

**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)



Editorial Board

Dr. K B Manoj, **Managing Editor**
Principal, Sree Narayana College, Kollam

Dr. Ambili Raj D B **Chief Editor**
Dr. V. L. Pushpa **Associate Editor**
Dr. S. V. Manoj **Associate Editor**
Mr. T. R. Sarunkumar **Associate Editor**

Members

Dr. K. Serji
Dr. Suma S
Dr. Smitha Sasidharan
Dr. S. Rijith
Ms. P. S. Asa
Ms. Reshma R
Mr. K. R. Jiju
Mr. Abhilash S.
Dr. Ambili S.
Dr. Vinod B. S.
Dr. Divya Dinesh

Printed & Published by : Dr. K B Manoj, Principal, Sree Narayana College, Kollam
ISBN 978-93-5268-873-9

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

Committees

Organizing Committee

Patron:	Sri. Vellapally Natesan
Chairman:	Dr. K. B. Manoj
Secretary:	Dr. V. L. Pushpa
Convenor:	Dr. Ambili Raj D B
Co-Convenor:	Dr. S. V. Manoj
Co-Convenor:	Sri. T. R. Sarunkumar

Members

Dr. K. Serji
Dr. Suma S
Dr. Smitha Sasidharan
Dr. S. Rijith
Ms. P. S. Asa
Ms. Reshma R
Mr. K. R. Jiju
Mr. Abhilash S.
Dr. Ambili S.
Dr. Vinod B. S.
Dr. Divya Dinesh

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

Computational Studies On Phytochemicals Against Asthma
Sooraj sabu¹, Arunkumar A², Pushpa V L^{*3}, K B Manoj³, sarithamol.s³,Induja P¹,Sunitha V R⁴

¹Department of Chemistry, S N College, Varkala ,²Department of Chemistry, S N College, Chengannur , ³Department of Chemistry, S N College, Kollam, ⁴ Department of Chemistry, MSM College, Kayamkulam.

drvlpushpa@gmail.com

ABSTRACT

Asthma is an anti-inflammatory lung disorder and no medicine is there to cure the condition effectively. Existing treatment are lifelong terms. So alternatives are suggested from plant world. 99 anti inflammatory phytochemicals were taken from Dukes Phytochemical Data Base and they were subjected to docking studies with JAK family proteins. Among these phytochemicals, Quercetin, Ellagic acid, Cynidin, Piperin are identified as the best candidates having wonderful docking scores (-7.27,-6.82,-6.83, -6.29 KJ/mol res.)and inhibition constant values are (5.53, 10.02, 9.87, 24.71 μ M res.) The docking score of the crystal ligand with the targets are, JAK 1(-5.3 KJ/mol), JAK 2(-6.04 KJ/mol), JAK 3(-6.61 KJ/mol) and TYK 2(-5.32 KJ/mol). A genomic study was also carried out on JAK1 gene. From this 11 deleterious SNPs are identified. Protein characterisation was done on JAK 1 proteins and 3EYG was selected as the best protein for molecular modelling studies. Through metagenomic study, effect of the microbes *Nocardia brevicatena* NBRC 12119and *Sanguibacteroides justesenii* strain OUH 308042 contig12 on JAK 1 gene is identified. By environmental analysis, the effects of chemicals such as [Methylprednisolone](#), [Acetaminophen](#) etc on the gene were detected. EDR analysis was done on the phytochemicals and Quercetin and hence got EDR value very close to the EDR of the drug Budesonide. The present study is concluded by pointing out the potency of phytochemicals, quercetin, ellagic acid and cyanidin as better lead for asthma.

INTRODUCTION

Asthma is a chronic inflammatory disorder that is managed with inhaled controller and reliever drugs. The existing anti asthmatic drugs have many side effects. It includes mood changes, forgetfulness, hair loss, easy bruising, a tendency toward high blood pressure and diabetes, thinning of the bones (osteoporosis), suppression of the adrenal glands, muscle weakness, weight gain, cataracts, and glaucoma. Here, a novel stratified approach for the treatment is reviewed, based upon identification of causal pathways, which focus on biologics. A systematic search of the literature revealed that asthma is associated with ***IL4JAK-STAT PATHWAY***. The present study focused on IL4-Jak-STAT signalling pathway and aimed to find out the essential features of a potential JAK inhibitor there by blocking the corresponding signalling system to reduce asthma. The Janus kinase (JAK) family, consisting of Jak1, Jak2, Jak3 and Tyk2, has gathered particular attention since JAK are essential for the signalling pathways of various cytokines. Through the present study, all the anti inflammatory phytochemicals available from literature has been studied using molecular docking with the