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## TATA CHEMICALS LIMITED

The Department of Chemistry, SSSIHL Prashanti Nilayam Campus, conducted a two-day international conference titled **Integrated Chemie CONFERENCE on Frontiers in Applied Chemistry – From Molecules to Materials - ICCON 2016** from **12 to 13 February 2016**. The conference was sponsored by Tata Chemicals Limited.

The format included **seven sessions** spread over the two days of the conference. The report will highlight each session and include the speaker abstracts for each talk.

### Day 1: Fri, 12 February 2016

#### INAUGURAL SESSION

Welcome Address by **Dr. B Sivakumar**, Asst. Professor, Dept. of Chemistry, SSSIHL.

Inaugural Address by **Prof. G Nageswara Rao**, Head, Dept. of Chemistry, SSSIHL.

Keynote Address by **Prof. V Chandrashekar**, Director, National Institute of Science Education and Research (NISER), Bhubaneswar.

**Title:** **Lanthanide complexes: New Examples of Molecular Magnets**

**Abstract:** There has been a renaissance in the chemistry of lanthanide ion complexes in view of their applications involving photophysical properties, magnetism and catalysis. Both homometallic and heterometallic (3d/4f) lanthanide complexes are being increasingly studied for their magnetic properties in general and as single-molecule

magnets in particular. In this talk we will present some of our work on trinuclear 3d/4f complexes which exhibit SMM properties.

#### References

- » Das S, Bejoymohandas K S et al. Chem. Eur. J. 2015, 21, 6449-6464
- » Goura J, Brambleby J, Goddard P, Chandrasekhar V. Chem. Eur. J. 2015, 21, 4926-30

Vote of thanks and Summary presentation by **Dr. R Sai Sathish**, Asst. Professor, Dept. of Chemistry, SSSIHL.

#### SESSION 1: PLENARY PRESENTATIONS

Chairperson: **Prof. Chelli Janardhana**, Professor (Hon.), Dept. of Chemistry, SSSIHL.

Address by **Prof. G Jayaraman**, Senior Professor, School of Biosciences and Technology, VIT University, Tamil Nadu.

**Title:** **Halotolerant organisms: A Potential Resource for Novel Metabolites**

**Abstract:** The salt stress response of four representative halotolerant bacterial species (*Halomonas hydrothermalis* VITP9, *Bacillus aquimaris* VITP4, *Planococcus maritimus* VITP21 and *Virgibacillus dokdonensis* VITP14) isolated from a previously unexplored solar saltern in Kumta, along the Arabian Sea coast in Karnataka, India was analysed using comparative metabolomics approach. Chemometric analysis of <sup>1</sup>H NMR spectra revealed salt-dependent increase in the levels of metabolites, mainly from the aspartate and glutamate family, that are directed from the glycolytic pathway, pentose phosphate pathway and citric acid cycle. The composition of the metabolites was found to be different with respect to the species and the type of growth medium. 2D NMR data revealed accumulation of two rare diaminoacids, N $\epsilon$ -acetyl- $\alpha$ -lysine and N $\delta$ -acetylornithine (by VITP21 and VITP4 strains respectively) apart from other well-known compatible solutes such as ectoine, proline, glutamate and glycine betaine upon salt stress. Metabolite profiles of species capable of synthesizing N $\epsilon$ -acetyl- $\alpha$ -lysine and N $\delta$ -acetylornithine suggested their biosynthesis from lysine and ornithine using aspartate and glutamate as their precursors, respectively.





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Address by **Dr. Narendra Reddy**, Professor and Ramalingaswami Fellow, Center for Emerging Technologies, Jain University, Bangalore.

**Title: Biopolymeric Materials for a Sustainable and Greener Future: Pursuing a Common Bond**

**Abstract:** Green and sustainable materials are in great demand in almost all industries and commodity products. Increased awareness on the environmental impacts of using petroleum based raw materials, decreasing source of petroleum and stringent rules on the use of the non-biodegradable petroleum based products, particularly in the developed countries, are the major factors for the demand in green and sustainable products. Although natural polymer based materials have been developed as substitute for petroleum based products, the higher cost, limited availability and inferior properties limit the use of biopolymeric materials. Compared to conventional biopolymers, agricultural residues such as straws and husks and coproducts such as soil meals, feathers are abundantly available at low cost and have unique properties. Green and sustainable products can be developed using these agricultural residues. However, chemical and physical modifications are necessary to make products from agricultural residues cost and quality-wise competitive to synthetic polymer based products. We will present the potential and possible applications of bioproducts from agricultural residues. Role of chemistry in developing the products will be highlighted.

## SESSION 2: TECHNICAL PRESENTATIONS

Chairperson: **Dr. S Jagadeeswara Rao**, Associate Professor (Hon.), Dept. of Chemistry, SSSIHL.

Address by **Dr. Dinesh Jagadeesan**, Ramanujan Fellow & Assistant Professor (AcSIR), Physical and Materials Chemistry Division, CSIR-National Chemical Laboratory, Pune.

**Title: Hydrogenation of Inorganic Carbonates – A potential route to recycle carbon**

**Abstract:** Inorganic carbonates, which occur abundantly on earth, constitute an inexpensive natural source of carbon. Direct conversion of

inorganic carbonates into hydrocarbons is of considerable importance to maintain the carbon neutrality. Thermal decomposition of metal carbonates with the composition  $M_1M_2(CO_3)_2$  (where  $M_1$  is a transition metal and  $M_2$  is an alkaline metal) in  $H_2$  shows that the transition metal ions are reduced to form catalytically active species that can convert in situ generated  $CO_2$  to valuable hydrocarbons. The scope of this reaction as a potential technology for carbon capture and utilization will be discussed with some examples.

### References

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- » D Jagadeesan, M Eswaramoorthy and C N R Rao ChemSusChem, 2009, 2, 878
- » D Jagadeesan, Y Sundarayya, G Madras, C N R Rao RSC Adv, 2013, 3, 7224
- » V K Jain, D Jagadeesan, (unpublished results)

Address by **Dr. Ramanathan V**, Asst. Professor, School of Chemical and Biotechnology, Sastra University, Tamil Nadu.

**Title: Old pill under new probe: Science behind a Siddha herbo-metallic drug**

**Abstract:** In this talk I am going to present the recent findings on the science behind the making and medicinal action of one of the herb-metallic drug from the Siddha repertoire. Siddha is a traditional medicinal system that has been in practice from ancient times in South Asia. Currently it is widely followed in Tamil Nadu and Sri Lanka and few other places. It has many similarities to Ayurveda except the fact that all documentation in Siddha literature was done in Tamil. Among the several drug formulations, herbo-metallic formulations are one of the major formulations which are widely used for various ailments. Among them, in this talk, I will be concentrating on one iron oxide based drug formulation namely kaantachenduram which is prescribed for hemolytic and arthritic complications. I will be talking about its scientific validation of the preparatory process, characterization of the drug and its efficacy using modern scientific methods.

Address by **Dr. Vinayak Sinha**, Associate Professor, Indian Institute of Science Education and Research (IISER), Mohali.

**Title: Contribution of post-harvest agricultural paddy residue fires in the N.W. Indo-Gangetic Plain to ambient carcinogenic benzenoids, toxic isocyanic acid and carbon monoxide**



**Abstract:** In the North West Indo-Gangetic Plain (N.W.IGP), large scale post-harvest paddy residue fires occur every year during the months of October–November. This anthropogenic perturbation causes contamination of the atmospheric environment such as benzene and toxic VOCs such as isocyanic acid. These gases and carbon monoxide are known to be emitted from biomass fires along with acetonitrile. Yet no long-term in-situ measurements quantifying the impact of this activity have been carried out in the N.W. IGP. Using high quality continuous online in-situ measurements of these gases at a strategic downwind site over a three year period from 2012 to 2014, we demonstrate the strong impact of this anthropogenic emission activity on ambient concentrations of these gases. This study makes a case for urgent mitigation of post-harvest paddy residue fires as the unknown synergistic effect of multi-pollutant exposure due to emissions from this anthropogenic source may be posing grave health risks to the population of the N.W. IGP.

#### References

- » A B P Chandra, Vinayak Sinha, Contribution of post-harvest agricultural paddy residue fires in the N.W. Indo-Gangetic Plain to ambient carcinogenic benzenoids, toxic isocyanic acid and carbon monoxide, Environment International, Volume 88, March 2016, Pages 187-197, ISSN 0160-4120. <http://dx.doi.org/10.1016/j.envint.2015.12.025>

#### Summary presentation

### SESSION 3: ORAL PRESENTATIONS

Chairperson: **Prof. G Nageswara Rao**, Head, Dept. of Chemistry, SSSIHL

Address by **Dr. (Ms.) V Prathyusha**, Asst. Professor (Hon.), Dept. of Chemistry, SSSIHL.

#### Title: Unusual Bonding in Molecules Containing Planar Tetracoordinate Centers

**Abstract:** Several research groups have shown that planar arrangement for the tetrahedral carbon is possible for molecules stabilized by electronic and structural constraints. Similar to carbon, isoelectronic species such as B-, N+, Al-, Si and P+ also prefer tetrahedral coordination. High level QC calculations were carried out on skeletally

substituted derivatives of one of the hydrocarbons  $C_5H_4$ , where the planar tetracoordinate carbon at the center is being replaced with the above mentioned isoelectronic species. The nature of the stationary points for both the planar and the tetrahedral systems for the above mentioned species were characterized based on the frequency calculations carried out on their optimized geometries. Interestingly, both the planar and the tetrahedral phosphonium ions ( $C_4H_4P^+$ ) are found to be a minima on the PES and also consistent by both DFT and MP2 methods, where the tetrahedral isomer was found to be more stable than the planar isomer. A TS corresponding to the interconversion between the two stereoisomers was identified. *Ab initio* MD calculations indicate that  $C_4H_4Si$  does undergo rapid interconversion between two identical tetrahedral structures through the planar transition state in the fs timescale. However,  $C_5H_4$ ,  $C_4H_4P^+$  and  $C_4H_4Al^-$  undergo irreversible ring opening during the simulations. Effect of substituents on the kinetic stabilization of the planar and tetrahedral tetra coordinate phosphorous center has been studied in detail.

Address by **Dr. P Suresh Kumar**, Asst. Professor, School of Chemical and Biotechnology, Sastra University, Tamil Nadu.

#### Title: Ultrafast, back-to-back electrochemical fabrication and electroanalysis: Template deposited copper nanostructures for hydrogen peroxide sensor

**Abstract:** Nobel metal NPs are of great interest in catalytic and electrocatalytic applications<sup>1</sup>. Herein we present a facile electrodeposition of copper nanostructures on pencil graphite lead substrate using anionic, cationic and non-ionic surfactant templates<sup>2</sup>. Influence of templates on the morphology and electrochemical catalytic activities of these copper electrodeposits are demonstrated using physical and electrochemical characterisation methods. These electrodes are shown to be excellent electrocatalyst for the fast detection of hydrogen peroxide. A maximum sensitivity of 104  $\mu A/mM$ , LOD of 6.88  $\mu M$ , response time of <2 seconds and a linearity in wide range of concentration from 60  $\mu M$  to 10 mM are observed. Our methodology enables one to analyse the sample using a freshly prepared electrode within five minutes without any complicated procedure, thereby demonstrating one of the fastest and cost effective method for hydrogen peroxide analysis with high sensitivity and selectivity. Studies have demonstrated that common electroactive species such as glucose, dopamine, ascorbic acid and uric acid contribute negligible interference





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to the hydrogen peroxide analysis.

References

- » A Decan M R, et al. Nature Commun. 2014, 5, 1–8.
- » Abass N A A, et al. Phys.Chem.Chem.Phys. 2014, 16, 4892–4899.

Summary presentation

Day 2: Sat, 13 February 2016

SESSION 4: PLENARY PRESENTATIONS

Chairperson: **Prof. V Chandrashekar**, Director, National Institute of Science Education and Research (NISER), Bhubaneswar.

Address by **Dr. D B Ramchary**, Associate Professor, School of Chemistry, University of Hyderabad

**Title: Organocatalytic Reductive Alkylation Reaction: Scope and Applications**

**Abstract:** The discovery of new reaction called 'Organocatalytic Reductive Alkylation' and application of this reaction to the synthesis of agrochemicals and pharmaceuticals will be discussed. My talk on 'Organocatalytic Reductive Alkylation' will be covering the combinations of enamine-, iminium-, self-, auto-, acid-, base- or/and CuSO<sub>4</sub>/Cu-catalyzed one-pot cascade reactions to generate the highly functionalized molecules, which have shown pharmaceutical applications.

References

- » D B Ramachary, and Y V Reddy, Eur. J. Org. Chem, 2012, 865-887.
- » D B Ramachary and S Jain, Org. Biomol. Chem., 2011, 9, 1277-1300.
- » D B Ramachary and M Kishor, J. Org. Chem., 2007, 72, 5056-5068.

Address by **Dr. Nanduri Srinivas**, Associate Professor, Department of Medicinal & Process Chemistry, National Institute of Pharmaceutical Education and Research (NIPER), Hyderabad

**Title: Indian Pharma 2020: Way forward**

**Abstract:** The Indian Pharmaceutical Industry has witnessed enormous growth since Independence. From being the importer of all lifesaving drugs in the pre-independence era to the current position of to the world leader in generic pharmaceuticals production, supplying 20% of

affordable and quality pharmaceuticals to the developed and developing countries, the change has been phenomenal. With the enormous growth in the generic drug production, the Indian Pharmaceutical Industry has been making ambitious efforts to move from being generic players into innovation driven companies, contributing to new drug discovery. The presentation will outline the Salient features of the Indian Pharmaceutical Industry, opportunities, challenges and the way forward.

Summary presentation

SESSION 5: INDUSTRIAL PRESENTATIONS

Chairperson: **Prof. G Jayaraman**, Senior Professor, School of Biosciences and Technology, VIT University, Tamil Nadu.

Address by **Dr. Ramesh Sistla**, Lead Investigator, Head of CADD at Biocon BMS R&D Center (BBRC), Syngene International Ltd., Bangalore

**Title: Thermodynamic and Kinetic Aspects of Reactions in Drug Discovery**

**Abstract:** Thermodynamics and kinetics represent the 'whether' and 'how fast' of a reaction respectively. Hence the knowledge of these aspects can help us to design our reactions. In drug discovery, compounds are routinely tested in a variety of biological assays ranging from on target activity to metabolism and other off-target related safety assays. Of special significance is the metabolism of compounds, known as bio-transformation, the process in which covalent addition of a polar group occurs on the molecule. How much metabolism happens and how quickly represents the metabolic stability of compounds. The atom on which the addition of polar group happens is the metabolic soft spot. Computational studies can help in identification of metabolic soft spots in molecules as also estimate the thermodynamics and kinetic aspects related to the biotransformation. In this talk I will introduce and discuss the metabolism related aspects of small molecules and show through literature examples how computational calculations can predict the spots of metabolism as well as help understand the thermodynamic and kinetic aspects of metabolic transformations.

References

- » Sinha et.al. Chem. Res. Toxicol., 2014, 27 (12), pp 2052–2061.



Address by **Dr. Ravi K Ujjinamatada**, Group Leader-II, Dept. of Medicinal Chemistry, Aurigene Discovery Technologies Ltd., Bangalore.

**Title:** Discovery of RAR-Related Orphan Receptor (ROR) gamma inverse agonists for the treatment of autoimmune diseases

**Abstract:** The nuclear hormone receptor, RAR-Related Orphan Receptor (ROR) gamma controls the differentiation of Th17 cells that plays a role in a variety of autoimmune diseases including psoriasis, arthritis, lupus, multiple sclerosis, asthma and inflammatory bowel diseases. We have successfully designed and synthesized novel ROR gamma inverse agonists. Identified leads have showed excellent in vitro potency, good ADME properties and in vivo efficacy in multiple models including, asthma, psoriasis, experimental auto immune encephalomyelitis and collagen induced arthritis. Drug discovery process and a few interesting results of this invention will be presented.

Summary presentation

#### SESSION 6: TECHNICAL PRESENTATIONS

Chairperson: **Prof. G Jayaraman**, Senior Professor, School of Biosciences and Technology, VIT University, Tamil Nadu.

Address by **Dr. S Raghobama**, Chief Research Scientist, NMR Research Center, Indian Institute of Science, Bangalore

**Title:** 1D & 2D NMR Spectroscopy: Applications in Structure Biology

**Abstract:** NMR spectroscopy is a powerful tool to get information at molecular level in chemical and biological samples. Though NMR is least sensitive among various spectroscopic techniques, it has immense application potential in various scientific fields. Tremendous growth in methodological developments and sensitivity enhancement over the decades has boosted its utility factor.

Some of the important basic parameters in NMR, such as chemical shifts, spin-spin coupling, nuclear Overhauser effect, etc., have a direct correlation to biomolecular structure. Multi-dimensional homo - /

hetero nuclear experiments enhanced by polarization transfer technique provide a vast canvas of experiments to delineate chemical and biological structures. Current thrust area happens to be in solid state NMR and dynamic nuclear polarization (DNP). Yet another field which is catching up steadily using NMR is metabolomics which has a great promise in medical diagnosis.

The talk covers a broad outline of the above mentioned topics and attempts to show how NMR can be applied to derive structure information with some examples.

Address by **Mr. Subramanyam Santhanam**, Sr. Manager, Legal Affairs, IP Group at SABIC, Bangalore

**Title:** Intellectual Property – What, Why & How of it as a Business Enabler

**Abstract:** The talk would introduce Intellectual Property as a discipline covering some basics around the types of intellectual property and why it is required in the current age. It would be touching upon patents, copyrights, trademarks, trade secrets and establish a parallel between tangible and intangible properties. The manner in which intellectual property acts as a business enabler would be covered by citing a few case studies with special focus on the chemical industry. Some of key treaties/agreements in this domain like Patent Cooperation Treaty (PCT), Madrid Agreement, TRIPS Agreement and the nodal agencies dealing with IP policy like WIPO, USPTO, EPO & IPO would be briefly touched upon.

Address by **Dr. K Anil Kumar**, Principal Scientist & Head, Innovation Centre, Tata Chemicals

**Title:** Be clear, and the rest will follow

**Abstract:** The theme of his talk centered around the famous quote 'Think simple, the rest will follow'. He dwelled on three industrial cases that changed the outlook of the industry towards a problem. The first was the problem of fluoride removal from water to produce soda ash, in the Lake Magadi, Kenya. The principles of common ion effect, were used to remove the sodium fluoride in the water. The second case was that of agricultural pests in India. In order to eliminate the pests that bore the stem of the coffee tree, the company had developed a silica nanoparticles. The main feature of the particles was that the size of the particles was controlled such that the gut of the insect gets irritated upon ingestion.



At a time when the industry is focusing on costly and apparently complex solutions to problems, the speaker highlighted that the answer lies in simple basic chemistry. The third situation was that of providing a low oil absorbing batter to the Indian consumer. In conventional batter available, the particles are large and the interstitial spaces of the particles are occupied by the oil. If there was a way to mill the pulses such that small particle diameter was obtained, then the packing would be compact and the oil absorbed would be less. Another added benefit of the new developed batter was that it absorbed more water than usual, and this proved to be a boon for the consumer as it gave more bajjis for the same amount of batter used. All in all, the talk opened a new perspective of the listeners towards science. The cue lies in “simple living and high thinking”.

Summary presentation

#### SESSION 7: ORAL PRESENTATIONS

Chairperson: **Dr. Nanduri Srinivas**, Associate Professor, Department of Medicinal & Process Chemistry, National Institute of Pharmaceutical Education and Research (NIPER), Hyderabad.

Address by **Mr. K Nanaji**, SRF, Centre for Nano Materials, International Advanced Research Centre for Powder Metallurgy and New Materials (ARCI), Hyderabad

**Title: Porous Carbon materials for Energy Storage Applications: Lithium Ion Batteries and Supercapacitors**

**Abstract:** Lithium ion batteries (LIBs) and Electrochemical double layer capacitors or supercapacitors (SCs) are promising energy storage devices for powering electric and hybrid electric vehicles due to their high energy and power density characteristics respectively. In today's commercial rechargeable LIBs, graphite is the most commonly used anode material, owing to various properties. However, the storage capacity (372 mAh/g) and the rate performance of graphite are still need to be improved in order to achieve better performance. Therefore, many researches are focused on the development of new carbon materials that have fast kinetics of lithium ion insertion/de-insertion, high storage capacity, high cyclic and rate capability than graphite. In the commercial supercapacitors, activated carbon is the most commonly used electrode material due to its high surface area. Here, we synthesized different porous carbon materials such as ordered mesoporous carbons(OMCs), hierarchical porous carbon(HPC)

spheres as a high-rate anode material for lithium ion storage as well as an efficient carbon electrode for EDLCs. The HPCs are synthesized by a simple, low-cost, green, and scalable single step method using P123 surfactant and sucrose as template and carbon precursor, respectively. The OMCs are synthesized from a mesoporous silica template. When compared to commercial materials, the porous materials show better performance in terms of capacity, cyclic stability and rate capability. The high capacitance of EDLC for porous carbons is due to the quick formation of electrical double layer at porous electrode/ electrolyte interface, which accumulates more electrical charges on the electrode surface. The porous carbon helps in better electrolyte accessibility, ion transportation and electron conductivity. The unique structure of OMCs helps in ion accessibility in all the three directions. In the hierarchical porous carbon, the macropores act as electrolyte reservoirs which can minimize the diffusion distances of ions to the carbon spheres, and mesopores and micropores provide high surface area for lithium storage capacity and electrolyte ion adsorption. Porous carbon applications in LIBs & SCs.

#### References

- » J M Tarascon, M Armand, Nature, 2001, 41, 359.
- » Y Chen, Z Lu, L Zhou, Y W Mai, H Huan, Energy Environ. Sci., 2012, 5, 7898.

Address by **Mr. Bishnu Prasad Joshi**, Alumnus, Dept. of Chemistry, SSSIHL.

**Title: Synthesis, characterization and rapid schizontocidal activities of Dibenzylidenecyclohexanone derivatives as new antiplasmodial Pharmacophores exhibiting strong synergistic effects with artemisinin against chloroquine resistant *Plasmodium falciparum***

**Abstract:** Dibenzylidenecyclohexanone (DBC) derivatives were synthesized, characterized and screened for their in vitro antiplasmodial activities. SAR studies showed antiplasmodial activity in the order of 3-NO<sub>2</sub> (Ic) > 3-chloro (Ie) > 4-chloro (If) > 2-chloro (Id). 2,6-Bis(3-nitro-benzylidene) cyclohexanone (Ic) which exhibited the highest antiplasmodial activity (IC<sub>50</sub>: 0.95 μM) against CQ sensitive Pf3D7, and resistant PfDd2, (IC<sub>50</sub>: 1 μM) and PfINDO (IC<sub>50</sub>: 1.1 μM) strains of *P. falciparum* was further explored for its drug like features. Combination studies showed that Ic exhibits strong and moderate synergistic effects with artemisinin (ΣFIC<sub>50</sub>: 0.34 to 0.57) and chloroquine (ΣFIC<sub>50</sub>: 0.61 to 0.90) respectively. Drug exposure followed by drug withdrawal based



stage specific kill kinetic studies showed that Ic is shizontocidal within 3 hrs while the earliest killing actions against Trophozoites and Rings were seen at >3 and >6 hrs respectively. The drugability of Ic appears high since it shows high compliance with Lipinski rule of 5 and exhibits high selectivity index (105.3) against HeLa cell line. This indicates that Dibenzylidenecyclohexanones could serve as structural templates for lead optimization of compounds for further anti-malarial drug discovery programs.

#### References

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- » Smilkstein M, Sriwilaijaro N, Kelly J X, Wilairat P, Riscoe M, Simple and inexpensive fluorescence-based technique for highthroughput antimalarial drug screening. Antimicrob. Agents Chemother. 2004, 48, 1803–1806

#### Valedictory function

Vote of thanks and Conference Summary by **Dr. A Sunil**, Research Faculty, Dept. of Chemistry, SSSIHL.

The conference concluded with *Mangala Arati* to Bhagawan Baba and a photo session.

#### POSTER SESSIONS

During both the days of the conference, at tea time, there were a few poster sessions that took place.

The visually pleasing presentations highlighted research information and academic focus of ten individuals at the conference.

The three winners of the poster presentation were:

- » **Sri Dhyanesh Vernekar**, Doctoral Research Scholar, Physical and Materials Chemistry Division, CSIR-National Chemical Laboratory, Pune.
- » **Sri Tej Kiran, Student**, II M.Sc. in Chemistry, SSSIHL
- » **Sri Sai Giridhar Sarma Kandanur**, Doctoral Research Scholar, Dept. of Chemistry, SSSIHL





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Department of CHEMISTRY

Integrated Chemie CONference  
on Frontiers in Applied Chemistry – From Molecules to Materials

12-13 FEBRUARY 2016 @ PRASANTHI NILAYAM CAMPUS

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