

# **E-Proceeding**

Paradigm Shift towards Sustainable Growth in Chemical and Biological Sciences

11th & 12th January, 2024





Organized by Department of Chemistry and Forensic Science & Department of Life Sciences Bhakta Kavi Narsinh Mehta University, Junagadh (Gujarat) India Jointly organized with Indian Society of Chemists and Biologists, Lucknow (Uttar Pradesh) India

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29th ISCB International Conference ISCBC-2024











Proceedings of International Conference on Paradigm Shift towards Sustainable Growth in Chemical and Biological Sciences (11th & 12th January, 2024) organized by Department of Chemistry and Forensic Science & Department of Life Sciences, India Society of Chemists and Biologists (Junagadh Chapter), Bhakta Kavi Narsinh Mehta University, Junagadh, Gujarat, INDIA & Sponsored by Gujarat State Biotechnology Mission; Department of Science & Technology, Students Startup and Innovation Policy (SSIP), Anlon Healthcare Pvt. Ltd., SNJ Pvt. Ltd. and Krishna Scientific Traders.

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Compiled in India by: Meet Rupapara, Gautam Makwana, Ashish Rudani, Akhil Vaghasiya, Nihar Jagatiya Department of Chemistry and Forensic Science & Department of Life Sciences, India Society of Chemists and Biologists (Junagadh Chapter), Bhakta Kavi Narsinh Mehta University, Junagadh, Gujarat, INDIA

|                         |  |  |  | ISCBC-2024  |    |
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| ſ                       | DLS, BKNMU<br>Prof. Firoz Shaikh<br>DOL, BKNMU<br>Prof. Vishal Joshi | Dr. Sandi<br>DLS, Bk<br>Conve<br>Dr. Mrunal<br>DOCFS, E<br>OCCAL Organiz<br>Prof. Jaya<br>DSS, E<br>Dr. Jitendi<br>Systems Mar<br>Dr. Rajesh E | p Gamit<br>KNMU<br><b>Ener</b><br>Ambasana<br>3KNMU<br><b>Eing Commi</b><br>asinh Zala<br>3KNMU<br>ra Bhalodia | Dr. Rashmi Patel<br>DOCFS, BKNMU<br>ttee<br>Prof. Bhavsinh Dodiya<br>DOCM, BKNMU<br>Dr. Kirtiba Vaghela<br>Chief Account Officer, BKNM<br>Dr. V. T. Thanki, Principal | 1U |

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# Prof. (Dr.) Chetan Trivedi

Vice Chancellor, Bhakta Kavi Narsinh Mehta University, Junagadh



Bhakta Kavi Narsinh Mehta University Junagadh established under the GUJARAT ACT NO. 23 of 2015, has emerged as a premier educational institute for the learning and skill enhancement covering areas of science, arts, humanities, law and medical courses. It is also famous for its location where rich biological diversity of plants, animals and microorganisms sited in the lap of mountain Girnar as well as Gir Sanctury for lions.

Since, June 2017, five post graduate departments have been started in the university namely Department of Life Sciences, Department of Chemistry & Forensic Sciences, Department of Commerce & Management, Department of Social sciences, and Department of English. There are more than 150 affiliated colleges and more than 50,000 students are pursuing their degrees in various disciplines of sciences, commerce, and arts. Since inception, Bhakta Kavi Narsinh Mehta University is thriving for excellence in education through plethora of teaching-learning and research activities providing conducive environment for the students to create their future and placement opportunities.

The international conference (ISCBC-2024) organized by Department of Chemistry & Forensic Sciences and Department of Life Sciences, Bhakta Kavi Narsinh Mehta University, in association with Indian Society of Chemists and Biologist (Lucknow) entitled 'Paradigm Shift Towards Sustainable Growth in Chemical And Biological Sciences' aptly reflects the trends and needs of multidisciplinary research for the Sustainable Growth of the country.

I am sure that this international conference will provide a platform for students, experts, researchers, academicians, industry leaders, and aspiring young minds converge to explore, share, and celebrate the latest advancements in these intricate domains. At its core, this conference aims to transcend traditional disciplinary boundaries and foster an environment of collaboration to envisage the dream of 'Atma Nirbhar Bharat'.



**Prof. Anamik Shah** Ex-Vice Chancellor, Gujarat Vidyapeeth, Ahmedabad, Gujarat, INDIA President, ISCB



**Prof. P.M.S. Chauhan** Ex-Chief Scientist and Professor (AcSIR), CDRI, Lucknow, INDIA General Secretary, ISCB Editor-in-Chief, Chemistry and Biology Interface

It is a matter of great pleasure that Indian Society of Chemists and Biologists (ISCB) has entered in its 26<sup>th</sup> year of establishment. We are celebrating the 28 years of our international conference next year. With great pleasure ISCB announces the 29<sup>th</sup> ISCB International Conference (ISCBC-2025) on "Paradigm Shift Towards Sustainable Growth in Chemical and Biological Sciences " from 11<sup>th</sup> to 12<sup>th</sup> January 2024 at Vishal Lords Inn, Gir National Park, Malanka Gujarat India. with cultural heritage of Rajkot and Gujarat with world class infrastructure and facility. The 29<sup>th</sup> ISCBC will be jointly organized by ISCB Junagadh Chapter started in year 2023 by the faculties of Department of chemistry & Forensic Science and Department of Life Sciences, Bhakta Kavi Narsinh Mehta University.

This conference is going to discuss recent advances in the field of chemical and biological sciences, including organic and inorganic chemistry, medicinal Chemistry and drug Discovery biochemistry and molecular biology, biotechnology, microbiology and genetic engineering, environmental sciences and sustainability, analytical techniques, nanotechnology and nanomaterials, animal, and plant sciences.

Delegates and Scientists across the globe, especially from USA, UK, Belgium, Sweden, Korea, Middle East and many other will participate as keynote/invited speakers to address above mentioned themes. The entire conference will be in parallel sessions and this conference will be addressed by more than 25 senior scientists & professors as keynote/invited speaker while it will also attract more than 250 young researchers & post-doctoral researchers across the country, who will take part as oral/poster presentations. Young foreign delegates are also encouraged to attend this event.



# Prof. (Dr.) Atul H. Bapodra

Head,

Department of Chemistry and Forensic Science Bhakta Kavi Narsinh Mehta University, Junagadh

Department of Chemistry and Forensic Science (DOCFS) was established in June 2018, under Bhakta Kavi Narsinh Mehta University, Junagadh, a state university of Government of Gujarat (India). The department offers Post graduation and Ph.D. programme in Chemical Sciences. The Department of Chemistry and Forensic Science endeavours to be recognized for excellence in Teaching – Learning adjunct by empowering students to compete in and contribute to the developing needs of the society.

The department, right from its inception has given high priority for teaching-learning with upgraded syllabus to foster life skill as well as job skill for better placement of students.

Our Ph.D. program is aimed to maintain a culture of excellence in research and uphold the highest standards in chemical science. The faculty is actively engaged in cutting edge research in the frontier areas of analytical method developments, natural product chemistry, drug discovery and development, organometallic chemistry and physico-chemical study of materials. During last 3 years, the department has published more than 15 research paper in international journal of repute and has 3 patents to its credits.

The international conference (ISCBC-2024) on 'Paradigm Shift Towards Sustainable Growth In Chemical And Biological Sciences' jointly organized by Department of Chemistry & Forensic Sciences and Department of Life Sciences, Bhakta Kavi Narsinh Mehta University, in association with Indian Society of Chemists and Biologist (Lucknow) aimed to provide exposure and interaction platform where young researcher and students will share and exchange ideas with international researcher and propel their knowledge to a new height.

I wish to express my thanks to honourable Vice Chancellor, BKNMU for timely encouragement and financial support. I also extend my thanks to GSBTM, Anlon, Krishna scientific, SNJ Labs for financial assistance and sponsorship. I wish a great success for the conference.



# Prof. (Dr.) Suhas J. Vyas

Head, Department of Life Sciences, Bhakta Kavi Narsinh Mehta University, Junagadh

It is my distinct pleasure and honour to welcome you to the International Conference of Chemists and Biologists, organized jointly by the Department of Chemistry and Forensic Sciences and the Department of Life Sciences at Bhakta Kavi Narsinh Mehta University, Junagadh, in collaboration with the Indian Society of Chemists and Biologists (ISCB), Lucknow.

This conference, serving as a pivotal junction for experts, researchers, academicians, industry leaders, and aspiring young minds, is dedicated to exploring, sharing, and celebrating the latest advancements in the diverse realms of Chemical and Biological Sciences. Chemical and Biological Sciences, as you are undoubtedly aware, play a crucial role in leading innovation, shaping our understanding, and addressing global challenges. This conference has been meticulously organized to provide a dynamic and comprehensive platform for advancing knowledge and fostering collaboration in these intricate domains.

The program encompasses a wide spectrum of topics, ranging from Organic and Inorganic Chemistry to Biochemistry and Molecular Biology, and from Environmental Sciences to Sustainability. We believe that the diverse and rich tapestry of presentations, discussions, and interactions will contribute to the collective pursuit of pushing the frontiers of human understanding in Chemical and Biological Sciences. As we embark on this scientific journey, I extend my heartfelt best wishes to all participants, speakers, delegates, and presenters. May this conference be a remarkable and enriching experience, fostering intellectual exchange and collaboration that transcends disciplinary boundaries.

Your contributions and insights are invaluable to the success of this conference, and we anticipate that the interactions on this scientific platform will lead to innovative approaches and solutions for the challenges we face in the world of Chemical and Biological Sciences.

Thank you for your participation, and I look forward to witnessing the impactful outcomes of this gathering.

Warm regards,



#### Dr. Naval Kapuriya

President, ISCB @ Junagadh Chapter Associate Professor, Department of Chemistry and Forensic Science Bhakta Kavi Narsinh Mehta University, Junagadh

Indian Society of Chemists and Biologist Junagadh Chapter was started in year 2023 by the faculties of Department of chemistry and Forensic Science and Department of Life Sciences, Bhakta Kavi Narsinh Mehta University with the one of the objectives to promote research and development activities through organizing symposia, conferences and special lectures in different disciplines of science.

In that context, the international conference was envisaged on 'Paradigm Shift Towards Sustainable Growth in Chemical and Biological Sciences' which can serve as a pivotal junction where experts, researchers, academicians, industry leaders, and aspiring young minds can interact. Further it will facilitate interdisciplinary discussions and collaborations among researchers and professionals from various scientific backgrounds.

The themes of ISCBC-2024 is encompassed with a wide range of topics within Chemical and Biological Sciences, including Organic and Inorganic Chemistry, Biochemistry and Molecular Biology, Medicinal Chemistry and Drug Discovery, Biotechnology and Genetic Engineering, Environmental Sciences and Sustainability, Analytical Techniques in Chemical and Biological Sciences, Nanotechnology and Nanomaterials in Biomedical Applications, Synthetic Biology and Biomolecular Engineering, Plant Sciences, Animal Sciences and Microbiology.

The conference will feature a variety of engaging activities such as plenary talk by renowned international and national experts, poster presentations from researchers interdisciplinary panels discussion, showcasing of state-of-the-art technologies by industry partners and promotion activities of student startup and innovation.

In summary, the conference ISCBC-2024, I firmly believe, will not only enrich our understanding of Chemical and Biological Sciences but also catalyze collaborations that drive innovation and lead to tangible, real-world impacts.

I wish to express my sincere thanks to the invited speakers, the participants and my co-workers, the students, volunteers, officials of BKNMU, Junagadh. For the support rendered in successful conduct of ISCBC-2024.

#### **International Advisory Committee**

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# Schedule of 29th ISCB International Conference Day-1 (11th January 2024)

| 08:00 am to 09:45 am                                | Registrati   | on & Breakfast  |  |
|---|--|---|--|
| 09:45 am to 11:30 am                                |  |   |  |
| 11:30 am to 11:45 am                                |  | a Break   |  |
|   | Plenary Session (@Rajma  | hal Hall)   |  |
| <b>Plenary Session - I</b><br>11:45 am to 12:30 pm  | <b>Dr. Edmond Differding</b> ,<br>Consultant (medicinal chemistry and drug discovery), Retd. M D at<br>Differding Consulting based in Contern, Luxembourg.                     |   |  |
| <b>Plenary Session - II</b><br>12:30 pm to 01:15 pm | Prof. Nigel Richards,<br>Professor of Biological Chemistry, Cardiff University, UK.  |   |  |
| 01:15 pm to 2:15 pm                                 | Lun  | ch Break  |  |
|   | Parallel Session   |   |  |
|   | Chemical Sciences<br>(@Rajmahal Hall)  | Life Sciences<br>(@Theatre)   |  |
| <b>Parallel Session -I</b><br>02:15 pm to 02:45 pm  | <b>Prof. Diwan Singh Rawat,</b><br>Vice Chancellor,<br>Kumaun University, Nainital.<br>Senior Professor of Chemistry at<br>University of Delhi. New Delhi.                     | <b>Prof. Dipak Ramji,</b><br>Professor of Cardiovascular Science<br>and Deputy Head of the School of<br>Biosciences at Cardiff University, UK.                |  |
| <b>Parallel Session -II</b><br>02:45 pm to 03:15 pm | <b>Prof. Mahesh Lakshman</b> ,<br>Fellow of the Royal Society of<br>Chemistry<br>Department of Chemistry and<br>Biochemistry<br>The City College of New York<br>New York, USA. | <b>Dr. Saravanan Matheshwaran</b> ,<br>Professor,<br>Department of Biological Sciences and<br>Bioengineering,<br>Indian Institute of Technology Kanpur,<br>UP |  |
|   | <b>Prof. Erik Van der Eycken,</b><br>University of Leuven (KU Leuven)<br>Belgium.  | <b>Dr. Ramchand CN,</b><br>President and CEO of Saksin life<br>sciences Pvt. Ltd<br>and MagGenome Technologies Pvt<br>Ltd., Chennai, Tamil Nadu.              |  |
| <b>Parallel Session -IV</b><br>03:45 pm to 04:15 pm | <b>Dr. Bapurao B. Shingate,</b><br>Associate Professor,<br>Department of Chemistry,<br>Dr. Babasaheb Ambedkar,<br>Marathwada University,<br>Aurangabad, Maharashtra.           | <b>Dr. Dhaval Patel</b><br>Gujarat Biotechnology University<br>Gandhinagar  |  |
| 04:15 pm to 04:30 pm                                |  |   |  |
| <b>Poster Presentation</b><br>04:30 pm to 06:30 pm  | Best posters will be awarded in c<br>(CHE & LS)  | losing ceremony in both groups.   |  |
|   | Cultural Event (@Rajmahal Hall)  |   |  |
|   | Dinner and Networking  |   |  |

# Day - 2 (12th January 2024)

| 08:00 am to 09:00   | Breakfast  |  |  |
|---|--|--|--|
|   | Plenary Session (@Rajmal   | nal Hall)  |  |
| <b>Plenary Session - III</b><br>09:15 am to 09:45<br>am                     |  |  |  |
|   | <b>Prof. Nisheeth Desai</b> ,<br>Ex. Senior Professor, BSR Faculty Fellow, Department of Chemistry,<br>Bhavnagar University, Gujarat.                                    |  |  |
| Plenary Session - V<br>10:15 am to 10:45<br>am                              | <b>Prof. Barbara Zajc,</b><br>Department of Chemistry and Biochemistry,<br>The City College of New York.   |  |  |
| <b>Plenary Session - VI</b><br>10:45 am to 11:15<br>am<br>11:15 am to 11:30 | <b>Dr. Nikhil Bhatt,</b><br>Senior R&D professional, Governing council member of Quality circle forum<br>of India, Pharma wing, Ankleshwar, Gujarat.<br><b>Tea break</b> |  |  |
| 11.15 ani to 11.50  | Parallel Session   |  |  |
|   | Chemical Sciences<br>(@Rajmahal Hall)  | Life Sciences<br>(@Theatre)  |  |
| <b>Parallel Session -V</b><br>11:30 am to 12:00<br>pm                       | <b>Prof. Raghuvir Pissurlenkar</b> ,<br>Goa College of Pharmacy,<br>Panaji Goa.  | <b>Prof. Renu Pandey</b> ,<br>Head, Division of Plant Physiology,<br>ICAR-Indian Agricultural Research<br>Institute, New Delhi   |  |
| <b>Parallel Session -VI</b><br>12:00 pm to 12:30<br>pm                      | <b>Prof. H. M. Patel,</b><br>Department of chemistry<br>Member Royal Society of Chemistry<br>Sardar Patel University,<br>Vallabh Vidyanagar, Gujarat,                    | <b>Prof. Rajesh Patel,</b><br>Department of Biosciences<br>Veer Narmad South Gujarat<br>University<br>Surat, Gujarat.  |  |
| <b>Parallel Session -VII</b><br>12:30 pm to 01:00<br>pm                     | <b>Prof. Anil Mishra,</b><br>Professor and Head,<br>Department of Chemistry<br>University of Lucknow, Lucknow,<br>UP.  | <b>Dr. I Nengah Wirajana</b> ,<br>Department of Chemistry, Faculty of<br>Mathematics and Natural Sciences,<br>Udayana University, Jimbaran<br>Badung, Bali, Indonesia. |  |
| 01:00 pm to 02:00   | Lunch Break  |  |  |
| 02:00 pm onwards  | Valedictory Function (@Rajmahal ]  | Hall)  |  |

# EMINENT SPEAKERS



#### **Prof. Unnat Pandit**

Controller General of Patents, Designs & Trade, Indian Patent Office, New Delhi Professor at the JNU, New Delhi, INDIA E-mail: cgoffice-mh@nic.in, office@unnatpandit.com

#### RESURGENCE OF BHARATIYA VISION IN RESEARCH UNDER AMRIT KAAL

#### Abstract

The Indian approach is inherently holistic, striving to integrate various fields of academic institutions. Indian culture and philosophy have always respected nature and emphasized sustainable living. The resurgence of Bharatiya vision in research under Amrit Kaal has led to increased interest in better and sustainable livelihood as per Bharatiya knowledge systems. There has been significant growth in the last few decades in Healthcare Pharmaceutical, biotechnology, nanotechnology, IT and space research reflecting the Bharatiya vision of '*Vasudhaiva Kutumbakam*'. This characteristic is increasingly recognized in the international research community, emphasizing interdisciplinary research.

Research for the resurgence in Amrit Kaal is going to lead the growth of our country driving economic and social rejuvenation and while considering this role of intellectual and innovation lead knowledge economy is going to play a pivotal role. Time is going to show the shift in the research approaches through accurate decision-making processes, shaping public policy, and driving innovation. The Bharatiya Vision in research helps understand complex issues, identify potential solutions, and make appropriate predictions about future trends.

The government is trying to revamp the result-oriented research ecosystem through the National Research Foundation, Innovation Initiatives, and National Education Policy-like strategic initiatives. The future of research lies in collaborative, interdisciplinary efforts that harness the power of emerging technologies. Research is not just about collecting/compiling information, data, or publication but also about translating these insights and knowledge into actionable strategies for resurgence. It's about creating value that benefits individuals, communities, and societies at large.

### **Dr. Edmond Differding**

Independent consultant on medicinal chemistry and drug discovery, Retired Managing Director at Differding Consulting based in Contern, Luxembourg, EUROPE E-mail: edmond@differding.com



#### BIOTECHNOLOGY IN INDIA – AN ANALYSIS OF BIRAC-FUNDED PROJECTS

#### Abstract

A comprehensive analysis of over 2000 projects funded by India's Department of Biotechnology since 2005 through private-public partnerships, and as of 2012 through the 'Biotechnology Industry Research Assistance Council (BIRAC)' until BIRAC's tenth anniversary at the end of March 2022 reveals details of the science and technology underpinning past and current biotechnology research and development projects in the country. They are led by human healthcare projects, of which medical technology and therapeutics are the main drivers, ahead of vaccines, regenerative medicine, public health and others. Agricultural projects have mainly been driven by plant breeding and cloning, animal biotechnology, agri-informatics, aquaculture, and (bio)fertilizers. The key components of industrial biotechnology have been fine chemicals, environmental projects, clean energy and industrial enzymes. The talk will focus on selected areas of R&D across all sectors.

#### Prof. Erik Van der Eycken

Laboratory for Organic & Microwave-Assisted Chemistry, Department of Chemistry, KU Leuven Celestijnenlaan 200F, 3001, Leuven, BELGIUM E-mail: erik.vandereycken@kuleuven.be



#### SYNTHESIS OF SMALL COMPLEX HETEROCYCLES

#### Abstract

The recent upsurge in the development of mild reaction methodologies for the synthesis of small heterocycles has generated a lot of interest among synthetic organic chemist. To expand this area in organic synthesis, the challenge is to identify novel strategies for the formation of biologically or pharmaceutically important heterocycles under mild conditions as well as continuous flow chemistry to meet up the growing demand for pharmaceuticals as well as agrochemicals. Therefore, in this lecture, an overview will be given about recent synthetic work done in our laboratories regarding this topic. 1) This will include the synthesis of spiroindolines and spiroindoles, which are an important class of spirocyclic compounds present in a wide range of pharmaceuticals and biologically important natural alkaloids. New procedures will be described, including the use of nanoparticles as heterogeneous catalysts. 2) The Ugi-4CR is by far one of the most successful multicomponent reactions leading to high structural diversity and molecular complexity. As the reaction mostly affords a linear peptide backbone, post-Ugi transformations are an elegant solution to rigidify the Ugi-adduct into more drug like species. Not surprisingly, the development of these transformations, leading to new structural frameworks, has expanded rapidly over the last few years. We will comment on the use of homogeneous gold catalysis for performing post Ugi-4CR modifications (Scheme). 3) C-H bond activation/functionalization has demonstrated unprecedented avenues for the streamlined synthesis of pharmaceutically and industrially valuable molecules in a benign manner. This enables the formal functionalization of a C-H bond, which is arguably the most prevalent "functional group" in organic chemistry. We will comment on our recent research regarding this topic. 4) Finally an introduction to our recently started up photo-redox chemistry will be given.



#### **Prof. Diwan Singh Rawat**

Vice Chancellor, Kumaun University, Nainital Senior Professor of Chemistry at University of Delhi, New Delhi, INDIA E-mail: dsrawat@chemistry.du.in

#### FROM BASIC TO TRANSLATIONAL RESEARCH: STORY OF DISCOVERY OF A CLINICAL CANDIDATE FOR PARKINSON TREATMENT

#### Abstract

In order to address the issue of drug resistance and improve the ADME properties of a drug molecule concept of molecular hybridization was put forward wherein two or more distinct pharmacophores are covalently linked into a single molecule. This approach may lead to a molecule with improved efficacy and may solve the problem of drug resistance and reduce the undesired side effects [1,2]. The development of such molecular frameworks with synthetic selectivity and economic viability is still a challenging task for the pharmaceutical industry. Drugs developed through this approach can be used for the cure of infectious diseases where treatment is limited to few drugs and the known drugs have limitations such as toxicity, pharmacokinetics, pharmacodynamic and drug resistance. The benefit of using molecular hybrid is to activate different or same targets by a single molecule, and increase the therapeutic efficacy and to improve the bioavailability. Molecular hybridization approach has resulted many drug candidates with improved activity profile and some of these compounds are in clinical trials. We have utilized this concept in designing antimalarial molecules and many molecules with aminiquinoline and pyrimidine phamacohpore showed low nano molar activity. Later a massive multi-institutional collaboration was started and over 700 new molecules were studies for Nurr1 activation, a potential target for Parkinson disease model and identified 15 hits out of which 3 compounds have cleared pre-clinical trials and technology has been transferred to NURRON pharmaceuticals for further development [3-15]. These molecules activate the Nurr1 enzyme which is essential for the survival of the dopamine neurons, stops the aggregation of  $\alpha$ synuclein protein in the brain, and promotes autophagy. Systematic studies demonstrated that these compounds can cures the Parkinson induced mice model at 5 mg/kg body weight without any toxicity. The molecule has entered in phase I clinical trials and the story was covered by The Wall Street Journal and Bollomberg.



#### **Prof. Nisheeth Desai**

Ex. Senior Prof & Head, BSR Faculty Fellow, Department of Chemistry, Bhavnagar University, INDIA E-mail: dnisheeth@rediffmail.com, dnisheeth@gmail.com

#### RESEARCH AND PUBLICATION STRATEGIES FOR BUILDING ACADEMIC CAREER

#### Abstract

A well-considered publication strategy can help maximize academic impact, support career development, and aid the production of an optimal portfolio of research outputs. For early career academics (ECAs), who are under growing pressure from higher education institutions for greater research output and publications, the adage "publish or perish" is still relevant. With the introduction of the National Education Policy - 2020 and the need for encouraging domestic citation, quality publications are considered to be the height of academic excellence. Research and publications are given utmost importance more than before. Over and above, the government incentivizes publication platforms/hosting for data storage to academic/research institutes. In today's globalized world, research publication strategy is equally crucial, which is why it is still the main topic of discussion on every academic platform. Researchers must write and publish high-quality research papers for a variety of reasons, prominent among them being the promotion of their academic careers and the advancement of empirical knowledge through the dissemination of research findings. Publications are also a gauge of the scholarly output required for advancement. Another reason is that most researchers become authorities in the field in which they work, and when they actively add to the literature and enhance the pool of empirical knowledge, their colleagues acknowledge and validate this expertise. The successful writing of the title, abstract, keywords, literature review, introduction, methods, results and discussion, conclusion, output of the major findings, and references are only a few of the significant components of publications that will be covered in this lecture. Researchers are finding difficulties encountering the issues of plagiarism, which is a crucial factor for publishing as well, and this key issue will be discussed with several illustrations.



# **Prof. Nigel Richards**

Professor of Biological Chemistry, Cardiff University, UK E-mail: RichardsN14@cardiff.ac.uk

#### THE ENZYMOLOGY OF FORMYCIN BIOSYNTHESIS

#### Abstract

There is renewed interest in the synthesis and clinical application of modified nucleosides and nucleotides. Notably, the effectiveness of remdesivir in treating SARS-CoV-2 infections has prompted a re-evaluation of the clinical utility of C-nucleosides; compounds in which the nucleobase is connected to the sugar by a C-C rather than a C-N bond. Inn this lecture, I will describe recent progress in understanding the structural and mechanistic enzymology of the biosynthetic pathway that is used to produce formycin, a C-nucleoside with antiviral and anticancer properties.

#### Dr. Nikhil Bhatt



Senior R&D professional, Governing Council member, Quality circle forum of India, Pharma wing, Ankleshwar, Gujarat, INDIA E-mail: nikhilbhatt86@hotmail.com, bhatt99@yahoo.com

#### **ENVIRONMENT AND HEALTH HAZARDS OF N-NITROSOAMINES**

#### Abstract

Nitrosamines are a group of organic compounds containing the nitroso functional group. They can be found in water, food, tobacco, pesticides, or plastics, but received public attention in mid-2018, when they were also found in medicinal products Nitrite and nitrosamine intake are associated with risk of gastric cancer and esophageal cancer. N-nitrosamines are so potent mutagenic carcinogens that they are referred to as the "cohort of concern" by the International Council for Harmonisation of Technical Requirements for Pharmaceuticals for Human Use (ICH) guideline on assessment and control of DNA reactive (mutagenic) impurities in pharmaceuticals to limit potential carcinogenic risk.

#### Dr. I Nengah Wirajana

Lecturer, Department of Chemistry, Faculty of Mathematics and Natural Sciences, Udayana University, Jimbaran Badung Bali, INDONESIA E-mail: nengah\_wirajana@unud.ac.id



#### COMPARATIVE METAGENOME ANALYSIS OF HOT SPRINGS OF BALI, INDONESIA FOR THE VALUABLE THERMOPHILES

#### Abstract

The ecology of hot springs is quite interesting as a potential source of new extremophiles. Identifying the microbial profile is essential to understanding thermophile survival mechanisms and biotechnology potential. As Indonesia is located at the intersection of several tectonic plates, its unique geomorphological feature is that it has many hot springs. Hot springs in Indonesia are rich reservoirs of microbiological life. Therefore, a microbiome study was conducted on the hot springs in Angseri (An), Banjar (Bj), and Batur (Bt) in the Indonesian province of Bali. In this work, we use a metagenomics technique with 16s rRNA gene amplicon sequencing by the GridION Nanopore platform to assess the bacterial diversity of three hot springs in Bali. The physicochemical analysis of all the water samples suggested the presence of several metals in hot springs. In Angseri and Batur, the most common metal is calcium, but in Banjar, aluminum is more common. Thirteen distinct metals were found in the hot springs of Banjar. MEGAN, MetagenAssist, and STAMP tools were used after the Kraken2-based analysis. There were 44 phyla found in Batur Hot Springs, 51 in Angseri, and 54 in Banjar overall. In contrast, species were found in Banjar, Angseri, and Batur in numbers of 2064, 1730, and 1373, respectively. Acinetobacter predominates in Batur hot spring; Methylophilus is predominant in Angseri; and Paucibacter is abundant in Banjar. All three metagenomes' core microbiomes were made up of nine distinct phyla, with the proteobacteria phylum dominating. All three samples performed hierarchical cluster analysis, which showed that the Angseri is more diversified than the Batur and Banjar. The microbiome's phenotypic characteristics indicate that the aerobic community predominates in all hot springs, with a significant presence of thermophiles and hyperthermophiles. Heterotrophs, chemolithotrophs, chemoheteotrophs, and methylotrophs are the dominant organisms in all hot springs. Nitrogen- and sulfate-metabolizing microbial species are present in all hot springs. Additionally, the presence of different hydrolase enzyme producers and xenobiotic-degrading bacteria has been identified. Hot spring microbiomes hold promise for biotechnological applications. Additional research on the culturalomics method is necessary for identifying the important species.



#### Prof. Mahesh Lakshman

Fellow of the Royal Society of Chemistry Department of Chemistry and Biochemistry The City College of New York 160 Convent Avenue New York, USA E-mail: mlakshman@ccny.cuny.edu

#### *N*-DIRECTED C–H BOND ACTIVATION AND ACYLATION OF 6-ARYLPURINE NUCLEOSIDES

#### Abstract

Remote functionalization *via* the use of directing groups is an efficient and cost-economical approach for late-stage functionalization of complex organic compounds. In this context, nucleosides are a highly privileged class of compounds. These important biomolecules have served as scaffolds for the design of diverse novel compounds, ranging from those that are physiologically and medicinally important, to others that are used to probe biomolecular structure and function, to fluorescent molecules that are used as probes of local environment in DNA and RNA. Nucleosides contain a polynitrogenated base and multiple oxygen atoms in the saccharide unit and in some bases. These Lewis basic centers are capable of metal sequestration in metalcatalyzed reactions. Also, nucleosides contain an acid and thermally labile glycosidic bond. Despite these challenging aspects, remote functionalization of nucleosides has been studied.<sup>1-9</sup> This presentation will describe *N*-directed remote acylation of C6 aryl purine ribo and 2'- deoxyribonucleosides and mechanistic considerations of the underlying chemistry.

## Dr. Bapurao B. Shingate

Associate Professor, Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad, Maharashtra, INDIA E-mail: bapushingate@gmail.com, bbshingate\_chem@bamu.ac.in



#### **EXPLORATIONS OF CLICK CHEMISTRY**

#### Abstract

In recent years, click chemistry has emerged as a fast and powerful approach to the synthesis of novel compounds with desired properties. The concept of "click chemistry" was coined by Sharpless to describe a set of "near perfect" bond-forming reactions which were very selective, high yielding, and wide in scope and describes chemistry tailored to generate substances quickly and reliably by joining small units together. In 2022, the Nobel Prize in Chemistry was jointly awarded to Carolyn R. Bertozzi, Morten P. Meldal and K. Barry Sharpless, "for the development of click chemistry and bioorthogonal chemistry". 1,2,3-Triazoles are important class of target molecules due to their interesting biological properties such as anti-allergic, anti-bacterial, and anti-HIV activity. We were encouraged to combine 1,2,3-triazole moieties with phenol, coumarins, isatin, benzothiazinone, acetophenone, quinoline, 2,4-thiazolidinedione and acid hydrazide in a single molecular framework. All the diversely functionalized molecules were synthesized from commercially available starting materials in minimum steps with high overall yield and screened for antitubercular, antioxidant, antimicrobial, anti-inflammatory and cytotoxic activities and will be discussed.



Prof. Deepak Ramji

Professor of Cardiovascular Science and Deputy Head of the School of Biosciences at Cardiff University, Cardiff, UK E-mail: Ramji@cardiff.ac.uk

#### PROTECTIVE ACTIONS OF NUTRACEUTICALS IN ATHEROSCLEROTIC CARDIOVASCULAR DISEASE AND OTHER INFLAMMATORY DISORDERS: FOCUS ON MOLECULAR MECHANISMS USING *IN VITRO* AND *IN VIVO* MODEL SYSTEMS

#### Abstract

Atherosclerosclerotic cardiovascular disease (ACVD) is responsible for a third of all global deaths. Although a reduction in morbidity and mortality from ACVD has been achieved recently by lifestyle changes and pharmaceutical intervention, this is expected to reverse in the future because of global increase in risk factors such as hypercholesterolemia, obesity and diabetes. Current pharmaceutical therapies against ACVD are associated with substantial residual risk for the disease together with other issues such as side effects. In addition, pharmaceutical agents against many promising targets have proved disappointing in clinical trials. It is therefore essential that the molecular basis of ACVD is fully understood, and new therapeutic/preventative agents or targets are identified and validated. The major focus of recent research in my laboratory is to understand the molecular mechanisms underlying the protective actions of natural products in ACVD using a combination of *in vitro* and *in* vivo model systems together with biochemical, molecular biology, pharmacological and immunological approaches. Our research has provided novel insights into the mechanisms underlying the protective actions of several nutraceuticals, including fatty acids, polyphenols and probiotic bacteria. In addition to the beneficial effects on ACVD, our studies have revealed protective actions against other inflammatory disorders, particularly non-alcoholic fatty liver disease. Our findings on the mechanisms underlying the beneficial actions of key nutraceuticals will be presented.

#### Dr. Saravanan Matheshwaran

Assistant Professor, Department of Biological Sciences and Bioengineering, Indian Institute of Technology Kanpur, UP, INDIA. E-mail: saran240478@gmail.com



#### TARGETING MYCOBACTERIAL "SOS" RESPONSE- A STRATEGY TO TOGGLE ANTIMICROBIAL RESISTANCE (AMR)

#### Abstract

The "SOS" response is an essential systematic mechanism against DNA damage in bacteria. It is indispensable for its regulatory role in maintaining genome integrity and in gaining fitness advantage by developing useful mutations to tolerate genotoxic stress, leading to the development of antimicrobial resistance. LexA and RecA are the key players regulating the global network of stressresponsive and damage-repair genes involved in this pathway. In an era of expanding drug resistance, targeting such non-traditional yet non-compromising pathways can provide useful answers in tackling global health hazards such as Tuberculosis (TB). The potential of targeting the "SOS" response is gathering increasing support to strengthen therapeutic efficacy. RecA inhibitors have been reported from chemical screening assays conducted in E.coli and Mycobacterium tuberculosis (Mtb), the latter being the causative agent of TB. However, RecA bears homologs not only across prokaryotic but also eukaryotic organisms, posing a challenge for specific action. Consequently, a shift in gears has taken place with scientists switching to the other master regulator, LexA, which does not possess any eukaryotic counterpart. An academic-industry partnership successfully delivered the first-of-its-kind inhibitors targeting E.coli LexA autoproteolysis. Such efforts have not yet been extended to Mtb and addressing this gap forms a major objective of our study. Here, we report potential inhibitors of Mtb LexA. We have elucidated the kinetic parameters of interaction and generated a homology model to obtain an idea of possible drug-binding sites in Mtb LexA. Our studies involve characterizing such compounds with the broader aim of improving the existing arsenal of anti-TB therapeutics. Characterizing such inhibitors of Mtb LexA autoproteolysis can be effective in stalling "SOS" induced mutagenesis and AMR in mycobacteria.

#### Prof. Barbara Zajc

Department of Chemistry and Biochemistry, The City College of New York, New York, USA E-mail: bzajc@ccny.cuny.edu



#### FLUORINATED HETEROARYL SULFONES, BUILDING BLOCKS FOR FLUOROORGANICS: FROM SYNTHESIS TO APPLICATIONS

#### Abstract

The unique properties of fluorinated organic compounds make them attractive in various fields, such as agrochemical, pharmaceutical, medicinal, and materials fields, and as NMR probes and radiochemicals. From the first fluorinated drugs, fludrocortisone and fluorouracil, to the blockbuster drugs Prozac and Lipitor, their number has been constantly increasing, and according to recent reviews more than 50% of the current most widely prescribed drugs contain at least one fluorine atom. About 35% of potential new drugs undergoing phase II and III clinical trials contain a fluorine atom, and in 2018–2022 period, the US FDA approved 58 new fluorinated drugs. Despite this importance of fluorinated organic compounds, regio and stereoselective introduction of fluorine atom continues to be challenging and there is a constant need for new synthetic approaches. We have been involved in a modular synthesis approach to fluorinated compounds *via* fluorinated building blocks. This talk will focus on the synthesis of fluorinated sulfones, including those with stereogenic centers. Their application for modification/synthesis of biologically relevant molecules, such as fluorinated nucleoside and amino acid analogs, will be presented.

# Prof. Anil Mishra

Head, Department of Chemistry, University of Lucknow, Lucknow, UP, INDIA E-mail: mishraanil101@hotmail.com



#### CHEMISTRY OF MANAGING STRESS FOR MENTAL WELL-BEING

#### Abstract

The "chemistry of stress" refers to the physiological and biochemical changes that occur in the body when an individual experiences stress. When a person encounters a stressful situation, the body's stress response, often referred to as the" fight or flight" response, is activated. This response involves a complex interplay of hormones and neurotransmitters. The chemistry of stress can have both shortterm and long-term effects on the body. Short-term stress can be adaptive, helping an individual react to a threat. However, chronic stress can lead to health issues, such as high blood pressure, weakened immune system, and mental health problems. Understanding the chemistry of stress is crucial for managing and mitigating its negative impacts on health and well-being. Understanding the complex chemistry of stress and its impact on the body underscores the importance of stress management techniques such as mindfulness, exercise, social support, and seeking professional help when necessary, to mitigate its negative effects on physical and mental wellbeing. It's important to manage stress not only for immediate well-being but also for long-term health. Adopting a holistic approach to stress management can have a positive impact on both your mental and physical health, ultimately supporting a robust immune system. Stress management plays a pivotal role in maintaining good mental health. In today's fast-paced world, stress has become a common concern, and its impact on mental well-being cannot be underestimated. High levels of stress can lead to anxiety, depression, and other mental health issues. Effective stress management helps prevent and mitigate these conditions. Stress affects the human body mainly by weakening our immune system and making our body prone to diseases. Stress starts from worry which is caused if we are unable to solve the problems. This leads to anxiety and then to stress. Stress is just an accumulation of worry. If we could stop it at the worry level stress can be controlled. There are several ways to control worry. In the Practical Approach emphasis is on how easily a person can manage his/her own life by following some basic principles which we usually tend to forget. These are Acceptance and Gratitude. Usually we do not remember these when it comes to our own problems. Here methods and examples will be given as to how these principles can be easily applied for one's own betterment. People apply acceptance unknowingly plenty of times but the important thing is to apply it knowingly and this will help in having a life with lesser stress. Meditation also plays an important role in controlling our thoughts. Conscious Breathing, the simplest form of meditation also plays an important role in reducing stress. Overall these simple methods can be used to manage stress in our life and make it more peaceful.



#### Prof. Raghuvir Pissurlenkar

Goa College of Pharmacy, Panaji, Goa, INDIA E-mail: raghuvir@pissurlenkars.net

#### NOVEL LEADS AGAINST BREAST CANCER TARGET ESTROGEN RECEPTOR ALPHA: A COMPUTATIONAL STUDY

#### Abstract

Breast cancer holds the distinction of being the most frequent type of cancer among women when compared to other forms of cancer. Estrogen regulates a variety of biological functions through Estrogen Receptors (ER) in the body. Estrogen Receptors can exert significant influence over cell growth, development, reproduction, and other important biological functions with its ability to modulate gene expression. Estrogen Receptors are found to be over-expressed in breast cancer events which cascades into deregulation of estrogen signaling pathways resulting into aberrant cell growth and proliferation. The primary focus of this research work was to identify potential virtual candidates to fuel the experimental studies in the discovery and development of therapeutic agents in the treatment of breast cancer through the application of various approaches under computational chemistry. Beginning with large virtual chemical libraries of diverse small organic compounds, winding the way through virtual screening and ADME / toxicity filtration and QSAR studies, a focus library was identified with excellent binding potential against Estrogen Receptor alpha (ER-a). The identified molecules belong with various structural heterocyclic classes such as benzimidazoles, indoles, benzothiazoles etc. The binding of these compounds was validated using molecular dynamics simulations for structural stability and Energy fluctuations using MMPBSA. Through successful collaborations these compounds possess the potential for further experimental validations.



#### Prof. Hitendra M. Patel

Department of chemistry Sardar Patel University, Vallabh Vidyanagar, Gujarat, INDIA. Elected member of the Organic Division Council, Royal Society of Chemistry E-mail: hm\_patel@spuvvn.edu

#### SYNTHESIS OF SMALL HETEROCYCLIC SCAFFOLDS AND THEIR ANTIPROLIFERATIVE TARGETS

#### Abstract

A sustainable approach for small heterocyclic scaffolds is a key precursor for medicinal and pharmaceutical applications. Diversified reaction protocols will be explored for highly functionalized heterocyclic scaffolds such as pyrazolodihydropyridine (PDHPs), Monstral analogues, pyridone-3,5-dicarbonitriles (PCNs), pyrano[2,3-c]pyrazoles (PPs) and Spirohetero cycles (SHs). This manifestation will focus ahead on various approaches taken to enhance the valuable sustainable chemistry with constructive ideas for the above-said heterocyclic scaffolds via selective multiple C–C, C-O and C-N bond formation under identical reaction conditions. The mentioned protocol works efficiently, tolerates different substituent's present in reactants, has a simple equipped procedure, provides excellent reaction yield in a short time, and uses a recyclable catalyst. The synthesized scaffolds will increase the impact towards the antiproliferative targets including diversified biological applications.

#### **Dr. Ramchand CN**

President and CEO of Saksin life sciences Pvt. Ltd, and MagGenome Technologies Pvt Ltd, Chennai, Tamil Nadu, INDIA E-mail: ramchand@maggenome.com



#### DISCOVERY AND DEVELOPMENT OF SYNTHETIC ANTI-VEGF FAB FOR TREATING WET-MACULAR DEGENERATION AND DIABETIC RETINOPATHY

#### Abstract

Wet age-related macular degeneration (wet-AMD) is a progressive neurodegenerative disease of the retina, affecting the central vision. Wet-AMD and Diabetic Retinopathy (DR) is a leading cause of irreversible vision loss, worldwide affecting the population older than 50 years. Products that significantly addresses market access representing a global ocular market of >\$25B and >200M patients globally. The vision behind FAB201 development is to provide an efficacious and cost-effective treatment for wet-AMD patients. Currently approved anti-VEGF drugs like Lucentis and Eylea in the market are expensive and not widely accessible in developing countries. Keeping this in mind to meet the unmet medical needs and to provide affordable treatment to developing countries. We have developed an anti-VEGF Fab molecule (FAB201 and FAB293) for wet-AMD and DR, filed US patent, successfully finished the discovery, proof of concept, development, pre-clinical toxicity studies and cGMP manufacturing for our proprietary molecule. FAB201, that is close to going to Phase-1 trails in US and Australia for wet AMD and DR. FAB201 and FAB293 are 48kDa synthetic human anti-VEGF Fab (Fragment Antigen Binding). It is a novel biologic (has unique CDRs in light chain & heavy chain) expressed in microbial system (E. coli BL21). FAB201and FAB293 has been developed using Phage display library with several rounds of affinity maturation for selection of clones with highest binding affinity, followed by site directed mutagenesis in CDRs for improved antigen binding towards hVEGF (Vascular Endothelial Growth Factor).Both the molecules were engineered to express at a higher level and the downstream processing was optimised to minimise losses during purification. Developmental process of molecular biology where, gene coding for FAB201 and FAB293 was inserted in a modified pBR322 vector and has pho A promoter sequence. E. coli BL21 Pho based expression system offers an efficient and economic system to produce recombinant proteins. Bioreactor and scale-up cultivation was done up to 200L fermentation for the large-scale production of FAB201. The anti-VEGF FAB201 purifications and orthogonal analytical tests were performed. The recombinant protein was extracted from the cell before subjecting for purification, for which a series of steps are performed in sequence so as to efficiently extract the expressed protein from the cell and also maintaining the stability of the protein molecule at the same time inactivating or denaturing any unwanted process related impurities. The Downstream Process for purification was optimised and was performed by a series of three chromatography steps to reduce impurities. Lysate was homogenized and clarified followed by purification by series of column chromatography. The quality of the product from all three purification steps were assessed by various analytical techniques. The purified drug substance was formulated by buffer exchange & concentration of the drug substance with the formulation buffer. The accelerated stability and stress stability studies are confined to temperature stability studies at ambient temperature and 37°C. Bioanalytical studies included several assays like Quantitation, In-process impurities analysis, Product related impurities and Sterility were performed. Biochemical & Biophysical characterization, analysis of batch consistency. In-vitro binding affinity, In-vitro efficacy study for batch release assay and In-vivo efficacy studies were performed. MTD and preclinical studies were done as per the regulatory guidelines. cGMP material was generated for the clinical studies. US FDA IND filing was done, and the molecule is ready for Phase-1 clinical trial.

# **Prof. Rajesh Patel**

Department of Bioscience Veer Narmad South Gujarat University, Surat, INDIA E-mail: raj252000@gmail.com



#### AMR: A ONE HEALTH BATTLEGROUND WHERE CHEMISTS AND BIOLOGISTS JOIN FORCES

#### Abstract

Antimicrobial resistance (AMR) poses a significant threat to One Health, with the overuse and misuse of antimicrobials contributing to a global burden that jeopardizes the effectiveness of existing treatments. This looming threat, highlighted by the COVID-19 pandemic, calls for a comprehensive and multidisciplinary approach, particularly within the framework of One Health.

This scientific talk aims to shed light on the collaborative efforts of chemists and biologists in the battle against AMR. The global landscape of AMR extends beyond human health, encompassing animals and the environment, creating reservoirs of resistance in each sector. The emergence of AMR raises the alarming prospect of a return to a pre-antibiotic era, where common infections become life-threatening.

In response to this crisis, chemists and biologists unite to forge a holistic strategy. Chemists, armed with their understanding of molecular interactions, embark on the design and development of novel antibiotics. This includes exploration into drug repurposing, targeted therapies, and innovative delivery systems, aiming to outsmart evolving pathogens and combat resistance head-on.

On the other front, biologists leverage their expertise in life sciences to become the eyes and ears on the battlefield. They delve into the intricate mechanisms of resistance, mapping microbial adaptation and predicting future threats. Through advanced diagnostics and surveillance, they guide the precision deployment of our antimicrobial arsenal.

The collaborative synergy between chemists and biologists manifests in the formation of interdisciplinary teams. These teams seamlessly integrate chemical and biological data, providing comprehensive insights into the multifaceted nature of AMR. Surveillance efforts span both realms, monitoring the environmental presence of antimicrobials and tracking the prevalence of resistant strains. Educational initiatives further prepare a workforce capable of navigating the complexities of AMR.

This talk acknowledges the challenges faced in the battle against AMR, including bacterial evolution, limitations in therapeutic options, and the specter of antimicrobial misuse. However, it also instills hope by showcasing the power of interdisciplinary collaboration. Chemists and biologists are called to join forces, combining their unique expertise to forge a future where the miracle of healing prevails over the darkness of resistance.

The fight against AMR is not just a battle for human health; it is a crucial endeavor that preserves the interconnected fabric of our world. This talk invites participants to witness the meeting of minds, the forging of alliances, and the dawn of a new era in the relentless fight against antimicrobial resistance. Together, through the collaborative efforts of chemists and biologists, we can fortify the global response to this critical One Health battleground.

#### Prof. Renu Pandey

Head, Division of Plant Physiology, ICAR-Indian Agricultural Research Institute, New Delhi, INDIA E-mail: renu\_pphy@iari.res.in

#### MECHANISMS OF ENHANCED PHOSPHORUS UPTAKE IN PLANTS: ROOT PROTEOME REVEALS POTENTIAL CANDIDATES

#### Abstract

Phosphorus (P) deficiency is widespread with most of the arable soils globally exhibiting high Pretention potential thereby leading to its low bioavailability for plant uptake. Plants possess several physiological mechanisms to cope with the low P availability. Among them, carboxylate efflux from roots is a crucial and differential response of plants, particularly, legumes to low P stress. We studied diverse panel of soybean for induced exudation of carboxylic acids including oxalate, citrate, succinate and fumarate under low P stress in P-efficient soybean genotypes. Physiological characterisation of a soybean panel comprising 116 genotypes exhibiting contrasting total carbon exudation (<sup>14</sup>CO<sub>2</sub>) revealed that traits such as root length, surface area and volume coupled with higher activity of TCA cycle enzymes significantly contributed to enhanced P acquisition efficiency. To understand the molecular basis of carboxylate efflux, the root proteome of contrasting genotypes (P-efficient: EC-232019 and P-inefficient: EC-113396) was compared. Among a total of 325 spots, 105 (32%) were differentially abundant proteins (DAPs) between sufficient (250 µM) and low P (4 µM) levels. Abundance of 44 (14%) proteins decreased by more than two-fold under low P stress, while 61 (19%) proteins increased by more than two-fold. Protein identification and annotation revealed that the DAPs were involved in a myriad of functions including carboxylic acid synthesis, carbohydrate, protein and lipid metabolism. Proteins with significant abundance included malate dehydrogenase, isocitrate dehydrogenase, phosphoglucomutase, phosphoglycerate mutase, fructokinase, enolase, phosphoglycerate kinase, triosephosphate isomerase, alcohol dehydrogenase, glucan water dikinase, glutamine synthetase and argininosuccinate lyase. Inferences from proteomic investigations suggest the crosstalk between various metabolic pathways implicated in conferring superior P acquisition efficiency under stress. Characterisation of the 17 proteins with unknown function might reveal roles of novel genes under low P stress. Further, the identified genotypes have potential to be used as donors in crop improvement programs to develop high-yielding P-efficient cultivars which may be an asset to low-input sustainable agriculture.



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## SPECTROPHOTOMETRIC ESTIMATION OF TOLFENAMIC ACID IN PHARMACEUTICAL & VETERINARY FORMULATIONS

Hardik L. Varu, Mrunal A. Ambasana Department of Chemistry and Forensic Science, Bhakta Kavi Narsinh Mehta University, Junagadh, Gujarat, INDIA E-mail: hardikvaru5@gmail.com & ambasanamrunal@gmail.com

## Abstract

The present work describes the development of molecular iodine mediated facile and sensitive method for the spectrophotometric estimation of tolfenamic acid in pharmaceutical and veterinary formulations. Here, in the presence of iodine, the secondary amine of tolfenamic acid coordinates with the lone pair of available electrons with iodine, which results in the formation of hyper iodine complex of tolfenamic acid. The newly formed coloured ion complex showed the absorbance maximum at 359 nm. The method was validated as recommended in ICH guidelines. The method was linear over the concentration range of  $0.01-0.07 \mu g/ml$  (r2 = 0.9998) with the limits of detection and quantitation of 0.002 and 0.006  $\mu g/ml$ , respectively. Intra-day (mean recovery of 99.7%) and inter-day (mean recovery of 100.9%) method precision was determined. The mean recovery of the accuracy study is between 99.0–100.5%. The method was found to be robust and suitable for assay of tolfenamic acid in pharmaceutical and veterinary formulations.

## SOLVENT FREE SYNTHESIS OF NEW 2-AMINO-4H-CHROMINES; INVITRO A-AMYLASE ACTIVITY AND INSILICO STUDIES

Savankumar R. Chothani<sup>\*</sup>, Naval P. Kapuriya Department of Chemistry and Forensic Science, Bhakta Kavi Narsinh Mehta University, Junagadh, Gujarat, INDIA E-mail: savanchothani143@gmail.com

### Abstract

In the quest for the novel and safer a-amylase inhibitors, a series of 2-amino-7-(bis(2-hydroxyethyl)) amino)-4(phenyl)-4H-chromene-3-carbonitrile derivatives has been designed and synthesized by incorporating bis(2-hydroxyethyl) amino skeleton with the chromene ring system to evaluate their antidiabetic activity as a-amylase inhibitors. To achieve targeted 2-amino-4H-chromenes, a solventfree synthetic protocol has been developed through multicomponent reaction of various substituted benzaldehydes, malononitrile and 2,2'-((3-hydroxyphenyl) azanediyl) bis(ethan-1-ol) using catalytical piperidine (15 mol%) at room temperature to generate corresponding 2-amino-7-(bis(2hydroxyethyl) amino)-4(phenyl)-4H-chromenes (5a-i) in excellent yields (65-90%) within short reaction time. The molecular structures of the newly prepared chromenes were established by various spectroscopic techniques including IR, mass, <sup>1</sup>H & <sup>13</sup>C NMR and elemental analysis. The dosedependent in vitro a-amylase inhibition study revealed that, most of these compounds exhibited significant antidiabetic activity having more than 50%  $\alpha$ -amylase inhibition at the dose of 10 mg/mL. Among these, compound 5b was more potent than acarbose with 91% inhibition of a-amylase and IC50 of  $3.60 \pm 0.01$  mg/mL. Further, in silico studies of targeted compounds were investigated to evaluate their drug-likeness properties and putative binding mode with receptor site of a-amylase. We demonstrated that the in vitro potency of the synthesized 2-amino-4H-chromene derivatives well correlated with their binding energy and drug-likeness properties. The in silico predicted properties of compound 5b regarded as non-toxic and safer antidiabetic agent.

## METAL FREE SYNTHESIS OF 2-AROYL 7-AZAINDOLES VIA THERMALLY INDUCED DENITROGENATIVE INTRAMOLECULAR ANNULATION OF 3-(TETRAZOLO[1,5-A] PYRIDIN-8-YL) PROP-2-EN-1-ONES

Chirag A. Chamakiya\*, Naval Kapuriya Department of Chemistry and Forensic Science, Bhakta Kavi Narsinh Mehta University, Junagadh, Gujarat, INDIA E-mail: drchiragchemist@gmail.com

### Abstract

A facile and metal-free intramolecular denitrogenative annulation strategy for the preparation of novel 2-aroyl 7-azaindoles has been developed from corresponding 3-(tetrazolo[1,5-a] pyridin-8-yl) prop-2-en-1-one in the presence of deep eutectic solvent Dowtherm A. The valuable features of the protocol included short reaction time, absence of metal catalyst, utilization of eutectic solvent easy product isolation, and very good yields of novel 2-aroyl 7-azaindoles.

# SELECTIVE DETECTION OF IODINE ION FROM CATALYST USING AZIDO-PYRAZOLE-CHALCONE BASED FLUOROSCENCE SENSOR

Rupal J. Joshi\*, Atul H. Bapodra Department of Chemistry and Forensic Science, Bhakta Kavi Narsinh Mehta University, Junagadh, Gujarat, INDIA E-mail: rupal.joshi1857@gmail.com

#### Abstract

Present study disclosed the synthesis of iodine (I-) ion fluorescence sensor based on azido pyrazolechalcone derivatives for selective detection of iodine in pure form. The azido pyrazole-chalcone derivatives was obtained from condensation reaction of 5-azido-3-methyl-1-phenyl-1H-pyrazole-4carbaldehyde and various acetophenones under alkaline methanol. The developed fluorescence sensors shown selective fluorospectrometric recognition of I-, while the various competitive anions (N3-, BrO3-, OH-, SO3-, CN-, Br-, NO3-, CO3-2, HPO4-, CH3COO-, SCN- and NO2-) did not led to any noticeable interference. The iodine showed linear correlation with fluorescence intensity of developed fluorescence sensor over the concentration range 7.5 to 37.5 mM. The correlation coefficient value of the method is 0.9906 with 2.5 mM detection limit of iodine. The synthesized compound 4A was also capable to detect iodine in various forms including KI or TBAI catalyst. The outcomes of the method showed that synthesized fluorescence sensor (4A) was selective and sensitive detector of iodine in aqueous solution.

## DESIGN, SYNTHESIS, AND BIOLOGICAL EVALUATION OF QUINOLINE-THIOZOLIDINEDIONE CONJUGATES AS POTENTIAL α -AMYLASE INHIBITORS

Sheetal B. Karmur\*, Atul H. Bapodra

Department of Chemistry and Forensic Science, Bhakta Kavi Narsinh Mehta University, Junagadh, Gujarat, INDIA E-mail: karmursheetal@gmail.com

#### Abstract

In the current study, the quinoline-thiozolidinedione conjugates were design, synthesized and evaluated against Type 2 diabetes mellitus, through  $\alpha$ -Amylase inhibition.  $\alpha$ -Amylase inhibition has been considered as a highly effective therapeutic approach against typical Type-2 diabetes mellitus. Furthermore, to evaluate the  $\alpha$ -Amylase inhibition abilities of synthesized conjugates, Acarbose drug was considered as a reference standard. It was further found that most of the synthesized compounds exhibited  $\alpha$ -Amylase inhibition activity compared to reference standard, moreover compound BO-SK-101, BO-SK-106, BO-SK-107, BO-SK-108, BO-SK-110, BO-SK-112, BO-SK-114 shows highly potent activity with IC50 value 5.00 -6.02  $\mu$ M. To calculate ligand receptor interaction; 1RPK barley  $\alpha$ -Amylase isozyme was used as a receptor in silico molecular docking studies of synthesized compounds. The docking scores of synthesized compounds were compared with the docking score of Acarbose. The results of the docking studies were indicated the synthesized compounds are potential as  $\alpha$ -Amylase inhibitors.

## SYNTHESIS AND CHARACTERIZATION OF SOME NEW HYBRIDS OF 2-CHLOROQUINOLINE AND BENZIMIDAZOLE CHALCONES AS ANTIBACTERIAL AGENTS

Manisha B. Karmur\*, Jasminkumar J. Bhalodia Department of Chemistry and Forensic Science, Bhakta Kavi Narsinh Mehta University, Junagadh, Gujarat, INDIA E-mail: karmurmanisha45@gmail.com

### Abstract

New scaffold designed by the combination of 2-chloro-3-(chloromethyl) quinoline and acetyl benzimidazole. Some novel 2-chloro-3-(chloromethyl) quinoline based benzimidazole chalcone derivatives were synthesized by multistep reaction steps and evaluated for antibacterial activity. Acetyl benzimidazole were reacted with aromatic aldehyde in presence of methanol to furnish substituted chalcones. These chalcones were further treated with 2-chloro-3-(chloromethyl) quinoline to get targeted compounds. The structure of newly synthesized compounds were characterized by IR, mass, 1H NMR and 13C NMR. The synthesized compounds were screened for their antibacterial activity against selective gram positive bacteria (Staphylococcus aureus, Bacillus cereus, Clostridium rubrum) and gram negative bacteria (Salmonella typhi, E. coli, Klebsiella pneumoniae, Pseudomonas aeruginosa) compared to standard antibiotic i.e., Tetracycline. Among all the synthesized compounds MK-103, MK-105, MK-106, MK-107, MK-108, MK-109, MK-111 were found to be the most active compounds.

## ANALYTICAL METHOD DEVELOPMENT, VALIDATION STUDIES OF NITROFURANTOIN IN BULK AND IN MARKETED PRODUCTS BY HIGH PERFORMANCE LIQUID CHROMATOGRAPHY

Rajesh A. Jadav, Atul H. Bapodra Department of Chemistry and Forensic Science, Bhakta Kavi Narsinh Mehta University, Junagadh, Gujarat, INDIA E-mail: jadavrajesh055@gmail.com

#### Abstract

Nitrofurantoin is used to treat lower urinary tract infection and it works as an antimicrobial drug. It is produced potent toxicity and causes damages to multiple organs if overdose or chronic use. So, it is must be in require dose in commercial formulation. This method can be quantified the nitrofurantoin by this proposed method. In this method caffeine was used as an internal standard. Some force degradation products of Nitrofurantoin were probably identified by mass spectra.

## TEOA-IL'S CATALYZED MULTICOMPONENT SYNTHESIS OF 2-AMINO-4H CHROMENE: A STRATEGY FOR GREEN AND SUSTAINABLE CHEMISTRY

Mayur Vala\*, Naval Kapuriya Smt V.M. Chandera Science College, Loej, Gujarat, INDIA E-mail: valamayur121@gmail.com

#### Abstract

In the Green Chemistry perspective, the evolution of a new era in chemical research has been entered by ionic liquids (IL's) as potential 'Green Designer Solvents' as new replacement for volatile organic solvents. The main advantages of ionic liquids are their negligible volatility, their non-flammability, the control of their properties due to the composition, and their high compatibility with various organic compounds and other materials. Additionally, they can be easily recycled due to their immiscibility with a range of solvents. In this study, various types of substituted chromene have been synthesized. Initially, benzaldehyde, malanonitrile and  $\alpha$ -naphthol were reacted using IL'S. The desired 2-amino 4-H chromenes were obtained in high yield.

## SUZUKI COUPLING REACTION BY CALIX [4] PYRROLE TETRABENZOHYDRAZIDE WRAPPED PALLADIUM NANOPARTICLES AND ITS APPLICATION AGAINST BREAST CANCER AND TUBERCULOSIS

Anilkumar S. Patel<sup>1</sup>, \*Nandan C. Pomal<sup>2</sup>, Keyur D. Bhatt<sup>2</sup>, Monil P. Dholariya<sup>1</sup>, Dinesh S. Kundariya<sup>3</sup>, Jaymin Parikh<sup>2</sup> <sup>1</sup>Department of Chemistry, Faculty of Science, Atmiya University, Rajkot, Gujarat, INDIA, <sup>2</sup>Department of Chemistry, Faculty of Science, Ganpat University, Kherva, Mehsana, Gujarat, INDIA <sup>3</sup>Department of Chemistry, Tolani College of Arts & Science, K.S.K.V. Kutch University, Bhuj, Gujarat, INDIA

E-mail: patelanil32@gmail.com & anil.patel@atmiyauni.ac.in

## Abstract

A facile synthesis of calix [4] pyrrole tetrabenzohydrazide wrapped-Palladium nanoparticles (CPTBH-PdNP's) and its characterization using UV-Visible, TEM, SAED, EDX, Zeta Potential, and DLS techniques confirmed the successful formation of CPTBH-PdNP's. These CPTBH-PdNP's were employed as catalysts in Suzuki coupling reactions under mild conditions, resulting in efficient C-C bond formations. Additionally, the CPTBH-PdNP's exhibited significant anti-cancer effects against the human breast cancer cell line MDA-MB-231, with an IC50 value of 38.86  $\mu$ g/mL, and exceptional efficacy against Mycobacterium Tuberculosis, with a minimum inhibitory concentration (MIC) value of 0.8  $\mu$ g/mL [1].

## SYNTHESIS AND STUDY OF MESOMORPHIC PROPERTIES OF LIQUID CRYSTALLINE COMPOUNDS INVOLVING LATERAL -OCH3 GROUP AND VINYL CARBOXYLATE CENTRAL LINKAGE

Gaurang P. Makavana\*, Neha K. Baku<sup>1</sup>, Jwalant J. Travadi<sup>2</sup> \*&<sup>2</sup>Chemistry Department, Kamani Science and Prataprai Arts College, Amreli, Gujarat, INDIA <sup>1</sup>Chemistry Department, Atmiya University, Rajkot, Gujarat, INDIA E-mail: gpmakvana2901@gmail.com

### Abstract

In the present investigation, a newly synthesized ester homologous series of mesogenic compounds having a vinyl carboxylate group as central linkage with two phenyl rings and a laterally substituted methoxy group as well as -CH=CH-COOC4H9 terminal end group was synthesized. Eleven homologues are synthesized. Among these eleven homologues first six derivatives C1 to C7 of the investigated series are nonmesomorphic by nature. Rest of the homologs are smectic by nature, among these C8, C10 and C12 homologues show monotropically smectic phase, while the last member of the series C14 show smectic phase enantiotropicaly. Thus presently investigated series is predominately smectogenic by nature without exhibiting nematic mesophase. Transition temperatures and textures of synthesized compounds were observed through an optical polarizing microscope equipped with a heating stage. The textures of smectogenic mesophase are focal conic fan-shaped. Some representative members were characterized by IR, 1HNMR, mass spectroscopy and elemental analysis. A phase diagram is obtained by plotting a graph of number of 'carbon atoms in the n-alkyl chain of the n-alkoxy terminal end group' versus 'transition temperatures'. Isotropic-smectic / smectic-isotropic transition curve behaves in a normal ascending manner. Thermal stability and other mesogenic characteristics are compared with other structurally similar homologous series. The mesogenic phase length ranges between 5° C and 24° C and is of middle-order melting type.

## SYNTHESIS AND BIOLOGICAL EVOLUTION OF BENZIMIDAZOLE CONTAINING NOVEL HYDRAZIDE-HYDRAZONE DERIVATIVES

Viralkumar A. Doshi\*, Dr. Yogesh S. Patel Department of Chemistry, Government Science College, Limkhedda Gujarat University, Ahmedabad, Gujarat, INDIA E-mail: viral\_doshi207@yahoo.com & dryspatel@gmail.com

## Abstract

New hydrazide-hydrazone derivatives (NIB 01- 15) were synthesized by reacting substituted Benzimidazole hydrazine derivative with substituted aromatic aldehydes. These derivatives underwent analysis using IR, NMR, and Mass spectroscopy. Utilizing the broth dilution method, their antifungal and antibacterial efficacy against three fungal and four bacterial stains was assessed. To forecast the pharmacokinetic characteristics (ADME) of the recently synthesised derivatives, an insilico analysis was also carried out. The results are statistically treated as its significance.

## DESIGN, SYNTHESIS AND CHARACTERIZATION OF 2,4,6-TRISUBSTITUTED PYRIMIDINE DERIVATIVES

Hina Jadav, Denish Viradiya\* Department of Chemistry, Shri Govind Guru University, Godhara, Gujarat, INDIA E-mail: hdjadav308@gmail.com

#### Abstract

Pyrimidines are the nitrogen containing heterocyclic molecules represents one of the most active classes of compounds possessing wide spectrum of biological activities like anticancer, anti-HIV, antifungal and antibacterial activities. In view of these finding in literature, we have synthesized some of 2,4,6-trisubstituted pyrimidine analogs. Initially, 2,4,6-trichloropyrimidine is synthesized by the reaction of barbituric acid with POC13. Further, trichloropyrimidine on ucleophilic substitution reaction with different amines/phenols gave targeted compounds. Structures of the synthesize compounds are confirmed by spectral techniques such as Mass and/or NMRs.

# METALLIC DEEP EUTECTIC SOLVENT AND THEIR ASSOCIATION WITH ALCOHOLS

Papu Kumar Naik<sup>1\*</sup>, Anjali Thakur<sup>1</sup> Department of Earth and Environmental Science, Parul Institute of Applied Sciences, Parul University, Vadodara, Gujarat, INDIA E-mail: papu.naik23945@paruluniversity.ac.in

#### Abstract

Zinc (II) chloride based deep eutectic solvents (DESs) were formed by mixing zinc (II) chloride with phosphoric acid. Densities, and speed of sound, of [ZnCl<sub>2</sub>] [phosphoric acid] 1:2.5 with methanol, ethanol, or propanol have been measured at T = (293.15, 303.15, 308.15, and 313.15) K and at atmospheric pressure. Excess molar volumes, isentropic compressibility, deviation in isentropic compressibility and intermolecular free length were calculated from the densities, and speed of sound, respectively. To fit the excess molar volumes and deviation in isentropic compressibility, the Redlich-Kister smoothing polynomial was used. Also, we have used perturbed chain statistical associating fluid theory equation of state (PC-SAFT EoS) for modeling the densities of the binary mixtures, and Schaaff's collision factor theory (SCFT) and Nomoto's relation (NR) were used for modeling the speed of sounds for the binary mixtures.

## SYNTHESIS OF 2-(4-((BENZO[d]OXAZOLE-2-YLTHIO) METHYL)-1H-1,2,3-TRIAZOLE-1-YL)-N-PHENYLACETAMIDE DERIVATIVES VIA CLICK APPROACH

Anjalee R. Khoyanee, Dr. Ranjan C. Khunt\*, Department of Chemistry, Saurashtra University, Rajkot, Gujarat, INDIA E-mail: anjalikhoyani1313@gmail.com

#### Abstract

In this study, we have illustrated here the synthesis of 2-(4-((Benzo[d]oxazole-2-ylthio) methyl)-1H-1,2,3-triazole-1-yl)-N-phenylacetamide derivatives by the reaction of suitable alkyne with various azides via [2+3] cycloaddition in the presence of Copper(I) as a catalyst and suitable solvent mixture of DMF:H2O:t-BuOH at room temperature. Above synthesized derivatives have remarkable interest due to their potential Antineoplastic activities. The study includes characterization with Mass, IR, 1H NMR, 13C NMR data providing valuable insights of molecular structure of the synthesized compounds. This aspect of the study aims to assess of the potential pharmacological properties of the synthesized compounds, which could have applications in drug discovery and medicinal chemistry.

## UNVEILING INNOVATIVE PURINE DIONE DERIVATIVES: A COMPREHENSIVE STUDY FOR ADVANCING MEDICINAL APPLICATIONS

Sanjay N. Bamaniya Department of Chemistry, Bhakta Kavi Narsinh Mehta University, Junagadh, Gujarat, INDIA E-mail: sanjaybamaniya6762@gmail.com

### Abstract

Purine derivatives have long been of interest in medicinal chemistry due to their versatile pharmacological properties. This research focuses on the design, synthesis, and characterization of novel purine dione derivatives, with a particular emphasis on the lead compound, Pentoxifylline, for its potential medicinal applications. The study encompasses a comprehensive investigation into the synthesis and structural analysis of these newly designed derivatives, using techniques such as NMR, Mass Spectroscopy, and IR Spectroscopy. Pharmacological evaluation of these compounds against various microbial strains, including E. coli, M. luteus, S. Typhi, S. aureus, and C. albicans, is conducted to assess their potential as antimicrobial agents. The results of this study provide valuable insights into the synthesis, structural attributes, and potential pharmaceutical applications of these purine dione derivatives, offering promising prospects for the development of novel therapeutic agents in the field of medicinal chemistry. The research highlights the importance of articulating these newly designed compounds for medicinal interest and lays the foundation for further exploration in drug development.

## SYNTHESIS AND CHARACTERIZATION OF THIAZOLE COMPOUNDS AS BIOLOGICALLY ACTIVE AGENT

Priyank M. Shah, Ranjan C. Khunt\* Department of Chemistry, Saurashtra University, Rajkot, Gujarat, INDIA E-mail: priyank9913@outlook.com

### Abstract

Thiazole derivatives have attracted a great deal of interest due to their association with various biological properties found in many potent biologically active molecules such as ritonavir (an antiretroviral drug), Sulfathiazol (an antimicrobial drug), etc. Due to its wide range of applications, thiazoles consist of a core structure for synthesizing a chemical library. We reported here the synthesis of thiazole derivatives (KMR-1 to KMR-5) by using a novel aldehyde, a scaffold from which a diverse range of other biologically important new chemical entities could be produced. This aspect of the study aims to assess the potential pharmacological properties of the synthesized compounds, which could be applied in drug development and medicinal chemistry.

## A CONCISE SYNTHESIS AND CHARACTERIZATION OF HETEROCYCLIC MOLECULES WITH NITROGEN AS ANTICANCER AGENT

Dharmesh K. Katariya\*, Ranjan C. Khunt, Manish K. Shah Chemical Research Laboratory, Department of Chemistry, Saurashtra University, Rajkot, Gujarat, INDIA E-mail: dk.katariya9395@yahoo.com

### Abstract

In the field of medicinal chemistry, heterocyclic compounds have gained attraction due to their potential as anticancer activity. By altering different cellular functions and interacting with essential biological substances including DNA and proteins, these compounds exercise their anticancer characteristics. Among them, heterocyclic molecules with nitrogen have attracted a lot of interest due to their many potential uses in cancer treatment. In this study, we have reported here the synthesis of tetrazole derivatives via the Ugi multicomponent reaction method. We further investigate the anticancer efficacy of these compounds against NCI-60 Cell lines. Future cancer therapies that are more accurate and effective may be made possible by tetrazole derivatives.

## CHALCONYL ESTER HOMOLOGOUS SERIES: SYNTHESIS AND CHARACTERIZATION WITH DISTINCT LATERAL AND TERMINAL GROUPS

Bharat H. Mevada\*, U.C. Bhoya Chemical Research Laboratory, Department of Chemistry, Saurashtra University, Rajkot, Gujarat, INDIA E-mail: mevadabharat23@gmail.com

### Abstract

A homologous series  $\alpha$ -4-(4'-n-alkoxy-3'-methoxy benzoyloxy) benzoyl- $\beta$ -naphthyl ethylene is synthesized and studied with a view to understand and establish the relation between molecular structure and mesomorphism. New homologous series consists of twelve homologues (C1-C8, C10, C12, C14 & C16) and show mesomorphic in nature. The members of the series were characterized by IR, NMR, Mass and Optical polarizing microscopy with heating stage. The mesomorphic properties of the present series are compared with other structurally related series.

## SYNTHESIS, SPECTROSCOPIC AND ANTIMICROBIAL STUDIES OF SOME NOVEL TRANSITION METAL BASED HETEROCHELATES

Parmar Jignasa<sup>1</sup>, Dr. Darshan Jani<sup>2</sup> Department of Chemistry, Shubhash University, Junagadh, Gujarat, INDIA E-mail: parmarjignasa275@gmail.com

#### Abstract

In the present work, we synthesized new Schiff base ligands and their transition metal complexes. The synthesized compounds were characterized and their antimicrobial activities were studied. Elemental analysis, IR, 1 H-NMR and mass spectrometry were done to fully characterize all the compounds. The ligands and their complexes were screened for in-vitro biological study against some Gram positive and Gram negative bacteria for the Zone of inhibition method. The complexes showed better activity than the ligands.

## FORMULATION AND CHARACTERIZATION OF POLYURETHANE FOAMS FROM NATURAL RENEWABLE RESOURCES

Tejas S. Gandhi1, Bharat kumar Z. Dholakiya1\* 1V.S. Patel College of Arts and Science college, Bilimora, Gujarat, INDIA 1\*Department of Applied Chemistry, Sardar Vallabhbhai National Institute of Technology-(SVNIT), Surat, Gujarat, INDIA E-mail: tejsvnit.ac.in@gmail.com

## Abstract

In the past, polyurethanes were usually made with petroleum polyols. With the dwindling and nonrenewable petroleum resource, some novel polyols made from vegetable and seed oil have been investigated for their potential of replacing the petroleum polyols. Of particular interest is a group of polyols derived from Cashew nut oil. These new polyols, however, have some major disadvantages limiting its applications when compared with petroleum polyols. Synthesis of polyols from CNSL as non-petroleum renewable resource and application in rigid polyurethane foam with better mechanical, thermal and fire performance.

## SYNTHESES AND BIOLOGICAL EVOLUTION OF SOME NOVEL CHLORO SUBSTITUTED PYRROLO [2, 3-d] PYRIMIDINE UREA DERIVATIVES

Mr. Ranjitkumar Ravatbhai Pada<sup>1\*</sup>, Dr. Jyotindra J. Bhatt<sup>1</sup> <sup>1</sup>Department of Chemistry, Faculty Block "A", KSKV Kachchh University, Mundra Road, Bhuj, Gujarat, INDIA E-mail: ranjit\_pada@yahoo.co.in & jyotindrajbhatt@gmail.com

### Abstract

Our area of interest is allied to study targeted antimicrobial agents. We focused on pyrrole fused chloro substituted pyrimidines. This ring system is tied up with carbamate in order to form corresponding urea derivative. The present study compiled syntheses, antibacterial and antifungal activity of some novel Chloro substituted Pyrrolo [2, 3-d] pyrimidines urea derivatives. The targeted compounds have been synthesized by condensation reaction between ((3R,4R)-1-(2-chloro-7Hpyrimidin-4-yl)-N,4-dimethylpiperidin-3-amine pyrrolo[2,3-d] and 4-nitrophenyl (4substitutedbenzyl) carbamate. The structures of synthesized compounds have been confirmed by various spectroscopic techniques like 13CNMR, 1H NMR, mass spectrometry (MS) and Infrared spectroscopy (IR). All the synthesised compounds have been screened in-vitro antimicrobial activities. Four different bacterial strains and two different fungal strains have been used. The standard drugs like Gentamycine, Ampicillin, Chloramphenicol, Ciprofloxacin and Norfloxacin have been used to compare antibacterial activities while two standard drugs Nystatin and Greseofulvin have been used to compare antifungal activities. The tabulated results are promising and encourage us for further expansion in our study.

## DESIGN SYNTHESIS OF MULTICOMPONENT, (3-(BENZO[d] [1,3] DIOXOL-5-YL)-7-CHLORO-3,4-DIHYDRO-2H-BENZO[b] [1,4] OXAZIN-2-YL) (PHENYL) METHANONE ANALOGUES

Mori Vijay G., Dr. J.M. Parmar Department of Chemistry, M. M. Science College, Morbi, Gujarat, INDIA E-mail: mori.vijay2015@gmail.com

#### Abstract

The green synthesis of (3-(benzo[d][1,3]dioxol-5-yl)-7-chloro-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-yl)(phenyl) methanone has been built using a novel green and efficient catalyst-free, mild one-pot, multicomponent synthetic strategy. In-situ Schiff-base formation, base-mediated alkylation with phenacyl bromide or substituted phenacyl bromide, and intramolecular cyclization are the steps in this isolated as single diastereomers in moderate to excellent yields (60-92%). The structures of the synthesized products were elucidated by IR, 1H NMR and 13C NMR spectroscopy and mass spectrometry. The synthesized hybrids were investigated for their antimicrobial activity against several bacterial and fungal strains, the synthesis of several functionally substituted benzoxazine scaffolds is also made possible by this novel flexible approach, which offers a large range of options. It can also be used as a component in the synthesis of complex molecular structures, particularly for pharmacological uses.

## SYNTHESIS, CHARACTERIZATION AND ANTIBACTERIAL ACTIVITY OF SOME NEW PYRIMIDINE DERIVATIVES FROM CHALCONE DERIVATIVES

Vala Manisha, Dr. Darshan Jani Department of Chemistry, Shubhash University, Junagadh, Gujarat, INDIA E-mail: valamanisha09@gmail.com

#### Abstract

This research syntheses chalcones as a starting material by aldehyde react with derivatives of aceophenone like 4-amino-acetophenone, 3-nitro-acetophenone and 4-nitroacetophenon. This chalcones react with urea and thiourea to produce pyrimidine derivatives. These compounds have been characterized by melting points, mass spectroscopy, IR spectroscopy, H1 NMR spectroscopy and thin layer chromatography technique (TLC) has been used for reactions steps and sequences. Antibacterial activity test of those derivative compounds.

#### **CELLULOSE IS AN EMERGING MATERIAL FOR THE FUTURE**

Jitubhai H. Morabiya\*, Dr. Hardik Bhatta S.E.T. college, Junagadha, Gujarat, INDIA E-mail: jitubhamorabiya@gmail.com

#### Abstract

Cellulose, a ubiquitous biopolymeric compound present in the walls of the cells of plants, is now at a time increasing attention as an emerging material with potential applications in the future. This poster explores the properties of cellulose that make it a promising compound for various industries, ranging from sustainable packaging to advanced biomedical applications. The renewable and abundant nature of cellulose, combined with its biodegradability also it an eco-friendly, cost-effective alternative to conventional materials. Additionally, advancements in nanotechnology have enabled the extraction of nanocellulose, opening new avenues for the development of high-performance materials with enhanced mechanical strength and flexibility. The biocompatibility of cellulose further extends its utility in biomedical research, where it also shows potential applications for drug delivery systems, tissue engineering, wound healing applications even electronic devices. This abstract focuses on the latest research and innovations that surround cellulose-based materials (CBM) and draws attention to their role in shaping a more sustainable and technologically advanced future. As researchers continue to explore the vast potential of cellulose, it is evident that this natural polymer is poised to play an important role in the development of innovative materials toward green chemistry, contributing to a more sustainable and environmentally conscious globally.

## O-HYDROXY KETONE BASED AZOMETHINE AS A SELECTIVE AND SENSITIVE CHEMOSENSOR FOR RARE EARTH METAL ION

R. S. Jani<sup>1\*</sup>, R. V. Zala<sup>2</sup> <sup>1</sup>Department of Chemistry, R. R. Lalan College, Bhuj, Gujarat, INDIA <sup>2</sup>Department of Chemistry, Kamani Science College & Prataprai Arts College, Amreli, Gujarat, INDIA E-mail: jani.rakesh71@yahoo.com

#### Abstract

A new o-Hydroxyketone based sensor N'-(1-(5-fluoro-2-hydroxyphenyl) ethylidene)-4anisoylhydrazine (3e) was designed, and its sensing ability towards various metal ions was assessed using UV-visible spectroscopy. The structure of 3e was spectroscopically characterized by UV-Visible, Infrared, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR spectroscopy and mass spectrometry. UV-Visible absorption spectral study showed selective sensing ability of 3e for Yb<sup>+3</sup> ion in presence of diverse rare earth metal ions. The results revealed that the detection limit for Yb<sup>+3</sup> was found to be 40 $\mu$ M. Moreover, the compound 3e was fully implemented for detection of Yb<sup>+3</sup> in simulated samples.

#### EFFECT OF BUTOXY ETHYL TERMINAL CHAIN ON MESOMORPHISM

<sup>a</sup>Chitra A. Padh, <sup>a</sup>Mikita Shah, <sup>b\*</sup>H. N. Patel, <sup>c\*</sup>Tarun M. Patel
<sup>a</sup>Department of Chemistry& Chemical Sciences, Sabarmati University, Gujarat
<sup>b\*</sup>Shree Maneklal M. Patel Institute of Sciences & Research Sector 15/23, Kadi Sarva Vishwavidhyalaya, Gandhinagar, Gujarat, INDIA.
<sup>c\*</sup>Sir P. T. Sciences College Department of Chemistry, Modasa, Gujarat, INDIA

E-mail: hement2patel@yahoo.co.in & drpatel16185@gmail.com

#### Abstract

A new mesogenic homologous series with butoxy ethyl terminal chain, butoxy ethyl 4(4'-nalkoxybenzoyloxybenzylidene) 4'-aminobenzoates has been synthesized by condensing an appropriate 4-n-alkoxy benzyloxy benzaldehyde with butoxy ethyl 4-amino benzoate. The synthesized, characterized compounds were by combination of elemental analysis and standard spectroscopic methods. First derivative is purely nematogenic. Ethoxy to n-hexyloxy derivatives exhibit enantiotropic smetic-A as well as nematic mesophases. n-heptyloxy to n-hexadecyloxy derivatives exhibit enantiotropic smatic-A mesophase. The phase transition properties of the present series were compared with structurally related other mesogenic derivatives to evaluate the effect of butoxyethyl tail and central schiff's base linkage on mesomorphism.

## DEVELOPMENT AND VALIDATION OF A SENSITIVE LC-MS METHOD FOR THE DETERMINATION AND QUANTIFICATION OF NITROSAMINES IN VILDAGLIPTIN AND METFORMIN DRUG PRODUCTS

Mehul Pathak\*, Dhara D. Patel Department of Chemistry, Sankalchand Patel University, Visnagar, Gujarat, INDIA E-mail: mehulpathak78@gmail.com

#### Abstract

N-nitrosamine impurities have been found in several drug products, showing a concern for regulatory aspects. The study presents the development and validation of a sensitive LC-MS/MS method for detecting eight nitrosamines in vildagliptin and metformin drug products. The developed method was specific and linearity was ranged 3.53 - 55.92 ppb for NDMA, 3.18 - 50.37 ppb for NMBA, 0.97 - 15.41 ppb for NDEA, 0.98 - 15.52 ppb for NEIPA, 1.00 - 15.86 ppb for NDIPA, 0.98 - 15.46 ppb for NDBA, 0.98 - 15.58 ppb for NMPA and 0.7 - 15.32 ppb for NDPA with correlation coefficient (r) was more than 0.98 and square of correlation coefficient (r2) was found to be greater than 0.96. The LOQ were obtained in the range of 0.97 - 3.53 ppb with %RSD in the range of 2.5 - 10.9 % for eight nitrosamines showed good sensitivity. Accuracy was found in the range of  $98.63 \pm 5.77 - 125.17 \pm 3.68$  % at LOQ level,  $74.77 \pm 0.83 - 88.17 \pm 0.15$  % at 50 % level,  $79.93 \pm 8.47 - 89.00 \pm 0.61$  % at 100 % level and  $74.67 \pm 2.31 - 84.03 \pm 0.93$  % at 150 % level for the eight nitrosamine impurities that were well within acceptance criteria of not less than 70.0 % and not more than 130.0 %. The method validation results demonstrated that the method is precise, accurate, and linear, can be applied to quantify the nitrosamines in vildagliptin and metformin drug products.

## WATER-MEDIATED SnAr SYNTHESIS OF SUBSTITUTED-4,6-DIMETHOXYPYRIMIDIN-2-AMINE DERIVATIVES: RATIONAL DESIGN AND MOLECULAR DYNAMICS EVALUATION OF NOVEL ANTICANCER AGENTS TARGETING LUNG CANCER

Dr. Jayesh Maru\*, Ranjit Dabhi Department of Chemistry, School of Sciences, Gujarat University, Ahmedabad, Gujarat, INDIA E-mail: jaymaru@gujaratuniversity.ac.in

#### Abstract

Heterocyclic compounds have shown significant potential for treating various diseases worldwide. This study presents the elucidation of a water-solvated aromatic nucleophilic substitution (SnAr) reaction followed by a Suzuki reaction for the synthesis of 2-aminopyrimidine derivatives (A1-A8), aided by a molecular dynamics study. We employed various solvents with different acids or bases at various temperatures to optimize the SnAr reactions, and we found that water is the most effective solvent, completing the SnAr reaction within an hour with a good yield. The synthesized compounds have been characterized using mass spectrometry, LC-MS, FTIR, and NMR spectroscopic analyses. The optimized substitution via nucleophilic attack on 2-chloropyrimidine enables easy isolation, a metal-free process, and environmentally approach in the initial step. While next coupling via Suzuki reaction using various halo-derivatives enhances the bio-potency towards A549 cells.

## INFLUENCE OF SUBSTITUTED ETHYL TAIL ON CENTRAL MESOGENIC CINNAMATE DERIVATIVES

<sup>a</sup>Sachin Ramchandra Vishe, <sup>a</sup>Mikita Shah, <sup>b\*</sup>H. N. Patel, <sup>c\*</sup>Tarun M. Patel
<sup>a</sup>Department of Chemistry & Chemical Sciences, Sabarmati University, Gujarat, INDIA
<sup>b\*</sup>Shree Maneklal M. Patel Institute of Sciences & Research Sector 15/23, Kadi Sarva Vishwavidhyalaya, Gandhinagar, Gujarat, INDIA
<sup>c\*</sup>Sir P. T. Sciences College, Department of Chemistry, Modasa, Gujarat, INDIA
E-mail: hement 2patel@yahoo.co.in & drpatel16185@gmail.com

## Abstract

A mesogenic derivatives of cinnamates with substituted ethyl tail: propoxyethyl[4(4-n-alkoxycinnamoyloxy) benzoates] has been synthesized by condensing an appropriate 4-n-alkoxycinnamoylchloride with propoxyethyl 4-hydroxybenzoate. The synthesized and characterized compounds were by combination of elemental analysis and standard spectroscopic methods. In this series all the compounds synthesized exhibit mesogenic. First three derivatives exhibit monotropic nematic mesophase. n-butyloxy to n-pentyloxy derivatives exhibit both enantiotropic smectic A as well as nematic mesophases. n-hexyloxy to n-hexadecyloxy derivatives exhibit only enantiotropic smectic A mesophase. The phase transition properties of the present series were compared with structurally related other mesogenic derivatives to evaluate the effect of propoxyethyl tail and cinnamoyloxy central linkage on mesomorphism.

## DESIGN, SYNTHESIS, AND CHARACTERIZATION OF 1, 3-DISUBSTITUTED-1,4-BENZODIAZEPINE DERIVATIVES

Satish M. Ghelani, Yogesh T. Naliapara Department of Chemistry, Bahauddin Science College, College Road, Junagadh, Gujarat, INDIA E-mail: satishghelani@yahoo.com

### Abstract

The 2-amino-4-flouro-benzophenone (1) that was reacted with chloroacetylchloride to afford 2-chloro-N-(2-(4'-fluorobenzoyl) phenyl)acetamide (2) was subsequently converted to 1,4-benzodiazepines (3) by the modification of the known hexamethylenetetramine based cyclization reaction developed by Blazevic and Kajfez. Thus, obtained product (3) was reacted with a variety of alkyl halide using KOH in DMF to give 1-substituted-5-(4-fluorophenyl)-1H-benzo[e] [1,4] diazepin-2(3H)-one (4a–b). To achieve 1, 3-disubstituted 1, 4-benzodiazepines (5a–t), 1-substituted-5-(4-fluorophenyl)-1H-benzo[e][1,4]diazepin-2(3H)-one (4a–b) was treated with various aromatic aldehydes in the presence of KOH in toluene.

## SYNTHESIS, CHARACTERIZATION AND LUMINESCENT PROPERTIES OF ZINC COMPLEXES BASED ON TETRADENTATE N<sub>2</sub>O<sub>2</sub>-DONOR PYRAZOLONE SCHIFF BASE

Jigneshkumar P. Sathvara\*, Rajendrasinh N. Jadeja\*\* Department of Chemistry, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat, INDIA E-mail: jsathwara96@gmail.com

### Abstract

The luminescent properties of Zinc (Zn) complexes based on tetradentate  $N_2O_2$ -donor Pyrazolone Schiff bases can be quite interesting and are an area of research in coordination chemistry. These complexes often exhibit Photoluminescence properties due to the presence of organic ligands, which can enhance or quench the emission of the Zn center, depending on the ligand's nature and coordination environment. To explore the photophysical properties of coordination compounds with new Zn (II) complex were synthesized based on a new Salen-type tetradentate  $N_2O_2$  ligands derived from 1-phenyl-3-methyl-4-formyl-5-pyrazolone. Through thermal characterization, this complex was proved to have good thermal stability. Photoluminescence spectra were recorded, both in solution and in the solid state, and the complexes showed noteworthy photoluminescence with a maximum in the blue region. Complexes have been characterized by ESI-mass spectroscopy, IR spectroscopy and thermal gravimetric analysis, UV–vis, emission and <sup>1</sup>H-NMR.

## SYNTHESIS OF NEW BIPHENYL ESTER SCHIFF BASE LIQUID CRYSTALLINE COMPOUNDS STUDY OF THEIR MESOMORPHIC BEHAVIOR AND DFT CALCULATIONS

Vijay K. Joshi\*, Dr Kiran Nakum\*\* Department of Chemistry, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat, INDIA E-mail: vkjoshi1996@gmail.com,

#### Abstract

A series of twelve new [1,1'-biphenyl]-4-yl (E)-4-(((4-(alkoxycarbonyl) phenyl) imino) methyl) benzoate, ABAE, biphenyl ester Schiff base liquid crystals have been prepared and investigated for their mesomorphic and photophysical properties. Each compound differ from each other by the alkoxy chain length varies between carbon n=2 to n=18. Proposed molecular structures of the prepared compounds were confirmed via FT-IR, and 1H NMR & 13C NMR, Mass, spectroscopy. The mesomorphic behaviour and thermal stability of all new compounds have been investigated by polarized optical microscopy (POM), differential scanning calorimetry (DSC) and thermal gravimetric analysis (TGA). Characteristic textures of smectic A and Nematic phase were observed for all new mesogenic compounds. Further, density functional theory (DFT) calculations were carried out to investigate thermal and geometrical parameters of all newly prepared mesogens.

## APPLICATIONS OF CHIRAL ARYLOXY CYCLOHEXANOLS IN DERACEMIZATION OF α-SUBSTITUTED CARBOXYLIC ACIDS BY DYNAMIC THERMODYNAMIC RESOLUTION

Atul Pandavadara\*, Ashutosh V. Bedekar\*\* Department of Chemistry, faculty of science, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat, INDIA E-mail: pandavadraatul001@gmail.com

#### Abstract

Derivatives of trans-2-aryloxycyclohexanol were synthesized, their enantiomers were separated by enzyme mediated kinetic resolution and their absolute configuration was established by synthesizing their diastereomers with esters of known chiral description. Chiral alcohols were then used as chiral auxiliaries for the preparation of esters by coupling with racemic  $\alpha$ -halo acids. The synthesised compounds characterised by IR and NMR spectroscopy. During the coupling reactions with DCC and a suitable base, an efficient dynamic thermodynamic resolution was observed and the products were isolated in high diastereomeric purity. The observed diastereoselectivity was in accordance with the relative energy profile of the products. The chirally pure  $\alpha$ -halo acid could be separated from the auxiliary, without any loss of optical purity of both components.

#### **ACID HYDRAZIDES: A NEW MILESTONE TO HYBRID DRUGS**

Nirajkumar A. Paghadar\*, Bhavesh H. Sarvaiya, Satish M. Ghelani Department of Chemistry, Bahauddin Science College, College Road, Junagadh, Gujarat, INDIA E-mail: paghdarneeraj@gmail.com

#### Abstract

The field of hybrid drugs is matter of exploration nowadays as it provides better alternative for existing drugs with improved properties. Acid hydrazides are known for their possible biological effects and are essential intermediates in the production of heterocyclic compounds. In order to achieve a dual mode of action, our work presents an effective method for accessing a hybrid molecule, an acid hydrazide with 4-methyl thiazole moiety. Our simplified process gives good yields under mild conditions with remarkable efficiency. The importance of acid hydrazides as useful intermediates for the synthesis of new bioactive heterocyclic compounds is highlighted by our research.

# SYNTHESIS, CHARACTERIZATION, ANTIBACTERIAL AND ANTIFUNGAL ACTIVITIES OF NOVEL 4-(ALKYL/ARYL AMINO)-2-(ETHYLTHIO)-6-(4-FLUOROPHENYL) PYRIMIDINE-5-CARBONITRILE

Jalpa H. Vadgama\*, Dr. Jayesh. J. Modha, Dr. Pragna H. Thanki\* Department of Chemistry, Maharshi Dayanand Science College, Porbandar, Gujarat, INDIA Bhakta Kavi Narsinh Mehta University, Junagadh Shri Natvarsinhji Arts and Science College Chhota Udepur, Gujarat, INDIA Shri Govind Guru University, Godhra, Gujarat, INDIA E-mail: jalpavadgama30@gmail.com & pragnathanki@gmail.com

#### Abstract

It is predictable that in 2050, antibiotic resistance will become one of the leading causes of death. Finding new antibiotics is crucial. Nitrogen-containing heterocyclic rings especially pyrimidines, 3,4-dihydropyrimidin-2(1H)-ones or dihydropyrimidinones (DHPMs) are lead molecules for research in this field due to their several pharmacological activities like antitumor, antiviral, anti-inflammatory, antidepressant, antimalarial and anticancer. Also, Aminopyrimidines have a unique position in medicinal chemistry because of their important clinical application. Literature survey reveals enough scope for achieving structural variations at the 4 and 6 positions in pyrimidine carbonitrile moiety. With an aim to explore better useful pyrimidine-5-Carbonitriles, newer 4-(alkyl/aryl amino)-2-(ethylthio)-6-(4-fluorophenyl) pyrimidine-5-Carbonitrile analogues has been prepared. Structural characterization of final synthesized compound was carried out using FTIR, 1H-NMR and mass analysis. Synthesized compounds were evaluated for their antibacterial and antifungal activities and some of the compounds showed good to excellent antibacterial activity for both gram positive bacteria and gram negative bacteria and also show good to modarate antifungal activity too.

# A RAPID ONE-POT SYNTHESIS AND BIOLOGICAL EVALUATION OF NOVEL 1,2,4-TRIAZOLO[1,5-a] PYRIMIDINES

Mayur L. Chandera, Jatin J. Upadhyay M.V.M. Science and Home Science College, Saurashtra University, Rajkot, Gujarat, INDIA. E-mail: chanderamayur419@gmail.com

#### Abstract

The synthesis of ten novel 1,2,4-Triazolo[1,5-a]-pyrimidine derivatives have been undertaken by involving Biginelli type three components reaction of 1-phenyl-3-aryl-1H-pyrazole-4-carbaldehydes, 3-amino-1,2,4-triazole and ethyl acetoacetate in DMF as per scheme-1. The constitution of all the compounds have been established by extensive use of analytical tools viz; IR, FT-IR, 1H-NMR, 13C-NMR, Mass spectra studies and elemental analyses. The antimicrobial activity against S. aureus MTCC-96 (gram-positive), E. Coli MTCC-443 (gram-negative) and antifungal activity against A. niger MTCC-282 and C. albicans MTCC-227 at different concentrations using micro-dilution broth method according to NCCLS standards. The antimicrobial activity was compared with Ampicillin, Chloramphenicol, Ciprofloxacin, Norfloxacin, Nystatin and Greseofulvin as standard drugs at same different concentration. The antimicrobial activity was measured in the zone of inhibition in m.m. The compounds such as MHV-1b, MHV-1d, MHV-1e, MHV-1f, MHV-1h, MHV-1i, MHV-1j showed moderate antibacterial activity against stapsylococcus aureus (gram positive) at the concentration of 250, 100, 250, 200, 250, 250, 250 µg/ml while MHV-1c, MHV-1f showed remarkable antibacterial activity against Streptococcus pyogenes (gram positive) at the concentration of 100 µg/ml. Moreover compounds MHV-1c, MHV-1i, found to be potent against Escherichia coli (gram negative) at the concentration of 62.5, 62.5 (µg/ml) and against Pseudomonas aeruginosa (gram negative) at the concentration of  $100 \,\mu\text{g/ml}$ .

# DESIGN AND SYNTHESIS OF 1, 4-DIHYDROPYRIDINE DERIVATIVES AS ANTI-CANCER AGENT

Denish Viradiya, Anamik Shah\* <sup>a</sup>Center of Excellence, National facility for drug discovery center, Department of Chemistry, Saurashtra University, Rajkot, Gujarat, INDIA. E-mail: djviradiya@gmail.com

## Abstract

A series of 1,4-dihydropyridine based compounds bearing benzylpyridinium moiety have been designed and evaluated for in vitro anticancer activity against (Caco2, A549 and U87 (MG)) cell lines using the MTT assay. Among these compounds, 7b, 7d, 7e, and 7f exhibited potent anticancer activity against the cell lines tested. The cytotoxicity of the synthesized derivatives was compared to standard drugs (gemcitabine, carboplatin, daunorubicin). Thus, synthesized DHPs can be considered as the encouraging molecueles for further drug development as anticancer agents.

# A GREEN SYNTHETIC APPROACH TOWARDS FEBUXOSTAT DERIVATIVES AS POTENT G PROTEIN-COUPLED RECEPTOR

Prasann Jogia<sup>a\*</sup>, Jayesh Modha<sup>a</sup> <sup>a</sup>Maharshi Dayanand Science College, Porbandar, Gujarat, INDIA E-mail: prasannjogia@gmail.com

#### Abstract

Febuxostat is a known xanthine oxidase inhibitor used to treat gout (disease of the king) and hyperuricemia (high uric acid in the blood). The design of the synthesized compounds has been done by securing febuxostat's pharmacophoric groups (isobutoxy, cyanide and thiazole ring). Also, T3P mediated ester derivatives of the febuxostat have been prepared in a greener way. These ester derivatives are then converted into 1,3-diketones and chalcones. Selected derivatives (Pyrrole, isoxazole, pyrimidine, flavone and 4H-pyran) which show good activity as G protein-coupled receptor as predicted by Swiss target prediction has been synthesized by a known reaction of 1,3-diketones and chalcones and chalcones and chalcones and chalcones.

# SYNTHESIS, CHARACTERIZATION, SPECTRAL STUDIES AND BIOLOGICAL ACTIVITIES OF SCHIFF BASE COMPOUNDS DERIVED FROM 1-BENZOTHIOPHENE-3-CARBALDEHYDE

Chandresh S. Vaya<sup>1\*</sup>, Dr. R.V. Zala<sup>2</sup> <sup>1</sup>GMB Polytechnic, Rajula, Gujarat, INDIA <sup>2</sup>Kamani Science College, Department of Chemistry, Amreli, Gujarat, INDIA E-mail: c.s.vaya2011@gmail.com

### Abstract

Schiff bases namely, 1-(1-benzothiophen-3-yl)-N-(4-methylphenyl)methanimine and 1-(1-benzothiophen-3-yl)-N-(2-nitrophenyl)methanimine have been synthesized and characterized by FT-IR, Mass and 1H-NMR spectroscopy. Schiff bases have been screened for Antimicrobial activity against bacteria and fungi by using MIC determination.

# BENZIMIDAZOLE-PIPERIDINE HYBRIDS AS ANTIMICROBIAL AGENTS: DESIGN, SYNTHESIS, AND IN VITRO ANTIMICROBIAL EFFICACY

Ms. Shantaben Kanabhai Kangad College of computer science and Information Technology, Junagadh, Gujarat, INDIA E-mail: shrutiahir7@gmail.com

#### Abstract

This research aims to investigate the antimicrobial potential of piperidine-benzimidazole derivatives and their significance as promising pharmaceutical agents. Benzimidazole derivatives have gained widespread attention for their versatility in therapeutic applications, serving as proton pump inhibitors, anticancer agents, anthelmintics, antihypertensives, and antifungals. To further explore their therapeutic capabilities, an efficient synthetic route was established to synthesize a diverse array of 2-(4-(1H-benzo[d]imidazol-2-yl) piperidin-1-yl)-N-phenylacetamide derivatives. Structural elucidation of the newly synthesized compounds was meticulously performed using advanced techniques, including 1H and 13C NMR, FT-IR spectroscopy, mass spectroscopy, and elemental analysis, ensuring accurate identification and characterization. The focus of this study was on evaluating the antimicrobial activity of these Piperidine-Benzimidazole derivatives against various microbial strains. The results reveal the significant antimicrobial and antifungal potential of these derivatives, showcasing their potential application in clinical settings. With potent activity against diverse microbial and fungal pathogens, these compounds present promising prospects as novel therapeutic agents for combating infectious diseases. This research offers valuable insights into the multifaceted therapeutic possibilities of Piperidine-Benzimidazole derivatives and paves the way for future investigations into their clinical implications in addressing microbial challenges.

## GREEN SYNTHESIS OF CHLORO CHALCONE DERIVATIVES BY SONOCHEMICAL METHOD

Kaneria Kelviben<sup>1</sup>, Chavda Presitaben<sup>2</sup>, Dr. Jagdish Movaliya<sup>3</sup>, Dipti L. Namera<sup>4</sup>, Kamlesh Khodbhaya<sup>5</sup> Department of Chemistry, Bahauddin Science College, College Road, Junagadh, Gujarat, INDIA E-mail: kelvikaneria10@gmail.com & chavdapresita77412@gmail.com

## Abstract

Green chemistry is an approach to the design, manufacture and use of chemical product to reduce or eliminate chemical hazards. It focuses on the reduction, reuse/recycle of the use of toxic and hazardous chemical. Sonochemistry will give a new opportunities for green chemistry. Sonochemistry is the application of ultrasound to chemical reactions and processes. Presently, sonochemistry is a simplistic pathway for a vast variety of syntheses in organic chemistry. Hence, significant features of the ultrasound technique compared with traditional methods are in higher yield, lesser reaction times, milder conditions, improved reaction rates, formation of purer products, easier manipulation and a role in waste minimization and energy protection. The present article will highlight the applications of sonochemical synthesis of chalcones using ultrasound via Claisen-Schmidt condensation.

# SYNTHESIS, CHARACTERIZATION AND ANTIMICROBIAL SCREENING OF (1E, 4E)-1-(3-METHYL-5-PHENOXY-1-PHENYL-1H-PYRAZOL-4-YL)-5-PHENYLPENTA-1,4-DIEN-3-ONE AND ITS DERIVATIVES

Kinjal J. Sabalpara\*, Jatin J. Upadhyay Matushri Virbaima Mahila Science & Home Science College, Rajkot, Gujarat, INDIA E-mail: kinjalsabalpara@gmail.com

#### Abstract

A series of novel pyrazole-based chalcones was synthesized by the reaction between (E)-4-(3-methyl-5-phenoxy-1-phenyl-1H-pyrazol-4-yl)but-3-en-2-one and various substituted aromatic aldehydes using Claisen–Schmidt condensation because chalcones containing pyrazole nucleus are of great interest as potent bioactive molecules owing to the presence of a reactive  $\alpha$ ,  $\beta$ -unsaturated carbonyl group in chalcones which is responsible for a wide spectrum of antiproliferative, antifungal, antibacterial, antiviral, antimalarial, etc. pharmacological properties. The newly synthesized heterocyclic moieties were characterized on the basis of their chemical properties and spectroscopic tools - IR, 1H NMR and Mass spectral analysis. The synthesized compounds were tested in vitro for their antimicrobial activity against standard bacterial strains like Escherichia coli, Staphylococcus aureus, Bacillus subtilis and standard fungal strains like Aspergillus niger and Candida albicans, by using the agar dilution technique and compared with Ofloxacin(antibacterial medication) and Clotrimazole(antifungal medication) as reference drugs. Some of the tested compounds showed significant antimicrobial activity.

## AQUA MEDIATED L-PROLINE CATALYZED SYNTHESIS AND STRUCTURE ANALYSIS OF CHROMEN DERIVATIVE

Dipti Namera<sup>\*</sup>, Jagdish Movaliya<sup>A</sup>

<sup>\*</sup>Department of Chemistry, Maharshi Dayanand Science College, Porbandar, Gujarat, INDIA <sup>A</sup>Department of Chemistry, Bahauddin Science College, Junagadh, Gujarat, INDIA E-mail: diptinamera22@gmail.com

## Abstract

9-phenyl-6,7-dihydrocyclopenta[b][1,3]dioxolo[4,5-g]chromen-8(9H)-one (Compound-I) C<sub>19</sub>H<sub>14</sub>O<sub>4</sub> and 9-(3,4- dichlorophenyl)-6,7-dihydrocyclopenta[b][1,3]dioxolo[4,5-g]chromen-8(9H)-one (Compound-II) C<sub>19</sub>H<sub>12</sub>Cl<sub>2</sub>O<sub>4</sub> were synthesized from sesamol, 1,3cyclopentadieneon and substituted aromatic aldehydes using L-Proline as a catalyst. An aqua mediated green reaction yields good yield and pure product. Both compounds were well characterized by IR and NMR spectroscopy. The structures of synthesized compounds were confirmed by Single Crystal X-ray Diffraction study. The X-ray study shows that Compound-I crystallizes in monoclinic P21/c (#14) space group with cell parameters a=5.4150(6)Å, b=15.413(2)Å, c=17.146(2)Å,  $\beta$ =92..152(3)o , V=1430.0(3)Å3 and (compound II) C<sub>19</sub>H<sub>12</sub>Cl<sub>2</sub>O<sub>4</sub> DM-208 crystallize in Triclinic P-1 (#2) space group with cell parameters a = 7.774(1) Å b = 9.706(2) Å c = 11.550(2) Å  $\alpha$  = 68.471(3) o  $\beta$ = 85.142(4) o  $\gamma$  = 78.692(4) o V = 794.8(2) Å3. CCDC 998772

# FLUORESCENCE ACTIVE SCHIFF BASE AND ITS RARE EARTH METAL COMPLEXES

Dharmil Jani Department of Chemistry, Shubhash University, Junagadh, Gujarat, INDIA E-mail: dharmil.2699@gmail.com

#### Abstract

Synthesis of rare earth metal complexes of fluorescence active Schiff base compounds derived from amine and aldehyde by condensation reaction. The synthesized compound were characterised by elemental analysis, UV–visible, FT-IR, 1H-NMR, MS spectral techniques. The spectral data were used to confirm that the formation of metal complexes with their proposed structure.

## SOLVATOCHROMISM OF SOME AZO DYES: SPECTROSCOPIC ARRAY CORRELATING THE ABSORPTION MAXIMA AND POLARITY OF SOLVENTS

Satabdi Panda, Raisarani Sharma, Sukalyan Dash\* Department of Chemistry, Veer Surendra Sai University of Technology, Burla, Odisha, INDIA E-mail: sukalyan\_dash@yahoo.com

#### Abstract

Azo dyes have been synthesized by the coupling reaction of resorcinol and salicylic acid with diazonium salts of aniline and derivative. Thirteen solvents with varying polarity were used to study the solvatochromic behaviour of the dyes. The abilities of azo dyes to sense the polarities of various categories of solvents have been demonstrated. Out of the two resorcinol-based dyes 1 and 2, dye 1 shows hypsochromic shift whereas dye 2 shows bathochromic shift in dipolar aprotic media. On the other hand, out of the two salicylic-acid based dyes 3 and 4, dye 3 shows bathochromic shift and dye 4 shows hypsochromic shift in polar protic solvent media. The changes in the spectral properties of the azo dyes have been correlated with the extent of stabilities of both the tautomeric forms of the probes, such as azo and hydrazo forms, in different solvent media. The relationship between the polarity of solvents and the hydrogen bond accepting and/or donating properties of the resulting azo dyes are substantiated through regression analysis method.

# STUDY OF PHASE BEHAVIOUR OF CASTOR OIL BLENDED DIESEL – TWEEN 80 + N-BUTANOL-WATER MICROEMULSIONS

Smriti Mishra\*, Raisarani Sharma, Biswajit Acharya, Sukalyan Dash Department of Chemistry, Veer Surendra Sai University of Technology, Burla, Odisha, INDIA E-mail: smriti.swastik.mishra@gmail.com

### Abstract

Phase behaviour of some microemulsions containing Castor oil blended Diesel-Tween 80-n-butanolwater will be studied. The microemulsions will comprise of castor oil blended with diesel as oil component, various proportions of Tween-80 surfactant and n-butanol cosurfactant as the emulsifier and water as the aqueous phase. Phase diagrams of the pseudo ternary systems with various proportions of the components will be constructed by using visual titration method. The three major sections of the pseudo-ternary phase diagrams i.e., oil in water (O/W), water in oil (W/O) and the bicontinuous regions will be demarcated. The turbid, clear and gel regions of the micro heterogeneous mixtures will be studied which will provide a definite idea over the proportions of the constituents for preparing a transparent microemulsion. Use of castor oil can be identified as a greener approach because it is accessible, non-toxic, renewable and can serve as an alternative to the conventional source of energy which emits less harmful gases. The flash point, pour point, cloud point, viscosity of the micro-emulsified fuel will be determined to understand the efficiency of the fuel.

## METAL CATALYST NITRENE ADDITION REACTION TO C-H BOND: A DFT STUDY

Shougaijam Premila Devi\*, Francis A. S. Chipem, \* R.H. Duncan Lyngdoh# Department of Chemistry, Manipur University, Manipur, INDIA Department of Chemistry North Eastern Hill University, Shillong, Meghalaya, INDIA E-mail: premila.devi.10@gmail.com

### Abstract

The purpose of this experiment is to computational study of nitrene inseration into C-H bond via catalysed pathway. Two different routes or mechanism are choosen fo the study and their feasibility is compared. Four different alkane namely methan, ethane, propane, and isobutene is used with three different azides. (R=H, Me and Ac) and here copper triflate is used as catalyst. Density functional theory (DFT) was used at B3LYP level along with a 6-31G\*\* basis set to study the two different pathways. Both the pathways occurs through the decomposition of azide and hydrogen abstraction. The difference in the both the pathways is the last two step. In this study it is found that mechanism 2 which is proceed through the binding of the alkyl radical with the copper nitrenoid.is the better pathway. For both the mechanism effect of the structure are also investigated.

# CHEMICAL PROFILING OF NON-POLAR COMPOUNDS IN CARICA PAPAYA LEAVES: A COMPREHENSIVE ANALYSIS USING GC-MS

Vishvraj V. Devmurari<sup>1\*</sup>, Swati C. Daki<sup>2</sup>, Kartik D. Ladva<sup>3</sup>, Pankajkumar B. Nariya<sup>4</sup> <sup>1,2,3</sup>Department of Chemistry, Shri M. & N. Virani Science College, Rajkot, Gujarat, INDIA <sup>4</sup>Department of Chemistry, Atmiya University, Rajkot, Gujarat, INDIA E-mail: vishvraj05@gmail.com

## Abstract

This study endeavors to extract and characterize non-polar chemical entities present in the leaves of Carica papaya, a plant traditionally employed in folk medicine for its medicinal properties. In this, investigation utilized the petroleum ether extract obtained from Carica papaya leaves. Through a sequential process involving saponification and methylation, to achieve fatty acid components and unsaponifiable matters. Following this, phytochemical constituents were isolated via chemical processes, and the resulting fractions underwent comprehensive analysis using thin-layer chromatography (TLC) and gas chromatography coupled with mass spectrometry (GC-MS). The comprehensive chemical analysis unveiled a diverse composition within the Carica papaya leaves, encompassing steroids, triterpenoids, and fatty acid methyl esters (FAMEs). Gas chromatography coupled with mass spectrometry (GC-MS) played a vital role to identifying 15 distinct fatty acid components in the saponifiable matter. Additionally, the unsaponifiable portion revealed the presence of two steroids (campesterol,  $\beta$ - or  $\gamma$ -sitosterol), one triterpene (squalene), and one diterpene (phytol). The outcomes underscore the richness of non-polar compounds inherent in the Carica papaya leaves. The emphasis on the GC-MS methodology in this study proved to be instrumental in efficiently identifying and characterizing these phytoconstituents. The established analytical method provides a direct and effective approach for the analysis of non-polar entities in plant materials. In conclusion, the findings contribute to the broader understanding of the chemical composition of Carica papaya leaves, specifically highlighting the abundance of non-polar compounds. The GC-MS method introduced herein holds significant promise for future research endeavors and applications, offering a reliable and direct means of analyzing non-polar constituents in diverse plant materials.

# GREEN SYNTHESIS, CHARACTERIZATION AND EVALUATION OF ANTI- MICROBIAL ACTIVITY OF SILVER NANOPARTICLES FROM METHANOLIC FRUIT EXTRACT OF PLANT TREMA ORIENTALIS L.

Indrani PrabirKumar Bhattacharya

Parul Institute of Applied Sciences, Parul University, Waghodiya, Vadodara, Gujarat, INDIA E-mail: indrani.bhattacharya82083@paruluniversity.ac.in

#### Abstract

Plants serve as an important source of medicine and provide suitable candidate compounds to produce eco-friendly therapeutic agents. Biomolecules present in plant extracts can be used to reduce metal ions to nanoparticles in a single-step green synthesis process. This study is based on the green synthesis of silver nanoparticles (AgNPs) by using methanolic fruit extract of plant Trema orientalis L. (MFETO) and evaluation of its anti-microbial activity against gram-positive bacteria (Staphylococcus aureus) and gram-negative bacteria (Escherechia coli). The synthesis of AgNPs was confirmed based on the change in the colour of the reaction mixture from pale yellow to dark brown, with absorbance range between 400-500 nm under UV-visible spectroscopy. It was further characterized by using different techniques such as fourier- transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), atomic force microscopy (AFM), transmission electron microscope (TEM) and energy-dispersive X-ray analysis (EDAX). FTIR analysis showed the involvement of different groups of biomolecules in the synthesis of AgNPs. XRD illustrates the formation of metallic nanoparticles with the face-centered cubic structure. TEM exhibited the size and shape of the green synthesized AgNPs. AFM showed the topological surface of AgNPs. Anti-microbial study of AgNPs was carried by using well-diffusion method which showed that the green synthesized AgNPs have antimicrobial activity against Escherichia coli and staphylococcus aureus. This work revealed that AgNPs synthesized from MFETO have more inhibitory effect on gram positive bacteria as compared to gram negative bacteria.

## SYNTHESIS AND CHARACTERIZATION OF THE HOMOLOGOUS SERIES OF CHALCONYL CINNAMATE ESTER WITH UNIQUE LATERAL AND TERMINAL GROUPS

Geeta M. Parmar\*, U.C. Bhoya Chemical Research Laboratory, Department of Chemistry, Saurashtra University, Rajkot, Gujarat, INDIA E-mail: parmargeeta742@gmail.com

#### Abstract

A homologous series  $\alpha$ -4-(4'-n-alkoxy-3'-methoxy cinnamoyloxy) benzoyl- $\beta$ -4"-isopropyl phenyl ethylene is synthesized and studied with a view to understand and establish the relation between molecular structure and mesomorphism. New homologous series consists of twelve homologues (C1-C8, C10, C12, C14 & C16) and show mesomorphic in nature. The members of the series were characterized by IR, NMR, Mass and Optical polarizing microscopy with heating stage. The mesomorphic properties of the present series are compared with other structurally related series.

# SYNTHESIS OF HOMOLOGOUS SERIES: 4-(4'-N-ALKOXY 3'-METHOXY CINNAMOYLOXY)-PHENYL-(BENZO[d]THIAZOL-2-YLIMINO) METHYL

A. H. Hadiya<sup>\*</sup>, S. B. Parmar, U. C. Bhoya Department of Chemistry, Saurashtra University, Rajkot, Gujarat, INDIA E-mail: hadiyaakhil@gmail.com

#### Abstract

Synthesis and study of new homologous series 4-(4'-n-alkoxy 3'-methoxy cinnamoyloxy)-phenyl-(benzo[d]thiazol-2-ylimino) methyl by condensing 4-n-alkoxy 3-methoxy cinnamic acid with (E)-4-((benzo[d]thiazol-2-ylimino) methyl) phenol in steglich esterification method. The homologous series consists of 12 homologues and study of liquid crystalline property. Work was planned to synthesize new liquid crystal material with a view to understand the effect of structural variation on liquid crystal or mesogenic character.

## BiMnO3 MODIFIED BaTiO3 (BTBiM5) - AN EXTREMELY HIGH DIELECTRIC CONSTANT CERAMIC NANOMATERIAL WITH A GOOD MAGNETIC PERFORMANCE

Debasish Mondal<sup>1</sup>, Julekha Khatun<sup>1</sup>, Debasis Dhak<sup>1\*</sup> <sup>1</sup>Nanomaterials Research Lab, Department of Chemistry, Sidho-Kanho-Birsha University, Purulia, West Bengal, INDIA E-mail: debasisdhak@yahoo.co.in & debasis.chem@skbu.ac.in

#### Abstract

The precursor solution decomposition method was used to create an ultrahigh dielectric constant covering BiMnO<sub>3</sub> modified BaTiO<sub>3</sub> (0.5BaTiO<sub>3</sub>-0.5BiMnO<sub>3</sub>, abbreviated as BTBiM<sub>5</sub>). A tetragonal phase with 32 nm crystallite size is present in the spherical morphological nanocrystalline ceramics. At low frequencies (1 kHz), the BTBiM<sub>5</sub> sintered pellet has an ultrahigh dielectric constant (108 order).) BTBiM<sub>5</sub>'s relaxor diffusive nature is characterized by its 1.37 diffusivity. BTBiM<sub>5</sub> shows non-Debye-type characterizations with only grain conductivity which is in good agreement with the single semicircular Nyquist plot. The room temperature magnetic performance of BTBiM<sub>5</sub> reaches saturation at 200 Oe. The high dielectric constant along with the evolution of magnetic character in the non-magnetic BaTiO<sub>3</sub> will make BMBiT<sub>5</sub> a leading candidate in the electrical and magnetic field soon.

## LOW-COST SAWYER TOWER CIRCUIT DESIGN AND STUDY OF P-E HYSTERISIS OF FERROELECTRIC MATERIAL

Binoy Das<sup>1</sup>, Julekha Khatun<sup>2</sup>, Moumita Patra<sup>1</sup>, Nityananda Das<sup>1\*</sup> <sup>1</sup>Department of Physics, J.K. College, Purulia, INDIA <sup>2</sup>Nanomaterials Research Lab, Department of Chemistry, Sidho-Kanho-Birsha University, Purulia, West Bengal, INDIA E-mail: ndas228@yahoo.com

#### Abstract

Sawyer Tower circuit is used to study the dielectric polarisation with variation of electric field. Generally, this study is done for polarisation study of ferroelectic ceramics. But this instrument is costly. We have designed this circuit for study of PE loop at 50 Hz. Firstly, a step-up transformer is designed to achieve 10 kV sinusoidal voltage variation. The secondary of the step-up transformer is so designed such the current is limited to few milli ampere. The output of the secondary is applied to the ferroelectric material through a proper arrangement. For measurement of the applied field one shunt resister is used such that voltage drop across this shunt does not exceed 20V. This is because the voltage drop across the shunt is fed to x- input of the digital storage oscilloscope (DSO) in XY mode. A high value (0.1 micro farad to 1 microfarad) capacitor (unpolarised) is used to get the voltage drop against this capacitor as a measurement of charge against the ferroelectric sample. This voltage drop is fed to Y input of DSO. The variation of polarisation with variation of electric field is observed on the DSO screen. By transferring the sampled data to a PC, the calculation of saturation polarisation, coercivity and retentivity is calculated.

# DEVELOPMENT OF POTENT GREEN CORROSION INHIBITOR FROM CARICA PAPAYA L. FEMALE LEAVES EXTRACT USING WEIGHT LOSS TECHNIQUE

Foram H. Vaghela, Hitendra S. Joshi Department of Chemistry, Saurashtra University, Rajkot, Gujarat, INDIA E-mail: foramvaghela1997@gmail.com

#### Abstract

Carica Papaya L. commonly known as papaya is one of the important crops grown in Kachchh region. Corrosion is deterioration or degradation of metal on its contact with environment. As per literature review annual world loss due to corrosion is estimated to 2.5 million US dollars and annual global market of corrosion inhibitor is about 825 billion US dollars. This study aims to develop potent green corrosion inhibitor from Carica papaya L. leaves. The diameter of aluminum plate is 2 mm. the samples were examined on the 2 hours and then pickled, dried and reweighed. In the 1M HCl Solution without inhibitor, maximum corrosion rates were shown. The inhibition efficiency of green corrosion inhibitor is 94.29%. Various types of corrosion inhibitors are known in the market, but green corrosion is beneficial due to its biodegradable, bio-compatible, renewable, and non-toxic characteristics. Also, the development of green corrosion inhibitor from Carica papaya L. leaves it may serve as a source of additional income to farmers as farmers have income from papaya trees twice a year during flowering and fruiting season.

# PHYSICO CHEMICAL ANALYSIS OF AVAILABLE POTASSIUM IN SOILS OF SOME VILLAGES OF IDAR TEHSIL DISTRICT: SABARKANTHA (GUJARAT) INDIA

Dr. Jitendra K. Parmar Department of Chemistry, Bahauddin Science College, Junagadh, Gujarat, INDIA E-mail: dr.jeetparmar@gmail.com

#### Abstract

Fertility of farmland soil is based on analytical results of various parameters like pH, electrical conductivity (EC), total organic carbon (OC), available nitrogen (N), available phosphorus (P2O5) and available potassium (K2O). Potassium can enhance plant to tolerate drought. This study leads us to the conclusion of the nutrient's quantity of soil of Idar tehsil, District- Sabarkantha, Gujarat (INDIA). Total 6063 farmland soil samples were selected from 26 villages of Idar tehsil for this the study. The available potassium in black soil varied from 322 to 425 kg ha-1 in surface layer. The higher value of available potassium indicated that these soils were added with sufficient quantities of potash fertilizers. The average fertility index for available potassium for this taluka is 6.92. This information will help farmers to decide the problems related to soil nutrients, thereby quality as well as quantity of fertilizers. Main objective of this soil analysis is to estimate available potassium in farmland soil as per Government of Gujarat Agriculture department lab manual under soil health card project.

# AROMATIC AMINES LINKED TO THIOBARBITURATES: DESIGN, MOLECULAR DOCKING TO SYNTHESIS AND IN VITRO CYTOTOXICITY, XANTHINE OXIDASE INHIBITION, ANTIMICROBIAL EVALUATION

Bhaveshkumar D. Dhorajiya<sup>\*1</sup>, Yogesh O. Bhola<sup>2</sup>, Tushar P. Sutariya<sup>3</sup>, Bharatkumar Z. Dholakiya<sup>4</sup>, Rafat M. Mohareb<sup>5</sup>, Vani Senthil<sup>6</sup>, David Sheng-Yang Wang<sup>6</sup> Department of Industrial Chemistry, V.P. and R.P.T.P. Science college, V. Vidhyanagar, Gujarat, INDIA E-mail: bhavesh.orgchem@gmail.com

#### Abstract

A simple and efficient one-pot synthesis of 5-[(arylamino)methylide]-2-thioxodihydropyrimidine- 4, 6-(1H,5H)-dione derivatives has been developed using multicomponent reaction approach. The newly synthesized adducts evaluated for their microbial activity against five bacterial strains (S. pyogenes MTCC 442, S. aureus MTCC 96 as the gram positive, E. coli MTCC 443, P. aeruginosa MTCC 424, K. pneumoniae MTCC 109 as the gram negative) and four fungal strains (C. albicans MTCC 227, A. clavatus MTCC 1323, T. rubrum MTCC 296, Penicillium wild strain).Moreover, these all compounds were also evaluated against seven cancer cell lines namely gastric cancer NUGC, colon cancer DLDI, liver cancerHA22T, liver cancerHEPG2, nasopharyngeal carcinoma HONEI, breast cancer MCF-7 and normal fibroblast cellsWI-38 as well as inhibitory effect towards the oxidation of xanthine to uric acid formation. Molecular docking simulations examining the inhibitory nature of the compound show an Antimalarial Activity & Anti-leukemia activity.

# A TURN-OFF" FLUORESCENCE MECHANISM FOR DUAL CHANNEL DETECTION OF Fe<sup>3+</sup> AND Ru<sup>3+</sup> METAL IONS BY USING NOVEL ISOINDOLINE-1,3-DIONE SUBSTITUTED SCHIFF BASE: COMPLETE THEORETICAL AND EXPERIMENTAL STUDY

Ankita Garg<sup>1</sup>, Aman Bhalla<sup>1</sup>, Savita Chaudhary<sup>1</sup> and Ahmad Umar<sup>2,3†</sup> <sup>1</sup>Department of Chemistry & Centre of Advanced Studies in Chemistry, Chandigarh, INDIA <sup>2</sup>Department of Chemistry, Faculty of Science and Arts, and Promising Centre for Sensors and Electronic Devices (PCSED), Najran University, Najran, Kingdom of Saudi Arabia <sup>3</sup>Department of Materials Science and Engineering, The Ohio State University, Columbus, OH, USA <sup>†</sup>Adjunct Professor at the Department of Materials Science and Engineering, The Ohio State

<sup>†</sup>Adjunct Professor at the Department of Materials Science and Engineering, The Ohio State University, Columbus, Ohio, USA E-mail: gargankita155@gmail.com

Abstract

A novel isoindoline-1,3-dione substituted fluorophore, 2-[1-benzyl-2-(4-methoxy-phenylimino)ethyl]-isoindole-1,3-dione (L), has been synthesized for the dual channel sensory recognition of Fe<sup>3+</sup> and Ru<sup>3+</sup> metal ions via turn-off fluorescence behaviour with the limit of detection value of 0.65  $\mu$ M and 0.26  $\mu$ M, for Fe<sup>3+</sup> and Ru<sup>3+</sup> respectively. The fluorophore (L), has been characterized by utilizing various spectroscopic techniques, including <sup>1</sup>H and <sup>13</sup>C NMR, FT-IR, elemental analyses, and highresolution mass spectrometry (HRMS). The binding stoichiometric verified from the fluorescence came out to be 1:1 for both Fe<sup>3+</sup> and Ru<sup>3+</sup> metal ions. The 'naked eye' response has further been utilized to develop fast, economical and simple on-site trace detection of Fe<sup>3+</sup> and Ru<sup>3+</sup> metal ions via preparing simple paper strips. A computational study using the DFT approach has further been carried out to incorporate new essence in terms of getting significant information regarding the complexation mode of (L) with Fe<sup>3+</sup> and Ru<sup>3+</sup> metal ions. The fundamental outcomes in this work will provide a new outlook for fabricating novel dual chemo-sensor that could further be employed on-site detection of metal ions with great selectivity and sensitivity. Details of the results of these studies1 will be presented and discussed.

# ENHANCED ADSORPTIVE EFFICACY OF BIOMASS RESIDUES VIA SYNERGISTIC INTERACTION WITH CAMELLIA SINENSIS FOR ADSORPTIVE REMOVAL OF HAZARDOUS TOXICANTS FROM WASTEWATER

Diksha Aggarwal, Sonal Singhal\* Department of Chemistry, Punjab University, Chandigarh, INDIA E-mail: aggarwaldiksha123@gmail.com

#### Abstract

One of the most pressing environmental issues facing the world is the availability of adequately clean water for human consumption. The release of various environmental contaminants in water bodies, both inorganic and organic, due to inflating urbanization and industrialization has a conspicuous effect on water quality standards. As water is uniquely vulnerable to pollution, water pollution control has received a considerable attention among the most critical environmental challenges. Nowadays, extensive efforts have been made to search for novel, cost effective and practical biosorbents derived from biomass resources with special attention to value added, biomass-based renewable materials. Recycling biomass waste to create goods with added value is a big step towards environmental sustainability. Upholding the statement, this work presents a study on synergistic integration of biomass derived materials with Camellia sinensis (spent tea leaves) for the adsorptive sequestration of toxic contaminants. Safranin O, Ciprofloxacin and Chlorpyrifos were chosen as the model pollutants for this investigation. The successful synthesis of the composites was established via characterization techniques such as XRD, FT-IR and FESEM. The obtained experimental data presented maximum adsorption capacity of 32.78 mg g-1 for SO, 24.87 mg g-1 for CF and 62.89 mg g-1 for CP, respectively. This work unveils the potential of fabricated materials as low-cost yet sustainable materials with high adsorption performance.

# MAGNETICALLY RETRIEVABLE G-C3N4/ZnO/NiFe2O4 TERNARY HETEROJUNCTION AS A PROSPECTIVE MATERIAL FOR PHOTOCATALYTIC DEGRADATION OF FLUOROQUINOLONES

Twinkle Garg, Sonal Singhal\* Department of Chemistry, Panjab University, Chandigarh, INDIA E-mail: twinkle42garg@gmail.com

#### Abstract

A novel direct dual Z-scheme g-C3N4/ZnO/NiFe2O4 (CZN) ternary heterostructure was manufactured by simple sonication-calcination strategy and the symphonized nanomaterial was maneuvered for the visible-light driven photocatalytic degradation of fluoroquinolones (FQs) antibiotics; i.e. levofloxacin (LVX), ciprofloxacin (CPF) and ofloxacin (OFL). The comparative appraisal of ternary composites with g-C3N4/ZnO was carried out for the degradation of FQs and augmented photocatalytic activity was observed by addition of NiFe2O4 nanoparticles to g-C3N4/ZnO (CZ) composite. The degradation studies for synthesized heterostructures were observed to follow pseudo first order kinetics and rate constant values for CZN2 (2:1 weight ratio of CZ and NiFe2O4) heterostructure were found to be 1.26, 1.14 and 1.67 times than that of g-C3N4/ZnO composite for LVX, OFL and CPF, respectively. Enhanced photocatalytic activity of ternary heterostructure was ascribed to dual Z- scheme charge transfer mechanism followed by heterostructure that resulted in amended visible light absorption capability, alleviated charge separation and diminished photo-induced electron-hole pair recombination rate. Also, recyclability and stability of the constructed Z-scheme heterostructure demonstrated the material to be a potential candidate for wastewater treatment. Thus, the fabricated heterostructures provides a new notion of contriving multifarious components to innocous system for environmental remediation.

## HIGHLY EFFICIENT METAL DOPED BIOCI NANO-ARCHITECTURE PHOTOCATALYSTS FOR VISIBLE-LIGHT DRIVEN PHOTOCATALYTIC DEGRADATION AND ANTIBACTERIAL BEHAVIOUR

Prerna<sup>a</sup>, Ganga Ram Chaudharya<sup>b</sup> <sup>a</sup>Department of Chemistry & Centre for Advanced Studies in Chemistry, Panjab University, Chandigarh, INDIA <sup>b</sup>SAIF/CIL, Panjab University, Chandigarh, INDIA E-mail: prernaattri30@gmail.com

#### Abstract

Herein, the fabrication of well-crystalline metal (Ni, Mo, Cd and Co) doped BiOCl nanoscale photocatalytic material (M-BiOCl; M = Ni, Mo, Cd, and Co) has been done by employing the solvothermal synthetic route. It was found that Ni doping results in remarkable improvement in photocatalytic and antibacterial behavior of BiOCl. The morphological investigation of typical samples by the field-emission scanning electron microscopy (FE-SEM) revealed that undoped BiOCl shows closely stacked thick discs like morphology, while doping with different metals resulted into nanosheet (Ni, Cd), nanoflowers (Mo) and nanodiscs (Co) like morphologies. Interestingly, doping of Ni metal led to a substantial transformation into large size nanosheets with (010) prominent facet and increased surface area (41.927 m2/g) along with improved porous structure. Similarly, highresolution transmission electron microscopy (HR-TEM) confirmed the formation of extended nanosheet like growth having dimensions ~ 287.16 x 179.14 nm for Ni-BiOCl photocatalyst along with nano-pores morphology that might serve as active sites during photocatalysis or antibacterial activity. Moreover, the inclusion of Ni into BiOCl nanostructure brings the band gap (Eg) shifted to 2.85 eV from 3.54 eV (pure BiOCI), while all other metal doped nanostructure exhibited nearly similar Eg. Meanwhile, the photo-induced charge carriers recombination behaviour analyzed by photoluminescence (PL) analysis shows diminished peak intensity for Ni-BiOCl as compared to pure BiOCl that can be directly correlated with minimum recombination of electron-hole during photocatalysis thus contributing for its excellent photocatalysis performance. In addition, we observed the excellent photocatalytic antibacterial activity of Ni-BiOCl against S. aureus bacteria under the visible light.

# SYNTHESIS, CHARACTERISATION AND ANTIBACTERIAL ACTIVITY OF SCHIFF BASES METAL COMPLEXES

Prashant Gajera<sup>\*1</sup>, Milan Vadodaria<sup>2</sup> <sup>1</sup>Department of Chemistry, Saurashtra University, Rajkot, Gujarat, INDIA <sup>2</sup>Department of Chemistry, Shri M. & N. Virani Science College (Autonomous), Yogidham Gurukul, Kalawad road, Rajkot, Gujarat, INDIA E-mail: gajeraprashant9@gmail.com

#### Abstract

The effects of ligands on structure and reactivity of transition metal complexes are very important study for research in organometallic chemistry. In this work, we have prepared Zn (II), Mn (II) and Cu (II) transition metal heterochelates. The prepared transition metal complexes have been characterized by various spectroscopic techniques like Mass spectroscopy, 1H NMR and thermal Analysis. Prepared transition metal complexes have been screened for various biological activities like anticancer, antifungal, antiviral, antitubercular and antibacterial.

# EMPOWERING PYRIMIDINE DERIVATIVE SYNTHESIS: MICROWAVE-ASSISTED GREEN CHEMISTRY APPROACH

Dr. Kaushik A. Joshi\*, Dr. Vipul N. Joshi, Dr. Haresh K. Ram <sup>1,2</sup>Department of Chemistry, D.K.V. Arts and Science College, Jamnagar, Gujarat, INDIA <sup>3</sup>Department of Chemistry, Tolani College of Arts & Science, Adipur, Gujarat, INDIA E-mail: joshikaushik24@gmail.com & vnjchem@gmail.com

## Abstract

Achieving an Effortless Microwave Synthesis of 1,2,3,4-Tetrahydropyrimidine Derivatives: Harnessing N-(2,4-bis(trifluoromethyl)phenyl)-3-oxobutanamide, Varied Aldehydes, and Urea in Ethanol with Trace Conc. HCl. Yielding High Purity Compounds sans Additional Purification. Structural Validation via FTIR, 1HMR, Mass Spectral Data, and comprehensive microbiological activity profiling of all compounds.

# DIRECT SYNTHESIS OF N-ARYL PYRROLES FROM BIOMASS-DERIVED FURAN AND NITROARENES OVER ZIRCONIUM BASED HYBRID SOLID ACID CATALYST

Meet Patel\*, Kalpana C. Maheria

Department of Chemistry, Sardar Vallabhbhai National Institute of Technology, Ichchhanath, Surat, Gujarat, INDIA

E-mail: kcm@chem.svnit.ac.in & patelmeet121343@gmail.com

#### Abstract

Given the wide applications of pyrroles in agriculture, pharmaceuticals, supramolecular and materials chemistry, a mild and eco-friendly route to produce functionalized pyrroles from bioderived feedstocks is highly desirable. A mild and convenient one pot method was developed to synthesize N-aryl pyrroles from biobased furan and nitroarenes using Zr-based phosphonic acid (ATMP=amino trimethylene phosphonic acid) (Scheme 1). The synthesized catalyst has been characterized by SEM-EDS, XRD, XPS, HR-TEM, FT-IR, and TGA analysis. Effect of various parameters on catalytic activity of Zr-ATMP has been investigated for the synthesis of N-aryl pyrroles. Good yields of the product has indicated high efficiency of ZrATMP catalyst. The catalyst has been found highly stable and reusable several times without loss of its catalytic activity.

## SYNTHESIS AND STUDY OF DONOR-ACCEPTOR CONJUGATED POLYMERS VIA METAL FREE ALDOL CONDENSATION POLYMERIZATION STRATEGY

Prerak R. Patel<sup>∓</sup>, Arun L. Patel<sup>\*⊤</sup> <sup>T</sup>Department of Chemistry, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat, INDIA E-mail: arunpatel\_5376@yahoo.co.in

#### Abstract

The development of donor-acceptor conjugated polymers is a challenge due to the involvement of costly transition-metal catalysts and hazardous reagents during the synthesis of such materials, which may potentially cause serious environmental problems. Aldol polycondensation is a promising, metal-free polymerization method to synthesize such donor-acceptor conjugated polymers. Herein, we report the synthesis of three new symmetrical diformyl functionalized thiophene-capped carbazole, fluorene and indolocarbazole moieties. The polymers, ACRBI, AFRBI and AICRBI, were synthesized by Aldol condensation reaction between the diformyl compounds and bis(indolinone). Photophysical, electrochemical, thermogravimetric analysis, gel permeation chromatography, DFT calculations and SCLC hole mobility measurements were performed for these polymers. The photophysical and electrochemical studies of these polymers revealed high visible light absorptivity with a HOMO energy level close to -5.5 eV and a low-lying LUMO energy level close to -3.35 eV. The SCLC hole mobilities of polymers ACRBI, AFRBI and AICRBI were determined to be 4.9  $\Box$  10<sup>-3</sup>, 6.7  $\Box$  10<sup>-2</sup>, and 1.7  $\Box$  10-3 cm<sup>2</sup>V<sup>-1</sup>S<sup>-1</sup>, respectively.

## CATALYZED SYNTHESIS OF THIAZOLIDINONE BASED BIOLOGICALLY POTENT MOLECULES VIA THREE COMPONENT BIGINELLI MULTICOMPONENT REACTION

Bilal Mansuri<sup>1\*</sup>, Ajay K. Dalai<sup>2</sup>, Kalpana C. Maheria<sup>1</sup> <sup>1</sup>Department of Chemistry, Sardar Vallabhbhai National Institute of Technology, Ichchhanath, Surat, Gujarat, INDIA <sup>2</sup>Department of Chemical and Biological Engineering, University of Saskatchewan, Saskatchewan, Saskatchewan, S7N 5N1, CANADA E-mail: kcm@chem.svnit.ac.in & mansuribilal81@gmail.com

#### Abstract

Thiazolidinone derivatives are traditionally known class of biologically active compounds. These derivatives possess significant biological activities such as COX-1 inhibition, anti-inflammatory, anti-proliferative, antihistaminic, and anti-HIV activities. In recent years, there is an increasing attention towards development of efficient synthesis of thiazolidinone derivatives. Several catalyzed synthetic protocols exist for their synthesis which involve use of various catalysts such as MCM-41/CuSO<sub>4</sub>, Pd-NPs, silica gel, alum, Fe<sub>3</sub>O<sub>4</sub> / SiO<sub>2</sub> / Salen / Mn, CoFe<sub>2</sub>O<sub>4</sub>@SiO<sub>2</sub>-/PrNH<sub>2</sub>, ammonium persulfate and La(NO<sub>3</sub>)<sub>3</sub>, etc. However, these reactions suffered from several drawbacks such as longer reaction times, the use of high boiling solvents, low yields, and use of toxic reactants/reagents etc. In this work an attempt has been made for one pot synthesis of thiazolidinone derivatives via MCRs over microporous and mesoporous zeolite H-BEA, HZBK1 (i.e. modified zeolite H-BEA via controlled desilication) as solid acid catalysts. The synthesized thiazolidinone molecules were characterized by elemental analysis, IR, Mass and <sup>1</sup>H-NMR spectroscopy. The mesoporous zeolite H-BEA was found catalytically more efficient than parent microporous zeolite H-BEA for the synthesis of thiazolidinone molecules, which may be due to its high surface area and improved pore accessbiilty.

## MICROWAVE ASSISTED GREEN SYNTHESIS OF QUINAZOLINONES OVER ION-EXCHANGE RESINS

Aayushi Lodhi<sup>1\*</sup>, Dhanendra Kumar<sup>1</sup>, Ayushi Patel<sup>1</sup>, Hemant Parmar<sup>2</sup>, Ajay K. Dalai<sup>3</sup>, Kalpana C. Maheria<sup>1</sup> <sup>1</sup>Department of Chemistry, Sardar Vallabhbhai National Institute of Technology, Ichchhanath, Surat, Gujarat, INDIA <sup>2</sup>Acume Chemicals Pvt. Ltd., Ankleshwar, Gujarat, INDIA <sup>3</sup>Department of Chemical and Biological Engineering, University of Saskatchewan, Saskatcon, Saskatchewan, S7N 5N1, CANADA E-mail: kcm@chem.svnit.ac.in & aayushilodhi9627@gmail.com

#### Abstract

The quinazolinone skeleton is a frequently encountered heterocycle in medicinal chemistry literature with various medicinal and pharmacological including antibacterial, analgesic, anti-inflammatory, antifungal, antimalarial, CNS depressant, anticonvulsant, anti-parkinsonism, and cancer activities. In the present endeavor, an attempt has been made to synthesize quinazolinones and its derivatives over Fe<sup>3+</sup> modified Amberlyst (solid acid catalyst) under microwave irradiations. Microwave synthetic approach offers several advantages in terms of reaction rate, production yield and improved energy efficiency. Due to the widespread curiosity in medicinal chemistry, in the present work, the heterogeneously catalysed construction of heterocycles under microwave irradiation is explored to reduce time and energy. The synthesised catalyst, Fe<sup>3+</sup>- Amberlyst has been characterized using various characterization techniques such as X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), N<sub>2</sub> sorption isotherms analysis, scanning electron microscopy energy dispersive X-ray analysis (SEM-EDX) and thermo-gravimetric (TG) analysis. The intended products were found in acceptable yields. The incorporation of Fe<sup>3+</sup> in Amberlyst-15 resulted in improved yield which may be due to enhanced Lewis acidity of the material. The most notable benefits of these process are their quick reaction times, simple workup, and more specifically, their environmental friendliness.

# DESIGN, DEVELOPMENT AND INVESTIGATION OF NOVEL BENZIMIDAZOLE DERIVATIVES AS POTENT ANTI-CANCER AGENTS

Pritesh P. Gajjar, Mrunal A. Ambasana Department of Chemistry and Forensic Science, Bhakta Kavi Narsinh Mehta University, Junagadh, Gujarat, INDIA E-mail: priteshgajjar2@gmail.com & ambasanamrunal@gmail.com

### Abstract

Herein we report the synthesis of benzimidazole derivatives through the reaction of heterocyclic chlorides with substituted amines in DMF under acid catalyzed reaction conditions. The employed method afforded good to excellent yields with excellent purity, as confirmed using chromatographic studies. Newly synthesized compounds were Characterized through IR, NMR, and MASS spectrometry analyses. The anti-cancer potential of these newly synthesized benzimidazole compounds (BO-PG-101 to BO-PG-110) was assessed against the Human Breast Adenocarcinoma (MCF-7) cell line. Notably, compounds BO-PG-101 to BO-PG-101 to BO-PG-100 exhibited significant anti-cancer activity, surpassing the standard Tamoxifen. Among these, BO-PG-109 and BO-PG-107 demonstrated particularly higher potency compared to other synthesized benzimidazoles.

# SYNTHESIS, SPECTROSCOPIC AND BIOLOGICAL STUDIES OF SOME NOVEL TRANSITION METAL BASE HETEROCHELATES SCAFFOLD

Dr. Darshan Jani\* Department of Chemistry, Noble University, Junagadh, Gujarat, INDIA E-mail: darshanjani09@gmail.com

#### Abstract

We created new Schiff base ligands and their transition metal complexes in this study. The compounds that were synthesized were characterized, and their antibacterial properties were investigated. To properly characterize all of the substances, elemental analysis, IR, <sup>1</sup>H-NMR, and mass spectrometry were used. The ligands and their complexes were tested in vitro against Gramm positive and Gramm negative bacteria using the Zone of Inhibition technique. The complexes outperformed the ligands in terms of activity.

# SYNTHESIS AND ANTICANCER ACTIVITY OF PYRROLO[2,1-B] THIAZOLE DERIVATIVES

Satishkumar Tala<sup>a</sup>, Ravi Chaniyara<sup>b</sup>, Te-Chang Lee<sup>b</sup>, Tsann-Long Su<sup>b</sup> <sup>a</sup>Department of Chemistry, Atmiya University, Kalawad Road, Rajkot, Gujarat, INDIA <sup>b</sup>Institute of Biomedical Sciences, Academia Sinica, Taipei, TAIWAN E-mail: satishtrada@gmail.com

#### Abstract

A series of benzo fused pyrrolo[2,1-b]thiazoles and their bis(alkylcarbamate) derivatives were synthesized for anticancer activity. The results of preliminary studies revealed that bis(hydroxymethyl) (9a-j) and their bis(alkylcarbamate) (10a-j & 11a-j) derivatives shows significant anticancer activity in inhibiting human leukemia and various solid tumor cell growth in vitro. The structure-activity relationship (SAR) studies of the synthesized compounds shows that bis(alkylcarbamates) derivatives are generally more effective than the corresponding bis(hydroxymethyl) counterparts against human lymphoblastic leukemia (CCRF-CEM) and other human solid tumor cell growths tested. Moreover, Multi-Drug Resistance (MDR) study revealed that these agents have little to no cross-resistance to Taxol or Vinblastine. Remarkably, complete tumor remission was observed in nude mice bearing human breast carcinoma (MX-1) xenograft by 4-F-Ph-(10b) and 4-Cl-Ph- (10c) carbamate derivatives, and more than 99% tumor suppression were observed by the corresponding bis(ethylcarbamate) derivatives at the maximal tolerated dose with relatively low toxicity (Weight loss study). In addition, these agents shows ability to interstrand cross-linking with DNA (alkaline agarose gel shifting assay). The present studies shows synthesis, DNA interstrand cross-linking, in vitro and in vivo studies of the compounds.

### BIOACTIVITY-GUIDED SEPARATION AND ISOLATION OF CARPAINE ALKALOID: EXPLORING THE WOUND HEALING POTENTIAL OF CARICA PAPAYA

 Vishvraj V. Devmurari<sup>1</sup>, Swati C. Daki<sup>2</sup>, Pankajkumar B. Nariya<sup>3</sup>, Harishkumar K. Madhyastha<sup>4</sup>, Kartik D. Ladva<sup>5</sup>
 <sup>1,2,5</sup>Department of Chemistry, Shri M. & N. Virani Science College, Rajkot, Gujarat, INDIA
 <sup>3</sup>Department of Chemistry, Atmiya University, Rajkot, Gujarat, INDIA
 <sup>4</sup>Department of Cardiovascular Physiology, Faculty of Medicine, University of Miyazaki, Miyazaki, JAPAN
 E-mail: dakiswati@gmail.com

#### Abstract

Carica papaya is a plant that has been used for medicinal purposes for a long time. It is known for its therapeutic properties in treating various diseases, especially dengue. In current study, we aimed to investigate the wound-healing potential of Carica papaya by examining its extracts; using different solvents, ranging from non-polar to polar (n-hexane, benzene, acetone, ethyl acetate, methanol and water), were employed to prepare extracts with varying polarities. The wound-healing activity of these extracts have been evaluated on the M5S cell line using the MTT assay for cell proliferation. Positive effects on the cell line were observed with hexane, ethyl acetate, acetone, and methanol extracts. Further the liquid-liquid extraction was employed to separate compounds from these active extracts. We observed positive cell proliferation results in the acetone-benzene fraction, acetonechloroform fraction, and methanol-chloroform fraction using partition techniques. The activity of these fractions was further validated by the cell-migration assay, revealing significant wound closure percentages, particularly in the methanol-chloroform fraction. The presence of secondary metabolites, specifically alkaloids in the active fractions, was confirmed, with isolation of an alkaloid accomplished through preparative HPLC. We have conducted extensive chromatographic and spectrographic analysis, including LC-MS and NMR, to elucidate the structure of alkaloid. The compound's structure, identified as carpaine, a known alkaloid, was ultimately confirmed; through a bioactivity-guided fractionation and isolation process. In conclusion, our study highlights the woundhealing potential of Carica papaya, specifically attributing this activity to the isolated carpaine alkaloid and opens future scope for further research on its application in wound healing activities.

# CHEMISTRY OF SCHIFF BASE METAL COMPLEXES AND THEIR BIOLOGICAL ACTIVITIES

Bansuri Nandaniya, Siva Prasad Das Saurashtra Education Trust, Junagadh, Gujarat, INDIA E-mail: nandaniyabansi2751@gmail.com

#### Abstract

Some novel Schiff base ligands & metal complexes of Mn(II),Ni(II),Cu(II),Zn(II) have been successfully synthesized from different aldehyde and amine derivatives, and confirmed with <sup>1</sup>H NMR, IR and Mass Spectral studies. We have synthesized a series of some new transition metal based heterochelates and characterize their properties. All the synthesized compounds were screened for their bioactivity. The heterochelates exhibit strong activities against Gram positive and Gram negative microorganisms in comparison with ligands. The heterochelates were found more active against one or more bacterial strain introducing a new class of metal based bactericidal agents for further research.

# CONTRIBUTION OF VEGETATION IN SUSTAINABILITY OF ENVIRONMENT, NATURAL RESOURCES CONSERVATION AND ROLE OF CARBON FOOT-PRINT & BLUE CARBON IN SMART CITY PROJECT - GANDHINAGAR, GUJARAT

Aanal Maitreya\*, Dr. Nainesh Modi

Department of Botany, Bioinformatics, Climate Change & Impacts Management, Ahmedabad, Gujarat, INDIA

E-mail: aanalmaitreya@gmail.com & nrmodi@gujaratuniversity.ac.in

#### Abstract

Different factors play important role in the Ecosystem, mainly the contribution of urban ecosystem is considered important in the development of any nation. Developing nations' modernization of cities has an important contribution relative to population. As a part of such modernization project of the Indian nation, the Smart City Project on June 2015, Gandhinagar, the capital of Gujarat, has also been included under the Smart City Mission, Gandhinagar city has many developments to maintain its importance in terms of development. The management of water, land and forests is also necessary for urban population. There are many projects like metro railway, gift city, railway station, Mahatma mandir, academic institutions, industrial units and offices are being constructed in connection with the general administration attached to the secretariat at the capital. The area of Gandhinagar Municipal Corporation, has been in existence since 2011. Many development works are required by removing previously planted trees, parks like Miyawaki forest, Aranya park, Punit van, Swarnim park, gardens in various sectors etc. have been constructed to avoid serious impact on the environment. Plants with different types of fruits and flowers, shrubs, trees, vines have been planted at the places of road dividers etc. So that the air pollution due to the transportation with heavy traffic of the city, industrial units and the people living in the roadside can be reduced. In order to prevent pollution, it is necessary to plan according to which clean air is available in the environment and efforts are also necessary to maintain water and lake or water habitats in the urban area. Many projects have been come up in Gandhinagar city over the last 50 years and have enhanced the city's area and growth. Necessary research work for environmental balance has been carried out and accordingly this research work has been presented.

# CRITICAL ASSESSMENT OF PAH CONTAMINATION IN THE GULF OF CAMBAY: ENVIRONMENTAL IMPACT AND EFFECTIVE BIOREMEDIATION STRATEGIES

Manisha Parmar, Haren Gosai\* Department of Biosciences, School of Science, Indrashil University, Rajpur-Kadi, Mehsana, Gujarat, INDIA E-mail: dh.haren@gmail.com & harengiri.gosai@indrashiluniversity.edu.in

#### Abstract

The rise in environmental pollution level is a result of human activities aimed at meeting energy demand. Polycyclic aromatic hydrocarbons (PAHs) stand out as the main contaminants due to their persistent and harmful nature. A comprehensive study was conducted to assess the impact of PAHs on human health in the coastal areas of Gujarat. The focus was also on quantifying the levels of these compounds. In the contaminated Alang-Sosiya Shipbreaking Yard in the Gulf of Cambay, 5 sediment samples were collected every four months over an 8-month period. The analysis revealed a significant PAHs contamination, with concentrations ranging from 1933 to 3844.31 ng g<sup>-1</sup> dw at various sites. Isomeric ratios and principal component analysis indicated pyrogenic PAHs inputs in polluted locations. Furthermore, natural groupings of detected PAHs were established, and an ecological risk assessment of PAHs at the Gulf of Cambay was performed. Additionally, PAHs degrading bacteria were isolated, demonstrating their effectiveness in breaking down multiple PAHs. The strain effectiveness was observed as follows: Pseudomonas stutzeri MP3 (67.86%), Stutzerimonas stutzeri MP4 (73.46%), and Stutzerimonas frequens MP8 (77.06%).

### MULTINATIONAL RECONNAISSANCE SURVEY REVEALED POSITIVE PERSPECTIVES AND ATTITUDES TOWARDS THE DIETARY APPLICATIONS OF SEAWEED-DERIVED SALT

Bhagirath Rakhasiya<sup>a\*</sup>, Rajkumar Dineshbhai Patel<sup>b</sup>, Andrei Savin<sup>c</sup>, Nguyen Van Nguyen<sup>d</sup>, Sunil K. Sahu<sup>e</sup>, Kapilkumar Nivrutti Ingle<sup>f</sup>, Rochak Mittal<sup>g</sup>, Tejal K. Gajaria<sup>h</sup>, Vaibhav A. Mantria<sup>I</sup>
<sup>a</sup>Csir-Central Salt and Marine Chemicals Research Institute, Gijubhai Badheka Marg, Bhavnagar, INDIA
<sup>b</sup>Government Medical College, Jail Road, Bhavnagar, INDIA
<sup>c</sup>University of The Aegean, Lesbos Island, Mytilene, GREECE
<sup>d</sup>Research Institute for Marine Fisheries, 224 Le Lai, Hai Phong, VIETNAM
<sup>e</sup>State Key Laboratory of Agricultural Genomics, Bgi-Shenzhen, Shenzhen, CHINA
<sup>f</sup>University of Szeged, Kozepfasor 52, H-6726 Szeged, HUNGARY
<sup>g</sup>University of Limerick, Castletroy, Co. Limerick, V94 T9px, IRELAND
<sup>h</sup>Navrachana University, Vasna-Bhayli Road, Vadodara, Gujarat, INDIA
<sup>I</sup>Academy Of Scientific and Innovative Research (Acsir), Ghaziabad, INDIA
E-mail: bhagirathrakhasiya@gmail.com

#### Abstract

The quantity of 'generally regarded as safe' common salt in daily diet a factor of concern, since excess consumption of it has increased the global hypertension burden to 1.28 billion. The voluntary salt restriction is hard to practice and therefore consumption of low-sodium salt substitutes is emerging as the feasible approach. The seaweed-derived salt is high in K (3792.74  $\pm$  541.23 mg 100 g-1) and low in Na (1541.51  $\pm$  231.79 g-1), besides the absence of pesticides, heavy metals, and coliforms makes it suitable for human consumption. We have conducted the reconnaissance survey in six different countries (India, Romania, Hungary, Ireland, Vietnam, and China), to understand the perspectives and attitudes toward the dietary applications of seaweed-derived salt. Results showed higher acceptance among government workers and other occupations (100%); 50 years and above the age (96%); education with less than a bachelor's degree (95.45%); eggitarian and vegetarian diet preference (94.44%); and females (94.41%). The lower consumption of salt (<5g day-1, 88%) was recorded in Romania and Vietnam. We found pickled food (35.56%) is the prime contributor to dietary consumption of salt. The highest Spearman correlation score (0.96) for perceptions and attitudes towards the use of seaweed-derived salt was reported between Hungary and Ireland. The outcome of this first-ever study is expected to shed light on consumer perceptions, which is necessary for branding, and strategic planning for promotions of emerging novel potential products, besides policy measures to reduce the hypertension burden with novel approaches.

### NEMATICIDAL AND MOLECULAR DOCKING INVESTIGATION OF AEGLE MARMELOS FRUIT EXTRACT AGAINST MELOIDOGYNE INCOGNITA

Krishna Trambadiya<sup>1\*</sup>, Riddhi Kanabar<sup>2</sup>, Manish Visavadia<sup>3</sup> <sup>1,2</sup>Department Of Zoology, Bahauddin Government Science College, Bhakta Kavi Narsinh Mehta University, Junagadh, Gujarat, INDIA <sup>3</sup>Government Science College, Gujarat University, Gandhinagar, Gujarat, INDIA E-mail: bhaktipatel2231998@gmail.com

#### Abstract

Meloidogyne incognita is a highly destructive plant-parasitic nematode that causes substantial damages in agricultural field. The aim of the current investigation was to assess the nematicidal efficacy of Aegle marmelos fruit extract against second-stage juvenile (J2) of M. incognita under invitro conditions. The investigation revealed that A. marmelos fruit extract exhibited the highest mortality rate 67.4% at 4% concentration. Employing liquid chromatography-mass spectroscopy (LCMS) analysis, marmesinin emerged as a key secondary metabolite in A. marmelos fruit extract. Molecular docking analysis elucidated the binding interactions of these secondary metabolites, particularly the robust affinity of marmesinin towards the targeted protein, acetylcholineesterase (AChE) in M. incognita. Impressively, the computed binding free energy of marmesinin revealing a strong affinity at -11 kcal/mol. This study signifies that the A. marmelos fruit has nematicidal potential that can be used to control M. incognita for sustainable agriculture. However, the practical applicability of these plant extract necessitates for extensive research and field trials with the ultimate goal of establishing environment friendly nematode control in agriculture.

# EXPLORING INTERTIDAL SPONGE NICHES: HABITAT PREFERENCES AND ECOLOGICAL ROLES IN THE COASTAL COMMUNITIES

Zalak Sabapara\*, Paresh Poriya Bahauddin Science College, Bhakta Kavi Narsinh Mehta University, Junagadh, Gujarat, INDIA E-mail: zgsabapara27@gmail.com

#### Abstract

Intertidal sponges play a crucial yet often overlooked role in coastal ecosystems, contributing to the dynamic balance of intertidal communities. Through field surveys and ecological assessments, the role of sponges is explained in this study; concerning the interactive effects with various habitats, for resolving the relationship between community dynamics and ecosystem functions in heterogeneous intertidal habitats. The study was conducted at the rocky intertidal areas of Gujarat. This study explores the ecological roles of intertidal sponges in the broader context of coastal community dynamics. We investigate their interactions with other organisms, such as algae, sponges, crustaceans, echinoderms, zoanthids, corals and molluscs, to assess their influence on community structure and ecosystem functioning. In this study, sponges mostly prefers rock pools, zoanthids bed, underneath of rock, shallow pool, coralline bed, caves-crevices and algal bed. The great majority of observed sponges were of encrusting in nature occurring in the cryptic habitats of caves and under surfaces of boulders. Under-surfaces of rocks and caves provide protection from temperature, water current, other extremes and trapping pools help reduce evaporation thus, reducing desiccation and salinity changes. The studied sponges exhibited mutualistic and also obligatory commensalism relationship with other organisms. So we concluded that, the coexistence of these organisms depends on factors such as habitat suitability, competition for resources, predation, and environmental conditions.

### NESTING HABIT AND HOST PREFERENCE OF BAYA WEAVER (PLOCEUS PHILIPPINUS LINN.) IN PENINSULAR REGION OF SAURASHTRA

Yusufkhan Pathan<sup>1\*</sup>, Arvindgiri Goswami<sup>1</sup> <sup>1\*&1</sup>Biology Department, M. V. M. Sci. & Home Science College, Saurashtra University, Rajkot, Gujarat, INDIA E-mail: pathanyn4@gmail.com

#### Abstract

The Baya Weaver (Ploceus philippinus) popularly known for excellent nest weaving skills, found across the Indian Sub-continent and Southeast Asia. The survey for the nesting habits of Baya Weaver was conducted at different sites of pennisular region of Saurashtra. A nest construction pattern, selection of host tree and the geographical condition around nest site showed that nest was constructed predominantly over the host tree located at agricultural land and nearby water to protect the offsprings against a predator. A total 841 nests carried out at various development stages of nest over the 11 different host plants of varied length among the 6 different families. The highest number of complete nests constructed over the babool tree Acacia nilotica (325 nests) followed by palm tree Phoenix sylvestris (220 nests) and royal palm tree Roystonea regia (101 nests). Among the various stages of nest 33.1% nest was successfully complete nest and 66.94% incomplete nest was observed during the six-month survey (June-November). The nesting population of Baya Weaver facing a various threat such as loss and modification of grassland in to human-dominated landscapes, lack of food availability and adverse weather.

# WINGS OVER WATER: INVESTIGATING THE IMPACT OF WATER PARAMETERS ON BIRD DIVERSITY AND ABUNDANCE

Vibhakar Jani\*, Chiragbala Gosai Government Science College, Veraval, Bhakta Kavi Narsinh Mehta University, Junagadh, Gujarat, INDIA E-mail: vibhakar.jani@gmail.com

#### Abstract

A wetland is an area of land where the soil is saturated with water either permanently or seasonally. It is very important part of ecosystem where many plant and animal species can flourish. It is one of the major habitat for birds because it supports the congregation of large number of resident and migratory birds. Physico-chemical parameters of wetland are known to influence on abundance of migratory and resident bird species. Present study is an effort to throw a spotlight on the interaction between biotic and abiotic factors of wetland near Dhandhusar village of Junagadh district of Gujarat state and its bird diversity. Site was visited once in a week for 18 months from December 2021 to May 2023 and bird census was carried out in each visit and water samples were also collected for documentation of physico-chemical changes over the time. Data revealed that bird density is negatively correlated with dissolved oxygen (DO) and water cover. Maximum migratory species of birds were noted during winter and maximum resident bird species were noted during post monsoon season. Density of Ducks is highest throughout the year. 101 bird species from 37 families were noted during this study.

# EXPLORING SALT TOLERANCE MECHANISMS: SEASONAL CARBOHYDRATE DYNAMICS IN SALT-TOLERANT PLANT SPECIES

Dhruvisha Mehta, Suhas Vyas\*

Department of Life Sciences, Bhakta Kavi Narsinh Mehta, University, Junagadh, Gujarat, INDIA E-mail: vsuhas.13@gmail.com

#### Abstract

Salt-tolerant plant species, including halophytes, mangroves, and seaweeds, flourish in saline environments, where they encounter osmotic and ionic stresses induced by high soil salinity. This investigation focuses on the adaptive strategies employed by these resilient plants, with a particular emphasis on the seasonal variations in carbohydrate content within their photosynthetic organs. A meticulous analysis was conducted, examining the total soluble sugars and starch in the leaves of representative halophytes and mangroves, as well as the thallus of seaweed species. The results of this analysis unveiled dynamic and nuanced patterns of carbohydrate accumulation in response to changing environmental conditions. The study offers valuable insights into the intricate salt tolerance mechanisms utilized by halophytes, mangroves, and seaweeds, thereby contributing to a deeper understanding of plant adaptation to saline environments.

### ASSESSING THE MACROFAUNA COMMUNITY: A COMPARATIVE ANALYSIS OF QUADRATE METHOD AND PHOTO QUADRATE TECHNIQUE

Dimpal Dodiya\*, Paresh Poriya Department of Zoology, Bahauddin Government Science College, Bhakta Kavi Narsinh Mehta

University, Junagadh, Gujarat, INDIA

E-mail: dodiyadimpal1995@gmail.com

#### Abstract

The present study applied both the quadrate method and the photo quadrate technique to assess the macrofauna community on the Adri coast. The quadrate sampling method was used to study seasonal fluctuations in the intertidal zone and the distribution of macrofauna populations. A 0.25 m<sup>2</sup> quadrate frame was systematically placed at 20-meter intervals using stratified random sampling to assess the macrofauna population, with data recorded for three ecological attributes: density, abundance, and frequency. For the first time, the advanced photo quadrate method was employed to conduct a quantitative assessment of the intertidal macrofaunal community's habitat on the Adri coast of Gujarat. Implemented on a rocky intertidal coast, the photo quadrate method involves capturing photographs and documenting the entire substrate, along with macrofaunal communities, at fixed locations. To assemble the photo quadrate frames, a stratified random sampling procedure was employed. Two photo quadrate frames were laid out in the middle intertidal zone and the other two in the lower intertidal zone. The Photo Quad software, which has a complete database of sessile benthos from the studied coast, considerably aided the advanced research approach. The photo quadrate method is different from the quadrate method; it provides a rapid and accurate quantitative assessment of the macrofauna community, establishing its distinctiveness compared to the traditional quadrate method.

# SUSTAINABLE LIPASE FROM A MARINE BACTERIUM: HARNESSING WASTE COOKING OIL AS AN INDUCER FOR ENHANCED BIOCATALYST PRODUCTION

Vaishnavi C. Goswami\*, Devayani R. Tipre Department of Microbiology and Biotechnology, School of Sciences, Gujarat University, Ahmedabad, Gujarat, INDIA E-mail: vaishnavigoswami5697@gmail.com & devayanitipre@hotmail.com

#### Abstract

Cooking oil undergoes various undesirable changes during the process of cooking, which restricts its further utilization. Disposal of this kind of polluting waste has become an increasingly distressing matter. Thus, proper waste management of waste cooking oil (WCO) is necessary. The present study concentrates on the use of WCO as an inducer for lipase production and optimization of process parameters from a marine bacterium isolate AS-17, which was isolated from the sediment sample of the coastline of Alang, Gujarat. Biolog® microbial identification system was used for the tentative identification as well as to study the metabolic profile of the isolate AS-17. One-factor-at-a-time approach was used for the optimization of various parameters such as salt concentration, oil concentration, pH, inoculum age as well and inoculum size. Lipase production was enhanced during the optimization process at 9% salt concentration, 2% WCO concentration, pH 7, 21 h old inoculum, and 2% inoculum size containing ~7 × 107 cells/mL. Optimization of these process variables resulted in a significant 1.3-fold increase in lipase production yielding a final production of 66.8 U/mL as compared to the unoptimized conditions which was 52 U/mL. The details will be discussed.

# FAECAL MATERIALS USED FOR DETERMINATION OF HABITAT UTILIZATION BY WILD ANIMALS AT GIRNAR WILDLIFE SANCTUARY, JUNAGADH

Riddhi Kanabar<sup>1\*</sup>, Krishna Trambadiya<sup>1</sup>, Manish Visavadia<sup>2</sup>, <sup>1</sup>Department Of Zoology, Bahauddin Government Science College, Bhakta Kavi Narsinh Mehta University, Junagadh, Gujarat, INDIA <sup>2</sup>Government Science College, Gujarat University, Gandhinagar, Gujarat, INDIA E-mail: riddhikanabar30@gmail.com

#### Abstract

Wild animals are often deposit their faeces in such dedicated sites, which may share by several animals. The present study was undertaken to determine habitat utilization by faecal materials of wild animals at Girnar Wildlife Sanctuary, Junagadh. The dominant forest type of the sanctuary area is mixed deciduous forest along with thorny scrub forest. The study area was divided in different habitat viz., grassland, woodland and scrubland. Woodland habitats were over utilized by herbivore like nilgai and sambar; scrubland habitats were over utilized by spotted deer. In carnivores like asiatic lion, grasslands were over utilized for defecation; leopards were often defecated at the same site used by herbivores like nilgai. The present study provides baseline information of defecation sites which may further used for monitoring or management strategies and to understand behavioural strategies of wild animals.

### UNVEILING THE POTENTIAL OF COLLEMA GENUS: A COMPREHENSIVE EXPLORATION OF CHEMICAL CONSTITUENTS AND BIOLOGICAL ACTIVITIES

Chhaya J. Bhatti, Sandip B. Gamit Department of Life Science, Bhakta Kavi Narsinh Mehta University, Junagadh, Gujarat, INDIA E-mail: chhayanil10@gmail.com

#### Abstract

Lichens are intriguing symbiotic organisms, combining a heterotrophic fungus and an autotrophic alga in a mutualistic relationship. The Collema genus is a notable example, featuring a gelatinous thallus composed of interwoven fungal hyphae and the cyanobacterium Nostoc. Flourishing in shaded environments, particularly with foliose, jellified, and ecorticate structures, Collema comprises over 75 species globally, with 16 identified in the Indian subcontinent. Among these, Collema crisatum stands out as a rare species. Chemically, Collema is rich in fatty acids, polar lipids, and aromatic compounds. Major polar lipids identified include diacylglyceryltrimethylhomoserine and phosphatidylcholine. Key unsaturated fatty acids like alpha-linolenic and oleic acids exhibit antiinflammatory properties. Many Collema species incorporate UV-absorbing substances such as scytonemin and mycosporine-glycine, along with the photo-protective mycosporine Collemin A, which demonstrates a dose-dependent prevention of UV-B-induced cell damage. Collema flaccidum stands out for its heteroglycan "Colleman" with potential immunomodulating effects. Extracts from Collema flaccidum contain compounds like bianthraquinone, colleflaccinosides, glycosides, cristazarin, usnic acid, depsidone, lichenin, protolichesterinic acid, and polyporic acid, showing promise in anticancer activities. Despite these remarkable metabolites, their applications in pharmaceutical and agrochemical industries are constrained by slow growth, limited biomass availability, and technical challenges associated with artificial cultivation. In antimicrobial activities, Collema cristatum, particularly in acetone extracts, demonstrates significant inhibitory effects against bacterial strains such as B. subtilis, E. coli, and S. aureus. Despite the potential applications of these unique metabolites, challenges in cultivation and biomass availability have hindered their widespread utilization in pharmaceutical and agrochemical industries.

### SUMMER GOLD; MADHUCA LONGIFOLIA VAR. LATIFOLIA – ECOLOGICAL, ECONOMIC AND ETHNOBOTANICAL ASPECTS

Kamlesh J. Gadhvi<sup>1</sup>, Suhas J. Vyas<sup>2</sup> <sup>1</sup>Gujarat Forestry Research Foundation, Gandhinagar, Gujarat, INDIA <sup>2</sup>Department of Life Sciences, Bhakta Kavi Narsinh Mehta University, Junagadh, Gujarat, INDIA E-mail: gadhvikj70@gmail.com

#### Abstract

A tree is integrated with human society in many ways and also plays an important role for other biodiversity. The present paper deals with how one tree species have the potential to gather all kind of different biological diversity in a holistic way. Madhuca longifolia var. latifolia is one of the most important tree in India commonly known as "Mahua tree". Ecological aspects of this tree most suitable host for epiphytic orchids and act as a bark nursery. Several bird species and IUCN listed species Indian giant flying squirrel (Petaurista philippensis) and Sloth bear (Melursus ursinus) which is mostly dependent on M. longifolia var. latifolia tree. Economic use of M. longifolia var. latifolia, especially during COVID-19 majority of tribal people dependent flowers of M. longifolia var. latifolia for financial support, when there was no employment, this tree became a source of livelihood for many people and it is even now. Seed used for oil extraction and trunk wood and braches is used to build a house. Local communities used dry felled leaves as manure for rice crops. Flowers, fruiting, seeds and emerging twig development these all phenological events completed in the summer season and especially during summer it is highly demanded, that's why "Summer gold" is entitled. Nowadays due to poverty local people cut trees and sell them in the local market, which directly threats both M. longifolia var. latifolia and its associated biological species. In the context of conservation forest department started conservation trough providing saplings to the villages.

### NEST IN THE CITY: A STUDY ON BIRD NEST SITE SELECTION IN URBAN HABITAT

Kalpesh Shankhala, Paresh Poriya Bahauddin Science College, Junagadh, Gujarat, INDIA E-mail: kalpeshpshankhala@gmail.com

#### Abstract

A study on nesting site selection in the Junagadh city (21.5222 °N, 70.4579 °E) located on the middle outskirts of Junagadh District was carried out for the first time to explore effect of urbanisation on nesting ecology of birds. A total of 23 sites were surveyed during the study period between March 2021 to February 2023. We recorded 96 bird species belongs 41 families under 18 orders from the study area. Only 12 sites were found to be selected by birds for nesting. The Agriculture University Campus was prime site for both migrant and resident bird species. The present study also provides a comprehensive checklist of avian fauna and birds nesting of Junagadh city, Gujarat.

# INVESTIGATING THE POTENTIAL USE OF WATER HYACINTH/ AQUATIC HITCHHIKERS BY PREPARATION OF VERMICOMPOSTING FOR SAVING THE TAPI RIVER FOR SUSTAINABLE ECONOMIC GROWTH IN SURAT

Ragini Dalal, Dr. Kailash Patel, Dr. Jagruti Barot Department of Bio-science, Veer Narmad South Gujarat University, Surat, Gujarat, INDIA E-mail: ragini.dalal@gmail.com

#### Abstract

The plant is a perennial herb (Eichhornia crassipes) which belongs to the family Pontederia, closely related to the Liliaceae (lily family) the mature plant consists of long, pendant roots, rhizomes, stolon, leaves, inflorescences and fruit clusters. (Herford, O sthagen and saelthun 1994) Water hyacinth growing in large scale in Surat region area of the Tapi river which is the main source of growth and development of industry in Surat and water density of fresh water decrease because of this water hyacinth.it absorbs maximum fresh water and became a big headache for hydraulic department of SURAT MUNICIPAL CORPORATION. every year after monsoon this water hyacinth covered whole cause-way area.so under the project called "The Tapi-Shuddhi Karan" Corporation is spending large amount of budget behind this cleaning of river from water hyacinth.

#### ANALYTICAL METHODS FOR ANTIMICROBIAL ACTIVITY

Chetana Rajyaguru<sup>1</sup>, Jatin Upadhyay<sup>2</sup>, S.P. Singh<sup>3</sup> <sup>1&2</sup>M.V.M. Science and Home Science College, Rajkot, Gujarat, INDIA <sup>3</sup>Bioscience Department, Saurashtra University, Rajkot, Gujarat, INDIA E-mail: chetanamrajyaguru1967@gmail.com

#### Abstract

This is a broad inter disciplinary aspect of research in which new chemicals are made by researchers in search of new medicines for diseases difficult to cure. It may be caused by bacteria, viruses, fungi, algae or Protozoa. Several diverse types of synthetic molecules are tested against Microbes to develop effective treatment for Microbial infections. These compounds are often targeted to work on Microbial cell to inhibit or kill them by several mechanisms affecting various active bio molecules and internal structures. The compounds may be organic, inorganic, polymers, peptides, proteins or Biocides. During the research work there were three analytical techniques helped in finding Antimicrobial Activity of the synthetic and biological organic compounds. Marine algae are used extensively for pharmaceutical products. In historical pages algae has proved medicine against goitre, nephritis and producing many antibiotics too. Several red algae were used to get the extracts of various types through certain chemical processes using solvents. Preparation of biological Extracts was tedious but avails pure extracts of lipids, sterols and fatty acids. The second technique, most extensively used to get MIC was Agar Dilution Procedure in which the antimicrobial agent is incorporated into the agar medium with each plate containing a different concentration of the agent. This technique has been proven the best in many of the case studies especially for prokaryotic organisms. The third, Quantitative Measurement of bacterial growth was done by using viable count technique and Direct Microscopic count. Determination of grown and survived bacteria was done by consideration of results of both the techniques. The exact amount of killed and survived microorganisms can be detected by these counts for each antimicrobial agent. In the conclusion of the work, varying responses were found with various microorganisms and some algal extracts were proven potentially active biological material against them. The significance of this work resides in making the path to study Damage to specific enzyme system and Understanding Molecular basis of MDR.

# MICROBIALLY INDUCED CALCITE PRECIPITATION AND FORMULATION OF BIOCEMENT

Megha S. Gadhvi\*, Dushyant R. Dudhagara Department of Lifesciences, Bhakta Kavi Narsinh Mehta University, Junagadh, Gujarat, INDIA E-mail: msgadhvi19@gmail.com

#### Abstract

One of the most prevalent minerals on Earth is calcite, or calcium carbonate (CaCO<sub>3</sub>). The MICP is a result of microbial metabolic processes as photosynthesis, denitrification, ammonification, and urea hydrolysis. Urea hydrolysis is the main pathway for MICP to form precipitated carbonates. MICP has the potential for the development of biocement, bioconcrete, and self-healing concrete. This research investigated the occurrence of ureolytic bacteria in saurashtra region. Samples were collected from calcareous bricks mine and coral reef sedimentary rocks and were used to isolate the indigenous ureolytic bacteria. Isolates were screened for urease activity on the urea base medium and urease producing isolates were found. Moreover, Calcite formation by isolates was performed in the YEurea medium and all urease producing isolates were precipitating calcite. Phenol-hypochlorite assay method through Enzyme activity of urease enzyme was determined. Maximum urease activity and calcite precipitation was found in bacterial isolate encoded as JCP-5. Therefore, this research showed an occurrence of indigenous bacteria in collected samples that can perform calcite precipitation (biomineralization) and thus can be helpful, if appropriately stimulated, in the preparation of biomortar, bio-concrete and for the remediation of cracks and gaps in the building materials.

# PROCESS MODELING AND OPTIMIZATION OF ANTICANCER L-METHIONINASE ENZYME FROM BACTERIUM ALCALIGENES AQUATILIS USING RESPONSE SURFACE METHODOLOGY AND ARTIFICIAL NEURAL NETWORK

Bhumi M. Javia\*, Dushyant R. Dudhagara Department of Life Sciences, Bhakta Kavi Narsinh Mehta University, Junagadh, Gujarat, INDIA E-mail: bhumijavia48@gmail.com

#### Abstract

The current study deals with the production of anticancer enzyme from bacterium Alcaligenes aquatilis via submerged fermentation. The statistical methods of Plackett Burman design and response surface methodology were used to optimize the nutritional factors for the production of L-methioninase by Alcaligenes aquatilis BJ-1. The regression models depicted considerably high R2 values of for L-methioninase activities, signifying that they are suitable for forecasting associations between KH<sub>2</sub>PO<sub>4</sub>, Na<sub>2</sub>HPO<sub>4</sub>, Glucose and L-methionine. In accordance with the model, the optimum condition for L-methioninase production were KH<sub>2</sub>PO<sub>4</sub> 1.0 g/L; Na<sub>2</sub>HPO<sub>4</sub> 8.0 g/L, Glucose 0.5 g/L and L-methionine 8 g/L. In the optimized condition Alcaligenes aquatilis BJ-1 produced L-methioninase with the activity of 8.21 U/ml which is 6.8 times superior to that produced in initial fermentation condition. Hence, this statistical technique enabled fast identification and combination of key medium factors for Alcaligenes aquatilis BJ-1, resulted in the high L-methioninase production. The significant nutrient factors and enzyme activity were incorporated in artificial neural network as input variables and output variable. The Levenberg algorithm was used for ANN training resulted in increased enzyme activity under the optimum condition as compared to response surface methodology.

### MULTIDIMENSIONAL EVALUATION OF SALT TOLERANCE IN GROUNDNUT GENOTYPES THROUGH BIOCHEMICAL RESPONSES

Rushita Parmar Devdasbhai Department of Life Science, Bhakta Kavi Narsinh Mehta University, Junagadh, Gujarat, INDIA E-mail: rushitaparmar8@gmail.com

#### Abstract

The present study explores the complex interplay between groundnut genotypes, salt tolerance and hormonal influence, shedding light on the dynamic responses of three specific groundnut genotypes, KDG-128, TG-37A and GG-20, to salt treatments and gibberellic acid (GA3). The study encompasses plant growth, total protein content and oil content as key parameters. Through comprehensive analysis, it identifies TG-37A and KDG-128 as salt-tolerant genotypes and GG-20 as salt-susceptible, highlighting the potential for targeted breeding efforts to develop more resilient groundnut varieties. Moreover, the quantification of protein and oil content under different treatments provides vital data for optimizing nutritional profiles in groundnut cultivars. Principal Component Analysis (PCA) underscores the significance of the first principal component (PC1) in explaining the majority of variance, capturing primary trends and differences in plant length. ANOVA and hierarchical analysis confirm the presence of statistically significant differences in protein and oil content among the genotypes. Pearson's correlation coefficient matrix analysis reveals strong positive correlations between plant length and protein content, plant length and oil content, and a moderate positive correlation between protein content and oil content. These findings provide valuable insights into groundnut physiology, salt tolerance, and nutritional composition, with implications for future research in sustainable agriculture and crop improvement.

### NEUROPROTECTIVE EFFECT OF FLURBIPROFEN ON NEUROINFLAMMATION AND BBB DISRUPTION IN MCAO RATS

Rajesh Ugale\*, Ankita Thul, Bhavesh Verma Department of Pharmaceutical Sciences, Rashtrasant Tukadoji Maharaj Nagpur University, Nagpur, Maharashtra, INDIA E-mail: ugale.rajesh@gmail.com

#### Abstract

Flurbiprofen is a nonsteroidal anti-inflammatory drug (NSAID) and a non-selective cyclooxygenase inhibitor. Flurbiprofen has shown neuroprotection against cerebral ischemia in rats by preventing apoptosis in earlier studies. However, the effect of flurbiprofen on neuroinflammation and disruption of the blood-brain barrier which results in neuronal damage, is yet unknown. Neuroprotective effect of flurbiprofen on neuroinflammation and BBB (Blood Brain Barrier) disruption in middle cerebral artery occlusion (MCAO) rats Adult Wistar rats (200-250g) were used for induction of cerebral ischemic stroke using middle cerebral artery occlusion. Following the blockage of middle cerebral artery (MCA) using 4-0 nylon filament, the animals underwent a 24-hour period of reperfusion. Beam walk testing and the neurological impairment score were used to measure behavior, and histological analyses (Evan's Blue and Nissl staining) were then conducted. Additionally, immunohistochemistry was used to analyze the molecular level of proteins (MMP9, CD86 & CD206). In this study, the flurbiprofen (10mg/kg; i.p.) administration improved neurological functional outcomes assessed by neurological deficit score and beam walk score. Furthermore, flurbiprofen enhanced Nissl substances that indicate neuronal recovery and lessened disruption of the BBB. Additionally, flurbiprofen significantly decreases the expression of the MMP9, CD86, and CD206 proteins representing BBB disruption and microglial inflammation respectively in MCAO rats. The present study demonstrated the neuroprotective effect of flurbiprofen on cerebral ischemic reperfusion injury in rat by decreasing neuroinflammation and BBB disruption.

# HPTLC FINGERPRINTING ANALYSIS AND ANTIOXIDANT ACTIVITY OF VALUABLE MEDICINAL PLANT DESMODIUM SPECIES

Jankiben Prajapati, Nidhi Kumari Ganvit Bhoomi Joshi, Illa Patel Department of Life Sciences, Hemchandracharya North Gujarat University Patan, Gujarat, INDIA E-mail: janki123va@gmail.com, ganvitnidhi277@gmail.com & illabotany@gamil.com

#### Abstract

Herbal medicine, also called botanical medicine or phytomedicine, refers to the use of any plant seed, leaves, roots, barks or flower for the medicinal purpose. From the ancient days the conventional medicine and herbalism is becoming more mainstream for the treatment of various chronic disease. The pharmacognostical studies of the plant Desmodium species, family Fabaceae were scientifically validated in this present study. Desmodium species is small shrub of tropical and subtropical region. It has been used in the Indian system of medicine for the treatment of number of diseases such as jaundice, rheumatism, fever, paralysis and inflammatory condition. It is one of the important constituents of Dashmool, a well- known mixture of 10 herbs used in many ailments including influenza, cough, cold and headache. It is also use as dietary supplements. Entire plant of various Desmodium species were explore randomly for curing several disease. Due to rich in secondary metabolites plants have number of pharmacological activities like anti-inflammatory, anti-diabetic, anti-ulcer and anti-cytoprotective but which species and part are more effective is not analyzed yet. So, this study focus on Quantitative analysis, HPTLC fingerprinting analysis of flavonoid from various parts of Desmodium species viz. D. gangeticum, D. triflorum, D. laxiflorum and D. oojeinense along with free radical scavenging activity. Work was conduct using CAMANG (Muttenz, switzerland) HPTLC system, using LINOMAT 5 applicator and vision CATS software and TLC visulizer for fingerprinting analysis. Chemicals like Toluene, methanol, ethyl acetate and formic acid used for mobile phase. 0.1 mM DPPH used to measure antioxidant activity. The conclusion put out is that all Desmodium species are rich source of flavonoid content. Leaf and root part of plant show maximum amount of antioxidant activities that may be future explore for drug industries.

### PHYTOCHEMICAL AND ANTIMICROBIAL ANALYSIS OF PHYLLANTHUS NIRURI

A.H. Pathak, H.H. Mehta\*

Department of Biotechnology, Smt. S.S. Patel Nootan Sciene and Commerce College, Sankalchand Patel University, Visnagar, Mehsana District, Gujarat, INDIA E-mail: hmehta089@gmail.com

#### Abstract

Indian Ayurveda system stands for long-lasting medicines derived from plants. There are so many plants that are used for medicinal purposes, and Phyllanthus niruri is one of them. Known for its various therapeutic applications. This plant holds the capability to produce natural alternative solutions for microbial infections. It contains various phytochemicals, which are the reason for its various health benefits like liver, kidney, cancer, viral, and fungal infections. In this study, we aimed to investigate the antimicrobial and antifungal potential of extracts derived from plants, as well as to explore various phytochemicals qualitatively by various biochemical tests. Our results demonstrated significant antimicrobial and antifungal activities of the P. niruri extracts. The extracts exhibited a broad spectrum of antimicrobial activity, inhibiting the growth of pathogenic bacteria. This study underscores the therapeutic potential of P. niruri as a source of natural antimicrobial and antifungal agents, which provides valuable insights into the effective way, which can guide the development of potential pharmaceutical and biotechnological applications.

# EFFECT OF COPPER STRESS ON SEED GERMINATION PARAMETER IN MURRAYA KOENIGII PLANT

Kumari Sunita\*, Dubey Supriya Umesh Kumar Plant Physiology and Biochemistry PGPR lab Department of Botany, DDU Gorakhpur University, Gorakhpur, UP, INDIA E-mail: ksunita78@gmail.com

#### Abstract

Copper is an important trace element for the growth and health of the plant, it play a vital role in various physiological process. Stress in plant refer to environment circumstances that have a negative impact on plant growth. This study investigates the impact of copper stress on the germination parameter of Murraya koenigii plant. Through controlled experiment we access how varying concentration of copper affect seed germination rates, emergence and overall seedling growth. Thus in this paper seeds of Murraya koenigii plant was collected and different parameters such as germination percentage, germination index, seed vigour index, and copper injury rate were examined in growth chamber at different level of copper metal stress at different concentration such as control, 2Mm, 5Mm, and 10Mm and our result showed that germination rate decline at higher concentration of copper radical length does not increase which results that copper stress affect the seed germination of Murraya koenigii by delay it's germination time.

### ASSESSMENT OF TP53 GENE MUTATION IN BREAST CANCER PATIENTS: A COMPREHENSIVE ANALYSIS OF MUTATION FREQUENCY

<sup>1</sup>Drashti A. Rao<sup>\*</sup>, <sup>2</sup>Dr. Sumitra Datta, <sup>3</sup>Dr. Hariom Sharma Department of Biochemistry, Gov. Medical College, Bhavnagar, Gujarat, INDIA E-mail: drashtirao4728@gmail.com

#### Abstract

Breast cancer remains a significant global health concern, necessitating comprehensive investigations into genetic factors that contribute to its pathogenesis. The TP53 gene, a crucial tumor suppressor, has been implicated in various cancers, including breast cancer. This study aimed to estimate the prevalence of TP53 gene mutations in breast cancer patients compared to a control group of healthy women. We conducted a case-control study comprising 150 breast cancer cases and 150 healthy controls. Genomic DNA was extracted from peripheral blood samples, and specific regions of the TP53 gene were amplified using polymerase chain reaction (PCR). Gel electrophoresis was employed for the identification of PCR amplicons, with a focus on detecting mutations in the TP53 gene. Among the 150 breast cancer cases, 20 individuals exhibited mutations in the TP53 gene, while no mutations were detected in the healthy control group. The observed mutations displayed diverse patterns, underscoring the heterogeneity of TP53 alterations in breast cancer. Our findings highlight a significant association between TP53 gene mutations and breast cancer, as evidenced by the absence of mutations in healthy controls. This study contributes valuable insights into the genetic landscape of breast cancer, emphasizing the potential diagnostic and prognostic relevance of TP53 mutations. Further exploration of the functional consequences of these mutations may pave the way for targeted therapeutic interventions. The identification of TP53 mutations in breast cancer patients underscores the importance of genetic screening for personalized treatment strategies and emphasizes the need for continued research in unraveling the intricate molecular mechanisms underlying breast cancer development.

### ELECTRO-OSMOTIC PUMP DESIGNED BY REVERSIBLE PROTON (de)INSERTION IN M0O3: MICROFLUIDIC OPERATIONAL USEFULNESS

Vidhiben Dave<sup>a,b</sup>, Govind Sethia,<sup>c,b</sup> Rajaram K. Nagaralea<sup>,b\*</sup>

<sup>a</sup>Membrane Science and Separation Technology Division, Electro Membrane Processes Laboratory, CSIR-Central Salt and Marine Chemicals Research Institute, Bhavnagar,

Gujarat, INDIA

<sup>b</sup>Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, INDIA <sup>c</sup>Inorganic Materials and Catalysis Division, CSIR-Central Salt and Marine Chemicals Research Institute, Bhavnagar, Gujarat, INDIA E-mail: rknagarale@csmcri.res.in

#### Abstract

The non-gassing, low-voltage electro-osmotic pump' s (EOP) ability to function depends on reversible proton (de)insertion and a high overpotential for oxygen and hydrogen evolution. Here, we present the synthesis, characterization, and application of the MoO3 electrode in an EOP operation. Because of reversible proton (de)insertion, the pump was operated well below the thermodynamic potential of water splitting. The active material was prepared through straightforward thermal oxidation of commercially available molybdenum (IV) sulphide. From the voltammogram, the calculated columbic capacity of the electrode was ~1300 C g-1 of MoO3. The detailed electrochemical characterizations revealed that the charge storage process was diffusion-controlled. EOP was assembled with a MoO3 electrode as both the cathode and anode were found to be effective in pumping water at 45.26 µL min-1 V-1 cm-2 electro-osmotic flux. The flow was linear with applied voltage; at 1 V, the obtained flow was 30 µL min-1 cm-2, whereas at 5 V, the obtained flow was 200 µL min-1 cm-2. In a continuous operation, the pump could deliver 1.28 mL of water in 160 min, which corresponds to 6862 water molecules per reacted proton. The practical applicability of the pump was demonstrated by its incorporation into an infusion device. The measured electro-osmotic flux for the device was 42.16 µL min-1 V-1 cm-2. To enhance the pump's functionality, we arranged multiple pumps in parallel mode and recorded their performance. The maximum flow rate with seven parallel pumps was 210 µL min-1 at 5 V, indicating the best utility in various microfluidic device application.

# FABRICATION AND CHARACTERIZATION OF SILVER NANOPARTICLES USING MARINE BROWN ALGAE ALONG WITH ITS ANTIMICROBIAL ACTIVITY

Disha Patel, Riya Desai, Mitu Patel, Illa Patel Department of Life Sciences, Hemchandracharya North Gujarat University Patan, Gujarat, INDIA E-mail: dishapatel4453@gmail.com & illabotany@gmail.com

#### Abstract

Nowadays, fabrication of silver nanoparticles using marine algae is gaining center of attention for research trend in compare to green synthesis from higher plants. The present study synthesized biocompatible and functionalized silver nanoparticles using an aqueous extract of abundantly available brown seaweed name Padina tetrastromatica (Hauck) as a reducing as well as stabilizing agent. Synthesis of nanomaterials by biological approach is innovative, cheaper and environmentally friendly and requires less- labor. The properties of prepared nanoparticles were characterized by UVvisible spectra, Fourier Transform Infrared Spectroscopy, X-ray diffraction analysis and Scanning electron microscopy (SEM) analysis. The formation of silver nanoparticles was confirmed by the presence of an absorption peak at 300-700 nm using UV-visible spectrophotometer. In the results Xray diffraction (XRD) pattern revealed face-centered cubic (FCC) structure of the formed Ag nanoparticles, whereas Fourier Transform Infrared (FTIR) spectrum analysis showed peaks between 400-4000 cm-1 which confirmed the presence of functional groups and other ligands required for the synthesis and stabilization of silver nanoparticles. The morphology of biosynthesized AgNPs as reported to be spherical in shape was documented by SEM. Thus, it can be concluded that marine seaweed Padina tetrastromatica can be used to fabricate AgNPs which have great antimicrobial activity against some pathogenic bacteria. The outcome of this research work is uses of marine sea weeds successfully generated AgNPs which can be explored in medicinal industry.

### STUDY ON SEWAGE WASTEWATER TREATMENT USING SEQUENTIAL BATCH REACTOR

Anjali Thakur, Kushal Bhagat Department of Earth & Environmental Sciences Parul Institute of Applied Sciences, Parul University, Gujarat, INDIA E-mail: anjali.thakur6736@paruluniversity.ac.in

#### Abstract

Our planet is called blue plant due to the fact it's far ruled with the aid of using water, it covers extra than 70% of the earth's area. Water is a primary need for living organisms. India's surface consists of 2.45% of land area and 4% of water of the world although it also includes 16% of the world population. Increasing in population is one of the major reasons for the high demand of fresh water and the generation of wastewater is also increasing. 99 % water carries domestic wastes generation from kitchen, bathing, and urine. The reuse of treated wastewater is important for agriculture development. The present study was carried out to analyse the impact of Sequential Batch Reactor based on Sewage Treatment Plant. The sample was collected from an inlet of Domestic Sewage treatment plant for three times. The plant appears removal effectiveness for limits pH, 7.55 to 8.12; COD, 472 to 62 mg/l.

### EFFICIENT MUNICIPAL WASTEWATER PURIFICATION USING AGRICULTURAL BIO-WASTE MATERIALS: A SUSTAINABLE TREATMENT EVALUATION

Vaishali G. Varsani\*, Suhas J. Vyas Department of Life Sciences, Bhakta Kavi Narsinh Mehta University, Junagadh, Gujarat, INDIA E-mail: vvarsani162@gmail.com

#### Abstract

This scientific study presents a comprehensive investigation into the purification of municipal sewage water through the utilization of agricultural waste materials (AHS, TAS and GHS). The treatment process involved a modified approach with 24hrs of aeration and the addition of 1 gm of agricultural waste biomaterials. The performance of the bio-coagulant was evaluated by monitoring the reduction of physico-chemical parameters. AHS exhibited remarkable turbidity removal efficiency of 93.37%, supported by pseudo-first and pseudo-second-order kinetic modelling. The application of agricultural waste materials significantly reduced key parameters, including solids (up to 70-80%), dissolved oxygen (DO) (50%), biological oxygen demand (BOD) and chemical oxygen demand (COD) (up to 90%). PCA showed the significant positive loading of PC1(84.71%) that influencing the dual treatments of wastewater. Statistical analysis (P<0.05) confirmed the effectiveness of agricultural biomaterials in sewage water treatment compared to pre-treated water. The turbidity coagulation pseudo-first-order and pseudo-second-order kinetic modelling also revealed the efficiency against turbidity reduction in municipal sewage water. The findings underscore the significance of utilizing agricultural waste materials for sustainable and efficient purification of municipal sewage water, addressing water pollution and enhancing wastewater treatment processes.

# STUDIES ON HALOTOLERANT AND HALOPHILES PLANT GROWTH-PROMOTING BACTERIA AND THEIR EFFECT ON GROUNDNUT PLANTS UNDER SALT STRESS

Devi J. Chhatrodiya<sup>1</sup>, Jignesh H. Kamdar<sup>1</sup> School of Science, R.K. University, Rajkot, Gujarat, INDIA E-mail: chhatrodiyadevi@gmail.com

#### Abstract

Unfortunately, the world's increasing environmental degradation and population pressures mean that global food production may soon be insufficient to feed everyone. Therefore, it is imperative to significantly increase agricultural productivity in the coming decades. Soil salinity is one of the most important abiotic stressors for plant growth in saline coastal soils. The coastal regions of Saurashtra Gujarat harbor a diverse group of microorganisms including halophilic and halotolerant bacteria that may have plant growth-promoting properties. In addition to eliciting plant defense responses against pathogens, the halotolerant microbes have the capacity to produce phytohormones (indole acetic acids, gibberellic acids, and cytokinin), and aid in plant growth in harsh salinity-filled environments. A total 100 morphological distinct colonies were isolated from veraval and kodinar region, represents the characteristics of halotolerant bacteria and further all of these strains were characterized by biochemical and morphological tools aiming to investigate their in-vitro and in-vivo plant growth promotion capabilities and metal tolerance abilities under saline stress condition. Furthermore, plant growth promoting field study and identification of isolates by polyphasic approches is in under progress. The study would be helpful for the increasing the soil fertility and plant productivity using the PGPB especially by halotolerant and halophilic strain.

# UNVEILING POTENTIAL ANTIVIRAL PHYTOCHEMICALS FROM TERMINALIA CHEBULA AGAINST SARS-COV-2: A MOLECULAR DOCKING EXPLORATION OF CATHEPSIN L INHIBITION

Urvisha Beladiya<sup>1\*</sup>, Rajesh Patel<sup>1</sup> <sup>1</sup>Department of Biosciences, Veer Narmad South Gujarat University, Surat, Gujarat, INDIA E-mail: urvishabeladiya3@gmail.com

#### Abstract

The unprecedented outbreak of SARS-CoV-2 has necessitated the development of novel therapeutic strategies. One promising avenue lies in harnessing the power of natural compounds, particularly phytochemicals from medicinal plants. In this study, we employed In vitro inhibition assay and molecular docking to investigate the potential of phytochemicals from Terminalia chebula, a renowned medicinal herb, as inhibitors of Cathepsin L. The crude extract of the Terminalia chebula exhibited moderate inhibitory activity against the Cathepsin L, with an average inhibition of 79.1%. One hundred plus phytochemicals from T. chebula were docked against the crystal structure of Cathepsin L to identify bioactive compounds. Binding affinities, interaction patterns, and druglikeness properties were meticulously analyzed. The study findings revealed several phytochemicals demonstrating promising binding potential and favorable druggability profiles. Punicacortein C, Chebulanin, Terchebulin, Terflavin B, Terflavin C, and Terflavin A emerged as the top contenders, exhibiting strong binding affinities and stable complex formation with Cathepsin L. The study also identified key amino acids involved in ligand binding such as Lys10, Ala214, Leu69, Trp7, Asp162 and Asp7. Molecular dynamics (MD) simulations was carried out to investigate the stability of Cathepsin L. drug complexes. The results showed strong and stable binding of phytochemicals towards Cathepsin. This in vitro and in silco study paves the way for further exploration of T. chebula's potent phytochemicals as potential antivirals against SARS-CoV-2. By harnessing the power of nature, we can potentially unlock new avenues for combating this global pandemic.

### RECENT ADVANCEMENTS AND FUTURE PROSPECTS OF AGRICULTURE: GATEWAY TO SMART AGROINFORMATICS.

Amarshi Prajapati<sup>\*</sup>, Harsha Motwani<sup>1</sup>, Saumya Patel<sup>1</sup>, Hitesh A. Solanki<sup>1</sup>, Rakesh Rawal<sup>2</sup> <sup>1</sup>Department of Botany, Bioinformatics and Climate Change Impacts Management, <sup>2</sup>Department of Life Science, School of Sciences, Gujarat University, Ahmedabad, Gujarat, INDIA. E-mail: amarshiprajapati13567@gmail.com

#### Abstract

Taking a note of consumption of healthy food and wholesome meals quality and quantity wise along with the human energy requirement, the agricultural activities have impacted the human health. Agriculture is facing significant pressure to meet the growing food demands of the increasing world population. Being a complex process, several tasks are involved in each stage of agriculture. In order to overcome the crucial challenges, a number of researchers have turned to using machine learning methods and computer vision technology for advancements in agriculture. The process of selecting types of crops to plant, planning the land, preparing the land for irrigation, preparing the seeds, and planting the seeds are all included in the cultivation phase. Monitoring and managing crop growth is the primary responsibility of farming after the cultivation stage and finally harvesting is done. Numerous Internet of Things (IOT) frameworks have been established to autonomously track and supervise agricultural areas with minimum human participation. By using AI approaches, issues related to different farming activities may be resolved. Artificial intelligence methods such as genetic algorithms, artificial neural networks, particle swarm optimization, and several more are being leveraged to the benefit of intelligent targeted farming. The classification accuracy of ResNet, VGG19, InceptionV3, NasNet-Mobile, MobileNet DenseNet121, and DenseNet169 for 28 different types of illnesses in 15 distinct crop species was upto 99.74%. The development of a general platform for all types of crops and animals, QoS (Quality of Service), the use of explainable artificial intelligence to monitor crop growth and disease prevention, and other technological and deployment breakthroughs are some of the upcoming developments in smart agriculture. As a result, the significance of information and communication technology (ICT) in promoting sustainable and smart agriculture is crucial.

# LEVERAGING BIOINFORMATICS FOR NEOANTIGEN-BASED CANCER IMMUNOTHERAPY: A COMPREHENSIVE REVIEW

Dharmendra Singh F. Rao\*, Himanshu A. Pandya<sup>1</sup>, Saumya K. Patel<sup>1</sup>, Rakesh M. Raval<sup>2</sup> <sup>1</sup>Department of Botany, Bioinformatics and Climate Change Impact Management, School of Science, Gujarat University, Ahmedabad, Gujarat, INDIA <sup>2</sup>Department of Life Sciences, School of Science, Gujarat University, Ahmedabad, Gujarat, INDIA

Department of Life Sciences, School of Science, Gujarat University, Ahmedabad, Gujarat, INDIA E-mail: raod12180@gmail.com

#### Abstract

The advent of cancer immunotherapy has transformed the landscape of cancer treatment, introducing novel avenues for tailored and precise interventions. A particularly promising approach centers on the identification and application of neoantigens, distinct non-self peptides originating from somatic mutations within cancer cells. These neoantigens, exclusive to tumor cells, are presented by HLA molecules, eliciting a T-cell response and can be harnessed to provoke an immune reaction against cancerous tissues. The evidence suggesting the effectiveness of employment of neoantigens in cancer immunotherapies has triggered the development of vaccines and adoptive T-cell therapies targeting them. However, only small fraction of tumor somatic mutations can be classified as neoantigen. Hence, identification of personalized neoantigens remains challenging. The demand for immunoinformatics methods capable of pinpointing optimal neoantigens from cancer genomes is substantial, yet the exploration of immunoinformatics tools for neoantigen identification remains underdeveloped. Moreover, we examine the present status of clinical trials and therapeutic applications involving neoantigen-based immunotherapies, along with the challenges encountered in translating bioinformatics-driven discoveries into clinical implementation. The review concludes by delineating prospective directions and emerging trends in the domain, including bioinformatics to enhance neoantigen prediction precision. This exhaustive inquiry underscores the fundamental role of bioinformatics in unlocking the complete potential of neoantigen-based cancer immunotherapy, fostering a deeper comprehension of the intricate interplay between computational methodologies and translational medicine, ultimately benefiting individuals affected by cancer.

### CRISPR-CAS9 PLANT GENOME EDITING ENHANCED BY BIOINFORMATICS PRECISION: A REVIEW

Nihar Garg\*, Amarshi Prajapati, Dharmendra Singh Rao Department of Botany, Bioinformatics and Climate Change Impacts Management, School of Sciences, Gujarat University, Ahmadabad, Gujarat, INDIA E-mail: niharg1627@gmail.com

#### Abstract

CRISPR/Cas9 requires expertise in tissue culture-based plant transformation as well as efficient genespecific single guide RNA (sgRNA) design, off-target effect prediction, and the use of vectors, promoters, Cas proteins, and terminators. Genome editing in eukaryotic systems using CRISPR-Cas9 has become popular for both basic and applied biological research. It has been noted that chromatin features and DNA methylation may contribute to notable variations in mutagenesis at particular loci with up to 250 bp for greater effectiveness. In order to develop new diagnostic tools for plant diseases, modern plant pathology uses bioinformatics techniques. Furthermore, new and effective methods for establishing long-lasting resistance are provided by crop genome editing technologies, specifically the CRISPR (clustered regulatory interspaced short palindromic repeats)/Cas9 (CRISPR-associated) system. Utilizing cutting-edge gene editing techniques to enhance plant health, such as CRISPR (clustered regularly interspaced short palindromic repeats)/Cas (CRISPR-associated nucleases), transcription activator-like effector nucleases (TALENs), mega nucleases (MNs), and zinc-finger nucleases (ZFNs). Cytokinins are widely used in agriculture for yield improvement and management due to their broad effects on plant growth, development, and physiology. The enzyme CKX gene encodes cytokinin oxidase/dehydrogenase (CKO/CKX), which catalyzes the irreversible breakdown of cytokinin. The CKX gene encodes enzyme cytokinin oxidase/dehydrogenase (CKO/CKX), which catalyzes the irreversible breakdown of cytokinin. New biotechnological tools (NBTs) like genome editing (GE), next-generation sequencing (NGS), markerassisted selection (MAS) and genetic transformation protocols can be employed in addition to conventional breeding techniques for crop improvement.

# A SYSTEMATIC REVIEW ON THE DEVELOPMENT OF NOVEL METHODOLOGY FOR DIABETES USING GENETICALLY ENGINEERED KIDNEY CELLS WITH THE APPLICATION OF BIOINFORMATICS

Khushal Purohit\*, Rohan A Pandey, Amarshi Prajapati Department of Botany, Bioinformatics and Climate Change Impact Management, School of Science, Gujarat University, Ahmedabad, Gujarat, INDIA E-mail: khushalp2407@gmail.com

#### Abstract

With more than 415 million cases worldwide, diabetes mellitus is becoming a major global health problem. High blood glucose levels are the cause of this chronic illness, which can have serious side effects. Although closed-loop management based on real glucose concentration is frequently absent from current medicines, their primary focus is on controlling insulin levels. By developing a human embryonic kidney 293 (HEK-293) cell line that secretes GLP-1 and insulin in response to blood sugar levels, this work closes this gap. Advanced bioinformatics tools like as TFsearch, KEGG Mapper, AutoDock Vina, CHARMM-GUI, AlignX, Phyre2, and Reactome are used to analyse data, predict protein structures and interactions, and create the modified cell line, A synthetic excitation transcription coupling system was used to pair a b-cell-mimetic cascade with human embryonic kidney cells using synthetic biology methods. This mechanism enables the cell line to directly react to the concentration of glucose employing calcium signalling, which in turn initiates the synthesis of GLP-1 and insulin. This study has a significant impact on the creation of closed-loop diabetes therapy systems. Because of its ability to detect and react to changes in blood sugar levels, the modified cell line may provide a more accurate and customized method of managing diabetes.

### SYNERGIZING BIOINFORMATICS IN COMPUTER-AIDED DRUG DISCOVERY: AN INCLUSIVE REVIEW

Drushya J. Barapatre\*, Nandan Dixit, Dharmendra Singh Rao. Department of Botany, Bioinformatics and Climate Change Impacts Management, School of Sciences, Gujarat University, Ahmadabad, Gujarat E-mail: drushya1204@gmail.com

#### Abstract

The integration of bioinformatics, a multidisciplinary field encompassing computational science and biology, has transformed CADD. Before CADD discovery it conventionally took 10-12 years to discover a drug which was time consuming and expensive. CADD does identification and optimization of drug candidates by illuminating the integration of genomic, proteomic, and systems biology data by using bioinformatics. Large volumes of biological data have been produced by the introduction of highthroughput technologies, offering knowledge of cellular functions, disease mechanisms, and drug-target interactions. The utilization of bioinformatics tools like Phyre and Phyre2, HHpred, CASTp, I-TASSER, Gromacs, Autodock, QSAR is essential for significant insights from the abundance of data. Advanced algorithms combined with proteomic and genomic databases make it easier to identify genes, pathways, and biomarkers linked to disease, which focuses on drug discovery. Bioinformatics in CADD allows selection of drug targets by predicting their draggability and assessing their relevance to specific diseases. The incorporation of bioinformatic analyses benefits molecular docking, virtual screening, and structurebased drug design, allowing researchers to prioritize potential lead compounds with greater precision. The importance of collaborative efforts among bioinformaticians, computational biologists, and medicinal chemists is emphasized, as are challenges such as data integration, standardization, and the need for improved predictive models. The studies discuss future directions, like the use of machine learning and artificial intelligence to handle complex biological data and make more accurate prediction. Finally, as technology advances, CADD is expected to incorporate virtual and augment technologies, the synergy between computational and biological sciences holds enormous promise for discovering new therapeutic avenues, addressing the challenges of developing effective and targeted drugs.

# A REVIEW ON "LEFLUNOMIDE" AS POTENT ARTIFICIAL ENZYME FOR THE TREATMENT OF RHEUMATOID ARTHRITIS

Rishabh K. Mishra\*, Rohan A. Pandey, Amarshi Prajapati Department of Botany, Bioinformatics and Climate Change Impact Management, School of Science, Gujarat University, Ahmedabad, Gujarat, INDIA E-mail: rishmishraisactivated@gmail.com

#### Abstract

An inflammatory autoimmune disease with an unclear etiology, Rheumatoid arthritis (RA) is typified by persistent inflammation of synovial tissues and blood-derived cell infiltration of the afflicted joints. This includes cells that exhibit symptoms of activation, such as memory T cells, dendritic cells, macrophages, and plasma cells. This typically results in the surrounding cartilage and underlying bone gradually eroding. It is thought that cytokine-induced damaging enzymes, especially those belonging to the matrix metalloproteinase family, are primarily responsible for joint degradation. This progressive disease has increased mortality, persistent impairment, diminished capacity to conduct daily activities, and chronic and acute morbidity. The Food and Drug Administration has recently approved leflunomide (Arava<sup>TM</sup>) for the treatment of rheumatoid arthritis (RA). Arava functions by inhibiting the inflammatory blood cells. It is an anti-inflammatory, Immunomodulatory drug as well as an artificial enzyme that acts by lessening illness severity and inflammation. Owing to the medication's ability to prevent structural joint degeneration, it has been categorized as a disease-modifying anti-rheumatic medication (DMARD). Leflunomide has a distinct mode of action and differs structurally from other medications now used to treat RA. Because of its immunomodulatory effect, it has proven to be protective in a number of animal models of autoimmunity and arthritis. This review is a summary of current in vivo and in vitro data, focusing primarily on the mechanism of action of leflunomide in Rheumatoid arthritis.

# A COMPREHENSIVE REVIEW OF THE APPLICATION OF METAGENOMICS TO HUMAN GUT MICROBIOME RESEARCH

Saara Lakum\*, Amarshi Prajapati, Rohan A. Pandey Department of Botany, Bioinformatics and Climate Change Impact Management, School of Science, Gujarat University, Ahmedabad, Gujarat, INDIA E-mail: saara.lakum248@gmail.com

#### Abstract

Human microbiota is a community of organisms that dwell and interact with body components which consists of trillions of bacteria that live in and on the body, is critical to sustaining health and impacting different physiological processes. There are important health consequences for humans from comprehending how the environment affects the gut microbiome's makeup and function. The intestinal microbiota, or gastrointestinal tract, is home to the most complex human microbial environment. Compared to the human genome, the intestinal microbiome, which is made up of many microbial populations, is thought to have a much greater genetic potential. The diversity and dysbiosis of the intestinal microbiome, as well as their connections to health and illness, can be studied using metagenomics. Additionally, functional metagenomics can detect interactions and co-evolution between the microbiota and host, as well as new functional genes, microbial pathways, genes for antibiotic resistance, and functional dysbiosis of the gut microbiome. Metabolomics is a huge addition to our understanding of the human gut microbiome.

### NOVEL HERBAL SOLUTIONS TO FIGHT ALZHEIMER'S DISEASE: A COMPREHENSIVE REVIEW

Tirtha R. Trivedi<sup>1\*</sup>, Dharmendra Singh F. Rao, Aafrinbanu M. Shaikh Department of Botany, Bioinformatics and Climate Change Impact Management, School of Science, Gujarat University, Ahmedabad, Gujarat, INDIA E-mail: tirthatrivedi22@gmail.com

#### Abstract

Alzheimer's disease (AD) is a deadly illness that primarily affects the elderly. It is typified by extracellular plaques in the hippocampal region that induce slow, progressive brain damage. In AD cells, aggregates of microtubule-binding proteins become twisted into tangles and are encased in plaques. A serious health concern is cognitive impairment, which is linked to age, stress, hypertension, and a number of neurodegenerative diseases. The most prevalent type of dementia and the primary cause of cognitive impairment is Alzheimer's disease. Alzheimer's disease therapy presents numerous therapeutic obstacles. The disease progresses unabated despite the pharmaceutical strategies currently in development. As safe substitutes for pharmaceutical treatments, herbal remedies and medicinal plants are becoming more and more popular as primary and supportive treatments for AD. Turmeric (Curcuma longa), Ashwagandha (Withania somnifera), bark of White Willow (Salix alba) and many more such herbs have antiinflammatory and anti-oxidant properties that may be beneficial in the treatment of Alzheimer's disease. When compared to pharmaceutical agents, medicinal plants are used to treat AD have lower levels of toxicity. The passage of herbal remedies through the blood-brain barrier presents an additional difficulty in reaching the brain, which is the target site of AD. Innovative alternative approaches to addressing the challenges of drug delivery across the blood-brain barrier are provided by nanomedicines. Nano-medicines have a variety of unique properties that allow them to deliver anti-AD drugs to particular regions in the brain. Nanomedicines possess the potential to lower dosage and frequency while also boosting patient compliance. This review focuses on novel delivery approaches for herbal medications used to treat Alzheimer's disease.

### **REVOLUTIONIZING BIOMARKER IDENTIFICATION WITH DEEP** LEARNING: A REVIEW

Taral Y. Patel, Sukanya Raval

Department of Botany, Bioinformatics and Climate Change Impacts Management, School of Science, Gujarat University, Ahmedabad, Gujarat, INDIA E-mail: taralpatel.y@gmail.com

#### Abstract

Biomarkers are the medical signs that mainly indicates the medical state of the particular person and it is measured in body to predict the incidence of the outcome or the disease, it is also useful in treatments, therapeutics procedure and even in unexpected environmental exposure like the chemicals or the nutrients. Bioinformatics emerges as crucial discipline in biomarker identification, providing computational tools for efficient analysis. Traditionally, the biomarker identification involves a range of laboratory techniques and enables the precise analysis of nucleic acid, protein and metabolites, offering insights into potential biomarker associated with health and disease. In-silico techniques have emerged as a powerful tools to analyze the large datasets by using advanced algorithms and statistical models and it can identify the potent biomarker in a cost effective and timely manner. Advancement in technology have pushed bioinformatics forward through the use of deep learning models. Whole slide images, are made which has shown promise in prediction of genetic biomarkers. The most often used deep learning methods are categorical classification and regression method. There is novel approach known as contrastively-clustered attentionbased multiple instance learning (CAMIL) a regression approach. These models predict the biomarker on the based of the WSI images. So, the deep learning for the identification of biomarker is rapidly evolving and the ongoing efforts in data sharing, collaborative research and methodological advancements are likely to contribute the research gaps in future.

# A HOLISTIC APPROACH THROUGH MULTIOMICS FOR UNVEILING THE INTRICACY OF BIOLOGICAL SYSTEMS: A REVIEW

Darshana Shashidhar Musini, Aafrinbanu M Shaikh, Rohan A. Pandey Department of Botany, Bioinformatics and Climate Change Impacts Management, School of Sciences, Gujarat University, Ahmedabad, Gujarat, INDIA E-mail: darshanamusini20@gmail.com

#### Abstract

The multiple levels of biology demand a more comprehensive and amalgamative solution to understand the interrelations of biomolecules and their functions. Multi-omics encompasses genomics, transcriptomics, epigenomics, proteomics and so forth. All the omics have interactions with one another, as a consequence providing an alternative to address any research topic. Discovering ways to improvise human health with understanding the molecular complexity multiomics approach can be followed. To comprehend the changes of a biologic system it is essential to study these processes as a whole. This is the point at which multiomics comes into work. This field includes all omics disciplines such as the genetic landscape, gene expression, the impact of epigenetic variations on proteome and quantification of protein through techniques like MS. In later stages it utilizes data analysis from various omics studies to comprehend an organism's natural and modified states. With elevated availability of integrative omics data from large datasets generated from high-throughput techniques several integration tools and methods can be understood. The multi-omics data repositories, visualization portals and further challenges can be considered. An overall understanding of the flow of information of underlying disease, host-pathogen interactions, complex non-communicable disease can be accomplished by this revolutionizing advancement.

# MULTI-TARGET QUANTITATIVE STRUCTURE ACTIVITY RELATIONSHIP IN DRUG DISCOVERY: A REVIEW

Muditha Dhananjana Bandara Rathnayake\*, Nandan Dixit Department of Botany, Bioinformatics and Climate Change Impacts Management, School of Science, Gujarat University, Ahmedabad, Gujarat, INDIA E-mail: dhananjanarathnayake123@gmail.com

#### Abstract

In the field of drug discovery, QSAR modeling is a computational approach to developing a mathematical model for determining the correlation between the chemical structure of the compound and its biological activities. The conventional approach is mainly based on targeting a single biological target, yet this method is challenged by the many complex interactions of targets in a biological system. Multi-target QSAR modeling is an advancement to conventional QSAR, considering it has the ability to predict multiple targets simultaneously. Multi-target QSAR models focus on different methodologies, data collection techniques, data preprocessing, feature selection, model development, model validation, hyperparameter tuning, and visualization techniques. A critique of QSAR-Co-X as the major open-source software tool and a general guide to other related repositories. Some linear and nonlinear models are analyzed to find out insights on the model's predictive performance based on different statistical parameters like root mean squared error (RMSE) or mean absolute error (MAE). The challenges in data collection, data preprocessing, complexity of the model and interpretability of results, overfitting, and generalization issues are addressed for a futuristic research approach. Multi-target QSAR is a successful predictive model that provides insights on drug-target interactions and a theoretical view on lead optimization in the drug discovery pipeline.

# **Places of Attraction**



Junagadh is famous for Girnar peaks with asia's longest ropeway and tourist attraction sites like Uperkot Fort, Ashoka's rock edicts, Mohabbat Maqbara, Darbar Hall Museum. Junagadh also have Sakkarbaug zoo with asiatic lions and rare animal and bird species.

Gir Sanctuary is home of the most endangered species of big cats - the Asiatic Lions. At Gir national park you can stay at luxurious resort with delicious food in home of lion. In jungle safari (Devaliya Park) you can encounter with lion as well as number of exquisite bird species.





Shree Somnath (Moon) is first among the twelve Aadi Jyotirlings of India and the place where lord Krishna took his last breath. Triveni Sangam of the three holy rivers Saraswati, Kapil and Hiran is a sacrosanct locale highly revered by Hindus as the Moksha Teerth.

Diu, union territory of India and coastal town was previously a Portuguese colony. At the bank of Arabian Sea it has attractive sites like Diu Fort, a 16th-century Portuguese citadel, lighthouse and canons, centuries-old Church, Naida caves and Nagao beach for water sports.





On Gujarat's Arabian sea coast, Madhavpur is a fantastic and sandy beach. Madhav Rao, a remarkable king, is the source of the name Madhavpur. According to the local's legend, Lord Krishna married Rukmini in the town of Madhavpur.

Porbandar is an important city which relates to famous people like Sudama, a friend of Lord Krishna and the birth place of father of nation Mahatma Gandhi. Porbandar is having chowpatty, the first planetarium of India and Sandipani-Sanskrit Pathshala of Pujya Rameshbhai Oza.





Dwarka is an ancient city for Hindu pilgrimage. The ancient Dwarkadhish temple is famous for carved entrance and a black-marble idol of Lord Krishna. The city was also called as 'Suvarna Dwarka' because it was all clad in gold, emeralds and jewels

Shivrajpur Beach received Blue Flag beach accreditation, is situated 12 kilometers from Dwarka (Gujarat) along the Dwarka-Okha Highway. It is the ideal place to spend the weekend. You might be fortunate enough to catch a glimpse of Dolphins or other lovely birds.



Department of Chemistry and Forensic Science | Department of Life Sciences Bhakta Kavi Narsinh Mehta University, Government Polytechnic Campus, University Road, Khadiya, Junagadh-362 263 (Gujarat) India.