

**NATIONAL SEMINAR ON
RECENT TRENDS IN ADVANCED
CHEMISTRY RESEARCH (RTACR - 2017)**

**(SPONSORED BY DST(SERB)& KSCSTE)
THURSDAY 25th AND FRIDAY 26th MAY 2017**



Organized By

**PG & RESEARCH DEPARTMENT OF CHEMISTRY
SREE NARAYANA COLLEGE, KOLLAM**

Affiliated to University of Kerala

(Re accredited by NAAC with 'A' grade)



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Welcome

Dear Participant,

On behalf of the organizing committee, it gives us great pleasure to extend a warm and hearty welcome to the participants of RTACR-2017.

Over the years, Chemistry has made major studies in many different disciplines. The influence of chemistry could be witnessed across disciplines such as Physics, Material science and Biology, in addition to others. It was therefore felt by the organizing committee to organize sessions based on different themes viz, Nano science, Photoscience, Computer aided drug design & Medicinal Chemistry and Material science, wherein chemistry has made major impact over the years. We do hope that this would be a helping hand for the researchers for further inclusive growth with interdisciplinary research.

We have arranged inaugural session, and invited lectures in different themes mentioned above. The lectures by the young researchers and poster sessions will also be held in the seminar hall of the college.

We wish you a professionally rewarding and enjoyable RTACR-2017 seminar.

Sincerely yours,

Dr. Ambili Raj D B (Convenor)

Dr. S. V. Manoj (Joint-Convenor)

T. R. Sarunkumar (Joint-Convenor)

PREFACE

The National Seminar on 'Recent Trends in Advanced Chemistry research-2017' (RTACR-2017) is being organized by The PG & Research Department of Chemistry, Sree Narayana College, Kollam on 25th & 26th May 2017 at S N College, Kollam. The RTACR-2017 seminar aims to focus on the current status and the future projections of research in various frontier areas in Chemistry. The organization of the seminar is based on the outstanding and significant research carried out by scientists from various parts of India. The Poster and Oral presentation sessions give ample opportunities to the young minds to interact with others and to benefit from exchange of ideas for the betterment of their research activity.

We thank the National Advisory Committee members of RTACR for their valuable suggestions in organizing the seminar. We also thank the sponsors of the symposium, SERB, Department of Science & Technology, Govt. of India and Kerala State Council for Science, Technology & Environment (KSCSTE), Govt. of Kerala for providing financial Support. On behalf of all the organizing committee members, it gives me great pleasure to wish all the participants an eventful and academically successful RTACR-2017 Seminar.

Dr. Ambili Raj D B

Covenor, RTACR-2017

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Contents

Surface morphology and spectral studies of CdS QDs encapsulated metal-organic frame works M.S. <u>Sreevidya</u> and A. Asif	2
Pharmacophore modeling studies on Indenopyrazole derivatives as Cyclin Dependent Kinase 4 Inhibitors <u>Divya. V</u> ¹ , V. L Pushpa* ² , Sunitha.V.R ¹ , K.B. Manoj	3
Oxovanadium(IV) Schiff base complex : Synthesis, spectral investigations and catalytic activity in hydroxylation of phenol. V. Arun and K. K. M. Yusuff	4
Highly Efficient Photoluminescence from 1-(2-Naphthoyl)-3,3,3-trifluoroacetate Complex of Eu ³⁺ with Bidentate Phosphine Oxide D. B. Ambili Raj , T. R. Sarunkumar , S. V.Manoj, and V. S. Vishnu	5
Magnetic Aromaticity of Benzene And Naphthalene Radicals: An Incisive Theoretical Study Using NICS Formalism Liz Francis, Archana Joseph, Sanjuna P Sunil, Renjith Thomas	6
A Theoretical Study on the effect of Magnetic Aromaticity on Orienting Effects in Aromatic Electrophilic Substitution Reactions Archana Joseph, Sanjuna P Sunil, Liz Francis, Renjith Thomas	7
Chemosensitization As A Strategy To Overcome Chemoresistance And Side Effects Of Docetaxel: An <i>In vitro</i> Study B S Vinod, Haritha H Nair, V Vinod , A Shabna, S Shabna And Ruby John Anto	8
Synthesis and characterization of Ethylenediammine-N,N,N',N'-tetrakis-4-methyl-benzoic acid Dr. Shyni Raphael M	9
Ideological Debate on Environmental Justice in India Abhilash.T	10
Recent Trends in Developing Highly Active Heterogeneous Photocatalysts Arathi. L, Nishana. N, Shukla. S, Kimberly A. Gray, Anas. S	12
Effect Of Curcumin On Metal Ions S R Arunima and C L Asha	15
Optimization on Preparation Conditions of Calcium-Crosslinked Alginate Nanoparticle (ALG) as Potential Matrix Material for Theophylline Sustained-Release and its Evaluation of Release Kinetics DeepaThomas, M.S Latha, K. Kurien Thomas	19
Influence Of Citric Acid As An Inhibitor On The Growth Of Kidney Stone (CaOx) Crystals Fathima R, Rejeena I, A Mujeeb, Ajeena R	23

A Comparative Study In The Structural, Surface Morphological And Optical Band Gaps Of Zinc Magnesium Oxide And Zinc Manganese Oxide Nanocomposites C R Indulal, R Biju, Deepak N and R Raveendran	26
Photocatalytic Activities of Polyaniline Based ZnO-NiO Nanocomposite Baiju V, Dedhila Devadathan, Raveendran R	30
Synthesis, Characterization and application of NiO/ZnO Heterostructured Photocatalyst Dedhila Devadathan, Baiju V, Raveendran R	34
Synthesis, Spectral studies and Antimicrobial studies of Co(II), Cu(II), Zn(II) Complexes of 2-(4-methoxyphenyl)benzothiazole Sarau Devi.A and Reena Ravindran	39
Vibrational analysis on solid state synthesized MV_2O_6 (M=Ba,Ca and Zn) ceramics using FT-Raman spectroscopy Hridya Rajan, Satheesh R	43
An Approach To Personalised Drug Design For Asthma Through Interleukin-4 As Target Bharath chandran, Sruthy.S .B, Dr. V.L. Pushpa, Dr. K. B. Manoj, Sarithamol. S, Sunitha. V. R, Induja P	46
Electrochemical Deposition Of Palladium: A Kinetic Study Renjini S, Pavitha P A, Anithakumry V	49
Synthesis Of Superparamagnetic Iron Oxide Nanoparticles And Its Functionilization Using A Chemotherapeutic Drug M R Anantharaman, S V Manoj and Smitha Sasidharan	52
Optical Studies of Iodine Doped Polyaniline synthesized via Green Method Smitha T.R* , Thushara Bhadrn, Vaishali Sankher and Prema K.H.	56
Synthesis And Characterization And Biocidal Activity Of Schiff's Base Transition Metal Complexes Derived From Salicylaldehyde S. Nidhila, M. Hareesh & R. Reshma	62
A Series of Calix[4]arene Peptoids: An Ugi pathway Sreeja Thulasi* and R. Luxmi Varma	65
Sugarcane Bagasse Ash: A Renewable Source Of Silica S. Chippymol, Dr. S Suma, Dr. Divya Dinesh, S K Aswathy	70
Preparation of Polyaniline-Ceria Nano-Hybrid Composite Deepa J.P., Abhilash S., Arija, Sandhya	73
Advanced polyelectrolyte modified biopolymer membranes for environmental applications	

P. Nikhil Chandra ^a , Charuvila T. Aravindakumar, Usha K.	79
2-D Qsar Studies On Janus Kinase 1 Inhibitors Against Asthma Arya Rajan P, Meenu S S, V.L.Pushpa, K B. Manoj, Sarithamol S, Divya V	83
2d-Qsar Study On A Series Of Cannabinoid Receptor Agonists For Asthma Sarath M R, Jeena J S, Dr. V L Pushpa, Dr. K B Manoj, Sarithamol S, Suchitra Surendran, Induja.P	86
Computational Studies On Phytochemicals Against Asthma Sooraj sabu, Arunkumar A, Pushpa V L, K B Manoj, Sarithamol.S, Induja P, Sunitha V R	90
Synthesis Of Biogenic Silica Nano Particles Priya S., Anagha P. J., S. Suma, Divya Dinesh	97
Probing Protein-Small Molecule Interaction S. Sreedhanya, Reshma Rajan, U. K. Aravind and C. T. Aravindakumar	101
Synthesis And Structural Studies Of Ni (Ii) Complex Of N, N, O-Donor Semicarbazone Layana. S. R, M. R, Sudarsanakumar	105
Physicochemical and Electrochemical Performance of Ti Based Electrocatalysts in Hydrogen Evolution Reactions: An Overview Sarika S and Rijith S	108
Graphene Based Adsorbents for the Removal of Thorium(IV) from Aqueous Media Rijith.S, Suma S, Karthika Lal, Silpa Seelan	109

2-D Qsar Studies On Janus Kinase 1 Inhibitors Against Asthma
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Abstract

Asthma is a chronic lung condition with ongoing airway inflammation resulting in breathing problems. There are lots of inhaled corticosteroids, bronchochodilators, and leukopterine modifiers to treat asthma. But their consumption can lead to vomiting weakness, boneless, slowing of growth etc. So the present studies focuses on 2D QSAR studies on biological assay taken from Brubeck et al. and its anti-asthmatic properties were studied. Statistically, regression models were build and squared correlation coefficient ($r^2=0.6522$), adjusted square correlation coefficient ($r_{adj}^2=0.5923$) of training set, cross validated correlation coefficient of test set, ($Q^2_{test}=0.602542$). Studies showed that positive ionization (POS), hydrogen bond donor sites (HBD), topological descriptors have a great influence on the biological activity of the compounds. The developed QSAR model was further checked for its prediction ability using external test set compounds within the same bioassay. It can be suggested to analyze and enhance anti-asthmatic activity of new set of molecules for drug synthesis.

Introduction

Asthma is a chronic lung disease characterized by variable obstruction, airway hyper responsiveness (AHR) and airway inflammation and remodeling. Histological studies show that Cytokines like IL-4 and IL-12 binds to its receptor sites to activate JAK protein which activates STAT (Signal transducer and Activator of Transducer) through tyrosine phosphorylation. This allows stat protein to dimerise and move to nucleus to mediate change in gene expression by binding specific DNA elements. As IL-4-JAK1-STAT6 signaling is responsible for asthma over-expression, the investigation will focus on finding JAK1 inhibitors against asthma. (1) There are many treatments for asthma such as corticosteroid inhalers, leukopterine and bronchochodilators. But they do have side-effects such as vomiting, restless, nausea, growth retardation etc. So an alternative method is required as JAK1 inhibitors against asthma.

QSAR (Quantitative Structure-Activity Relationship) approach helps to correlate biological activity of molecules with properties in terms of descriptors. This determine the activities of untested compounds quantitatively. A set of 95 molecules were taken that showed nanomolar inhibition towards JAK 1. QSAR models were created and statistical studies were done using the software Build QSAR. Superior set (training set) molecules were then used to generate candidate set (test set). (2 & 3)