

2<sup>nd</sup> International Conference on  
**PHARMACEUTICAL CHEMISTRY AND DRUG DISCOVERY**  
June 12-13, 2019 | Bangkok, Thailand

PHARMA CHEM CONGRESS 2019



**SCIENTIFIC TRACKS & ABSTRACTS**  
**DAY 1**

# DAY 1 SESSIONS

## JUNE 12, 2019

### Pharmaceutical Chemistry

#### SESSION CHAIR

Jose-Luis Diaz-Ortega  
National Institute of Public Health, Mexico

#### SESSION INTRODUCTION

**Title:** Design, synthesis, pharmacological screening, molecular docking and toxicity studies on 7-(2-(benzo[d]thiazol-2-ylamino) ethoxy)-4-methyl-2Hchromen-2-one derivatives for atypical antipsychotic activity  
**Ashish A Gawai**, Anuradha College of Pharmacy, India

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Ashish A Gawai, J Pharm Chem Chem Sci 2019, Volume 3

## DESIGN, SYNTHESIS, PHARMACOLOGICAL SCREENING, MOLECULAR DOCKING AND TOXICITY STUDIES ON 7-(2-(BENZO[D]THIAZOL-2-YLAMINO) ETHOXY)-4-METHYL-2H-CHROMEN-2-ONE DERIVATIVES FOR ATYPICAL ANTIPSYCHOTIC ACTIVITY

**Ashish A Gawai**

Anuradha College of Pharmacy, India

Typical antipsychotics are used to treat a mental, baffling, severe disorder called Schizophrenia. The present study focuses on design and synthesis of some novel derivatives. The novel series 7-(2-(benzo[d]thiazol-2-yl-amino)ethoxy)-4-methyl-2H-chromen-2-one (4a-4k) was designed and synthesized by refluxing 2-amino benzothiazole substituted derivatives (3a-3k) with 7-(2-chloroethoxy)-4-methyl-2H-chromen-2-one(2) in dry pyridine. All the synthesized compounds were screened and evaluated for their dopamine D2 and serotonin 5HT2 antagonistic activity as a measure of typical antipsychotic property. Compounds 4b, 4c, 4e, 4g and 4i have shown good preliminary pharmacological activity. Some of the better activity compounds were selected for determination of acute toxicity (LD50) studies by OECD guidelines and also for effective dose (ED50) determination by probit log scale method. The therapeutic index (TI) of the selected compounds was determined for selection of safer and better compounds. These synthesized derivatives were screened by molecular docking method. The compounds were sketched using ChemBioDraw Ultra 12 and subjected for all possible conformation of compounds interacting with receptors. Molecular docking was performed with the Glide 7.6, Maestro 11.3 of Schrodinger 2017. PDB for Dopamine receptor 6CM4 and for serotonin 5TUD were obtained from Brookhaven Protein database. The ligand-protein hydrogen bond network was obtained and total energy was minimized by employing OPLS 2005 force field. The docking poses were ranked according to GlideScore. From all above data results, compounds with electron withdrawing substitution like 4e and 4b has shown better atypical antipsychotic profile.

## BIOGRAPHY

Ashish A Gawai is an Associate Professor at Department of Pharmaceutical Chemistry at Anuradha College of Pharmacy, India. He had completed his Master of Pharmacy in Pharmaceutical Chemistry from Bharti Vidyapeeth University, Poona College of Pharmacy, India and PhD in Pharmaceutical Sciences at Department of Pharmaceutical Sciences, Dibrugarh University, India. He has 12 years of teaching, 1.5 years of industrial experience and having more than 30 research papers and 50 research publications. He has also crashed Maharashtra Public Service Commission and Union Public Service Commission examination for Pharmacy post. He has attended to the invited conference at South Korea as well as several in India also. He has one published book entitled "A TEXTBOOK OF MEDICINAL CHEMISTRY" in his credit also. He is a potential reviewer for prestigious research journals like *Bentham Science*, *Indian Journal of Pharmaceutical Sciences* and many more. 24 students were completed Post-Graduation under his guidance. His research area is drug synthesis, drug design (Molecular modeling and docking study), toxicity studies and quality assurance.

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**SCIENTIFIC TRACKS & ABSTRACTS**  
**DAY 2**

# DAY 2 SESSIONS

## JUNE 13, 2019

### Pharmaceutical Chemistry

#### SESSION CHAIR

**Cho Min Naing**  
International Medical University, Malaysia

#### SESSION INTRODUCTION

- Title:** [The hypertension risk of iron brakes with release of particulate matter](#)  
**William J Rowe**, University of Toledo, USA
- Title:** [Regulatory approval of new drug delivery systems: Bridging the gaps](#)  
**Ripal Gharia**, Cliantha Research Ltd., India

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William J Rowe, J Pharm Chem Chem Sci 2019, Volume 3

## THE HYPERTENSION RISK OF IRON BRAKES WITH RELEASE OF PARTICULATE MATTER

**William J Rowe**

University of Toledo, USA

Of 12 moon walkers, James Irwin on day after return from Apollo 15 mission, showed extraordinary bi-cycle(B) stress test(ST) hypertension (275/125mmHg) after three minutes exercise, supervising >5000 maximum treadmill ST, author never witnessed ST blood pressure approaching this level. Symptom limited maximum B stress test showed "cyanotic fingernails", possibly venous blood trapped peripherally, supporting author's "Apollo 15 Space Syndrome", postulating that severe fingertip pain during space walks, triggered by plasma fluid, trapped distally; mechanism could be related to endothelial dysfunction, providing "Silent ischemia" warning. Neil Armstrong returned to Earth with severe diastolic hypertension (160/135 mmHg), consistent with ischemic left ventricular dysfunction, 50mm increase in comparison with resting BP 110/85 mmHg. With inhalation of lunar dust, brought into habitat on space suit with high lunar iron (I) this dust inhalation, along with reduced(R) space flight transferrin, R antioxidant, calcium(Ca) blocker-magnesium, conducive to severe oxidative stress, Ca overload with potential endothelial injuries. Using moon walker studies as example, author's recent editorials shows that iron dust, released from brakes, with over 90% of brakes made of iron, is a major hypertension factor and may also contribute to myocardial infarctions.

## BIOGRAPHY

William J Rowe is a board certified specialist in Internal Medicine at Fellow British Interplanetary Society (FBIS), Fellow American College of Nutrition, Retired Fellow Royal Society of Medicine (FACN). He received his MD at the University of Cincinnati and was in private practice in Toledo, Ohio for 34 years. During that time he supervised over 5000 symptom-limited maximum hospital-based treadmill stress tests. He studied three world class extraordinary endurance athletes and published their exercise-related magnesium deficiencies. This triggered a 20 year pursuit of the cardiovascular complications of space flight. He has published in LANCET that extraordinary, unremitting endurance exercise can injure a perfectly normal heart. Of only four space syndromes, he has published two: "The Apollo 15 Space Syndrome" and "Neil Armstrong Syndrome."

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Note:

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Ripal Gharia, J Pharm Chem Chem Sci 2019, Volume 3

## REGULATORY APPROVAL OF NEW DRUG DELIVERY SYSTEMS: BRIDGING THE GAPS

**Ripal Gharia**

Cliantha Research Ltd., India

Bringing a new drug through discovery, clinical testing, development and regulatory approval is currently estimated to take a decade and cost well over \$120 million. Scientists are working on different aspects to reduce this cost. New Drug Delivery System (NDDS) refers to the formulations, systems and technologies for transporting a pharmaceutical compound in the body as it is needed to safely achieve its desired therapeutic effects. NDDS technologies usually combine already approved drugs with different delivery system for either same or different indication and/or route of administration. Regulatory approval process requires less preclinical and clinical studies compared to NCE, but more than generics. NDDS can pose challenges regarding their classification for authorization by regulatory agencies, particularly with respect to nanomedicine and nanotechnology. There are currently no specific requirements from the regulatory agencies (FDA and EMA) for the preclinical and clinical testing of nanoparticle based drug delivery systems and only reflection papers providing guidelines on the pharmaceutical development of a specific type of nanoparticle based drug delivery systems have been published and to date the evaluation process follows a similar path as for small-molecule drugs. The development of a new drug starts with preclinical testing followed by the submission of an Investigational New Drug (IND) application in order to initiate the clinical trials. Intended therapeutic benefits needs to be taken into account for designing preclinical and clinical studies. Application of quality by design concepts early in the development will help the developer to build quality in and will ultimately improve clinical translation.

## BIOGRAPHY

Ripal Gharia currently working as Assistant General Manager at Cliantha Research Ltd., she has about 12+ years of working experience in clinical research. She is working as safety expert, medical monitor and medical writer mainly in therapeutic areas of oncology, cardiology, dermatology, ophthalmology, urology, pain medicine, obstetrics and gynecology and respiratory for various regulatory submissions such as FDA, EMA and DCGI. She was also conducted training programs for project teams located in India and USA. She has a close rapport with KOLs and subject experts in various therapeutic areas. She is a part of more than 70+ studies in different phases of drug development. She is interested in the areas of medical and regulatory affairs, pharmacovigilance, NDDS, medical devices and vaccines.

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Note: