

# Scientific Program



14<sup>th</sup> World Congress on

## Medicinal Chemistry and Drug Design

&

8<sup>th</sup> World Congress on

## Mass Spectrometry

June 10-11, 2019 | Edinburgh, Scotland

UK: Conference Series LLC Ltd  
47 Churchfield Road, London, W3 6AY  
Toll Free: +0-800-014-8923

# DAY-1

June 10, 2019

Meeting Hall: **Gifford**

08:30-09:30 Registrations

*Opening Ceremony* ..... **09:30-09:50**

## KEYNOTE FORUM

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09:50-10:00 Introduction

10:00-10:30 **Title: Polyamides as multifaceted molecules for medicinal chemistry**  
**James K Bashkin**, University of Missouri-St. Louis, USA

10:30-11:00 **Title: Design and synthesis of DapE inhibitors as potential antibiotics with a new mechanism of action**  
**Daniel P Becker**, Loyola University Chicago, USA

## GROUP PHOTO

**Networking & Refreshments 11:00-11:20 @ Dunedin Bar Area**

11:20-11:50 **Title: A knowledge-based approach for drug target and bioactivity prediction**  
**Orazio Nicolotti**, University of Bari, Italy

## WORKSHOP

11:50-12:50 **Title: Approach to GABA-A receptor isoform-selective allosteric agonists**  
**Karol S Bruzik**, University of Illinois, USA

**Lunch Break 12:50-13:40 @ Westview Restaurant**

**Sessions: Anti-Cancer Agents | Anti Microbial and Infectious Agents | Chemical Biology | Drug Delivery Targeted Drug Delivery | Computer-Aided Drug Design | Drug Design | ADME- Drug Chemistry | Clinical Diagnostic | Biological Mass Spectrometry**



**Chair: Orazio Nicolotti**, University of Bari, Italy

**Chair: Daniel P Becker**, Loyola University Chicago, USA

## INTRODUCTION

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13:40-14:05 **Title: Diazeniumdiolates as HNO/NO donors: Synthesis and biological activity**  
**Daniela Andrei**, Dominican University, USA

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- 14:05-14:30** **Title: Novel phenyldiazenyl fibrate analogues as PPAR agonists: Design, synthesis and pharmacological evaluation**  
Letizia Giampietro, University of Chieti, Italy
- 14:30-14:55** **Title: Isomers and diastereomers of C-methylated spermidine and spermine: Synthesis and biochemical application**  
Alex R Khomutov, Russian Academy of Sciences, Russia
- 14:55-15:20** **Title: Synthesis and cytotoxicity evaluation of novel amide and sulfonimide PPARa antagonists**  
Alessandra Ammazalorso, University of Chieti, Italy
- 15:20-15:45** **Title: Antibacteria, antiparasitic and *in silico* studies of dichapetalum madagascariense**  
Poire  
Mary Anti Chama, University of Ghana, Ghana
- 15:45-16:10** **Title: Broad-spectrum binding to human papillomavirus DNA**  
James K Bashkin, University of Missouri-St. Louis, USA
- Networking & Refreshments 16:10-16:30 @ Dunedin Bar Area**
- 16:30-16:55** **Title: Proteomic strategy for identification of proteins responding to DNA damage by platinum anticancer drugs**  
Fuyi Wang, Chinese Academy of Sciences, China
- 16:55-17:20** **Title: The development of small and less power TOF-MS in space exploration**  
Rongxin Yan, Beijing Institute of Spacecraft Environment Engineering, China
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## Panel Discussion

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# DAY-2

June 11, 2019

Meeting Hall: **Gifford**

## POSTER PRESENTATIONS 11:00-12:00 @ DUNEDIN BAR AREA

**Poster Judge:** Daniela Andrei, Dominican University, USA

- MCMS-01** **Title: Off-Label human trials of chloroquine formulations as topical Anti-Human Papillomavirus (HPV) treatments for high- and low-risk HPV-derived disease: Anecdotal studies**  
James K Bashkin, University of Missouri-St. Louis, USA
- MCMS-02** **Title: Design, synthesis and molecular modeling of isothiochromanone hybrids bearing N-benzyl pyridinium moiety as dual binding site acetylcholinesterase inhibitors**  
Jinyi Xu, Pharmaceutical University, China
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- MCMS-03** **Title: Combined prodrugs: Dual action against HIV and HCMV**  
Anastasia Khandazhinskaya, Engelhardt Institute of Molecular Biology, Russia
- MCMS-04** **Title: Synthesis and anti-tumor evaluation of C-23 modified novel 23-hydroxybetulinic acid derivatives**  
Shengtao Xu, Pharmaceutical University, China
- MCMS-05** **Title: Structure-guided identification of a small molecule that inhibits anaerobic choline metabolism by human gut bacteria**  
Maud Bollenbach, Harvard University, USA
- MCMS-06** **Title: Isomers and diastereomers of C-methylated spermidine and spermine: Synthesis and biochemical application**  
Alex R Khomutov, Russian Academy of Sciences, Russia
- MCMS-07** **Title: Proteomic profiles of melanoma-derived exosomes (MTEX) from the plasma of melanoma patients – A preliminary study**  
Monika Pietrowska, Maria Skłodowska-Curie Institute – Oncology Center Gliwice Branch, Poland
- MCMS-08** **Title: Proteomes of exosomes from HPV(+) or HPV(-) Head and Neck Cancer cells: Different enrichment in immunoregulatory proteins**  
Marta Gawin, Maria Skłodowska-Curie Institute – Oncology Center Gliwice Branch, Poland

## Awards & Closing Ceremony

Lunch Break 12:00-13:00 @ Westview Restaurant

## Bookmark your Dates

15<sup>th</sup> World Congress on  
**Medicinal Chemistry and Drug Design**

June 22-23, 2020 | Rome, Italy

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9<sup>th</sup> World Congress on  
**Mass Spectrometry**

June 10-11, 2020 | Frankfurt, Germany

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