

**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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Quantitative Structure Activity Studies on the Bioassay of JAK1 for Asthma

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ABSTRACT

A series of Cycloalkylnitrile pyrazole carboxamides as Janus kinases inhibitors based new heterocyclic have collected from the United States Patent (10) Brubaker et. Al. All the compounds listed have potent antiasthmatic activity. To explore the potency of these compounds, quantitative structure activity relationship study was carried out. Statistically significant ($r^2 = 0.6099$) and predictive ($Q^2 = 0.5207$) QSAR model was developed. It is evident from the QSAR study that the inhibitory property of the compounds was highly correlated with molecular properties driven by topological indices. Molecular solubility and shadow descriptors, influence the biological activity significantly. Positive contribution of molecular shadow descriptors suggests that molecules with bulkier substituent are more likely to enhance anti-asthmatic activity. Since the model developed is found to be statistically significant and predictive, they can be applied for predicting anti-asthmatic activity of new molecules prior to synthesis.

INTRODUCTION

Asthma is a common long term inflammatory disease which affects the airways of the lungs. It is characterized by the variable and recurring symptoms, reversible airflow obstruction, and bronchospasm. Symptoms include episodes of wheezing, coughing, chest tightness and shortness of breath. Asthma is thought to be caused by a combination of genetic and environmental factors. Environmental factors include exposure to air pollutants and allergens. Diagnosis is usually based on the pattern of symptoms, response to therapy over time, and spirometry. There is no permanent cure for asthma. Symptoms can be prevented by avoiding triggers, such as allergens and irritants or by inhaling corticosteroids. Side effects created by the treatments urged the research world to think of alternatives in the field of medications. The present study is aimed at IL4-JAK-STAT signaling pathway as potential target for the concerned analyses. Quantitative structure activity relationship (QSAR) is one of the most widely used tools to design new candidates for several therapeutic areas. It provides useful insights into the structural features which are responsible for the biological activity and help to generate a mathematical model which can predict activity of new molecules. Present work focused on the structure activity studies on JAK1 inhibitors for giving better contributions in the field of drug designing for asthma.

EXPERIMENTAL

Data Set In the present study molecules were selected from United States Patent Brubaker et. al. One hundred and seventeen compounds were divided into training and test set, in the ratio