru), INSA (New Delhi) and NAST (Lrayagraj).



Llace: Bengaluru Date: 19-09-2022

Phone

L. K Das Chairman, Science Education **Lane**l

INDIAN ACADEMY OF SCIENCES, C. V. RAMAN AVENUE, POST BOX No. 8005, RAMAN RESEARCH INSTITUTE CAMPUS, SADASHIVANAGAR P.O., BENGALURU 560 080, INDIA Commemorating the monumental occasion "75 years of India's Independence: Azadi ka Amrit Mahotsay"

Certificate of Participation

This is to certify that,

JAY SHANKAR PRASAD SAHU

has successfully participated and completed a project in ARIES Training School in Observational Astronomy (ATSOA) - 2023, held from 17th - 28th April, 2023.

Date : 28th April, 2023

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Dr. Kuntal Misra Co-ordinator ATSOA-2023

Amrit Mahotsav

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Commemorating the monumental occasion "75 yoars of India's Independence: Azadi ka Amrit Mahotsav"

Certificate of Participation

This is to certify that,

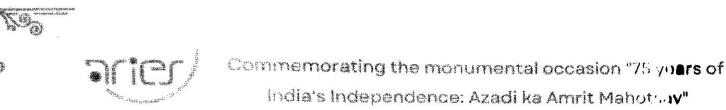
NIRAJ KUMAR SAHU

has successfully participated and completed a project in ARIES Training School in Observational Astronomy (ATSOA) - 2023, held from 17th - 28th April, 2023.

Date : 28th April, 2023

Kintal Nisra

Dr. Kuntal Misra Co-ordinator ATSOA-2023





This is to certify that,

UNNATI PANDEY

has successfully participated and completed a project in ARIES Training School in Observational Astronomy (ATSOA) - 2023, held from 17th - 28th April, 2023.

Kintal Misra

Dr. Kuntal Misra Co-ordinator ATSOA-2023

Date : 28th April, 2023

Commemorating the monumental occasion "75 years of India's Independence: Azadi ka Amrit Mahotsuv"

Date: 28th April, 2023

the af Participation

This is to certify that,

YOJASHWI DEWANGAN

Kintal Nisr

Co-ordinator A SUA

Dr. Kuntal Misra

has successfully participated and completed a project in ARIES Training School in Observational Astronomy (ATSOA) - 2023, held from 17th - 28th April, 2023.



Report on 'Karuna Project'

The two month internship programme was organized by SoS in Psychology, Pt. Ravishankar Shukla Univversity, Raipur (C.G.), in the collaboration with the 'Karuna Project', a National organization working for spreading awareness about Mental Health. At first, students were given seven days training for this programme. Where, they learned to sensitized adolescents for their mental health and techniques to keep it maintained. After completion of the internship the certificate and monetary prize of 2500 rupees given to those students who participated in internship programme based on mental health awareness by 'Karuna Project' and did field work. Students were facilitated by certificate by Mrs. Nidhi Nathaniel (America), Director of 'Karuna Project' programme and notable alumni of the SoS. Under this national project **2**7 students of the department, visited 75 schools of Chhattisgarh state and spread awareness about mental health among 4000 students.

Prof. Prabhavati Shukla Head, SoS in Psychology, Pt. Ravishankar Shukla University, Raipur (C.G.)

> Professor & Head · School of Studies in Psychology Pt. Ravishankar Shukla University RAIPUR (C.G.)

WWW.projectkaruna.org





1 of 2

Letter of Collaboration

To,

Dr. P. Shukla HOD Psychology Pt. Ravishankar University Raipur, CG

Madam,

We would like to extend a collaboration proposal with your prestigious department. If given this opportunity we would like to offer an internship program for your students to create an ongoing community outreach program on mental health awareness & wellbeing.

This program will equip your students to take up responsibility as young citizens in creating awareness in the community.

Here are the details of the internship.

<u>Purpose</u>: To create an outreach internship program to reach out to the high schoolers of our city (and nearby towns in CG) and educate them about mental health awareness and wellbeing.

www.projectkaruna.org

The volunteers will be given in-person and online training by the team of Project Karuna. The volunteers will be conducting in-person educational sessions in the schools of Raipur and designated/chosen cities.

<u>Timeline</u> : 3-month internship, The trainees can work at their own pace. <u>Honorarium</u>: The volunteers will be given 800 rupees for each school they cover. This will be provided at the end of their internship.

<u>Process</u>: The internship step-by-step guide is attached to this letter for the details.

<u>Certificate:</u> A collaborative certificate of completion will be provided at the end of the academic year.

We eagerly look forward for a positive response from your end.

Thanks & Regards,

Widhi Nathanel

Nidhi Nathaniel Founder - Project Karuna <u>info@projectkaruna.org</u> <u>www.projectkaruna.org</u> Date: 1/5/2023

Accepted by:

Dr. P. Shukla HOD (Psychology) Pt. Ravishankar University Raipur, CG Date: 1/5/2023

Project Karuna

Transforming Mental Health through Education, Counseling and Nutritional Healing

Mission : H: HEALTH E: Education A: Awareness L: Living

Karuna seeks to establish a strategic research and evidence based mental health awareness, prevention and early intervention program among various school age children ranging between 13-17 years of age.

Statistics show that the onset of major psychological disorders like depression and anxiety starts at this age which may lead to serious issues in later part of their lives. Therefore, Karuna seeks to bring this program to various educational institutions with focus across this age group.

Much work has been done towards cure and prevention of mental health, yet there exists a huge gap between the need and the provision.

This is in part, due to the lack of awareness and education regarding both the prevention and detection of mental health issues as well as the available solutions. Karuna seeks to fill this gap.

Karuna uses a two-pronged approach to mental health. Our core belief hinges on the mind body connection- a sound mind resides in a sound body and vice versa.Karuna seeks to target detection of neurotic disorders at early age and intervene before these become major issues in adult life.

Karuna recognizes the need to refer out to specialized professionals, when interventions outside its scope are required.

1

PROJECT KARUNA 2023 SCHOOLS COVERED

CHANDAN (10)

1. दिन बुधवार, दिनांक ०५/०७/२०२३, समय १३:५० से १४:५८

शाला का नाम _ सरस्वती शिक्षा मन्दिर हायर सेकेण्डरी स्कूल, छत्तीसगढ़ नगर टिकरापारा रायपुर छत्तीसगढ़ ४९२००१

2. दिन: शुक्रवार, दिनांक: 14/07/2023, समय: 03:45 से 05:00pm

School: Shasakiy uchhtar Madhyamik Shala Pyarelal Hindu High School Raipur Chhattisgarh

3.दिन: शनिवार, दिनांक: 15/07/2023, समय- 12:00- 13:35

School: MMD english higher secondary school chhattisgarh nagar Raipur

4. दिन: मंगलवार, दिनांक: 18/07/2023, समय: 04:00 से 05:00,

School: J.N. Pandey, Raipur

5.दिन: ब्धवार, दिनांक: 19/07/2023

School: नूतन शासकीय उच्चतर माध्यमिक विद्यालय, रायपुर

6.Date: 08/08/2023, School: Govt. H. S. School, Sanjay Nagar

Bhulla Professor & Head Professor & Head dies in Psychology kar Shukla University School of Stu Pt. Ravishan

7.दिन: शनिवार,Date: 12/08/2023, School: A.K memorial school, Byranbajaar

8.Date: - 12/08/2023, School name: - Sant Paul hr. Sec. School Byron bazar Raipur, no. Of students: - 42

9.School name: - Disha convent school Dunda, date: - 21/08/2023,No. Of students:- 23

10.Day - Wednesday, Date - 06/09/23, School name - St. Paul Higher Secondary school, Raipur

ANURAG (3)

1.दिनः शनिवार,दिनांकः 08/07/2023, समयः 10:30 से 11:40 शालाकानामः पवनपुत्रविद्यामंदिरउच्चतरमाध्यमिकविद्यालय ,कृषकनगर , जोरा, रायपुर , छत्तीसगढ़

2.दिनःमंगलवार, दिनांक: 18/07/2023,पालियों कीसंख्याःदोपालीमेंपहलीपाली (विज्ञानएवंकृषिकेछात्र)

दूसरीपाली(वाणिज्यएवंकलाकेछात्र)समयः 12:00 से 01:15 एवं 01:50से 03:10,School: शासकीयउच्चतरमाध्यमिकविद्यालयजोरा, रायपुर , छत्तीसगढ़ 3.दिन: बुधवार, दिनांक: 23/08/2023,School:कामधेनुपब्लिकस्कूल, तुलसीडीह, रायगढ

TANU (3)

1.Day: Monday, Date: 10/07/2023, Time: 3 to 4 pm,

School:Dr. Ram Manohar Lohia Govt. Higher Secondary school, Santoshi Nagar, Raipur

2.Day: Satuday, Date: 22/07/2023, School: Govt. H. Sec. School,
Beterenga, Raipur, Session 1- 9am -10.30, Session 2- 10.45-1130. am
3.Day: Tuesday, Date: 04/09/2023, School: Higher Secondary School
Mathpurena

Aadya (2)

1.Day: Wednesday, Date: 12/07/2023, Time: 01:00 to 02:10 pmSchool: KB Girls H.S. School, Santoshi Nagar Chowk, Old Dhamtari Road, Raipur(CG)

2.Day: Thursday, Date: 20/07/2023, Time: 02:15 to 03:30

School: शासकीयहाईस्कूल, डूण्डा, रायपुर

Pradipti (2)

1.दिनः गुरुवार,दिनांकः 13/07/2023, समयः 02:30 से 04:00 शालाकानामः गणपतसिंधीशासकीयविद्यालय , पुरानीबस्ती , रायपुर , छत्तीसगढ़ 2.दिनः शुक्रवार,दिनांकः 14/07/2023,समयः 02:00 से 03:55 School: Government higher secondary school MathparaRaipur Chhattisgarh

Reena (3)

1.दिनः शुक्रवार, दिनांकः 14/07/2023, समयः 01:00 pm School: डॉशोभारामदेवांगनशासकीयउच्चतरमाध्यमिकविद्यालयधमतरी 2.दिनः शनिवार, दिनांकः 15/07/2023, समयः 08:30 School: Nutan higher Secondary School Dhamtari 3.दिनः शनिवार, दिनांकः 15/07/2023, समयः 10: 30 School:शासकीयनत्थूजीजगतापनगरपालिकनिगम उ माध्यविधमतरी

Sheetal (3)

1.Day: Saturday, Date: 15/07/23, Time: 01:00 to 02: 30 School: शास. हाईस्कूलमलपुरीकलाविख़.धमधा . जि. दुर्गछ.ग. 2.Day: Saturday, Date: 15/07/23,Time: 09:00 to 10:00 School: Govt Higher secondary school kapasada Durg .C.G 3.Day: Saturday, Date: scheduled for 09/09/23 School: Maharshi Dayanand Arya Hr.Sec. School Tatibandh, Raipur (C.G.)

Sushma (3)

1.दिन: शनिवार, दिनांक : 15/07/2023, समय: 03:00 से 04:00

School:माधवरावसप्रेशासकीयउत्कृष्टहिन्दीमाध्यमविधालयबूढापारा, रायपुर

2.Day: Saturday, Date: 05/08/2023, School: Saraswati sishuH.S.School, DDU nagar Raipur

3.Day: Friday, Date: 08/09/2023, शासकीयउच्च. माध्य. विधालय प.

रविशंकरशुक्लविश्वविद्यालयपरिसर, रायपुर (छ.ग.)

Kesari ji (3)

1.Day: Saturday, date: 14/07/2023, Time: afternoon School: Shivom vidhyapeeth Raipur.

2.Day: Saturday, Date: 22/07/2023, School: Pt. Girja Shankar school Raipur.

3.Day: Tuesday, Date: 08/08/2023School: R.D. Tiwari School, Amapara

Purneshwari (2)

1दिनःमंगलवार,Date: 18/07/2023,School: शासकीयउच्चतरमाध्यमिकशालागुमा, धरसीवा 2दिन: मंगलवार, Date: 18/07/2023School: शासकीयउच्चतरमाध्यमिकविद्यालयहौरापुर

Manisha (3)

1.दिन: मंगलवार, Date: 18/07/2023

School: Municipal Corporation H. Sec School , Tikrapara , Raipur

2.Day: Friday, Date: 21/07/2023, Time: 01:30 School: pt Girja Sankar govt H. Sec. Raipur.

3.Day: Saturday, Date: 22/07/2023, Time: 12.30-1.30, School: Dakshina Murti Vidyapeeth Changorabhata Raipur

Supriya (2)

1.दिन: ब्धवार, Date: 19/07/2023,समय: 04:00

School: Laxminarayan Girl's Higher Secondary School, Gurukul parisar ,kalibadi Road , Raipur (C.G.)

2.Day: Wednesday, Date: - 20/09/2023, School Name: Leela's public school, Motipura (jamgaon Road), Durg (C.G.)

Pinky (3)

1.दिन- बुधवार, दिनांक- 19/07/23, school- शास. उच्च. माध्य. विद्या. जांजग, सक्ती

2.दिन- गुरुवार, दिनांक- 20/07/23, समय- 12:30, School- शास. हाईस्कूल,नवापाराकुर्द, सक्ती

3.दिन- शुक्रवार, दिनांक- 21/07/23, समय- 12:30, School- शास. हाईस्कूल, टेमार, सक्ती

Shruti (3)

1.Day: Friday, Date: 21/07/2023, Time: 12:45pm, School: Vardhman the school Krishna Nagar

2.Day: Thursday, Date: 27/07/2023, School:स्वेताविद्यामंदिर

3.दिन: शुक्रवार, तारीख: 22/09/2023, School:

पूर्वमाध्यमिकशालाभाठागांवरायपुरछत्तीसगढ़.

Adyasa (2)

1.Day:शनिवार, Date: 22/07/2023, School: Mother Teresa School (Katora Talab)

2.Day: Wednesday, Date: 13/09/2023, School: Chhattisgarh Public Hr Secondary School.

Priyanka (2)

1.Day: Monday, Date: 24/07/2023, School: Govt. RMSA High School SirrikalaFingheshwar date -24/07/23

2.Day: Tuesday, Date: 22/08/2023, School: govt. higher secondary School Atari (Raipur)

Akash Minj (2)

Day: Tuesday, Date: 25/07/2023, School: Govt. H.H.S Saraitikra
 Day: Tuesday, Date: 25/07/2023School: Govt. Hr. Sec. school
 Rampur

Sweta (3)

1.Day: Monday, Date: 25/07/2023, Address: Maa Bharti Vidyalaya Gudhiyari Raipur Chhattisgarh 2.Day: Thursday,Date : 27/07/23,School : SashishalaNagar Nigam
Kanya Uchhattar Madhyamik Shala Gudhiyari Raipur Chhattisgarh
3.Day: Saturday, Date: 16/09/2023, Name of the school - Govt.
Higher Secondary School Trimurty Nagar Raipur CG

Sudarshan (3)

1. First schools:Day- Wednesday, Permission date- 24-07-23, Session date26-07-23

Time 12.30 to 1.30, Govt. H. S. School Ghumka

2. Second school:Day-Wednesday, Permission date-26-07-23, Session date-26-07-23

Time- 3 to 4 o'clock, Govt. H. S. School Patewa

3.Day: Wednesday, Date: 13/09/2023, School: Govt H School Harduva, Rajnandgaon

Sanchita (1)

1.Day: Saturday, Date:05/08/2023, School Name - Holy Mother Hr Sec School, Sunder Nagar.

Pravin

1.Date_07-08-2023 ,Day: Monday, Time_11am-12.05pm, School_G. H. S. S. Jhalmla(झलमला) Balod. 2.Day: Friday Date: 15/09/2023, Time- 12.30--1.30pm, School-स्वामीआत्मानंदउत्कृष्टहिंदीमाध्यमविद्यालयबलोद

Tejaswani (2)

1.Day -Monday, Date - 14/08/2023, Time 11:00 to 12:00School - Bharat Devangangovt higher secondary school KharoraRaipur Chhattisgarh

2.Day – Monday, Date - 21/08/ 2023, Time - 01:00 to 02:00 pm

School - Govt. High School Boriya Khurd RaipurChhattisgarh

Dhaneswari (2)

1.Day: Tuesday,Date: 22/08/2023School: Govt. H. S. School, Rakhi, Raipur

2.Day: Wednesday, Date: 23/08/2023, School: High secondary school pardadaraipur

Krishna ma'am (2)

1.Day: Friday, Date: 25/08/2023, School: Sant DyaneshwarVidyalay, Raipur Chhattisgarh 2.Day: Saturday, Date: 09/09/2023, Name of School :Model English Higher Secondary School, civil lines, Raipur, CG.

Muralidhar (2)

1.Day: Monday, Date: 28/08/2023, School: Vinayam Hr Sec School, Gudhiyan Raipur

2.Day: Tuesday, Date: 29/08/2023School: Novnihal Public School, Ekta Nagar, Gudhiyari, Raipur

Anushka (3)

1.Day: Tuesday, Date: 05/09/23

School: Sunbeam Convent Senior Secondary School, Anuppur, Madhya Pradesh

2.Day: Friday, Date: 08/09/2023,School: Eklavya Model Residential School, Anuppur, MP

3.Day: Saturday, Date: 09/09/2023

School: Bethel Mission Senior Secondary School, Anuppur, MP

Kajal (3)

1. Day: Monday, Date: 11/09/23, School: Govt School Amleshwar, Patan, Durg.

2.Day: Thursday, Date: 14/08/2023, School: Govt H.S. School Sankara, Patan, Durg.

3.Day: Saturday, Date: 16/09/2023

School: Swami Atmanand Excellence English Medium School, Amleshwar, Patan, Durg.















































Workshop on Improvised Pedagogies for Effective Teahcing & Learning with reference to Natioal Education Policy 2020

Organized by Department of Teacher Education, Pt. Ravishankar Shukla University, Raipur In Consultation With State Council of Educational Research & Training (SCERT) Chhattisgarh, Raipur January 27-30, 2023

Workshop Schedule

Day 1		
Time	Topics/ Agenda	Facilitation
09.30-10.30	Registration	
10.30 -10.45	Welcome, Context and Objectives	Prof. C.D. Agashe Director, Department of Teacher Education Pt. Ravishankar Shukla University, Raipur, Chhattisgarh
10.45-11.15	Inaugural Speech	Prof. K.C. Verma Vice Chancellor, Pt. Ravishankar Shukla University, Raipur
11.15-11.30	Tea Break	
11.30-01.00	Nava Jatan (Competency Based Education in Schools)	Shri Sunil Mishra, Senior Faculty, SCERT
01.00-02.00	Lunch	
02.00-03.30	Essential Components of the Pedagogy of Science	Smt. M.Vijaya Lakshmi, HoD, Pedagogy of Physical Sciences & Assistant Professor, CTE, Raipur
03.30-04.00	Open Discussion/ Suggestions/ Queries	Faculty Members, Department of Teacher Education, RSU, Raipur
la se la castra	Close of Day 1	• • • • • • • • • • • • • • • • • • •

Director \$2 Institute of Teachers Education Pt. Ravishankar Shukla University Raipur (C.G.)



Day 2				
Time	Topics/ Agenda	Facilitation		
10.00-11.00	Pedagogical Leadership	Shri Alok K Sharma, State Nodal Officer, Implementation of NEP 2020 & Senior Faculty, SCERT		
11.00 -12.00	Experiential Learning & 21 st Century Skills	Dr. Neelam Arora, Senior Faculty, SCERT		
12.00-01.00	Conceptualizing the Art Based Pedagogy	Smt. Preeti Singh, Senior Faculty, SCERT		
01.00-02.00	Lunch			
2.00-03.30	An Instructional Working Model (TLM) for Teaching Learning Strategies	Smt. Preeti Jain, Lecturer, Govt. HSS, Nagpura, Durg		
03.30-04.30	The Culture of Assessment: Preparation of common norms, standards and guidelines for assessment and evaluation as per NEP 2020	Smt. Vidya Dange, Senior Faculty, SCERT		
04.30-05.00	Open Discussion/ Suggestions/ Queries	Faculty Members, Department of Teacher Education, RSU, Raipur		
Close of Day 2				

Day 3

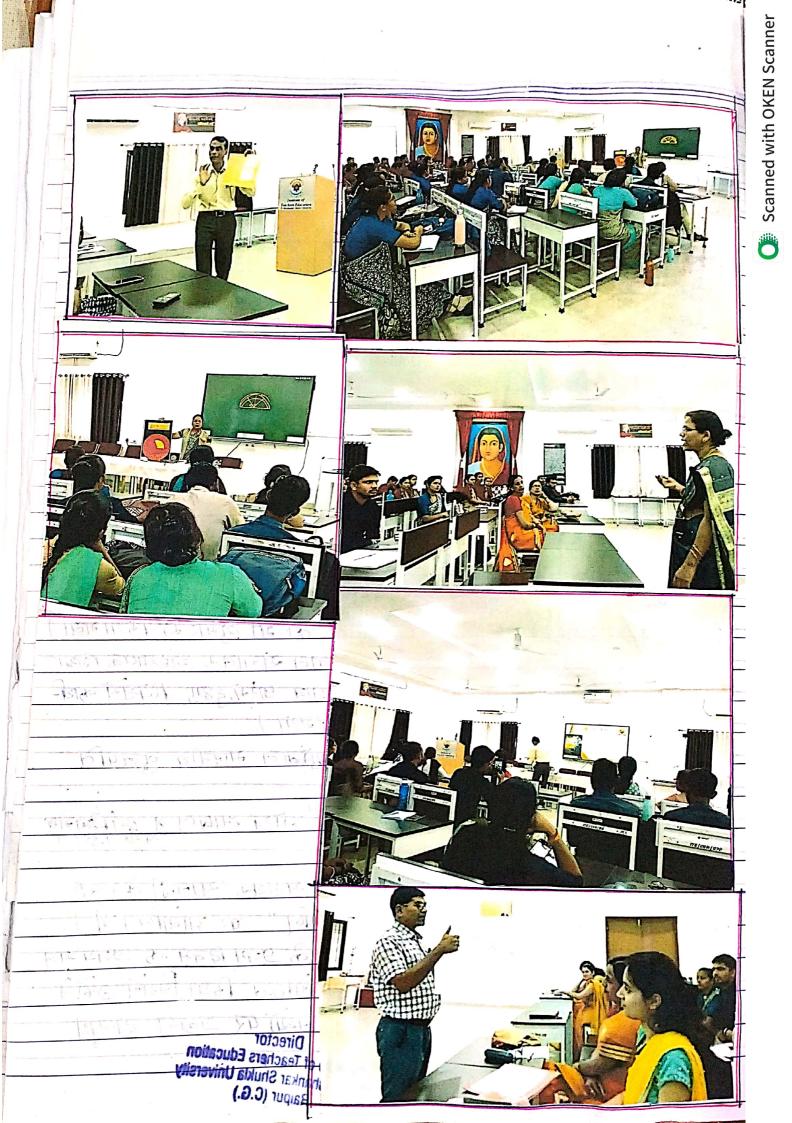
Time	Topics/ Agenda	Facilitation
10.00-12.00	Online Teaching and Learning in the 21st century; Integration of Technology for learner-centric and Open Educational Resources	Shri Alok K Sharma, State Nodal Officer, Implementation of NEP 2020 & Senior Faculty, SCERT
		Shri Saurav Mohanti, Consultant, TISS Mumbai
12.00 -01.00	Theories and Techniques of Teaching of Language	Dr. B. Raghu, Assistant Director, District Education Office, Durg
01.00-02.00	Lunch	
02.00-03.30	Essential Components of the Pedagogy of Mathematics	Shri C K Verma Lecturer, J R Dani Govt. Girls Higher Secondary School, Raipur
03.30-04.00	Open Discussion/ Suggestions/ Queries	Faculty Members, Department of Teacher Education, RSU, Raipur
04.00-04.30	Way Forward & Valediction	
V star a	Close of Day 3	Ito

Director Department of Teacher Education Pt. Ravishankar Shukla University Raipur, Chhattisgarh

Time	Topics/ Agenda	Facilitation
10.00-12.00	Online Teaching and Learning in the 21st century; Integration of Technology for learner- centric and Open Educational Resources	
12.00-12.30	Open Discussion/ Suggestions/ Queries	Faculty Members, Department of Teacher Education, RSU, Raipur
	Close of Day 4	NA.

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Director Department of Teacher Education Pt. Ravishankar Shukla University Raipur, Chhattisgarh







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CERTIFICATE OF PARTICIPATION

Mr. / MS. HEENA

M.Ed 2nd SEM.

Participated in 3 days workshop on

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"Improvised model construction for

Teaching aids"

27th to 29th January 2023

Organized by Institute of Teachers Education, Pt. Ravishankar Shukla

University Raipur,

In collaboration with S.C.E.R.T. Raipur, (C.G.)

Prof. C.D. Agashe Director Institute of Teachers Education