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PROCEEDINGS

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

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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 oppurtunities 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 fortheir 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 he 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

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Contents

Computational Studies On Phytochemicals Against Asthma

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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 µM 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

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